Controlled Reductive C-C Coupling of Isocyanides Promoted by an Aluminyl Anion

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General Experimental Procedures

All manipulations were performed under dry nitrogen or argon using standard Schlenk-line techniques, or in a conventional nitrogen-filled glovebox. Hexane, toluene, diethyl ether (Et_2O), and tetrahydrofuran (THF) were obtained from a PureSolv MD 5 system and stored over activated 5 Å molecular sieves for 24 hours prior to use. NMR spectra were recorded using a Jeol JNM-ECZ500S 500 MHz spectrometer equipped with a ROYAL digital auto tune probe S, operating at 500.1 (^{1}H) and 125.8 (^{13}C). Spectra were recorded at 294 K (unless stated otherwise) and proton and carbon chemical shifts were referenced internally to residual solvent resonances. Coupling constants are quoted in Hz. Elemental analyses were performed by the Elemental Analysis Service at London Metropolitan University. K[Al(NON)] was prepared according to the literature procedures.[1] All other chemicals were purchased from Sigma-Aldrich and used without further purification.

Experimental details for K[Al(NON)(H)(CN)] (1a) / K[Al(NON)(H)(NC)] (1b)

A solution of *tert*-butyl isocyanide (23 mg, 0.28 mmol) in toluene (~5 mL) was added to a stirred solution of K[Al(NON)] (76 mg, 0.14 mmol) at room temperature. The reaction mixture was allowed to stir for *ca.* 1 hr to give a white suspension. The volatiles were removed *in vacuo* and the residue dissolved in THF. Crystals suitable for single crystal X-ray diffraction experiments were grown at room temperature *via* slow evaporation. Yield 46 mg, 58 %.

An isomeric mixture exists in solution. Overlap in the ^{1}H NMR spectrum causes most of the peaks to be indistinguishable between the two isomers. However, a noticeable shift is observed between the Si*Me*$_2$ signals that has been used to calculate the relative ratio between each isomer as 4:1.

The ^{13}C{^{1}H} NMR spectrum also shows two signals for a the Al–*C*N / Al–N*C* ligands and has also been used to distinguish the two isomers. In the ^{13}C{^{1}H} NMR spectrum, signals associated with the minor isomer are denoted with an asterisk (*).

^{1}H NMR (500 MHz, THF-D_8): δ 6.93 (d, J = 7.5, 3H, C$_6$*H*$_3$), 6.79 (t, J = 7.5, 2H, C$_6$*H*$_3$), 4.09 – 4.00 (m, 4H, C*H*Me$_2$), 1.30 (d, J = 6.8, 6H, CH*Me*$_2$), 1.22 – 1.14 (m, 18H, CH*Me*$_2$), 0.11, 0.02 (s, 6H, Si*Me*$_2$).

SiMe$_2$ *^{1}H NMR signals for each isomer: 0.11 (s, 6.0H,* ***Major****), 0.11 (s, 1.5H,* ***Minor****), 0.02 (s, 6.0H,* ***Major****), 0.01 (s, 1.5H,* ***Minor****).*

^{13}C{^{1}H} NMR (126 MHz, THF-D_8): δ 174.2* (Al–N*C*, **Minor**), 147.9*, 147.7, 147.6*, 146.1*, 146.0 (*C*$_6$H$_3$), 141.0 (Al–*C*N, **Major**), 123.8, 123.6*, 123.5, 123.4*, 122.1, 122.0* (*C*$_6$H$_3$), 28.0, 27.7, 27.5*, 27.1*, (*C*HMe$_2$), 26.9, 26.8, 26.0, 25.9*, 25.7*, 25.6 (CH*Me*$_2$), 3.1*, 3.0, 2.6, 2.6* (Si*Me*$_2$).

IR (solid, cm^{-1}): 2119 (υ_{CN}), 1755 ($\upsilon_{Al\text{-}H}$).

Figure S1 ^{1}H NMR spectrum (500 MHz, THF-D_8) of K[Al(NON)(H)(CN)] (**1a**) / K[Al(NON)(H)(NC)] (**1b**)

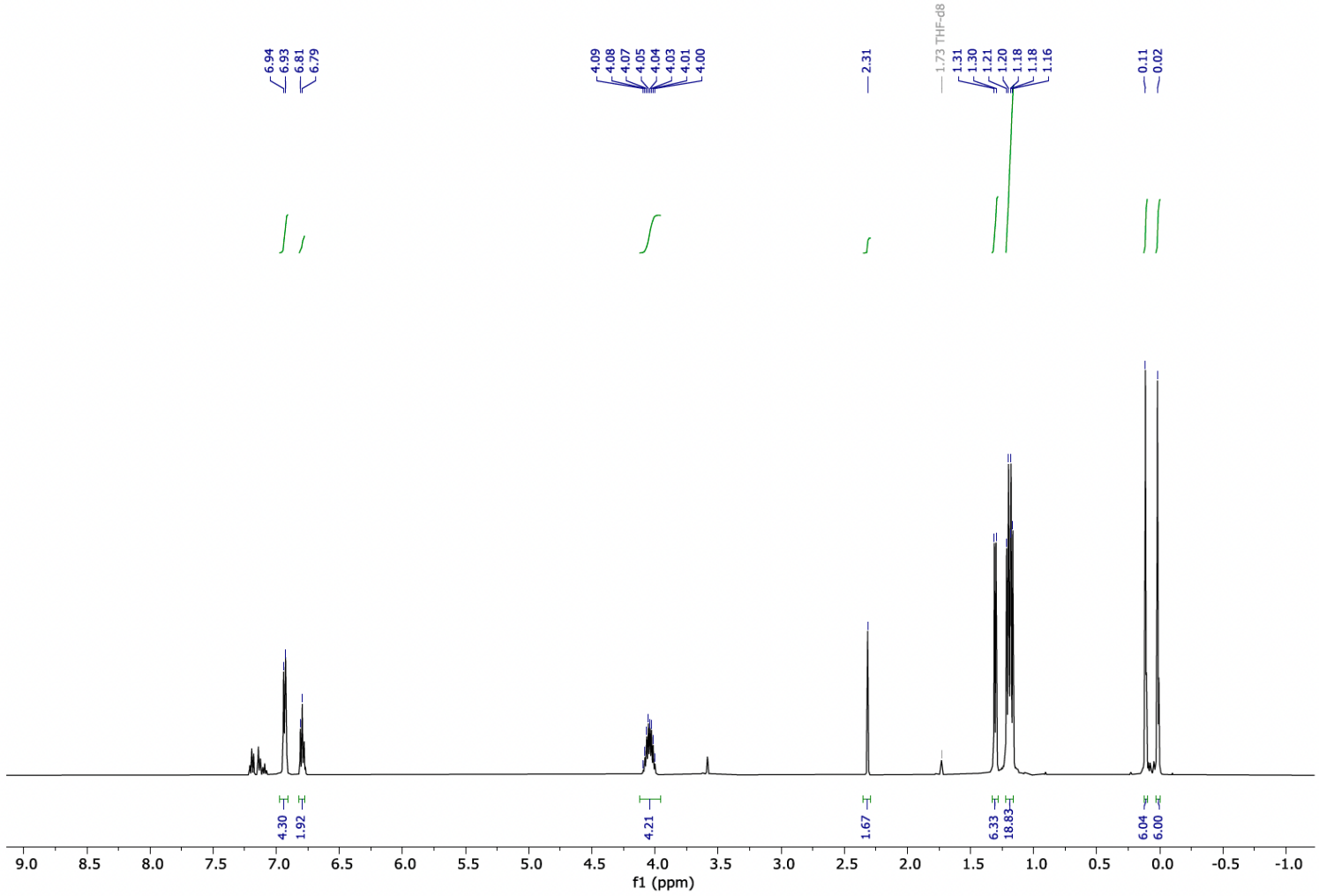


Figure S2 Expansion of Si*Me*$_2$ region of the ^{1}H NMR spectrum (500 MHz, THF-D_8) of K[Al(NON)(H)(CN)] (**1a**) / K[Al(NON)(H)(NC)] (**1b**)

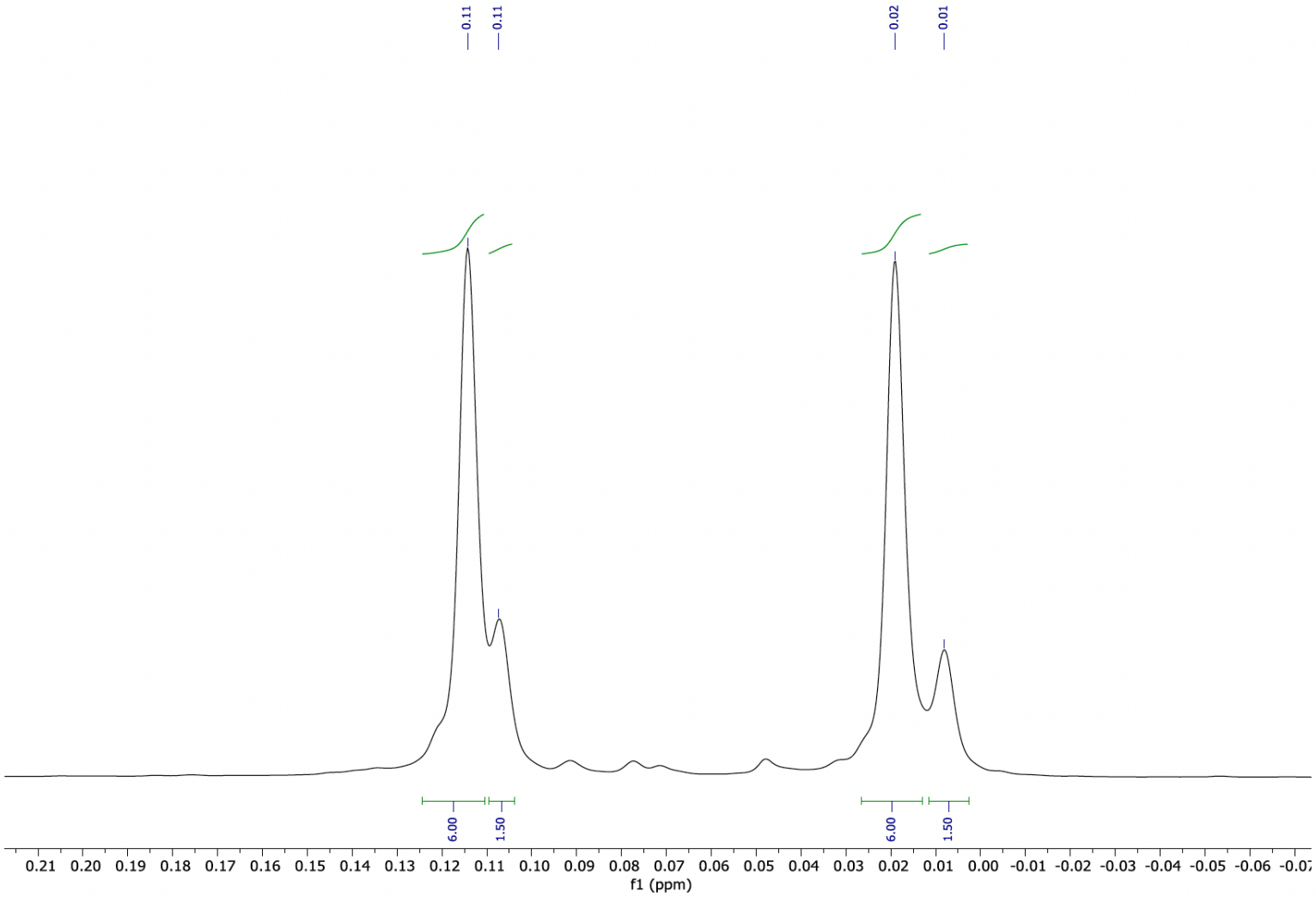


Figure S3 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, THF-D_8) of K[Al(NON)(H)(CN)] (**1a**) / K[Al(NON)(H)(NC)] (**1b**)

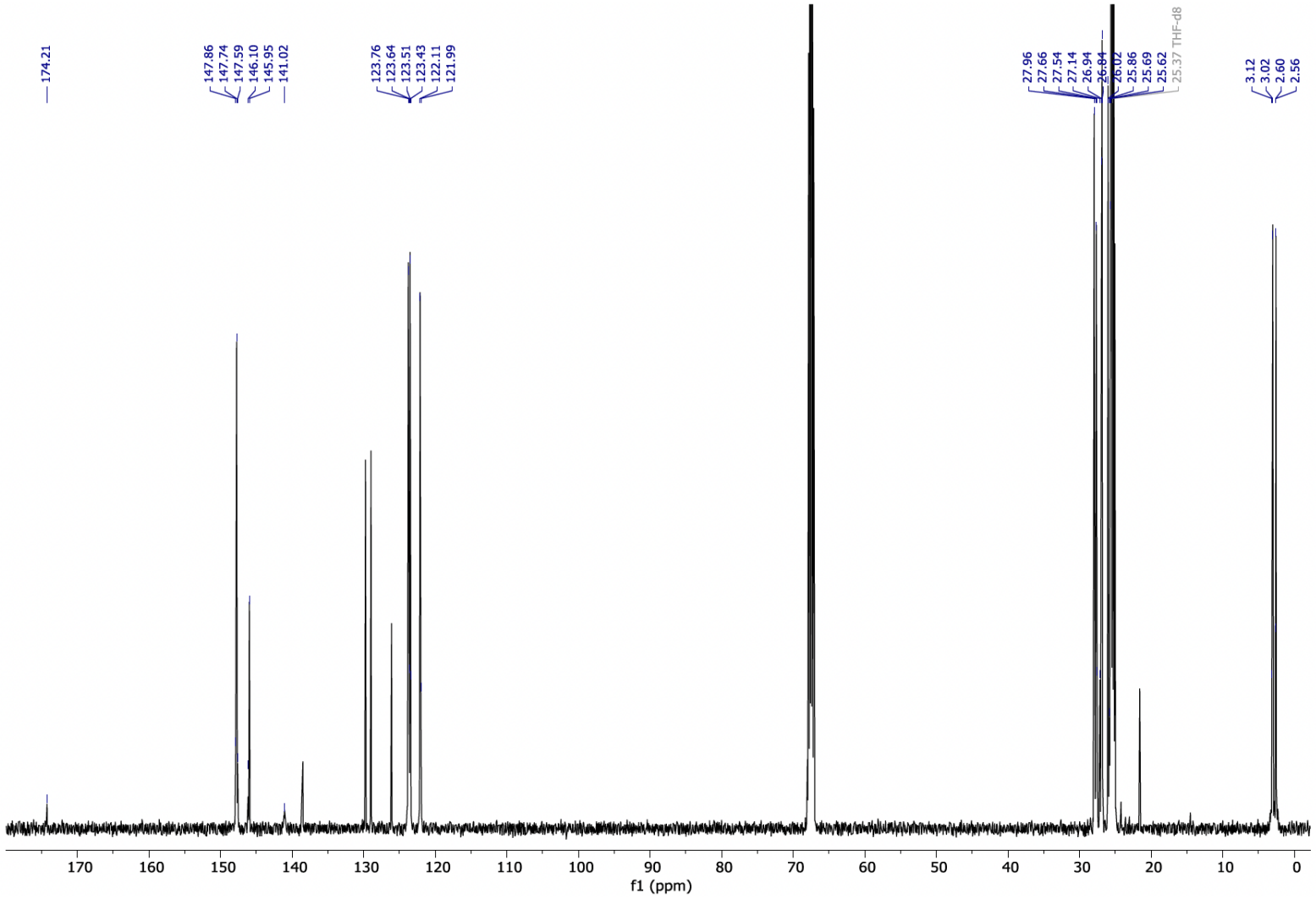


Figure S4 Expansion of Al–*C*N / Al–N*C* region of $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, THF-D_8) of K[Al(NON)(H)(CN)] (**1a**) / K[Al(NON)(H)(NC)] (**1b**)

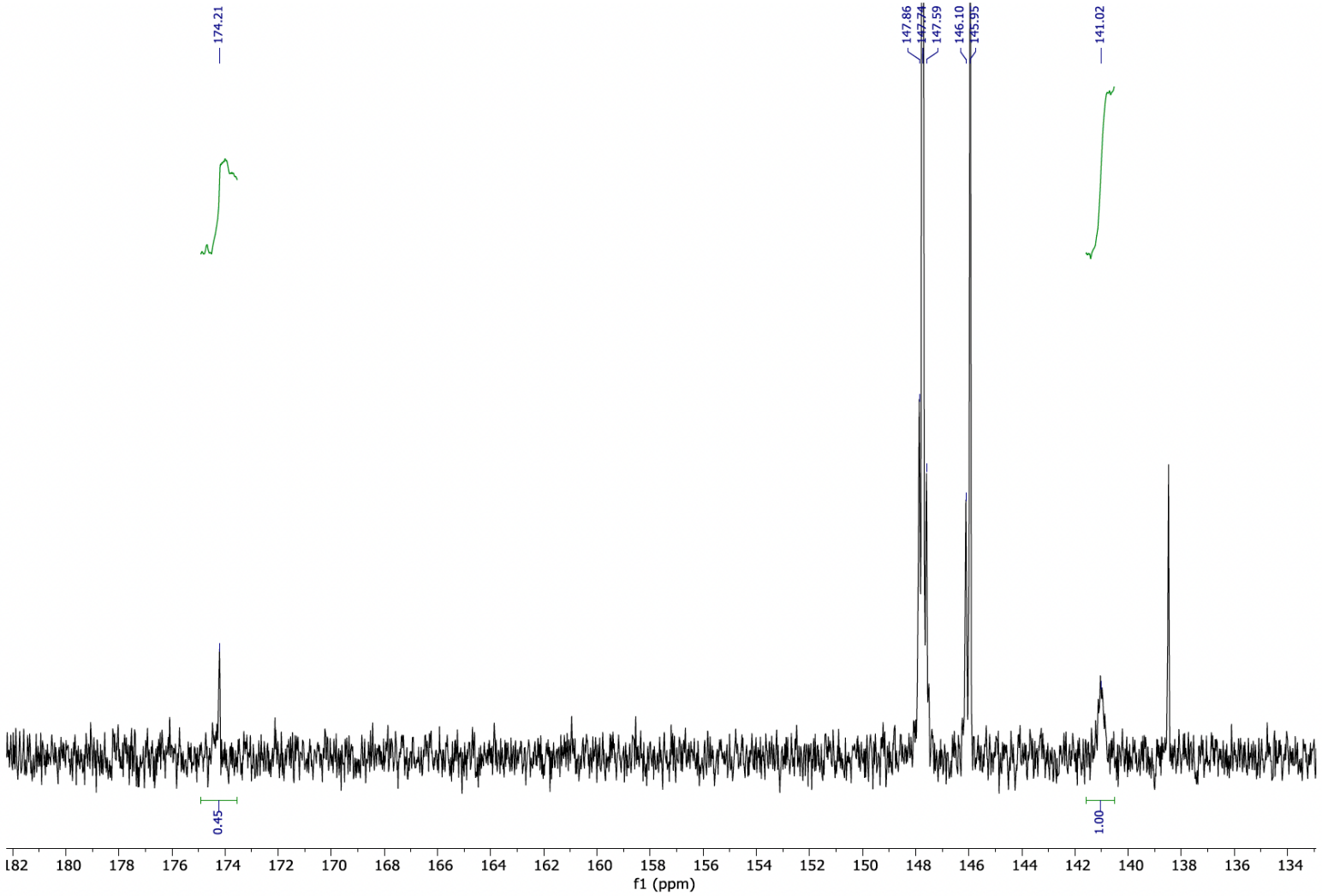


Figure S5 IR spectrum (solid, cm^{-1}) of K[Al(NON)(H)(CN)] (**1a**) / K[Al(NON)(H)(NC)] (**1b**)

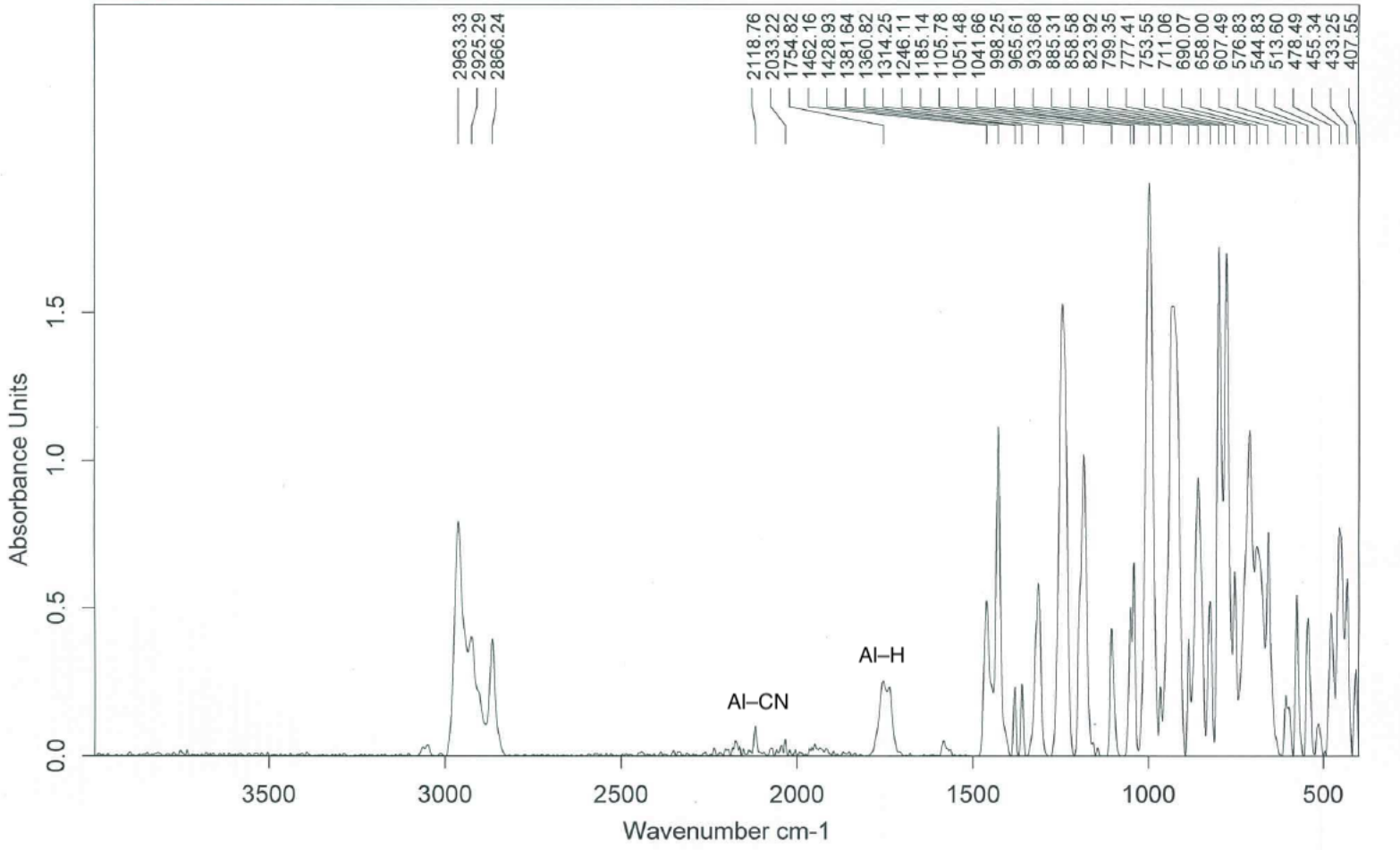
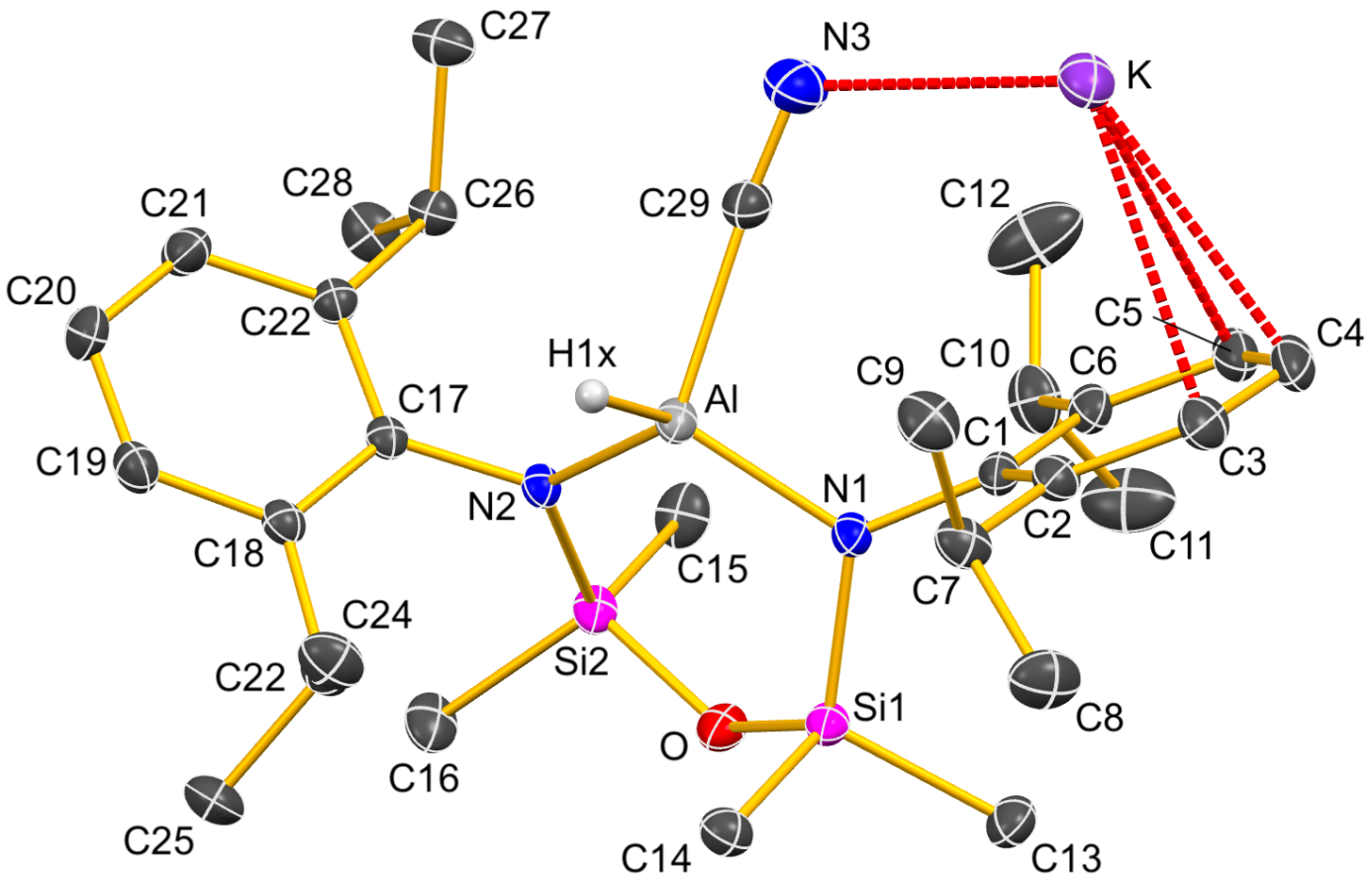


Figure S6 Displacement ellipsoid plot (30 %, H-atoms except Al*H* omitted) of K[Al(NON)(H)(CN)] (**1a**) (*asymmetric unit*)



Experimental details for [K(2.2.2)crypt][Al(NON)(H)(CN)] (1a·crypt) / [K(2.2.2)crypt][Al(NON)(H)(NC)] (1b·crypt)

A solution of *tert*-butyl isocyanide (15 mg, 0.19 mmol) in THF (~3 mL) was added to a stirred solution of K{Al(NON)}] (102 mg, 0.19 mmol) in THF (~3 mL) at room temperature. The reaction mixture was allowed to stir for *ca.* 1 hr and 222-cryptand (70 mg, 0.19 mmol) was added. The volatiles were removed *in vacuo* and the residue dissolved in boiling toluene (~3 mL). Crystals suitable for single crystal X-ray diffraction experiments were grown at room temperature *via* slow evaporation. Yield 134 mg, 76 %.

An isomeric mixture exists in solution. Overlap in the ^{1}H NMR spectrum causes most of the peaks to be indistinguishable between the two isomers. However, a noticeable shift is observed between the $SiMe_2$ signals that has been used to calculate the relative ratio between each isomer as 5:3.

Anal. Calcd. for $C_{47}H_{83}AlKN_5O_7Si_2$ (*951.53*): C, 59.27; H, 8.79; N, 7.35 %. Found: C, 58.64; H, 8.91; N, 7.04 %.

^{1}H NMR (500 MHz, THF-D_8): δ 6.97 – 6.85 (m, 4H, C_6H_3), 6.75 (t, J = 7.2, 2H, C_6H_3), 4.14 – 4.10 (m, 4H, C*H*Me_2), 3.49 (s, 12H, crypt-CH_2), 3.50 – 3.42 (m, 12H, crypt-CH_2), 2.46 – 2.49 (m, 12H, crypt-CH_2), 1.30 (d, J = 6.8 Hz, 6H, CHMe_2), 1.21 – 1.14 (m, 16H, CHMe_2), 0.10, –0.02 (s, 6H, SiMe_2).

$SiMe_2$ ^{1}H NMR signals for each isomer: 0.11 (s, 6.0H, ***Major****), 0.10 (s, 3.6H,* ***Minor****), –0.02 (s, 6.0H,* ***Major****), –0.03 (s, 3.6H,* ***Minor****)*.

^{13}C{^{1}H} NMR (126 MHz, THF-D_8): δ 179.3 (Al–N*C*, **Minor**),* 148.3, 148.2, 147.6, 147.5, 146.5, 146.4, 123.6, 123.5, 123.5, 123.4, 121.9, 121.8 (C_6H_3), 71.3, 68.5, 54.8 (crypt-*C*H_2), 27.9, 27.7, 27.7, 27.6, 27.5, 27.1, 27.1, 26.0, 26.0, 25.9, 25.9, 25.6 (*C*HMe_2 and CHMe_2), 3.3, 3.1, 2.7, 2.6 (SiMe_2).

* The ^{13}C{^{1}H} NMR spectrum only shows a signal for the Al–N*C* ligand (Al–*C*N not observed due to coupling with ^{27}Al nuclei).

IR (solid, cm^{-1}): 2106 (υ_{CN}), 1792 ($\upsilon_{Al\text{-}H}$).

Figure S7 ^{1}H NMR spectrum (500 MHz, THF-D_8) of [K(2.2.2)crypt][Al(NON)(H)(CN)] (**1a·crypt**) / [K(2.2.2)crypt][Al(NON)(H)(NC)] (**1b·crypt**)

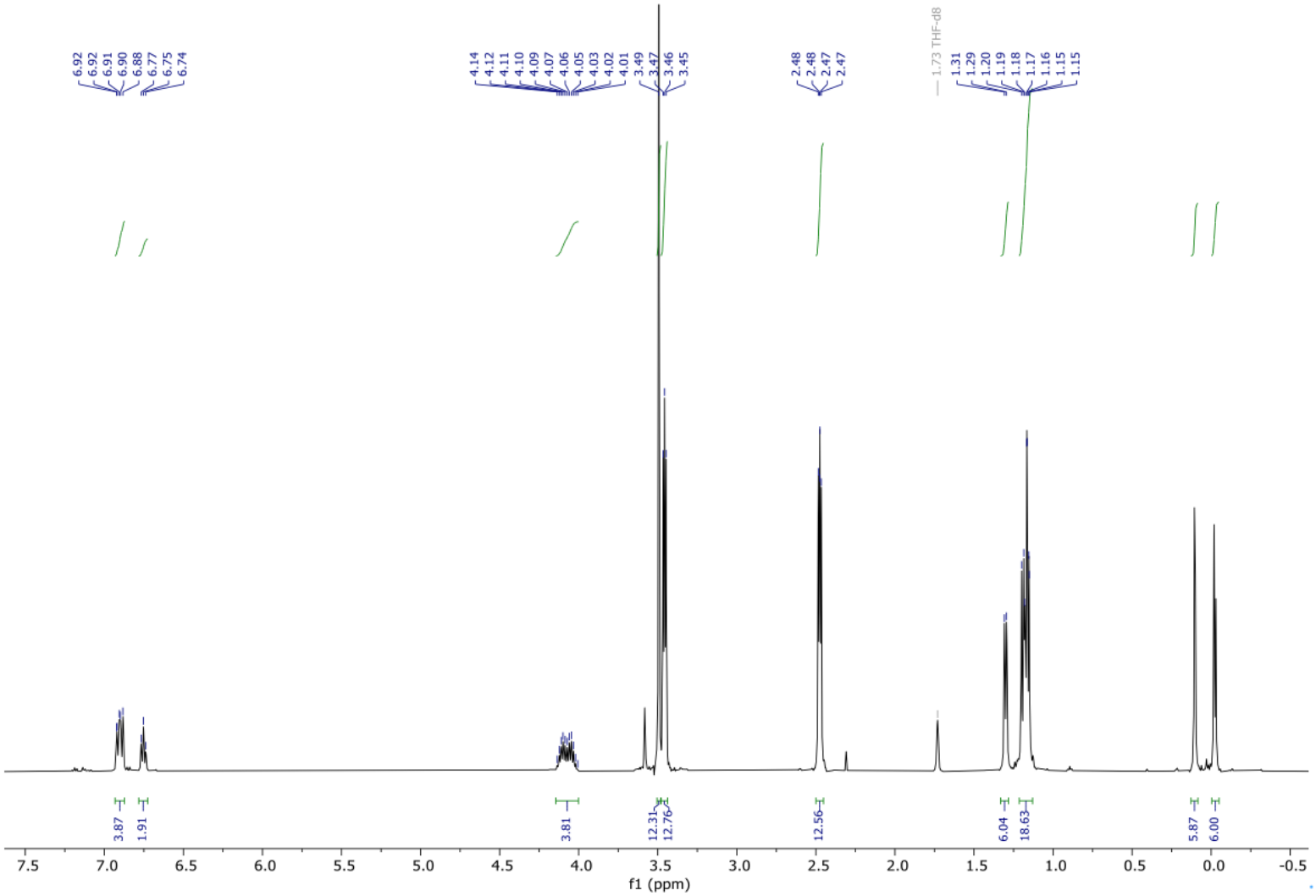


Figure S8 Expansion of Si*Me*$_2$ region of the ^{1}H NMR spectrum (500 MHz, THF-D$_8$) of [K(2.2.2)crypt][Al(NON)(H)(CN)] (**1a·crypt**) / [K(2.2.2)crypt][Al(NON)(H)(NC)] (**1b·crypt**)

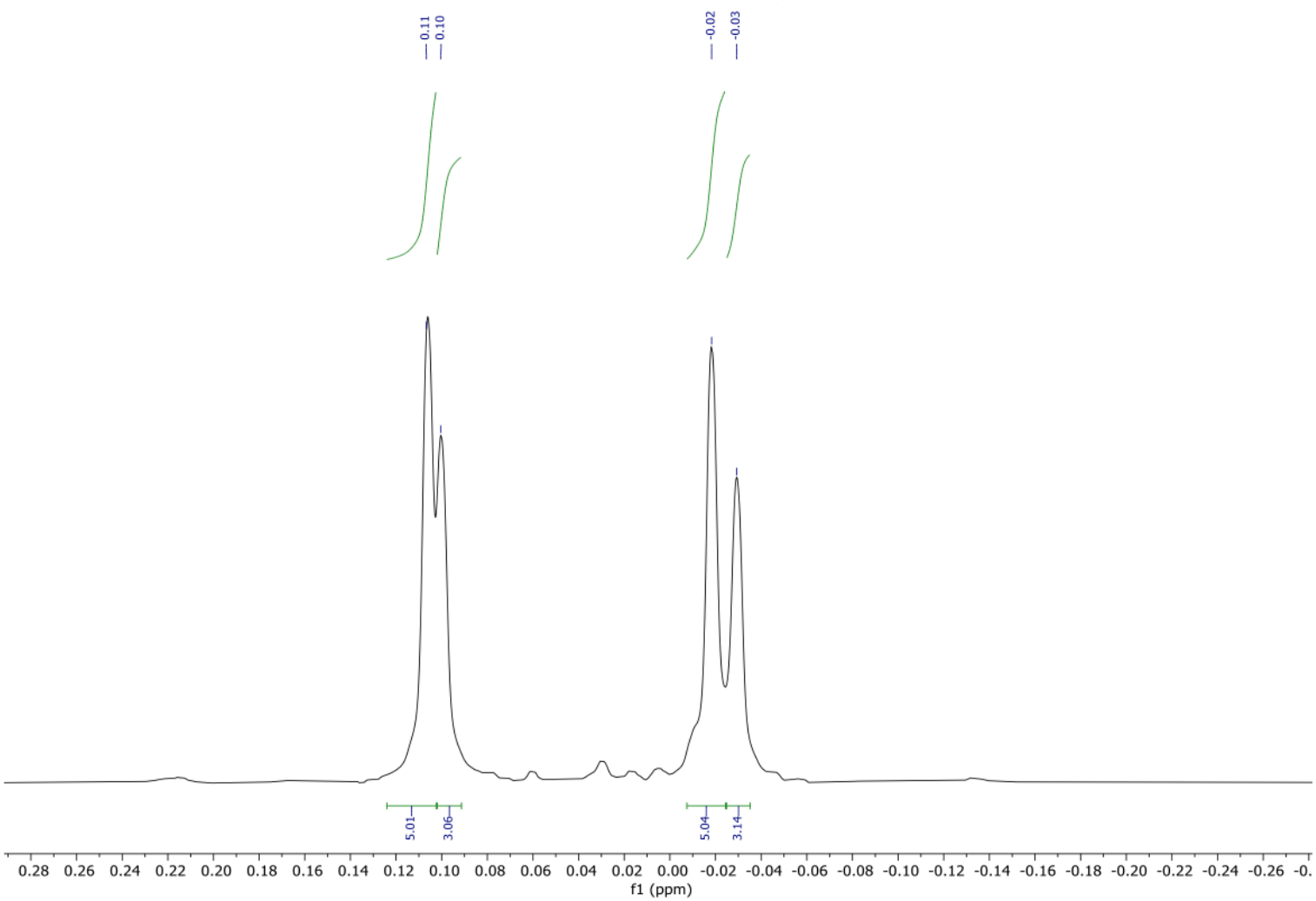


Figure S9 $^{13}C\{^{1}H\}$ NMR spectrum (500 MHz, THF-D_8) of [K(2.2.2)crypt][Al(NON)(H)(CN)] (**1a·crypt**) / [K(2.2.2)crypt][Al(NON)(H)(NC)] (**1b·crypt**)

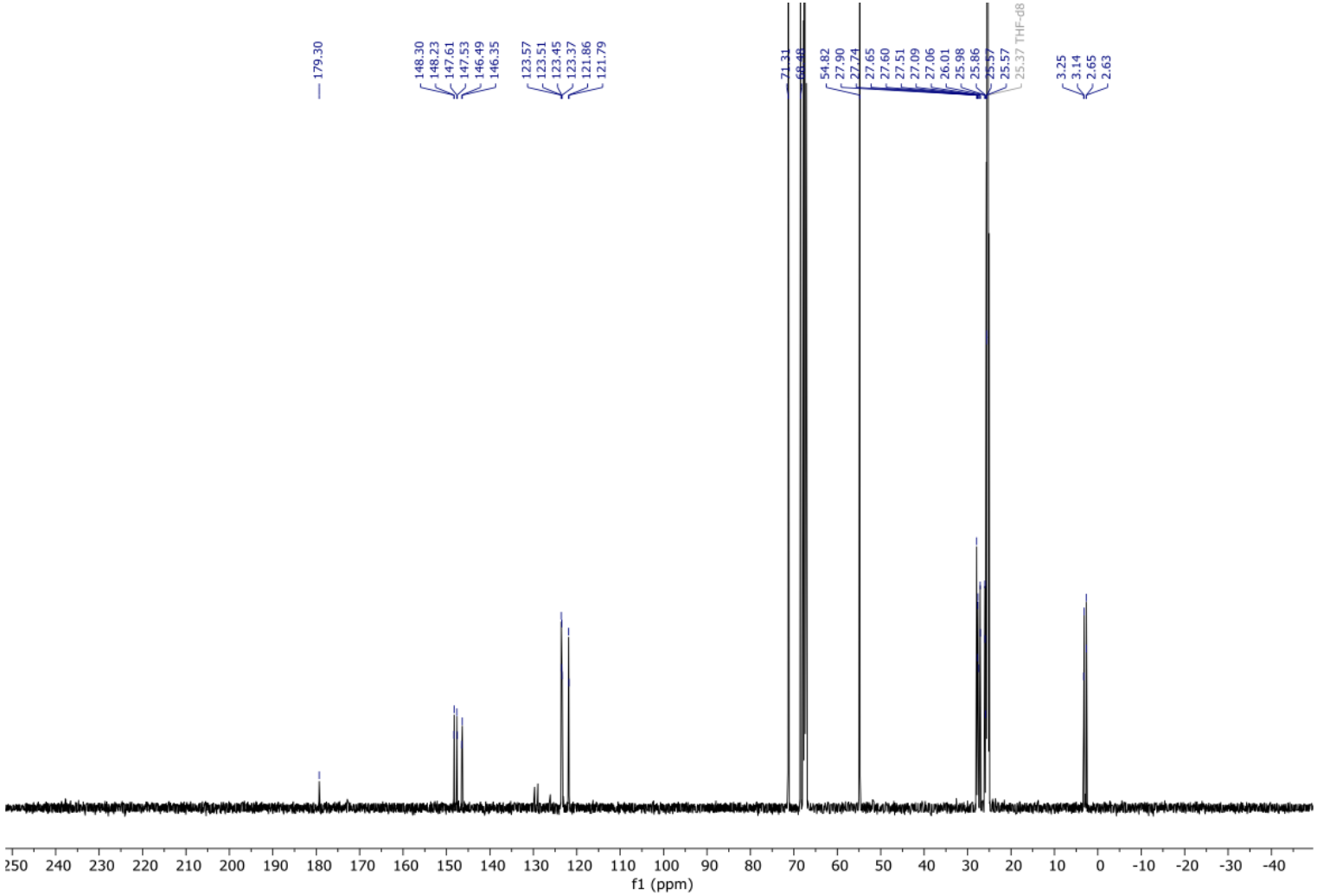


Figure S10 IR spectrum (solid, cm^{-1}) of [K(2.2.2)crypt][Al(NON)(H)(CN)] (**1a·crypt**) / [K(2.2.2)crypt][Al(NON)(H)(NC)] (**1b·crypt**)

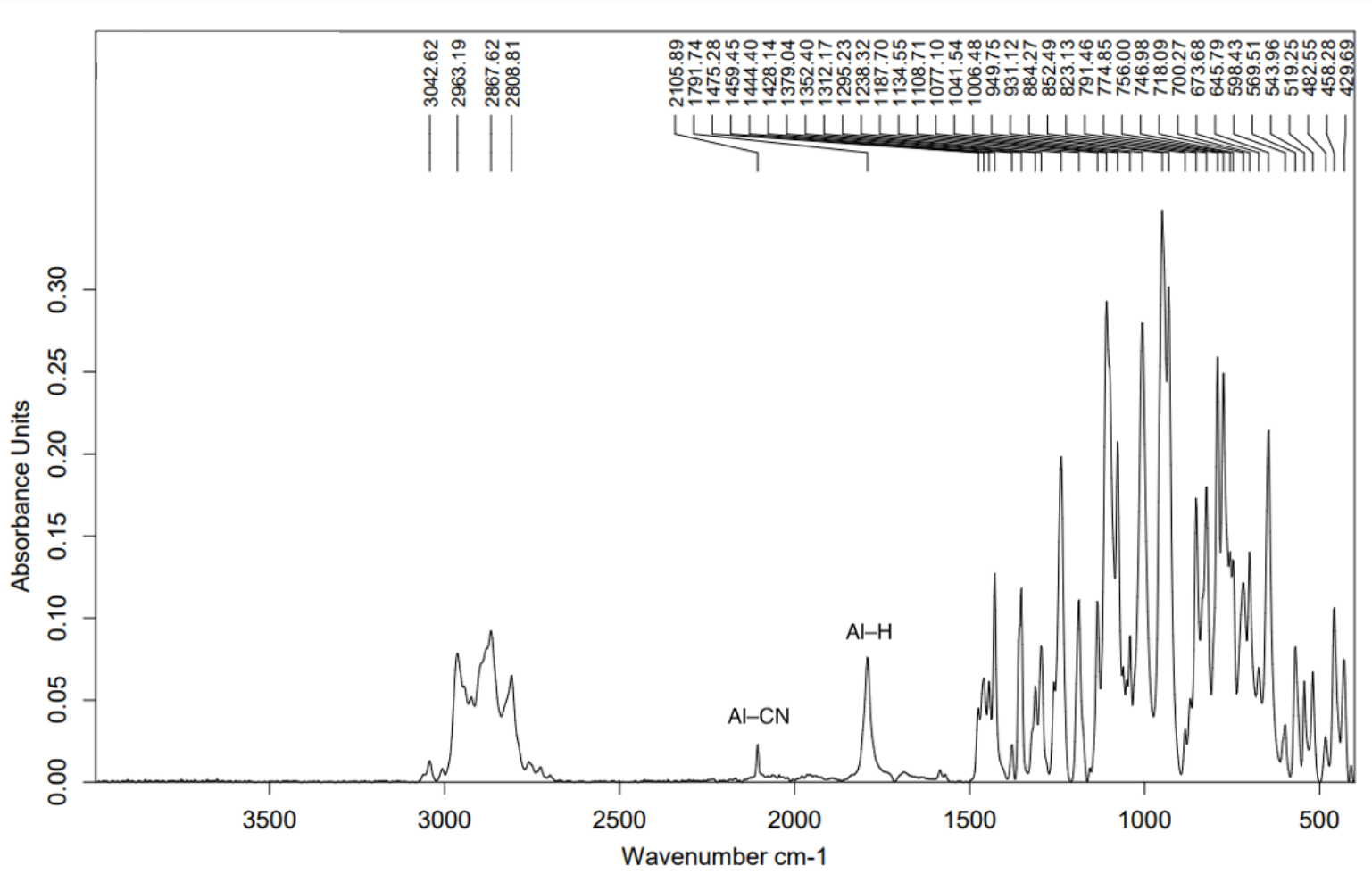
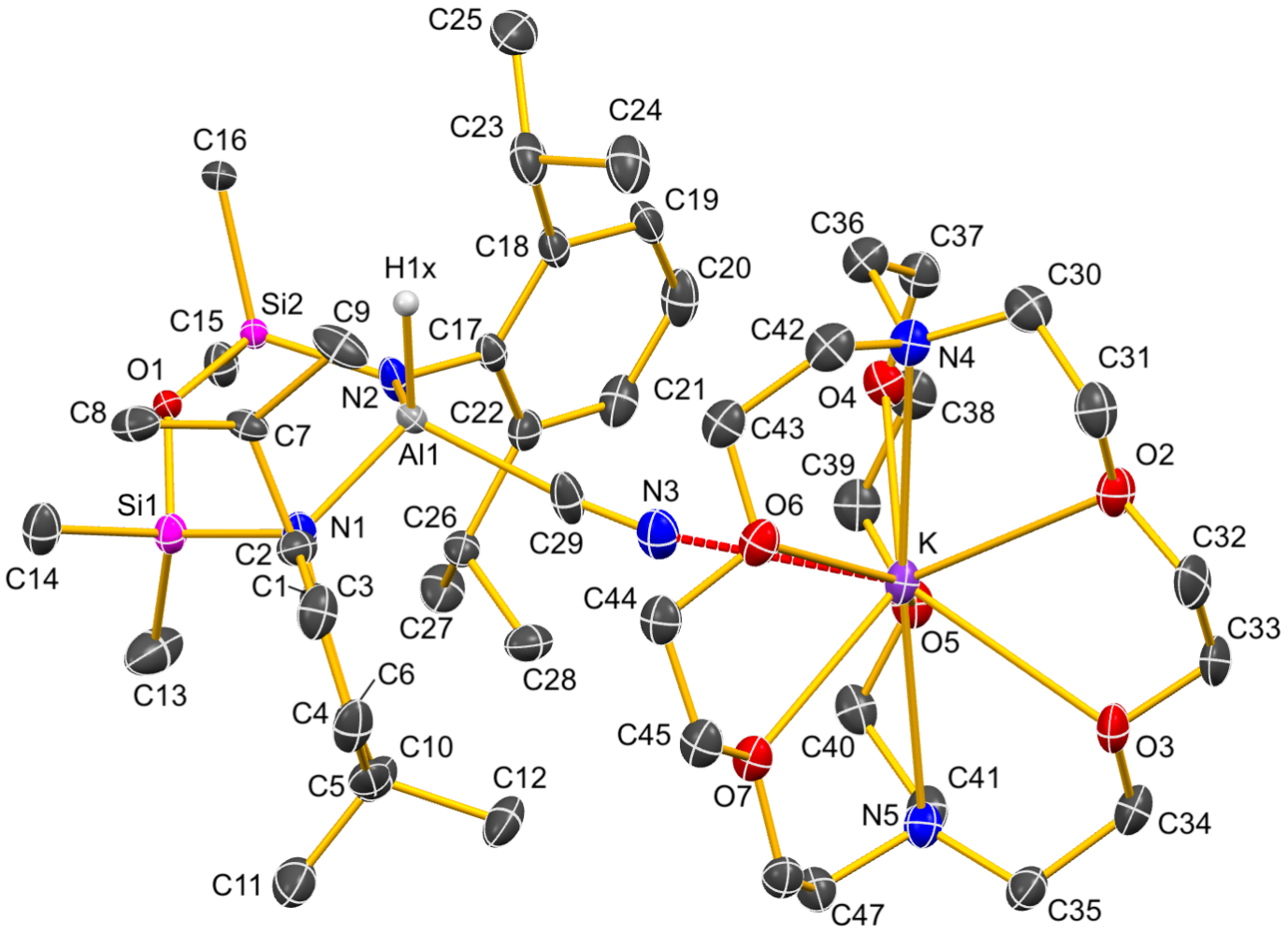


Figure S11 Displacement ellipsoid plot (30 %, H-atoms except Al*H* and disordered atoms omitted) of [K(2.2.2)crypt][Al(NON)(H)(CN)] (**1a·crypt**) (*asymmetric unit*)



Experimental details for [K(Et$_2$O)$_2$][Al(NON){(DmpNC)$_2$(DmpNC*)}] (2·Et$_2$O) (* = ring-activated DmpNC)

A solution of 2,6-dimethylphenyl isocyanide (130 mg, 0.99 mmol) in toluene was added drop wise to a stirred solution of K[Al(NON)] (182 mg, 0.33 mmol) in an ampoule at –78 °C. The resulting dark red/purple mixture was allowed to warm to room temperature and the volatiles removed *in vacuo*. Crystallisation was achieved from a solution of toluene or diethyl ether *via* slow evaporation at room temperature. An analytically pure purple powder was obtained by washing the crystals with hexane (5 x 2 mL). Yield 211 mg, 68 %.

Anal. Calcd. for $C_{63}H_{93}AlKN_5O_3Si_2$ (*1089.63*): C, 69.38; H, 8.60; N, 6.43 %. Found: C, 68.50; H, 8.45; N, 6.50 %.

^{1}H NMR (500 MHz, THF-D$_8$): δ 6.98 (d, *J* = 7.8, 1H, C$_6$*H$_3$*), 6.95 (d, *J* = 7.7, 1H, C$_6$*H$_3$*), 6.89 (m, 3H, C$_6$*H$_3$*),‡ 6.87 – 6.79 (m, 2H, C$_6$*H$_3$*), 6.76 (t, *J* = 7.5, 1H, C$_6$*H$_3$*), 6.47 (d, *J* = 7.3, 1H, C$_6$*H$_3$*), 6.44 (d, *J* = 7.3, 1H, C$_6$*H$_3$*), 6.33 (t, *J* = 7.4, 1H, C$_6$*H$_3$*), 5.79 (d, *J* = 6.0, 1H, C$_6$*H$_3$*),* 5.71 – 5.62 (m, 2H, C$_6$*H$_3$*),* 4.02 (sept, *J* = 7.3, 1H, C*H*Me$_2$), 3.69 – 3.54 (m, 3H, C*H*Me$_2$), 3.39 (q, *J* = 7.0, 4H, Et$_2$O),¥ 2.53 (s, 3H, C$_6$H$_3$*Me$_2$*), 2.22 (s, 3H, C$_6$H$_3$*Me$_2$*), 1.95 (s, 3H, C$_6$H$_3$*Me$_2$*), 1.39 (d, *J* = 6.5, 3H, CH*Me$_2$*), 1.36 (s, 3H, C$_6$H$_3$*Me$_2$*), 1.24 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.15 (d, *J* = 6.7, 3H, CH*Me$_2$*), 1.12 (t, *J* = 7.0, 6H, Et$_2$O),¥ 1.06 (d, *J* = 4.2, 3H, CH*Me$_2$*), 1.05 (d, *J* = 4.2, 3H, CH*Me$_2$*), 0.95 (s, 3H, C$_6$H$_3$*Me$_2$*),* 0.93 (s, 3H, C$_6$H$_3$*Me$_2$*),* 0.77 (d, *J* = 6.5, 3H, CH*Me$_2$*), 0.72 (d, *J* = 6.8, 3H, CH*Me$_2$*), 0.40 (d, *J* = 6.8, 3H, CH*Me$_2$*), 0.38 (s, 3H, Si*Me$_2$*), 0.26 (s, 3H, Si*Me$_2$*), –0.13 (s, 3H, Si*Me$_2$*), –0.15 (s, 3H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, THF-D$_8$): δ 167.4 (C=*C*=N), 156.3,* 152.6, 151.3, 148.5, 148.0, 147.9, 147.3, 144.3, 143.2 (*C$_6$*H$_3$), 135.1 (C=*C*=C), 133.6,* 131.3, 129.1, 128.9, 128.8, 128.8, 128.5, 128.4, 128.1, 127.5, 124.7, 124.6, 124.4, 123.8, 123.5,* 123.3, 123.1, 122.4,* 122.3,* 120.5 (*C$_6$*H$_3$), 66.4 (Et$_2$O),¥ 63.4 (*C$_6$*H$_3$),* 29.8, 28.8 (CH*Me$_2$*), 28.6 (*C*HMe$_2$), 28.6 (C$_6$H$_3$*Me$_2$*), 28.2 (CH*Me$_2$*), 28.0 (*C*HMe$_2$), 27.8 (CH*Me$_2$*), 27.6, 27.3 (*C*HMe$_2$), 27.1, 26.3, 25.9, 24.0 (CH*Me$_2$*), 21.1, 20.1, 19.8, 18.2, 18.1 (C$_6$H$_3$*Me$_2$*), 15.7 (Et$_2$O),¥ 5.4, 5.1, 1.4, 1.3 (Si*Me$_2$*).

* activated ring system; ‡ overlapping signals causing observed splitting pattern; ¥ one equivalent of Et$_2$O present after crystals dried under vacuum.

Figure S12 ^{1}H NMR spectrum (500 MHz, THF-D_8) of [K(Et_2O)$_2$][Al(NON){(DmpNC)$_2$(DmpNC*)}] (**2·Et_2O**) (* = ring-activated DmpNC).

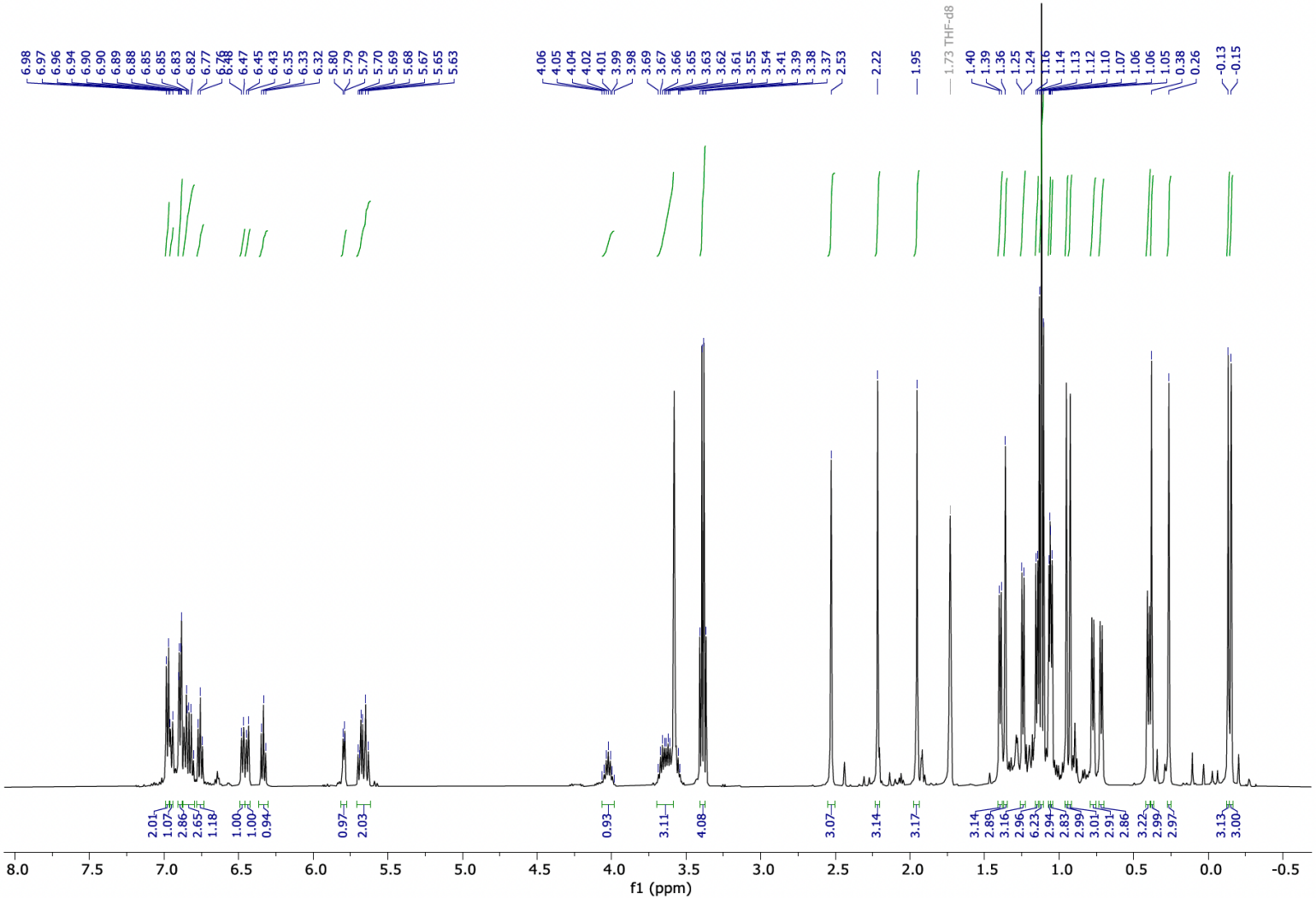


Figure S13 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, THF-D_8) of $[K(Et_2O)_2][Al(NON)\{(DmpNC)_2(DmpNC^*)\}]$ (**2·Et₂O**) (* = ring-activated DmpNC).

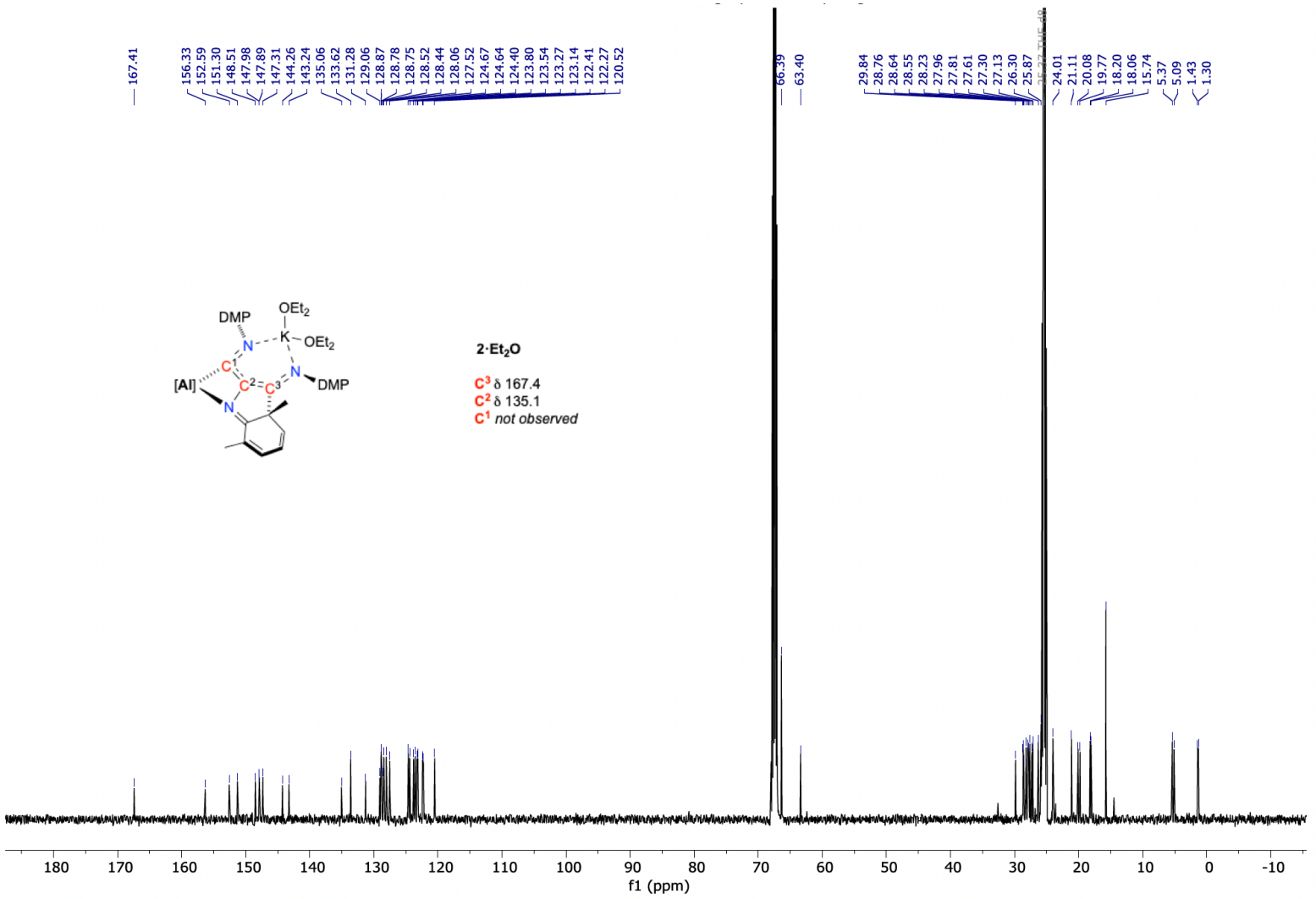


Figure S14 Displacement ellipsoid plot (30 %, H-atoms omitted) of $[K(Et_2O)_2][Al(NON)\{(DmpNC)_2(DmpNC^*)\}]$ (**2·Et₂O**) (* = ring-activated DmpNC).

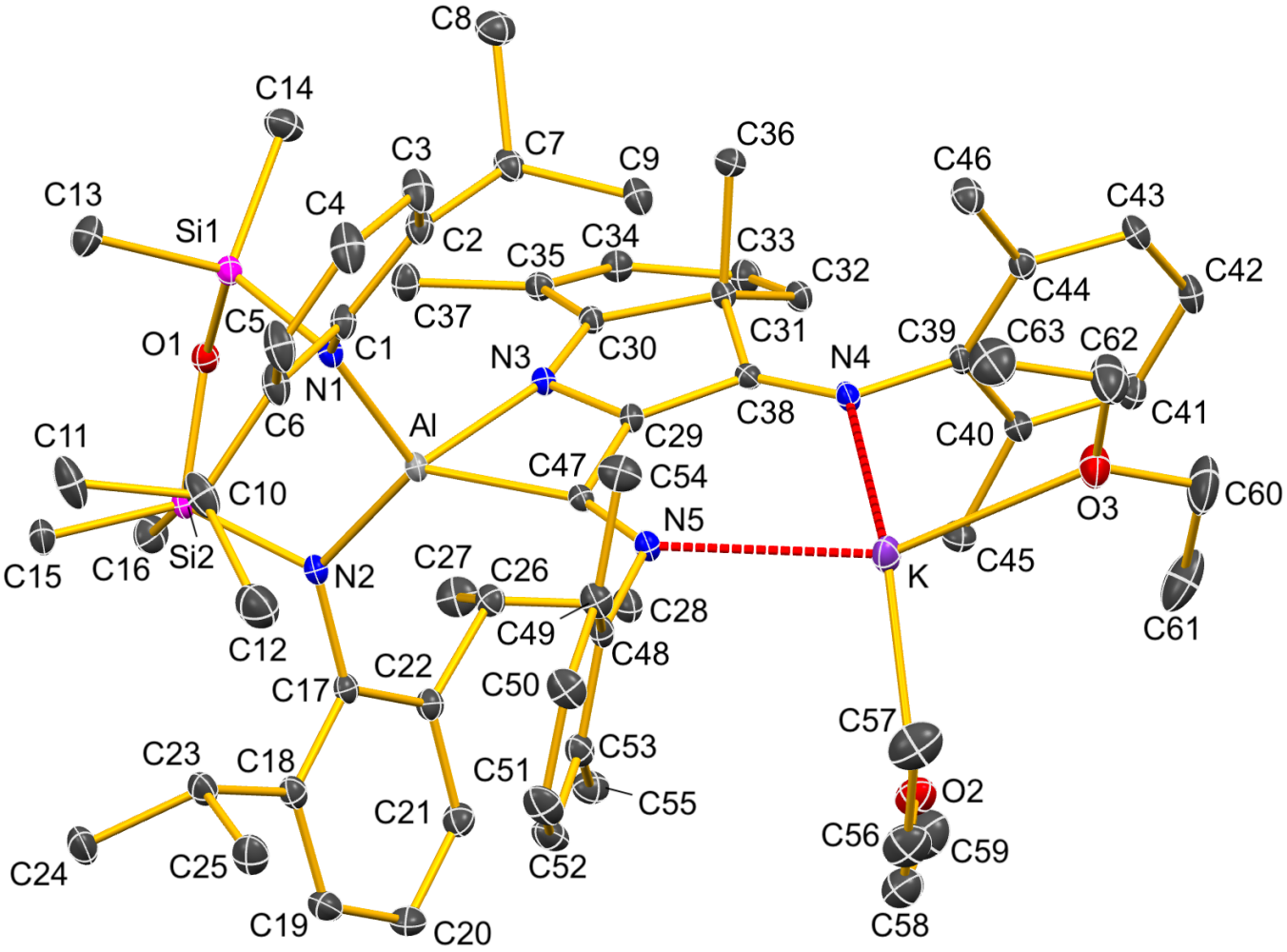
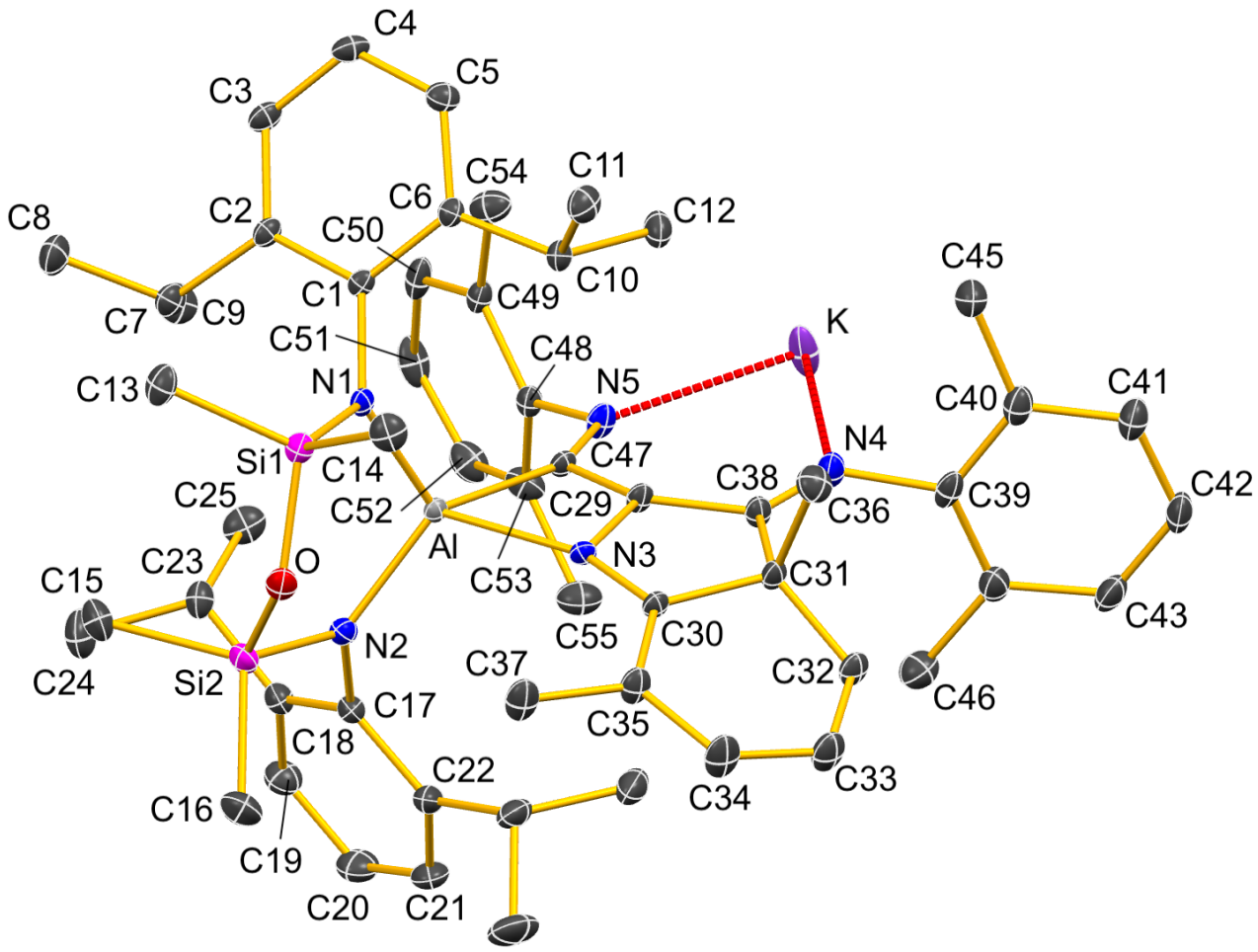


Figure S15 Displacement ellipsoid plot (30 %, H-atoms , disordered atoms and toluene solvate molecules omitted) of K[Al(NON){(DmpNC)$_2$(DmpNC*)}] (**2·toluene**) (* = ring-activated DmpNC).



Experimental details for [K(Et$_2$O)][Al(NON)(AdNC)$_2$] (3·Et$_2$O)

A solution of 1-adamantyl isocyanide (52 mg, 0.32 mmol) in toluene (~5 mL) was added to a stirred solution of K[Al(NON)] (89 mg, 0.16 mmol) at room temperature. The reaction mixture was allowed to stir for *ca.* 1 hr to give a bright yellow solution. The solvent was removed *in vacuo* and the residue dissolved in diethyl ether. Crystallisation was achieved by slow evaporation of a diethyl ether solution stored at room temperature. Yield 120 mg, 85 %.

Anal. Calcd. for $C_{54}H_{86}AlKN_4O_2Si_2$ (*944.57*): C, 68.60; H, 9.18; N, 5.93 %. Found: C, 69.87; H, 8.89; N, 5.49 %.

^{1}H NMR (500 MHz, Toluene-D$_8$, 373 K*): δ 7.13 – 7.09 (m, 3H, C$_6$*H$_3$*), 6.84 (d, *J* = 7.6, 1H, C$_6$*H$_3$*), 6.78 (d, *J* = 7.6, 1H, C$_6$*H$_3$*), 6.62 (t, *J* = 7.6, 1H, C$_6$*H$_3$*), 4.20 – 3.92 (m, 4H, C*H*Me$_2$), 3.27 (q, *J* = 7.0, 14H, Et$_2$O), 1.91 (br s, 4H, Ad), 1.81 (br s, 2H, Ad), 1.74 – 1.67 (m, 16H, Ad), 1.61 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.56 (s, 2H, Ad), 1.54 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.46 (br d, *J* = 11.0, 2H, Ad), 1.38 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.36 – 1.30 (m, 2H, Ad), 1.29 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.23 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.07 (t, *J* = 7.0, 20H, Et$_2$O), 0.97 (br d, *J* = 11.0, 2H, Ad), 0.74 (s, 3H, Si*Me$_2$*), 0.65 (s, 3H, Si*Me$_2$*), 0.08 (s, 3H, Si*Me$_2$*), –0.14 (s, 3H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, Toluene-D$_8$, 373 K*): δ 196.1 (C=*C*=N), 151.1, 149.4, 149.2, 147.3, 146.1, 145.8, 124.0, 123.8, 123.2, 123.1, 122.1 (*C$_6$*H$_3$), 65.9 (Et$_2$O), 55.3,‡ 45.4,‡ 43.8,‡ 37.7,‡ 31.1, 30.8 (Ad), 28.7,‡ 27.9, 27.4 (*C*HMe$_2$), 27.1, 26.8, 26.3, 25.9, 25.7, 25.6, 25.5, 24.8 (CH*Me$_2$*), 15.5 (Et$_2$O), 5.2,‡ 1.1, 0.1 (Si*Me$_2$*).

* NMR spectra recorded at 373 K due to poor solubility in toluene-D$_8$; ‡ overlapping signal correspond to more than one ^{13}C peak; Al–*C* resonance not observed.

Figure S16 ^{1}H NMR spectrum (500 MHz, Toluene-D_8, 373 K) of [K(Et_2O)][Al(NON)($AdNC)_2$] (**3·Et_2O**).

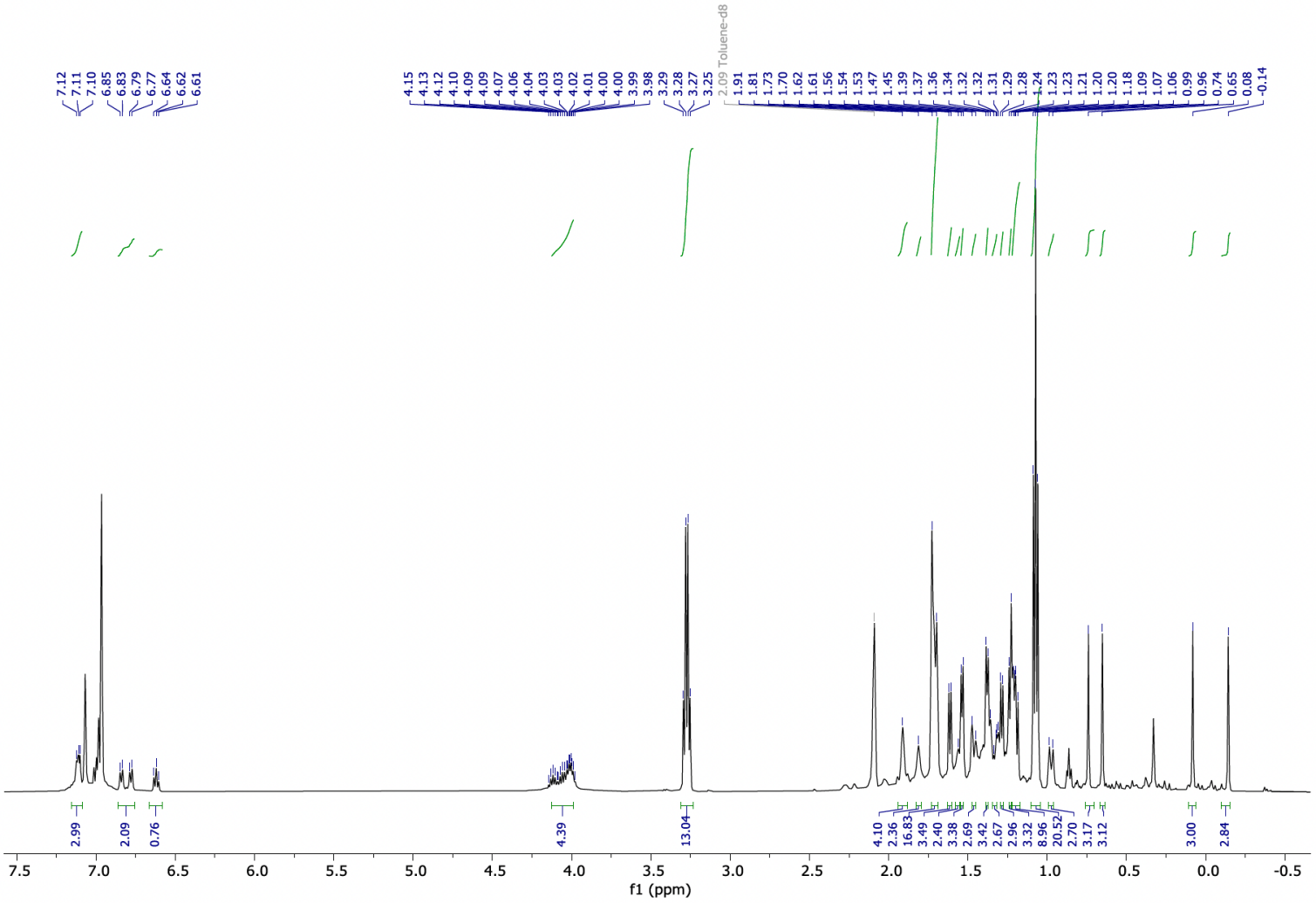


Figure S17 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, Toluene-D_8, 373 K) of $[K(Et_2O)][Al(NON)(AdNC)_2]$ (**3·Et$_2$O**).

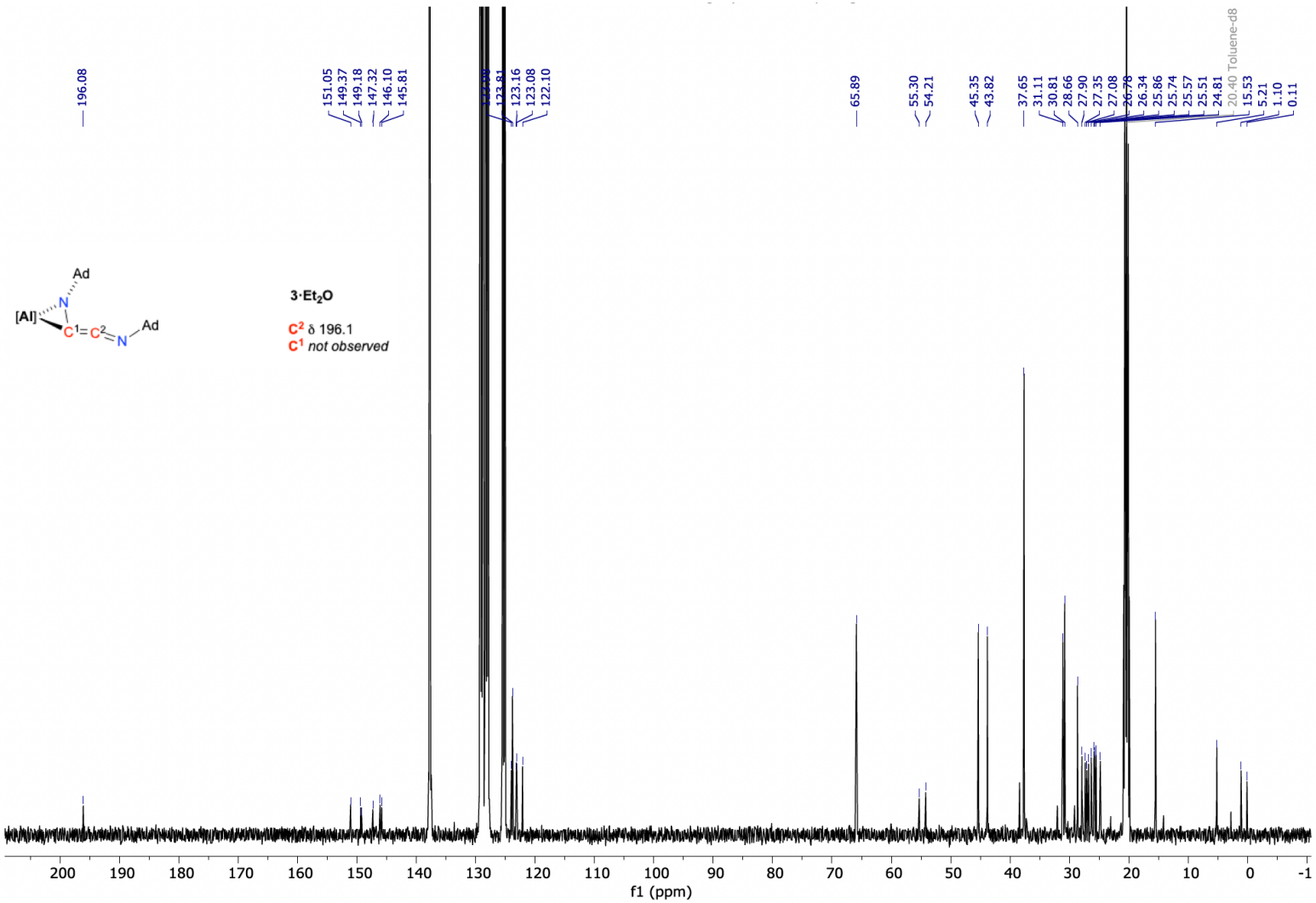
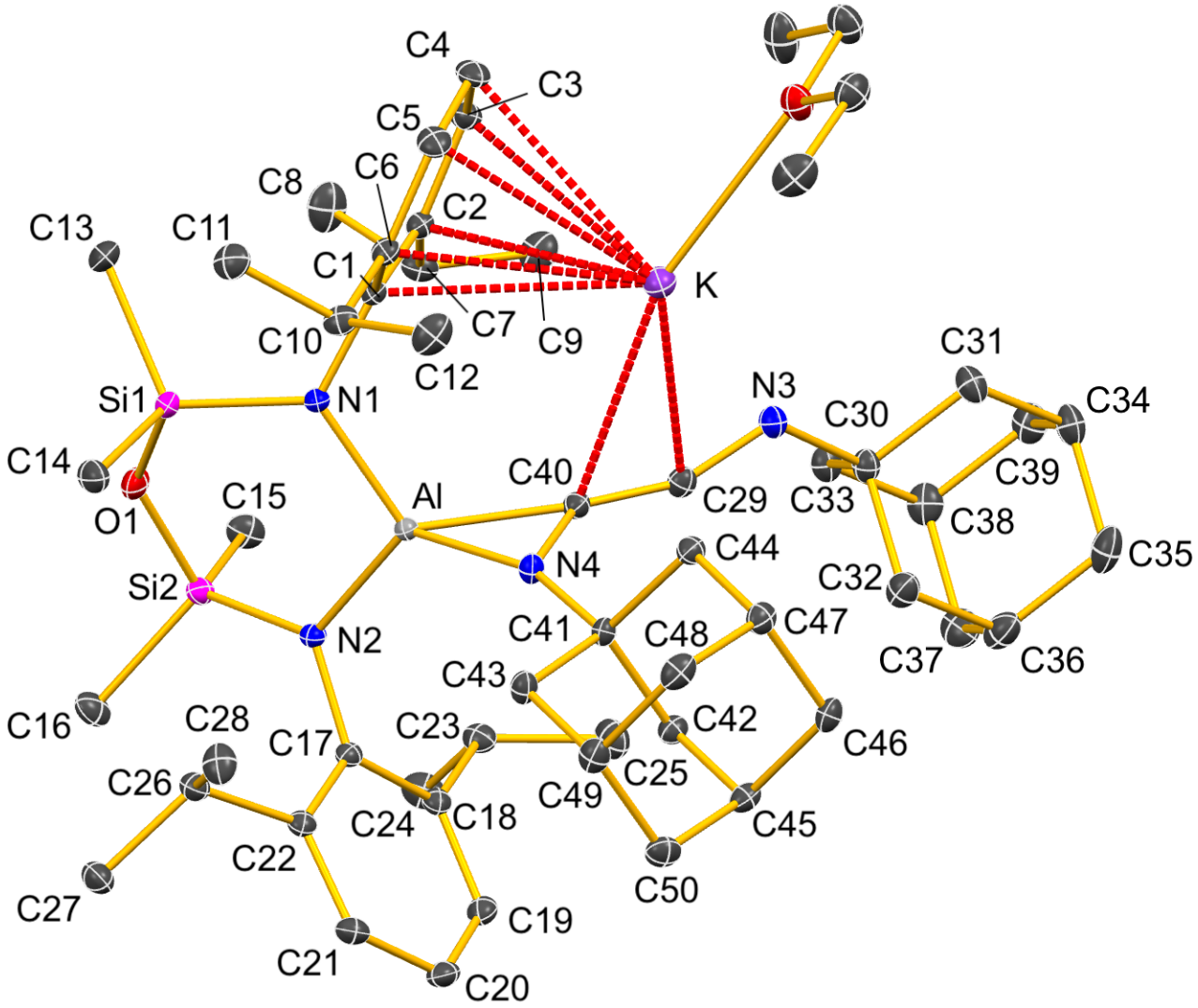


Figure S18 Displacement ellipsoid plot (30 %, H-atoms omitted) of $[K(Et_2O)][Al(NON)(AdNC)_2]$ (**3·Et$_2$O**)



Experimental Details for $[K(THF)_2][Al(NON)(AdNC)_2(DmpNC)]$ (4·THF)

A solution of $[K(Et_2O)_2][Al(NON)(AdNC)_2]$ (76 mg, 0.09 mmol) in THF-D_8 was added to a solution of 2,6-dimethylphenyl isonitrile (12 mg, 0.09 mmol) in a J Youngs fitted NMR tube. The mixture was allowed to react for 18 hours to give a dark red solution. The solution was transferred to a scintillation vial and the solvent removed *in vacuo*. Crystallisation was achieved by slow evaporation from a hexane/diethyl ether mixture stored at room temperature. Yield 70 mg, 75 %.

While the broadness of signals in the NMR spectra thwarted accurate spectroscopic characterisation, the observed signals do agree with the proposed structure determined from single crystal X-ray diffraction experiments.

Anal. Calcd. for $C_{67}H_{101}AlKN_5O_3Si_2$ (*1145.70*): C, 70.18; H, 8.88; N, 6.11 %. Found: C, 70.01; H, 8.74; N, 5.93 %.

^{1}H NMR (500 MHz, THF-D_8): δ 6.94 – 6.84 (m, 4H, C_6H_3), 6.76 – 6.67 (m, 2H, C_6H_3), 6.49 (br d, *J* = 7.3, 2H, C_6H_3), 6.32 (t, *J* = 7.3, 1H, C_6H_3), 4.10 (br sept, 4H, CHMe_2), 1.86 – 1.76 (m, 6H, *Ad*), 1.70 – 1.15 (m, 48H, *Ad*, CHMe_2, $C_6H_3Me_2$), 1.08 (br d, 6H, CHMe_2), 0.31 (s, 3H, SiMe_2), 0.26 (s, 3H, SiMe_2), 0.10 (s, 3H, SiMe_2), –0.02 (s, 3H, SiMe_2).

^{1}H NMR (500 MHz, THF-D_8, 333 K): δ 6.91 (dd, *J* = 14.8, 7.4, 4H, C_6H_3), 6.74 (t, *J* = 7.4, 2H, C_6H_3), 6.49 (d, *J* = 7.4, 2H, C_6H_3), 6.34 (t, *J* = 7.4, 1H, C_6H_3), 4.23 (br sept, 2H, C*H*Me_2), 4.02 (br sept, 2H, C*H*Me_2), 1.83 (br s, 6H, *Ad*), 1.59 – 1.40 (m, 22H, Ad, $C_6H_3Me_2$), 1.33 – 1.05 (m, 32H, Ad, CHMe_2),* 0.16 (br s, 12H, SiMe_2).

* overlapping doublets: 1.28 (d, *J* = 6.6), 1.20 (d, *J* = 6.7), 1.12 (d, *J* = 6.6).

^{13}C{^{1}H} NMR (126 MHz, THF-D_8): 209.5, 153.0 (N*C*), 148.5, 146.8, 127.0, 124.1, 123.9, 123.4, 121.7, 119.4 (C_6H_3), 59.0, 51.3, 43.6, 43.2, 38.0, 37.6, 31.1, 28.5, 28.3, 27.9, 27.7, 27.5, 18.9 (*Ad*, *C*HMe_2, $C_6H_3Me_2$), 4.8, 4.2, 3.5, 2.7 (SiMe_2).

Figure S19 ^{1}H NMR spectrum (500 MHz, THF-D_8) of [K(THF)$_2$][Al(NON)(AdNC)$_2$(DmpNC)] (**4·THF**).

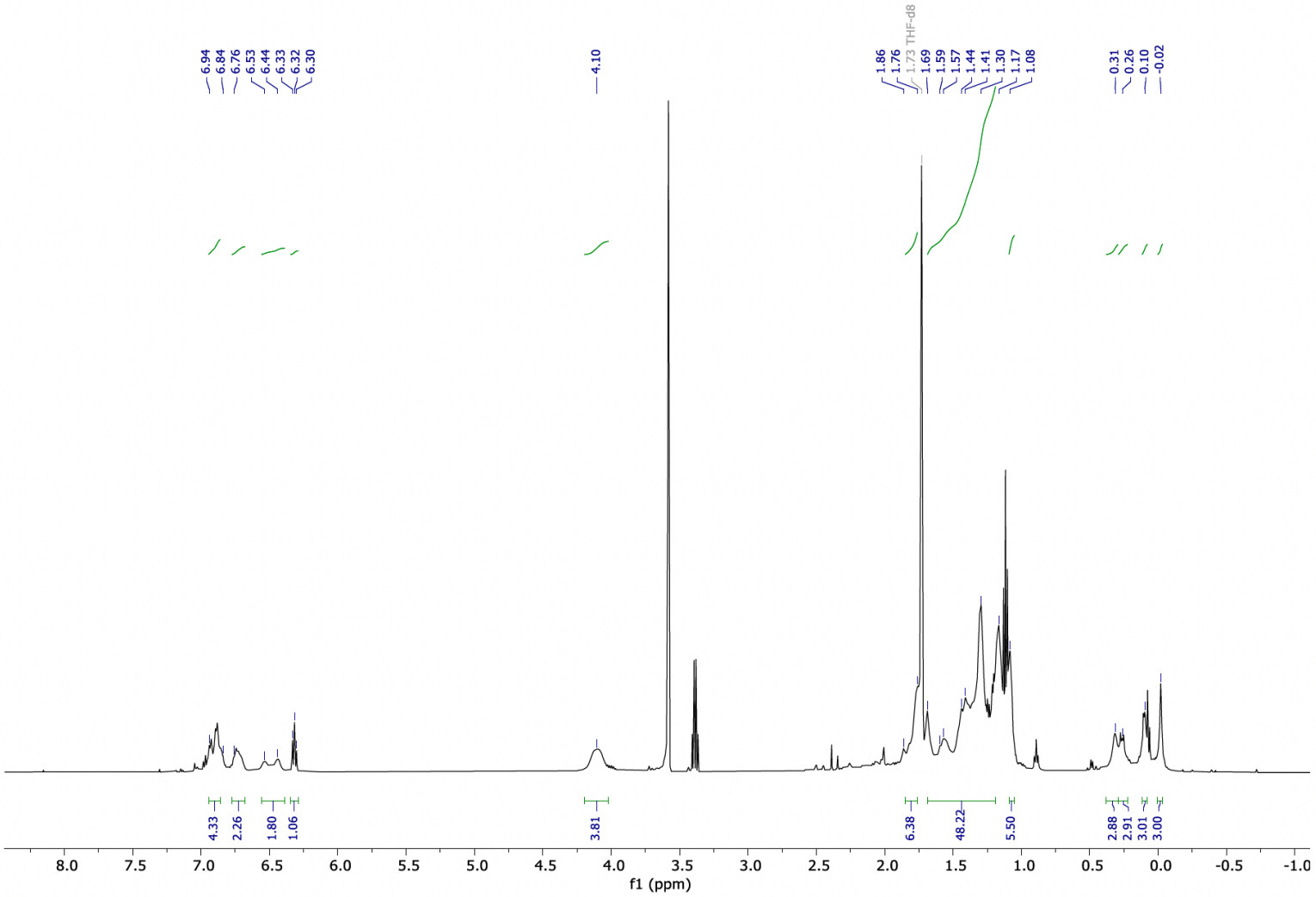


Figure S20 ^{1}H NMR spectrum (500 MHz, THF-D_8, 333 K) of $[K(THF)_2][Al(NON)(AdNC)_2(DmpNC)]$ (**4·THF**).

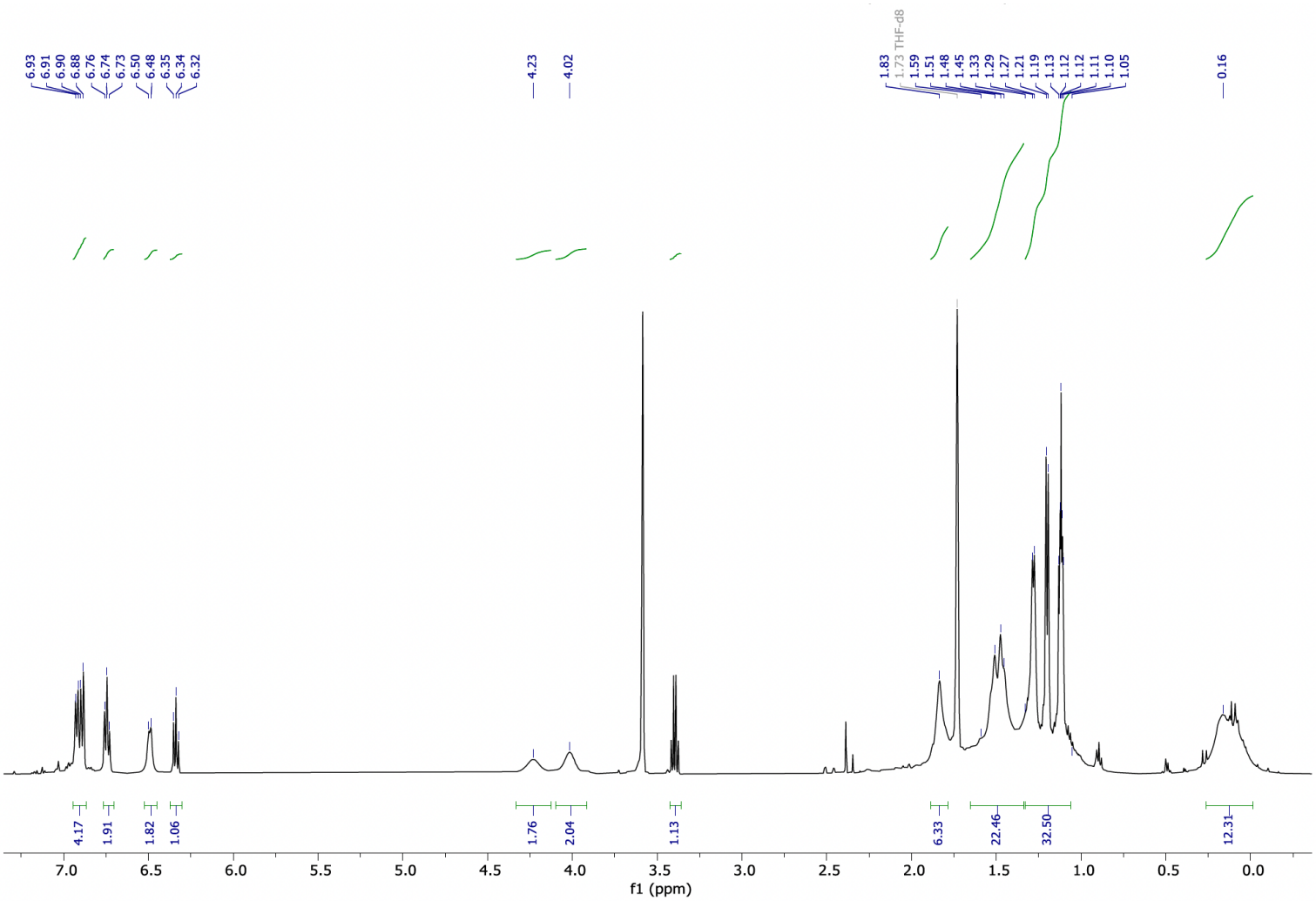


Figure S21 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, THF-D_8, 333 K) of $[K(THF)_2][Al(NON)(AdNC)_2(DmpNC)]$ (**4·THF**).

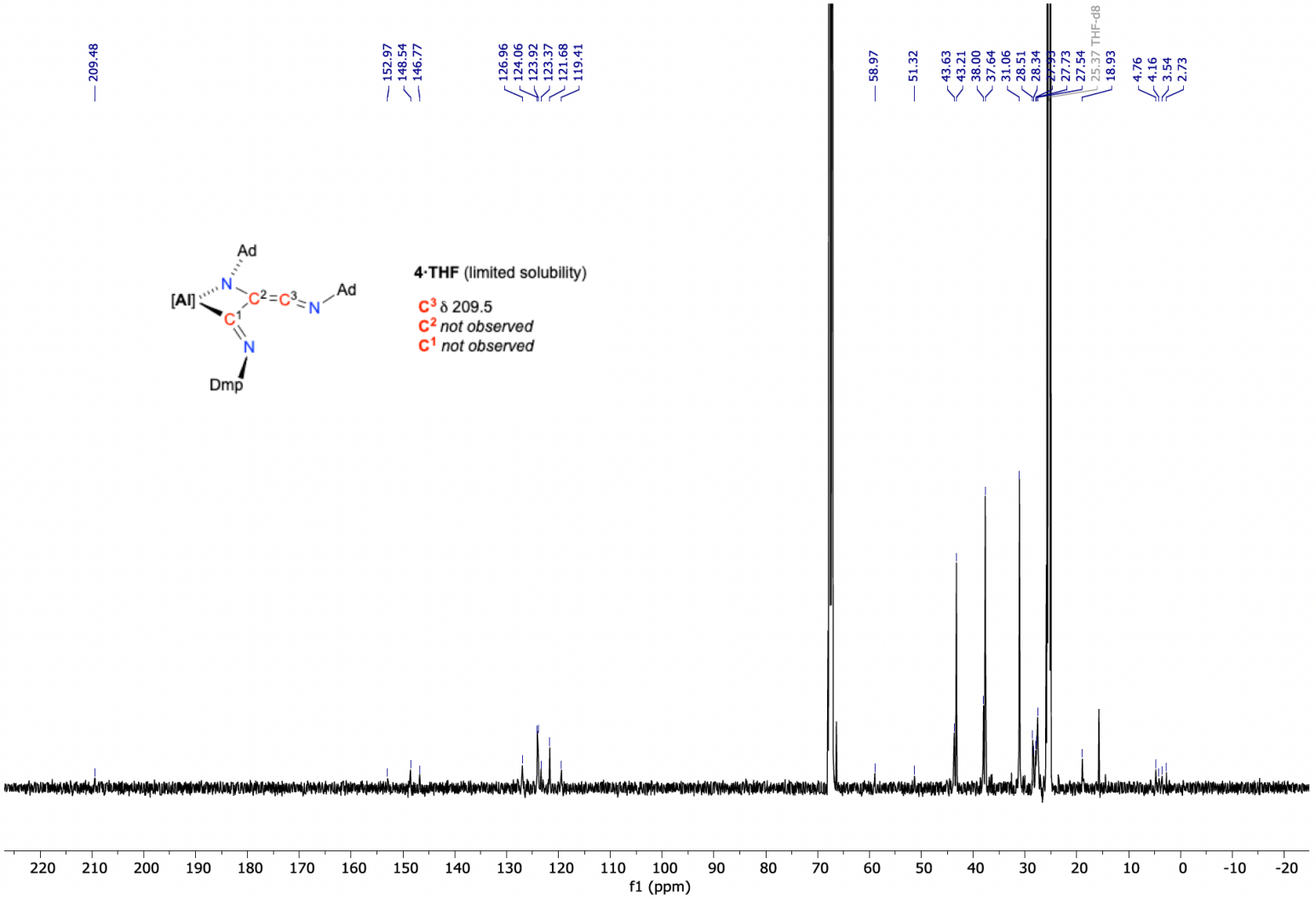
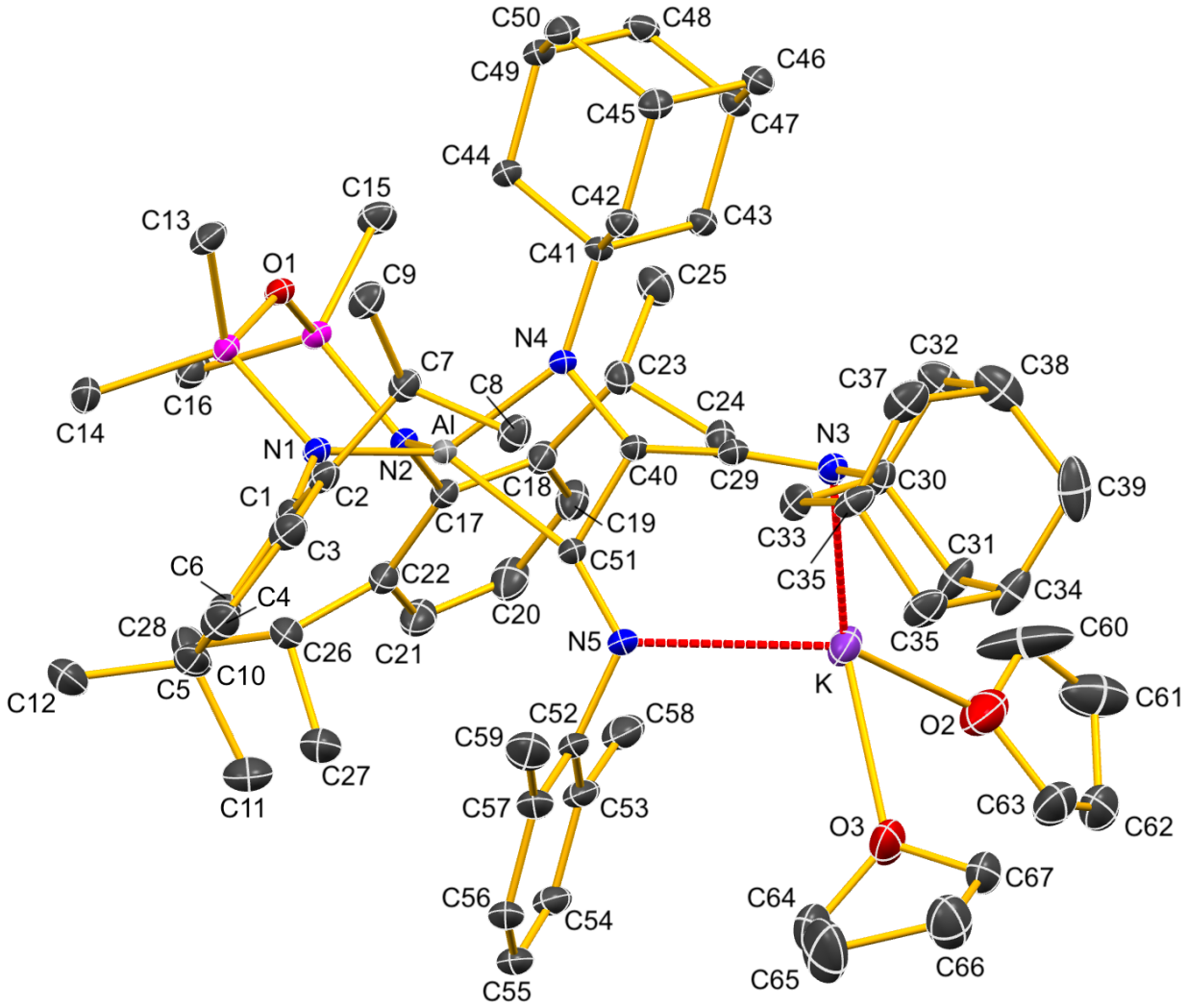


Figure S22 Displacement ellipsoid plot (20 %, H-atoms and disordered components omitted) of $[K(THF)_2][Al(NON)(AdNC)_2(DmpNC)]$ (**4·THF**).



Experimental Details for [K(toluene)][Al(NON)(AdNC)$_3$] (5·toluene)

A solution of 1-adamantyl isocyanide (49 mg, 0.30 mmol) in THF (~5 mL) was added to a stirred solution of [K{Al(NON)}]$_2$ (54 mg, 0.10 mmol) at room temperature. A dark red intermediate was observed upon addition of the reagents. The solution was allowed to stir for *ca.* 1 hour to give a bright orange solution. Crystallisation was achieved from a THF/toluene mixture stored at –30 °C for 18 hours. Yield 66 mg, 61 %.

Anal. Calcd. for $C_{68}H_{99}AlKN_5OSi_2$ (*1123.68*): C, 72.62; H, 8.88; N, 6.23 %. Found: C, 72.54; H, 8.57; N, 6.65 %.

^{1}H NMR (500 MHz, THF-D$_8$): δ 6.98 – 6.94 (m, 2H, C$_6$*H$_3$*), 6.92 – 6.88 (m, 2H, C$_6$*H$_3$*), 6.78 (d, *J* = 7.6, 1H, C$_6$*H$_3$*), 6.75 (d, *J* = 7.6, 1H, C$_6$*H$_3$*), 4.10 (sept, *J* = 6.8, 1H, C*H*Me$_2$), 4.02 – 3.92 (m, 2H, C*H*Me$_2$), 3.82 (sept, *J* = 6.8, 1H, C*H*Me$_2$), 3.62 (s, 4H, THF), 2.16 (br t, 3H, Ad), 2.08 – 1.94 (m, 10H, Ad), 1.85 – 1.71 (m, 18H, Ad, THF), 1.70 – 1.63 (m, 6H, Ad), 1.62 – 1.52 (m, 6H, Ad), 1.34 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.26 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.23 (d, *J* = 11.7, 5H, Ad), 1.19 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.17 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.15 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.16 – 1.12 (m, 3H, Ad), 1.10 (d, *J* = 6.8, 3H, CH*Me$_2$*), 1.08 (d, *J* = 6.8, 3H, CH*Me$_2$*), 0.99 (d, *J* = 6.8, 3H, CH*Me$_2$*), 0.78 – 0.71 (m, 3H, Ad), 0.30 (s, 3H, Si*Me$_2$*), 0.23 (s, 3H, Si*Me$_2$*), 0.20 (s, 3H, Si*Me$_2$*), –0.02 (s, 3H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, THF-D$_8$): δ 226.6 (C=*C*=C), 212.6 (C–*C*=N), 148.7, 147.7, 147.4, 147.4, 145.8, 145.0 (*C$_6$*H$_3$), 129.7, 129.0, 124.2, 124.1, 123.9, 123.8, 122.1, 121.9 (*C$_6$*H$_3$), 108.5 (C–*C*=C), 68.3 (THF), 61.0, 58.3, 50.7, 45.2, 45.0, 42.3, 38.0, 37.5*, 31.2*, 30.5 (Ad), 29.9, 29.3, 29.2, 28.3 (CH*Me$_2$*), 27.9, 27.9, 27.5* (*C*HMe$_2$), 27.4 (CH*Me$_2$*), 26.4 (THF), 26.2, 26.0, 25.9 (CH*Me$_2$*), 7.2, 6.7, 5.9, 3.3 (Si*Me$_2$*).

*overlapping ^{13}C signal (appearing as a single signal).

Figure S23 ^{1}H NMR spectrum (500 MHz, THF-D_8) of [K(toluene)][Al(NON)(AdNC)$_3$] (**5·toluene**)

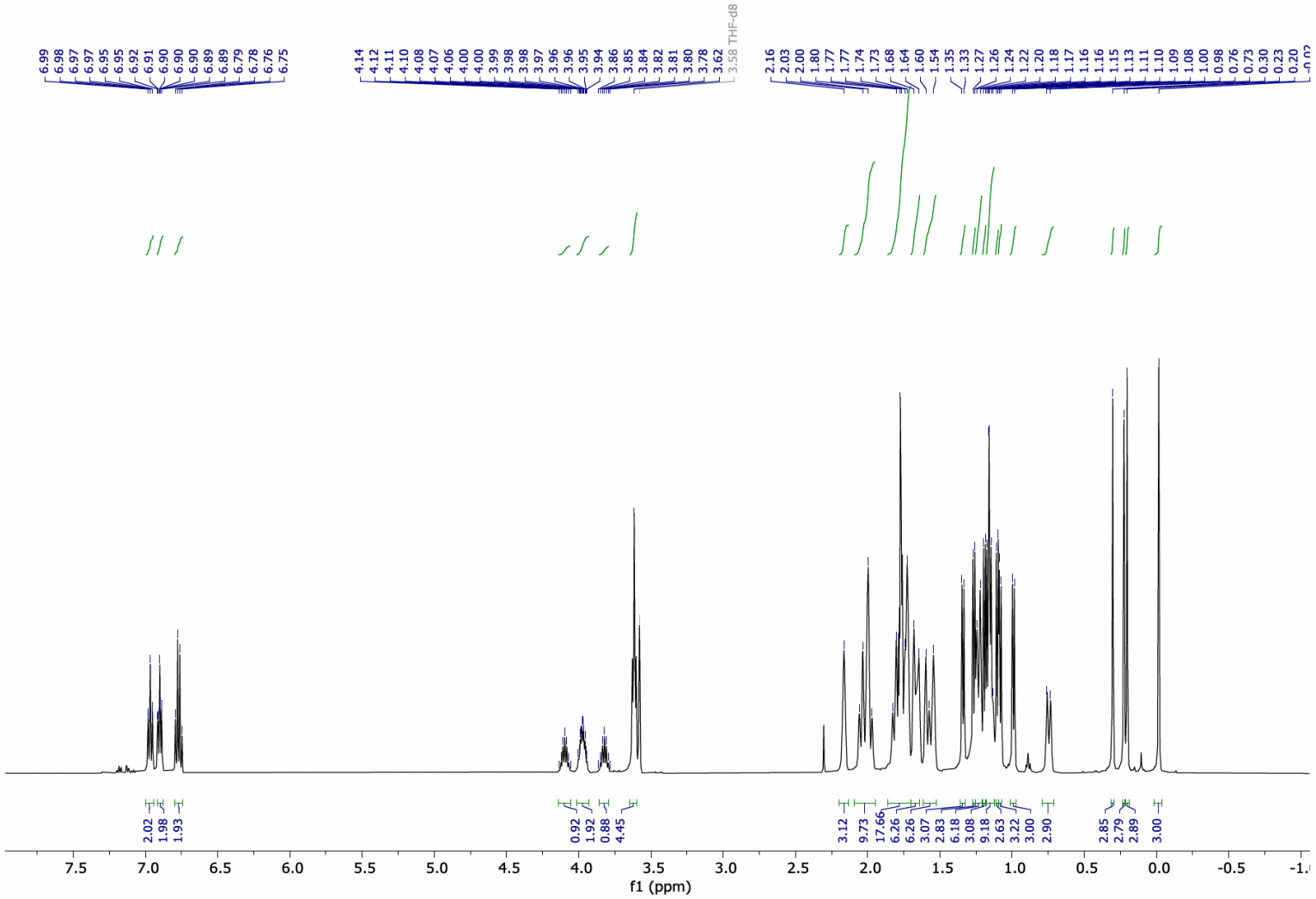


Figure S24 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, THF-D_8) of [K(toluene)][Al(NON)(AdNC)$_3$] (**5·toluene**)

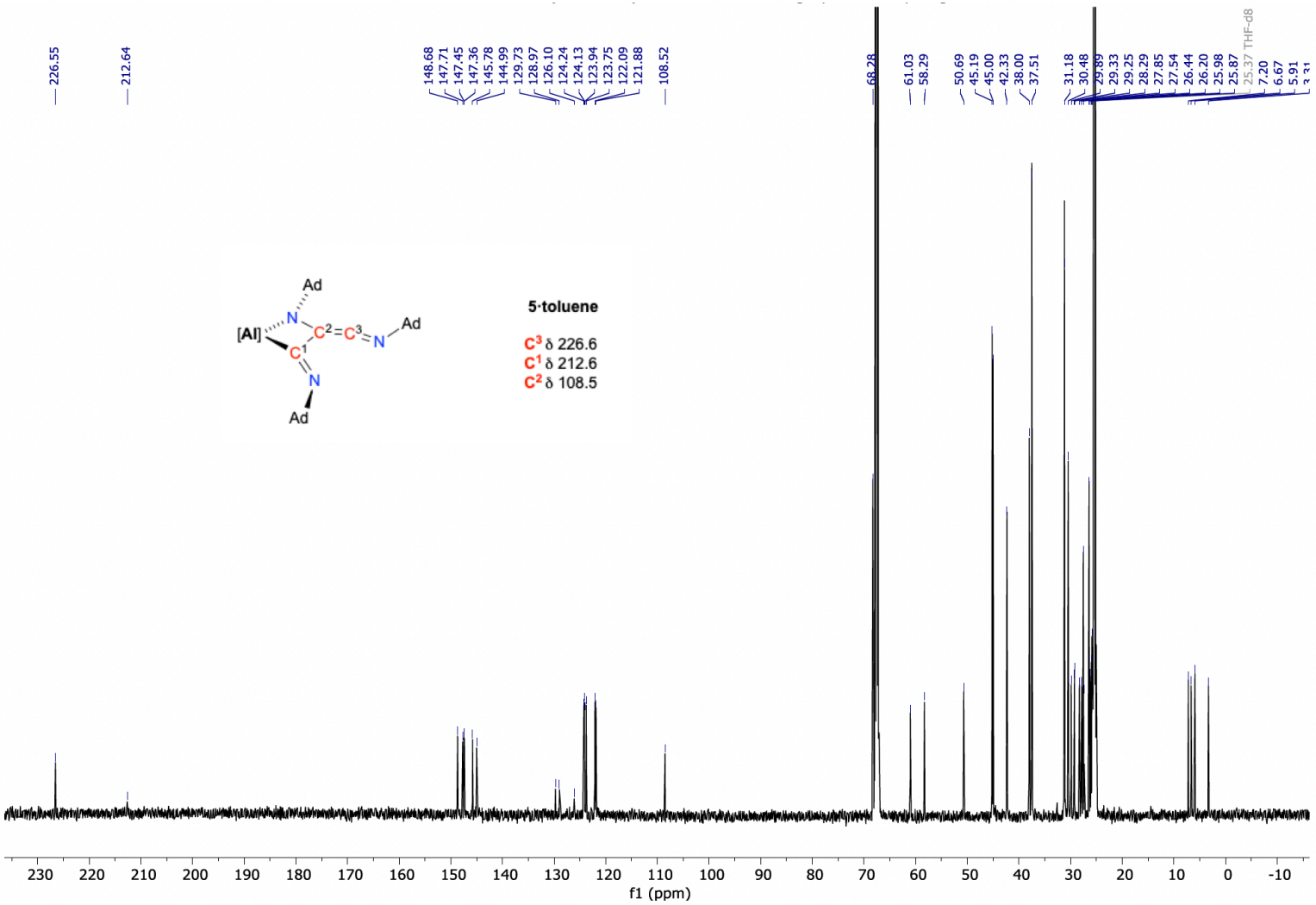
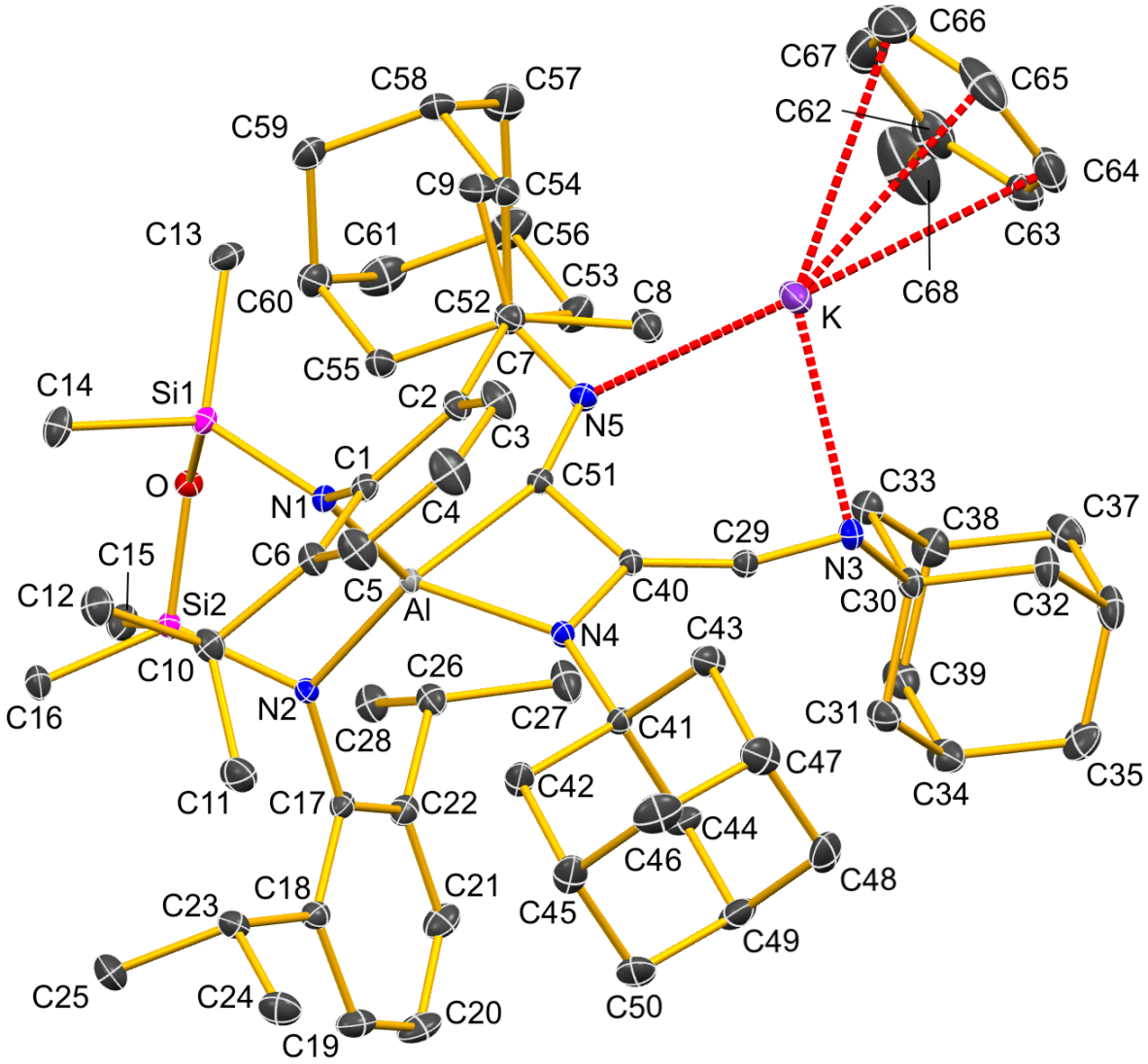


Figure S25 Displacement ellipsoid plot (30 %, H-atoms omitted) of [K(toluene)][Al(NON)(AdNC)$_3$] (**5·toluene**).



Crystallographic Details

Crystals were covered in inert oil and suitable single crystals were selected under a microscope and mounted on an Agilent SuperNova diffractometer fitted with an EOS S2 detector. Data were collected at 120 K (unless indicated otherwise) using focused microsource Cu Kα radiation at 1.54184 Å. Intensities were corrected for Lorentz and polarisation effects and for absorption using multi-scan methods.[2] Space groups were determined from systematic absences and checked for higher symmetry. All structures were solved using direct methods with SHELXS,[3] refined on F^2 using all data by full matrix least-squares procedures with SHELXL-97,[4] within the WinGX[5] program. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in calculated positions or manually assigned from residual electron density where appropriate, unless otherwise stated. The functions minimized were Σ*w*(*F2*o-*F2c),* with *w* = [σ2(F2o) + *a*P2 + *bP*]-1, where *P* = [max(Fo)2 + 2F2c]/3. The isotropic displacement parameters are 1.2 or 1.5 times the isotropic equivalent of their carrier atoms.

Additional Details:

*K[Al(NON)(H)(CN)] (**1a**)*: The unit cell contains a half of a poorly defined THF solvent molecule that lies on a 2-fold rotation access. A suitable model for this could not be developed and so it was treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. Details included in the .cif.

*[K(2.2.2)crypt][Al(NON)(H)(CN)] (**1-crypt**)*: The Al(H) unit is disordered over two positions located above and below the approximate plane of the ligand, with some additional disorder modelled in the iPr and Si-O-Si components of the ligand. Due to this disorder, the hydride ligands could not be located on the Al atoms. They were placed in calculated positions for a tetrahedral metal (HFIX 13) and the Al–H distance contained to be 1.6 A (in accordance with related structures).

K[Al(NON){(DmpNC)$_2$(DmpNC)]·2(C_7H_8) (**2·toluene**)*: A residual electron density peak from the diffraction located between 3 × alkyl groups was assigned to a low occupancy position for the potassium cation. The disordered toluene (about an inversion centre) forms a π-interaction with this low occupancy K^+, and is located between the 1-D chains that are formed when the major occupancy K^+ interacts with the oxygen atom of the ligand scaffold in an adjacent molecule.

*[K(THF)$_2$][Al(NON)(AdNC)$_2$(DmpNC)] (**4·THF**)*: There is significant disorder in the molecule due to the presence of either THF / Et2O at one of the coordination sites of potassium. This was modelled as THF (67.4%) and Et2O (30.6%), leading to the non-integer value for the number of hydrogen atoms in the asymmetric unit. This substitution caused additional disorder in the molecule which was modelled for the major components but ignored for the minor components (leading to the Alert Level B concerning the large Ueq(max)/Ueq(min) or carbon).

Table S1 Crystal structure and refinement data for K[Al(NON)(H)(CN)] (**1a**), [K(2.2.2)crypt][Al(NON)(H)(CN)] (**1-crypt**), [K(Et_2O)$_2$][Al(NON){(DmpNC)$_2$(DmpNC*)] (**2·Et_2O**, * = ring activated DmpNC) and K[Al(NON){(DmpNC)$_2$(DmpNC*)]·2(C_7H_8) (**2·toluene**, * = ring activated DmpNC).

	1a	**1·crypt**	**2·Et_2O**	**2·toluene**
Empirical formula	$C_{31}H_{51}AlKN_3O_{1.5}Si_2$	$C_{47}H_{83}AlKN_5O_7Si_2$	$C_{63}H_{93}AlKN_5O_3Si_2$	$C_{131}H_{170}Al_2K_2N_{10}O_2Si_4$
CCDC Number	2247345	2247346	2247347	2247348
M_r	612.00	952.44	1090.68	2161.28
T [K]	150.0(1)	120.1(2)	120.01(10)	120.01(10)
Crystal size [mm]	0.34 × 0.26 × 0.22	0.25 × 0.21 × 0.12	0.24 × 0.14 × 0.09	0.20 × 0.09 × 0.08
Crystal system	Monoclinic	Triclinic	Monoclinic	Triclinic
Space group	I2/*a* (alternative No.15)	$P\bar{1}$ (No.2)	$P2_1/c$ (No.14)	$P\bar{1}$ (No.2)
a [Å]	18.16775(17)	12.3130(3)	11.59172(14)	11.0552(3)
b [Å]	13.05007(9)	12.5109(3)	22.52352(17)	11.8345(3)
c [Å]	30.7237(2)	19.2634(5)	24.5925(2)	23.9671(7)
α [°]	90	104.783(2)	90	82.310(2)
β [°]	102.7091(8)	105.037(2)	96.0048(9)	76.873(2)
γ [°]	90	99.317(2)	90	80.547(2)
V [Å^3]	7105.83(9)	2687.05(13)	6385.53(11)	2997.04
Z	8	2	4	1
$D_{calc.}$ [mg m^{-3}]	1.144	1.177	1.135	1.198
Absorption coefficient [mm^{-1}]	2.41	1.85	1.57	1.65
θ **range for data collection [°]**	3.694 to 73.296	3.768 to 73.236	3.614 to 73.313	3.806 to 73.303
Reflections collected	48752	30839	45551	39077
Independent reflections	7138 [R_{int} 0.029]	10624 [R_{int} 0.023]	12745 [R_{int} 0.029]	11958 [R_{int} 0.048]
Reflections with $I > 2\sigma(I)$	6775	10030	11417	10186
Data/restraints/parameters	7138 / 0 / 351	10624 / 2 / 682	12745 / 0 / 698	11958 / 0 / 725
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.038, wR_2 = 0.111	R_1 = 0.081, wR_2 = 0.187	R_1 = 0.035, wR_2 = 0.089	R_1 = 0.090 wR_2 = 0.227
Final R indices (all data)	R_1 = 0.040, wR_2 = 0.112	R_1 = 0.084, wR_2 = 0.189	R_1 = 0.040, wR_2 = 0.092	R_1 = 0.102, wR_2 = 0.234
GOOF on F^2	1.027	1.12	1.003	1.101
Largest diff. peak/hole [e.Å^{-3}]	0.86 and –0.45	1.00 and –0.81	0.30 and –0.29	0.979 and –0.669

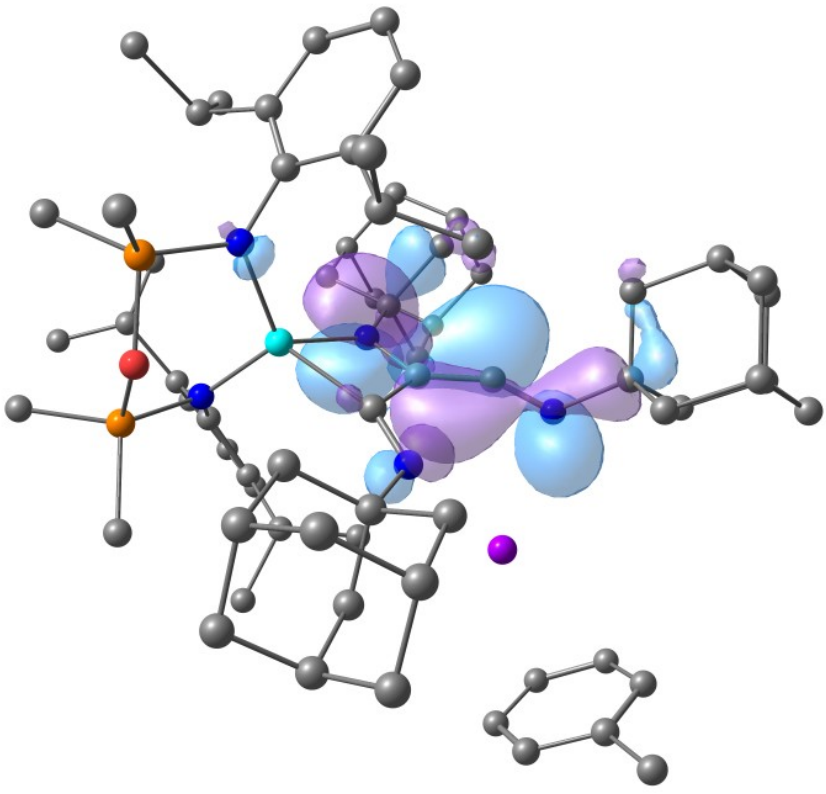
Table S2 Crystal structure and refinement data for $K(Et_2O)][Al(NON)(AdNC)_2]$ (**3·Et₂O**), $[K(THF)_2][Al(NON)(AdNC)_2(DmpNC)]$ (**4·THF**) and $[K(toluene)][Al(NON)(AdNC)_3]$ (**5·toluene**).

	3·Et₂O	**4·THF**	**5·toluene**
Empirical formula	$C_{54}H_{86}AlKN_4O_2Si_2$	$C_{67}H_{101.61}AlKN_5O_3Si_2$	$C_{68}H_{99}AlKN_5OSi_2$
CCDC Number	2247349	2247350	2247351
M_r	945.52	1147.4	1124.78
T [K]	125(7)	150.00(10)	150.00(10)
Crystal size [mm]	0.24 × 0.15 × 0.10	0.15 × 0.14 × 0.09	0.24 × 0.09 × 0.06
Crystal system	Orthorhombic	Triclinic	Monoclinic
Space group	Pbca (No. 61)	$P\bar{1}$ (No.2)	C*c* (No. 9)
a [Å]	22.07209(13)	12.7748(6)	36.4496(7)
b [Å]	19.95370(13)	14.6769(7)	12.44536(9)
c [Å]	24.45220(16)	19.1675(8)	20.2703(4)
α [°]	90	84.046(4)	90
β [°]	90	88.135(4)	136.513(3)
γ [°]	90	65.381(5)	90
V [Å^3]	10769.23(12)	3249.3(3)	6328.05(18)
Z	8	2	4
$D_{calc.}$ [mg m^{-3}]	1.167	1.173	1.181
Absorption coefficient [mm^{-1}]	1.176	1.1564	1.575
θ **range for data collection [°]**	3.490 to 73.461	3.806 to 73.238	3.524 to 73.290
Reflections collected	137184	43228	20829
Independent reflections	10812 [R_{int} 0.063]	12963 [R_{int} 0.042]	8059
Reflections with $I > 2\sigma(I)$	10149	10297	7878
Data/restraints/parameters	10812 / 0 / 591	12963 / 0 / 864	8059 / 2 / 716
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.035, wR_2 = 0.093	R_1 = 0.058, wR_2 = 0.143	R_1 = 0.024, wR_2 = 0.060
Final R indices (all data)	R_1 = 0.037, wR_2 = 0.095	R_1 = 0.075, wR_2 = 0.153	R_1 = 0.025, wR_2 = 0.061
GOOF on F^2	1.033	1.032	1.011
Largest diff. peak/hole [e.Å^{-3}]	0.30 and –0.47	0.57 and –0.67	0.20 and –0.21

Computational Methodology

DFT calculations were run with Gaussian 16 (C.01).[6] The Al, Si and K centres were described with the Stuttgart RECPs and associated basis sets,[7] and the 6-31G** basis set was used for all other atoms (BS1).[8] A polarization function was also added to Al (ζ_d = 0.190), Si (ζ_d = 0.284) and K (ζ_d = 1.000). Initial BP86 optimizations were performed using the 'grid = ultrafine' option,[9] with all stationary points being fully characterized via analytical frequency calculations as minima or transition states (all positive eigenvalues or one imaginary eigenvalue respectively), and with intrinsic reaction coordinate calculations confirming the connectivity of the reaction pathways. All energies were recomputed with a larger basis set featuring 6-311++G** basis sets on all atoms (BS2). Corrections for the effect of toluene (ε = 2.3741) solvent were run using the polarizable continuum model and BS1,[10] using the keyword "scrf=toluene" within Gaussian. Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[11] Natural Bonding Orbital (NBO7)[12] analyses were performed on the BP86-optmised geometries at the BP86/6-311++G** level, within Gaussian 16 (C.01).

Figure S26 Representation of the HOMO of [K(toluene)][Al(NON)(AdNC)$_3$] (**5·toluene**)



Breakdown of Energy Contributions

The following tables detail the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

$\mathbf{\Delta E_{BSI}}$	SCF energy computed with the BP86 functional with BS1
$\mathbf{\Delta H_{BSI}}$	Enthalpy at 0 K with BS1
$\mathbf{\Delta G_{BSI}}$	Free energy at 298.15 K and 1 atm with BS1
$\mathbf{\Delta G_{BSI/}}\boldsymbol{tol}$	Free energy corrected for toluene solvent with BS1
$\mathbf{\Delta G_{BSI/}}\boldsymbol{tol}\mathbf{+D3BJ}$	Free energy corrected for toluene and dispersion effects with BS1
$\mathbf{\Delta E_{BS2}}$	SCF energy computed with the BP86 functional with BS2
$\mathbf{\Delta G_{}}\boldsymbol{tol}$	Free energy corrected for basis set (BS2), dispersion effects and toluene solvent

In each case the final data used in the main article are highlighted in bold. Free energies are quoted in kcal mol^{-1}, and include all three single point corrections (for BS2, solvation and dispersion).

Table S3. Relative energies for computed structures(kcal mol^{-1}). Data in bold is at the same level as free energies used in the text. Free energies are quoted relative to **A**.

	ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/tol}$	$\Delta G_{BSI/tol+D3BJ}$	ΔE_{BS2}	ΔG_{tol}
A	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
B	-1.2	-0.4	7.3	7.9	-1.5	1.4	**1.1**
B′	-2.4	-2.1	3.2	3.6	-1.5	-0.2	**0.7**
C	-2.1	-1.2	11.0	11.9	1.0	1.4	**4.5**
TS(C-D)	-2.3	-1.3	11.6	12.5	-0.7	2.2	**3.8**
D	-2.6	-1.6	10.7	11.6	-2.8	2.2	**1.9**
E	-4.5	-3.3	14.8	15.4	1.0	2.3	**7.8**
TS(E-F)	3.5	4.5	23.7	24.6	6.4	9.4	**12.3**
F	-5.7	-4.1	15.8	17.4	-7.5	-0.3	**-2.1**
G	3.7	5.1	18.0	16.1	8.0	6.6	**10.9**
TS(G-H)	10.4	11.4	31.9	32.3	13.8	12.1	**15.5**
H	-48.0	-44.7	-22.2	-21.3	-45.1	-45.1	**-42.2**
G·Et$_2$O	0.2	1.7	19.0	17.9	4.0	4.0	**7.9**
TS(G·Et$_2$O-3·Et$_2$O)	1.0	2.7	33.9	36.3	5.1	6.1	**10.2**
3·Et$_2$O	-58.0	-54.4	-21.8	-18.9	-52.0	-52.7	**-46.6**
I	-45.3	-40.7	-2.3	0.0	-44.8	-37.9	**-37.3**
J	-55.7	-52.0	-18.9	-16.0	-46.5	-49.1	**-40.0**
TS(I-K)	-38.7	-35.3	3.9	5.0	-42.8	-31.0	**-34.1**
TS(J-K)	-16.0	-11.7	26.8	29.9	-14.3	-7.4	**-5.7**
K	-65.8	-59.8	-21.3	-21.7	-70.0	-56.8	**-60.9**
4·THF	-86.5	-79.1	-18.5	-14.1	-81.1	-72.3	**-66.8**
L	-38.4	-34.5	-3.1	-2.3	-41.9	-30.3	**-33.8**
TS(L-M)	-24.5	-20.1	-17.9	19.3	-27.5	-14.9	**-18.0**
M	-63.6	-57.6	-18.9	-18.2	-69.6	-55.9	**-59.9**
I′	-45.6	-41.1	-4.7	-2.5	-44.0	-37.9	**-36.2**
J′	-60.2	-56.4	-25.0	-21.6	-48.5	-53.0	**-41.3**
TS(I′-K′)	-39.9	-35.6	2.0	2.8	-47.5	-31.9	**-39.4**
TS(J′-K′)	-19.3	-15.7	21.1	24.3	-19.5	-9.9	**-10.6**
K′	-66.2	-60.4	-22.3	-21.8	-71.3	-56.5	**-61.6**
5·toluene	-73.3	-66.9	-19.4	-16.2	-74.0	-61.5	**-62.3**
L′	-46.9	-42.6	-10.3	-8.6	-43.2	-36.9	**-33.3**
TS(L′-K′)	-22.4	-18.2	18.7	19.9	-23.0	-13.4	**-14.0**

Figure S27 DFT computed free energy profile (BP86-D3BJ,(PCM=toluene)/BS2//BP86/BS1, in kcal mol^{-1}) for splitting the [K{Al(NON)}]$_2$ (**A**) dimer and coordination of Ad-NC.

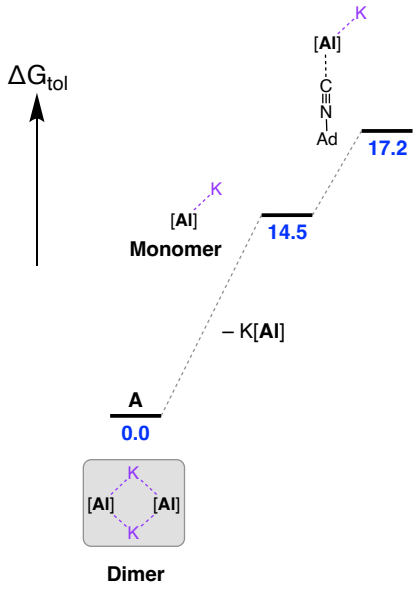


Figure S28 DFT computed free energy profile (BP86-D3BJ,(PCM=toluene)/BS2//BP86/BS1, in kcal mol^{-1}) for the coordination of three equivalents of Ad-NC to [K{Al(NON)}]$_2$ (**A**)

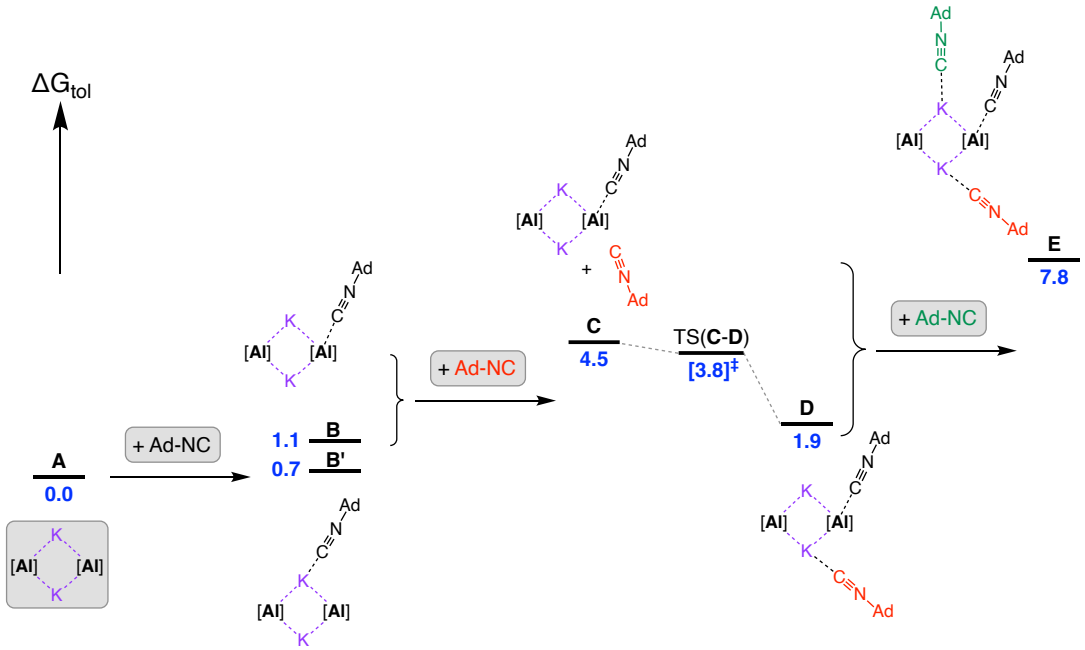


Figure S29 DFT computed free energy profile (BP86-D3BJ,(PCM=toluene)/BS2//BP86/BS1, in kcal mol^{-1}) for the Et_2O assisted coupling of two Ad-NC molecules.

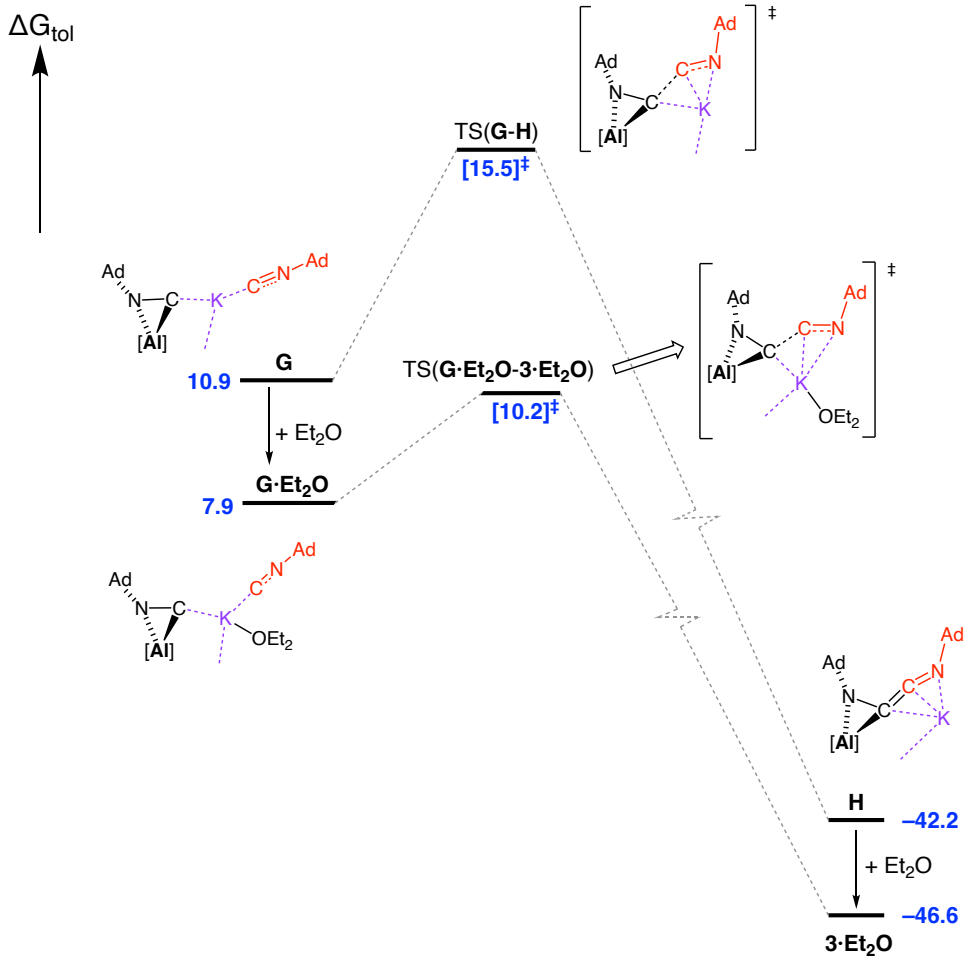


Figure S30 DFT computed free energy profile (BP86-D3BJ,(PCM=toluene)/BS2//BP86/BS1, in kcal mol^{-1}) for the formation of the hypothetical {$Ad_{am}Dmp_{ket}Ad_{im}$} isomer of K[Al(NON)$(AdNC)_2$(DmpNC)].

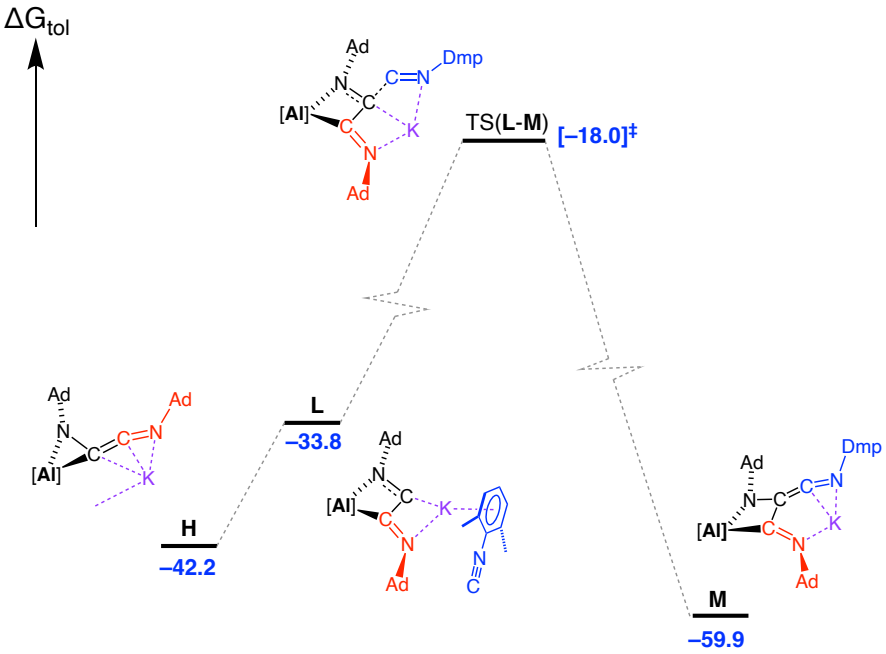


Figure S31 DFT computed free energy profile (BP86-D3BJ,(PCM=toluene)/BS2//BP86/BS1, in kcal mol^{-1}) for the formation of [K(toluene)][Al(NON)(AdNC)$_3$] (**5·toluene**).

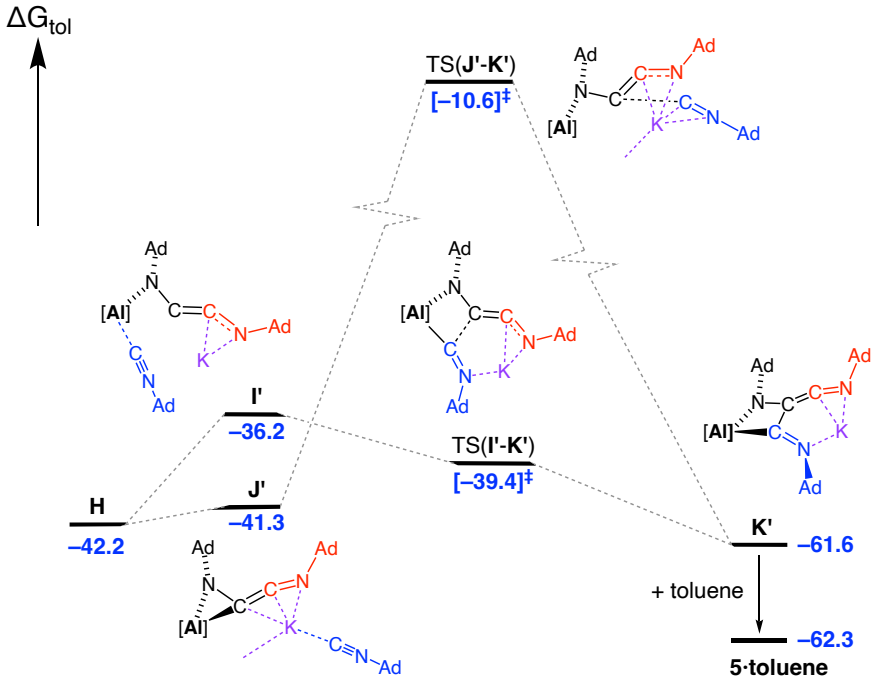
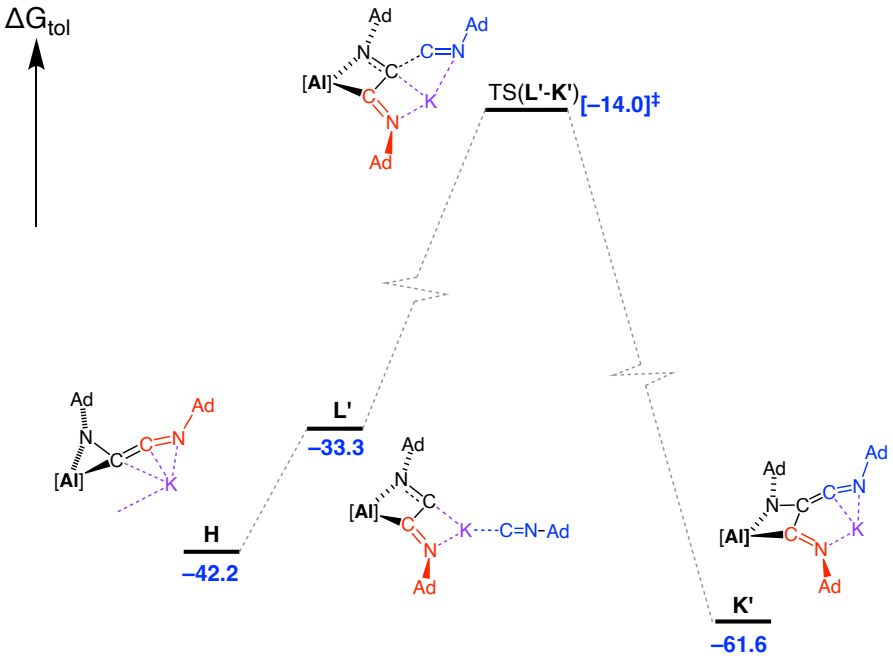


Figure S32 DFT computed free energy profile (BP86-D3BJ,(PCM=toluene)/BS2//BP86/BS1, in kcal mol^{-1}) for the formation of K[Al(NON)(AdNC)$_3$] via the third pathway.



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Cartesian Coordinates and Computed Energies [in Hartrees] for Calculated Structures

AdNC
SCF (BP86) Energy = -482.928833186
Enthalpy 0K = -482.694447
Enthalpy 298K = -482.684176
Free Energy 298K = -482.727013
Lowest Frequency = 132.0188 cm^{-1}
Second Frequency = 132.0192 cm^{-1}
SCF (BP86-D3BJ) Energy = -482.983068007
SCF (tol) Energy = -482.931714038
SCF (BS2) Energy = -483.043305574

N	0.00000	0.00000	2.49479
C	-0.00000	0.00000	3.68647
C	0.00000	0.00000	1.05755
C	-0.00000	1.46410	0.53700
H	-0.89040	1.98845	0.92948
H	0.89040	1.98845	0.92948
C	1.26795	-0.73205	0.53700
H	1.27685	-1.76533	0.92948
H	2.16725	-0.22312	0.92948
C	-1.26795	-0.73205	0.53700
H	-2.16725	-0.22312	0.92948
H	-1.27685	-1.76533	0.92948
C	-0.00000	1.45998	-1.01050
H	-0.00000	2.50569	-1.37038
C	1.26425	0.72992	-1.52446
H	1.28484	0.74180	-2.63063
H	2.17491	1.25568	-1.17939
C	1.26438	-0.72999	-1.01050
H	2.16999	-1.25284	-1.37038
C	-0.00000	-1.45983	-1.52446
H	-0.00000	-1.48360	-2.63063
H	-0.00000	-2.51137	-1.17939
C	-1.26438	-0.72999	-1.01050
H	-2.16999	-1.25284	-1.37038
C	-1.26425	0.72992	-1.52446
H	-1.28484	0.74180	-2.63063
H	-2.17491	1.25568	-1.17939

Ar'NC
SCF (BP86) Energy = -403.086260309
Enthalpy 0K = -402.936922
Enthalpy 298K = -402.926064
Free Energy 298K = -402.971842
Lowest Frequency = 104.0377 cm^{-1}
Second Frequency = 104.4888 cm^{-1}
SCF (BP86-D3BJ) Energy = -403.119812143
SCF (tol) Energy = -403.088797622
SCF (BS2) Energy = -403.186415552

N	1.82997	-0.00196	0.00004
C	3.02552	-0.00310	-0.00009
C	0.44090	-0.00048	0.00002
C	-0.23753	1.24578	-0.00005
C	-0.24018	-1.24530	0.00006
C	0.53634	2.54192	0.00004
H	-0.14541	3.40639	0.00088
H	1.19257	2.61861	-0.88474
H	1.19371	2.61783	0.88406
C	0.53093	-2.54308	0.00000
H	1.18816	-2.62039	-0.88400
H	-0.15266	-3.40610	-0.00086
H	1.18696	-2.62116	0.88481
C	-1.64281	1.21799	-0.00003
H	-2.19021	2.16677	-0.00005
C	-2.34285	0.00248	-0.00002
H	-3.43764	0.00365	-0.00004
C	-1.64540	-1.21452	0.00000
H	-2.19482	-2.16212	0.00001

Et_2O
SCF (BP86) Energy = -233.654981611
Enthalpy 0K = -233.521943
Enthalpy 298K = -233.514142
Free Energy 298K = -233.552232
Lowest Frequency = 64.8588 cm^{-1}
Second Frequency = 127.4962 cm^{-1}
SCF (BP86-D3BJ) Energy = -233.669091718
SCF (tol) Energy = -233.656181129
SCF (BS2) Energy = -233.719121473

O	0.00000	-0.00099	0.84706
C	-1.00272	-0.66248	0.06724
H	-1.41089	-1.45617	0.71844
H	-0.55431	-1.16692	-0.81492
C	-2.12608	0.28358	-0.37343
H	-1.74876	1.08285	-1.03404
H	-2.59416	0.75819	0.50446
H	-2.90411	-0.26972	-0.92834
C	1.00248	0.66219	0.06851
H	1.41052	1.45504	0.72087
H	0.55411	1.16820	-0.81280
C	2.12627	-0.28268	-0.37391
H	1.74946	-1.08078	-1.03627
H	2.59450	-0.75876	0.50310
H	2.90399	0.27234	-0.92749

THF
SCF (BP86) Energy = -232.447574761
Enthalpy 0K = -232.333967
Enthalpy 298K = -232.327978
Free Energy 298K = -232.363078
Lowest Frequency = 23.1459 cm^{-1}
Second Frequency = 275.4150 cm^{-1}
SCF (BP86-D3BJ) Energy = -232.461052284
SCF (tol) Energy = -232.448939410
SCF (BS2) Energy = -232.511411715

C	1.11953	0.49016	0.18507
O	-0.01624	1.21238	-0.30202
C	-1.14796	0.45256	0.13889
C	-0.75507	-1.04216	-0.02233
C	0.80213	-0.99935	-0.08328
H	2.01008	0.86631	-0.34439
H	1.25822	0.66776	1.27604
H	-1.37417	0.67882	1.20507
H	-2.01389	0.75889	-0.47051
H	-1.12708	-1.64979	0.81904
H	-1.17361	-1.46775	-0.94858
H	1.27911	-1.66696	0.65304
H	1.15943	-1.29360	-1.08365

Toluene (C_7H_8)
SCF (BP86) Energy = -271.559258300
Enthalpy 0K = -271.434922
Enthalpy 298K = -271.427572
Free Energy 298K = -271.465923
Lowest Frequency = 28.3294 cm^{-1}
Second Frequency = 202.7397 cm^{-1}
SCF (BP86-D3BJ) Energy = -271.581062958
SCF (tol) Energy = -271.560402015
SCF (BS2) Energy = -271.625271775

C	-0.92053	0.00004	-0.01165
C	-0.19617	1.20974	-0.00911
H	-0.74140	2.16116	-0.01831
C	1.20734	1.21260	0.00222
H	1.74901	2.16477	0.00117
C	1.91519	-0.00003	0.00875
H	3.01024	-0.00006	0.01406
C	1.20727	-1.21263	0.00222
H	1.74891	-2.16482	0.00117
C	-0.19622	-1.20972	-0.00911
H	-0.74149	-2.16111	-0.01832
C	-2.43510	0.00002	0.00929
H	-2.84731	0.89355	-0.48855
H	-2.82133	-0.00239	1.04566
H	-2.84735	-0.89122	-0.49263

A
SCF (BP86) Energy = -2635.74430418
Enthalpy 0K = -2634.413171
Enthalpy 298K = -2634.318262
Free Energy 298K = -2634.553383
Lowest Frequency = 8.2172 cm-1
Second Frequency = 11.6603 cm-1
SCF (BP86-D3BJ) Energy = -2636.19792467
SCF (tol) Energy = -2635.75267860
SCF (BS2) Energy = -5403.03948350

K	0.00010	2.32736	0.00027
Si	5.76066	1.17016	-1.04125
Si	5.76046	-1.17060	1.04091
Al	2.86534	-0.00002	-0.00016
O	6.40873	-0.00047	-0.00039
N	4.05657	1.40607	-0.60774
N	4.05630	-1.40635	0.60757
C	3.38831	2.65502	-0.75757
C	3.28766	3.55616	0.35895
C	2.50960	4.72646	0.24588
H	2.44198	5.40686	1.10299
C	1.83779	5.05128	-0.94244
H	1.25263	5.97413	-1.01679
C	1.95073	4.18821	-2.04192
H	1.44694	4.44659	-2.98142
C	2.71199	3.00127	-1.97778
C	4.00323	3.26550	1.67893
H	4.68539	2.42033	1.48387
C	4.84437	4.46174	2.17399
H	5.55075	4.80556	1.40026
H	5.42643	4.17583	3.06742
H	4.21313	5.32287	2.45790
C	3.00906	2.80971	2.77130
H	2.26120	3.59662	2.98293
H	3.53544	2.58589	3.71629
H	2.46910	1.89519	2.46049
C	2.80467	2.12447	-3.22670
H	3.43430	1.26010	-2.95996
C	3.48454	2.87769	-4.39284
H	2.87802	3.73814	-4.72831
H	3.62069	2.20881	-5.26081
H	4.47464	3.26597	-4.09989
C	1.42875	1.57458	-3.66331
H	0.98017	0.94976	-2.86952
H	1.53031	0.94446	-4.56445
H	0.72103	2.38789	-3.90791
C	6.02957	0.48655	-2.79449
H	7.08831	0.19910	-2.91675
H	5.78759	1.22691	-3.57517
H	5.41314	-0.41138	-2.97006
C	6.76706	2.76462	-0.84592
H	6.81335	3.08400	0.20759
H	6.32838	3.58726	-1.43613
H	7.80013	2.60534	-1.19916
C	6.02967	-0.48662	2.79395
H	7.08841	-0.19904	2.91587
H	5.78798	-1.22689	3.57480
H	5.41320	0.41127	2.96957
C	6.76650	-2.76534	0.84594
H	6.81305	-3.08471	-0.20756
H	6.32736	-3.58787	1.43597
H	7.79949	-2.60637	1.19954
C	3.38790	-2.65517	0.75765
C	2.71172	-3.00120	1.97801
C	1.95037	-4.18806	2.04242
H	1.44670	-4.44626	2.98204
C	1.83717	-5.05126	0.94307
H	1.25194	-5.97405	1.01763
C	2.50882	-4.72665	-0.24539
H	2.44101	-5.40716	-1.10240
C	3.28699	-3.55645	-0.35873
C	2.80460	-2.12418	3.22677
H	3.43439	-1.25998	2.95985
C	3.48432	-2.87727	4.39307
H	2.87765	-3.73753	4.72874
H	3.62060	-2.20822	5.26089
H	4.47436	-3.26580	4.10020
C	1.42877	-1.57395	3.66325
H	0.98032	-0.94919	2.86934
H	1.53043	-0.94369	4.56429
H	0.72090	-2.38709	3.90798
C	4.00245	-3.26606	-1.67884
H	4.68465	-2.42087	-1.48399
C	4.84352	-4.46242	-2.17371
H	5.54996	-4.80608	-1.39997
H	5.42551	-4.17672	-3.06726
H	4.21224	-5.32361	-2.45738
C	3.00822	-2.81047	-2.77123
H	3.53453	-2.58685	-3.71630
H	2.46830	-1.89587	-2.46058
H	2.26032	-3.59740	-2.98265
K	-0.00002	-2.32754	0.00003
Si	-5.76039	-1.16992	-1.04146
Si	-5.76050	1.17052	1.04094
Al	-2.86522	-0.00011	0.00051
O	-6.40873	0.00037	-0.00038
N	-4.05644	-1.40607	-0.60750
N	-4.05634	1.40631	0.60765
C	-3.38822	-2.65501	-0.75751
C	-2.71190	-3.00114	-1.97776
C	-1.95071	-4.18811	-2.04206
H	-1.44693	-4.44638	-2.98160
C	-1.83778	-5.05131	-0.94268
H	-1.25265	-5.97417	-1.01715
C	-2.50958	-4.72661	0.24567
H	-2.44200	-5.40713	1.10269

C	-3.28763	-3.55632	0.35888
C	-2.80453	-2.12415	-3.22656
H	-3.43409	-1.25977	-2.95969
C	-3.48446	-2.87714	-4.39281
H	-4.47460	-3.26538	-4.09990
H	-3.62056	-2.20812	-5.26068
H	-2.87802	-3.73759	-4.72841
C	-1.42857	-1.57430	-3.66310
H	-0.72091	-2.38762	-3.90783
H	-1.53008	-0.94403	-4.56414
H	-0.97992	-0.94964	-2.86922
C	-4.00332	-3.26587	1.67884
H	-4.68529	-2.42053	1.48390
C	-4.84478	-4.46211	2.17340
H	-4.21375	-5.32346	2.45712
H	-5.42690	-4.17636	3.06685
H	-5.55112	-4.80553	1.39946
C	-3.00925	-2.81061	2.77151
H	-2.46903	-1.89611	2.46107
H	-3.53575	-2.58694	3.71647
H	-2.26159	-3.59773	2.98305
C	-6.76683	-2.76444	-0.84683
H	-7.79974	-2.60521	-1.20056
H	-6.32780	-3.58701	-1.43688
H	-6.81361	-3.08390	0.20664
C	-6.02890	-0.48576	-2.79455
H	-5.41183	0.41175	-2.97004
H	-5.78759	-1.22615	-3.57541
H	-7.08744	-0.19749	-2.91657
C	-6.76651	2.76528	0.84599
H	-7.79948	2.60638	1.19967
H	-6.32729	3.58781	1.43595
H	-6.81312	3.08460	-0.20752
C	-6.02970	0.48641	2.79394
H	-5.41319	-0.41147	2.96946
H	-5.78801	1.22662	3.57485
H	-7.08843	0.19879	2.91586
C	-3.38799	2.65517	0.75760
C	-3.28705	3.55629	-0.35890
C	-2.50891	4.72653	-0.24569
H	-2.44108	5.40692	-1.10280
C	-1.83732	5.05131	0.94275
H	-1.25210	5.97412	1.01721
C	-1.95055	4.18827	2.04222
H	-1.44692	4.44662	2.98183
C	-2.71188	3.00138	1.97794
C	-4.00244	3.26567	-1.67900
H	-4.68466	2.42053	-1.48403
C	-4.84346	4.46195	-2.17415
H	-4.21216	5.32308	-2.45795
H	-5.42540	4.17609	-3.06768
H	-5.54995	4.80577	-1.40051
C	-3.00813	2.80986	-2.77122
H	-2.46825	1.89531	-2.46035
H	-3.53438	2.58605	-3.71629
H	-2.26021	3.59673	-2.98275
C	-2.80488	2.12458	3.22685
H	-3.43452	1.26026	2.95997
C	-3.48493	2.87784	4.39285
H	-4.47497	3.26616	4.09971
H	-3.62127	2.20897	5.26080
H	-2.87844	3.73827	4.72843
C	-1.42909	1.57458	3.66371
H	-1.53087	0.94445	4.56482
H	-0.98040	0.94975	2.86999
H	-0.72135	2.38783	3.90847

B

SCF (BP86) Energy = -3118.67687934
Enthalpy 0K = -3117.108814
Enthalpy 298K = -3117.003884
Free Energy 298K = -3117.257168
Lowest Frequency = 7.9080 cm^{-1}
Second Frequency = 11.1199 cm^{-1}
SCF (BP86-D3BJ) Energy = -3119.21463029
SCF (tol) Energy = -3118.68620809
SCF (BS2) Energy = -5886.07823998

K	-0.50237	-1.22639	1.94206
Si	4.62619	1.30869	2.74166
Si	4.94471	2.53612	-0.10508
Al	2.36034	0.71102	0.52970
O	5.38003	1.60748	1.24725
N	3.06991	0.55646	2.37422
N	3.20400	2.30827	-0.30364
C	2.35598	-0.22023	3.32748
C	2.52824	-1.65105	3.40202
C	1.75989	-2.41589	4.30460
H	1.91668	-3.50048	4.34650
C	0.81824	-1.82862	5.15847
H	0.24388	-2.43759	5.86461
C	0.64239	-0.44081	5.09953
H	-0.08224	0.03505	5.77120
C	1.38138	0.36993	4.21154
C	3.52553	-2.40282	2.51975
H	4.07899	-1.64281	1.94253
C	4.53857	-3.22556	3.34780
H	5.06241	-2.59868	4.08639
H	5.29764	-3.68013	2.68626
H	4.04589	-4.04938	3.89491
C	2.79135	-3.32503	1.51944
H	2.15670	-4.06086	2.04657
H	3.51284	-3.89451	0.90613
H	2.15280	-2.74303	0.83076
C	1.10108	1.87168	4.23863
H	1.74306	2.33043	3.46774
C	1.45005	2.48971	5.61255
H	0.77439	2.11595	6.40303
H	1.35050	3.58905	5.58322
H	2.48052	2.24694	5.91875
C	-0.37273	2.17786	3.88891
H	-0.62903	1.81786	2.87558
H	-0.56822	3.26346	3.91515
H	-1.06649	1.70119	4.60471
C	4.52775	2.96479	3.67671
H	5.52677	3.43482	3.68972
H	4.21296	2.82304	4.72396
H	3.82364	3.67031	3.20532
C	5.81299	0.19262	3.71561
H	6.13769	-0.66896	3.11096
H	5.34037	-0.18625	4.63791
H	6.71184	0.76347	4.00580
C	6.04317	1.87087	-1.50902
H	7.10337	1.98731	-1.22359
H	5.88522	2.42357	-2.45043
H	5.85620	0.80196	-1.69491
C	5.46601	4.34776	0.14712
H	5.07731	4.77221	1.08574
H	5.11835	4.97952	-0.68861
H	6.56779	4.40895	0.17681
C	2.42107	3.13406	-1.15376
C	2.16764	2.77156	-2.52536
C	1.30398	3.55709	-3.31827
H	1.12801	3.26544	-4.36092
C	0.68668	4.71060	-2.81683

H	0.03267	5.31609	-3.45280
C	0.94471	5.08635	-1.49152
H	0.48117	5.99676	-1.09291
C	1.79741	4.33425	-0.65750
C	2.82424	1.55415	-3.17646
H	3.53260	1.14604	-2.43764
C	3.61635	1.94102	-4.44578
H	2.95055	2.29206	-5.25451
H	4.17432	1.07113	-4.83572
H	4.34127	2.74601	-4.23990
C	1.79188	0.44942	-3.49805
H	1.31908	0.07010	-2.57343
H	2.27322	-0.40774	-4.00370
H	1.00086	0.82283	-4.17514
C	2.00828	4.81664	0.77607
H	2.77502	4.15798	1.21745
C	2.50233	6.27825	0.84732
H	3.41404	6.43145	0.24851
H	2.72898	6.55578	1.89200
H	1.73646	6.98558	0.48136
C	0.71880	4.65188	1.60724
H	0.88087	4.96410	2.65429
H	0.38823	3.59944	1.61940
H	-0.10256	5.26958	1.19886
K	-0.81013	2.09137	-1.13921
Si	-6.61809	0.38618	-0.82946
Si	-5.75566	-2.60774	-0.50546
Al	-3.46283	-0.27959	-0.10132
O	-6.80889	-1.29148	-0.67426
N	-4.88339	0.73117	-0.95738
N	-4.25437	-2.02037	0.23498
C	-4.37628	1.86435	-1.65945
C	-4.19685	3.13168	-1.00709
C	-3.56720	4.18916	-1.69701
H	-3.44178	5.15410	-1.19081
C	-3.11547	4.04206	-3.01583
H	-2.64114	4.87944	-3.53812
C	-3.30420	2.81289	-3.66392
H	-2.97119	2.69700	-4.70224
C	-3.93146	1.72726	-3.01982
C	-4.68400	3.37857	0.42063
H	-5.15449	2.44204	0.76046
C	-5.74602	4.50046	0.46919
H	-6.58662	4.29063	-0.21371
H	-6.15157	4.60781	1.49066
H	-5.31920	5.47691	0.17736
C	-3.52261	3.68637	1.39087
H	-2.96338	4.58987	1.08555
H	-3.90351	3.86235	2.41246
H	-2.81623	2.83818	1.44048
C	-4.11964	0.41912	-3.78894
H	-4.77659	-0.21408	-3.16825
C	-4.80310	0.62929	-5.15742
H	-4.16560	1.20219	-5.85460
H	-5.01397	-0.34439	-5.63348
H	-5.75647	1.17320	-5.05241
C	-2.78152	-0.33529	-3.95899
H	-2.33158	-0.57081	-2.97597
H	-2.93004	-1.28678	-4.50038
H	-2.05404	0.26763	-4.53388
C	-7.56592	0.96906	-2.36540
H	-8.64908	0.81259	-2.22494
H	-7.39824	2.04359	-2.55231
H	-7.25498	0.41189	-3.26381
C	-7.46120	1.10198	0.71671
H	-6.90834	0.82889	1.63154
H	-7.54953	2.20050	0.68219
H	-8.47895	0.68256	0.80011
C	-6.61613	-3.90329	0.57847
H	-7.49521	-4.31377	0.05299
H	-5.93766	-4.74073	0.81433
H	-6.96214	-3.46335	1.52757
C	-5.53763	-3.32527	-2.25341
H	-4.98334	-2.63058	-2.90691
H	-5.00192	-4.28924	-2.24576
H	-6.53108	-3.49398	-2.70420
C	-3.47468	-2.82926	1.11009
C	-3.64567	-2.72455	2.53445
C	-2.78349	-3.43340	3.39569
H	-2.92309	-3.34631	4.47957
C	-1.76532	-4.26161	2.90000
H	-1.11615	-4.81618	3.58587
C	-1.60844	-4.38543	1.51208
H	-0.82748	-5.04633	1.11640
C	-2.43996	-3.69087	0.60767
C	-4.74554	-1.85092	3.13995
H	-5.40347	-1.55388	2.30533
C	-5.59815	-2.60793	4.18110
H	-5.01490	-2.87096	5.08185
H	-6.44313	-1.97933	4.51233
H	-6.00898	-3.54237	3.76397
C	-4.16539	-0.55492	3.75109
H	-3.63216	0.04029	2.98567
H	-4.96814	0.07643	4.17208
H	-3.45424	-0.78263	4.56691
C	-2.21884	-3.89153	-0.89179
H	-2.97066	-3.27187	-1.40688
C	-2.44089	-5.36509	-1.30188
H	-3.43581	-5.72555	-0.99027
H	-2.36143	-5.48055	-2.39732
H	-1.68917	-6.03176	-0.84197
C	-0.82711	-3.40331	-1.35111
H	-0.70047	-3.56052	-2.43713
H	-0.69376	-2.32428	-1.15256
H	-0.01374	-3.95060	-0.83984
C	6.92335	-3.74605	-3.54582
H	7.75933	-3.07488	-3.27194
H	7.33771	-4.51956	-4.21942
C	5.81475	-2.94910	-4.27357
H	6.23308	-2.46333	-5.17451
C	6.33313	-4.40874	-2.27818
H	7.12331	-4.97234	-1.74840
C	5.78562	-3.31476	-1.33056
H	6.58747	-2.61879	-1.02441
H	5.37195	-3.76647	-0.41083
C	5.26438	-1.85185	-3.33152
H	4.47827	-1.26139	-3.83586
H	6.06551	-1.15045	-3.03580
C	4.66681	-2.51464	-2.05755
C	3.51890	-3.47952	-2.46921
H	3.08106	-3.93152	-1.56116
H	2.72017	-2.90047	-2.96720
C	4.66860	-3.90671	-4.67877
H	5.04979	-4.68117	-5.37062
H	3.87972	-3.35066	-5.22017
C	5.18624	-5.36712	-2.68024
H	5.57527	-6.16681	-3.33817
H	4.77014	-5.86250	-1.78234
C	4.07860	-4.57153	-3.41203
H	3.25459	-5.25214	-3.69593
C	3.72760	-0.64406	-0.46948
N	4.16095	-1.49438	-1.18285

B'

SCF (BP86) Energy = -3118.68086908
Enthalpy 0K = -3117.114231

Enthalpy 298K = -3117.007957
Free Energy 298K = -3117.270293
Lowest Frequency = 6.0377 cm^{-1}
Second Frequency = 8.1181 cm^{-1}
SCF (BP86-D3BJ) Energy = -3119.20494015
SCF (tol) Energy = -3118.69069946
SCF (BS2) Energy = -5886.08351248

K	-0.80777	1.13892	1.07006
Si	-3.41514	-4.41065	2.12197
Si	-3.15653	-5.13011	-0.89647
Al	-1.44739	-2.55427	0.25798
O	-3.72134	-5.28017	0.69583
N	-2.74235	-2.83464	1.67489
N	-1.70201	-4.11297	-0.88203
C	-3.02506	-1.63785	2.39654
C	-4.11001	-0.79224	1.98493
C	-4.28905	0.46138	2.60070
H	-5.11417	1.10429	2.27374
C	-3.44025	0.90457	3.62555
H	-3.60091	1.87980	4.09843
C	-2.40408	0.06573	4.05896
H	-1.76014	0.38921	4.88623
C	-2.18419	-1.20020	3.47462
C	-5.06628	-1.23150	0.87536
H	-4.89943	-2.31248	0.73036
C	-6.55000	-1.02176	1.24393
H	-6.79935	-1.50119	2.20538
H	-7.20218	-1.45492	0.46525
H	-6.81016	0.04916	1.32777
C	-4.73316	-0.54026	-0.46480
H	-4.83192	0.55646	-0.38113
H	-5.40942	-0.88727	-1.26732
H	-3.69353	-0.75599	-0.77513
C	-1.08092	-2.09254	4.04282
H	-1.05034	-2.99632	3.41195
C	-1.41269	-2.52500	5.49012
H	-1.43660	-1.65713	6.17367
H	-0.65257	-3.22982	5.87139
H	-2.39801	-3.01791	5.54808
C	0.31361	-1.43577	3.98017
H	0.59649	-1.19926	2.93864
H	1.08293	-2.11559	4.38680
H	0.35625	-0.50245	4.57036
C	-2.22344	-5.49110	3.13545
H	-2.62925	-6.51403	3.22139
H	-2.07462	-5.09806	4.15526
H	-1.23621	-5.55727	2.64787
C	-5.04664	-4.24800	3.07531
H	-5.83999	-3.81073	2.44811
H	-4.92388	-3.61059	3.96753
H	-5.38716	-5.24241	3.41106
C	-4.59820	-4.38678	-1.88823
H	-5.51025	-4.98565	-1.72058
H	-4.39354	-4.37682	-2.97212
H	-4.80770	-3.35202	-1.56987
C	-2.80652	-6.86998	-1.56626
H	-2.13635	-7.43412	-0.89820
H	-2.34051	-6.82637	-2.56542
H	-3.75077	-7.43401	-1.65525
C	-0.63672	-4.30762	-1.80632
C	-0.58857	-3.59419	-3.05345
C	0.54546	-3.71636	-3.88488
H	0.56769	-3.17158	-4.83669
C	1.63118	-4.53073	-3.53470
H	2.49623	-4.62209	-4.20005
C	1.58126	-5.24502	-2.32780
H	2.41964	-5.89670	-2.05569
C	0.47277	-5.15574	-1.46176
C	-1.74956	-2.71888	-3.52630
H	-2.51925	-2.76349	-2.73803
C	-2.36518	-3.26417	-4.83534
H	-1.64682	-3.21254	-5.67331
H	-3.25379	-2.67463	-5.12246
H	-2.67252	-4.31824	-4.72860
C	-1.34198	-1.23819	-3.69272
H	-0.98817	-0.81812	-2.73398
H	-2.20342	-0.63308	-4.02748
H	-0.54051	-1.11585	-4.44442
C	0.48436	-5.94769	-0.15348
H	-0.54502	-5.91403	0.24192
C	0.88062	-7.42644	-0.34787
H	0.25206	-7.91578	-1.11031
H	0.76403	-7.98009	0.60006
H	1.93454	-7.53678	-0.66076
C	1.39630	-5.27345	0.89648
H	1.39355	-5.83777	1.84619
H	1.05509	-4.24400	1.11717
H	2.44205	-5.22164	0.53984
K	1.90343	-2.00233	-1.21896
Si	6.30547	1.68608	0.18443
Si	4.56156	4.26947	0.03450
Al	3.04302	1.29962	0.02149
O	5.95203	3.31422	-0.12783
N	4.88412	0.72856	-0.26609
N	3.20429	3.19702	0.43191
C	5.00249	-0.55783	-0.85991
C	5.09610	-1.74544	-0.05561
C	5.09740	-3.01247	-0.67644
H	5.17825	-3.91060	-0.05189
C	5.01289	-3.14935	-2.06959
H	5.02474	-4.14133	-2.53324
C	4.93556	-1.99348	-2.86085
H	4.88962	-2.09282	-3.95194
C	4.93910	-0.70406	-2.28991
C	5.20837	-1.67326	1.46704
H	5.19354	-0.60383	1.73259
C	6.53956	-2.27919	1.96606
H	7.40780	-1.79964	1.48307
H	6.63973	-2.15048	3.05828
H	6.59833	-3.36177	1.75277
C	4.00723	-2.33767	2.17407
H	3.92573	-3.41091	1.92307
H	4.11024	-2.26087	3.27086
H	3.05942	-1.84357	1.89475
C	4.88284	0.51484	-3.21274
H	5.06351	1.39785	-2.57575
C	5.97319	0.47488	-4.30591
H	5.80769	-0.34807	-5.02442
H	5.97255	1.41692	-4.88164
H	6.97708	0.34018	-3.87011
C	3.48451	0.68442	-3.84969
H	2.70844	0.81704	-3.07226
H	3.45659	1.57074	-4.50833
H	3.21507	-0.19632	-4.46242
C	7.82387	1.23124	-0.85452
H	8.70870	1.78347	-0.49464
H	8.04529	0.15238	-0.79118
H	7.67029	1.48910	-1.91475
C	6.76612	1.57788	2.02677
H	5.88854	1.75315	2.67163
H	7.19257	0.59558	2.29088
H	7.52072	2.34826	2.26269
C	4.85292	5.57608	1.38141
H	5.63026	6.28766	1.05405

H	3.93196	6.14867	1.58603
H	5.18794	5.11654	2.32510
C	4.43936	5.17309	-1.63450
H	4.25158	4.46849	-2.46197
H	3.64912	5.94181	-1.64708
H	5.40235	5.67545	-1.83323
C	2.02201	3.70158	1.05517
C	1.86786	3.61941	2.48178
C	0.64379	3.98726	3.07530
H	0.53655	3.91585	4.16424
C	-0.43124	4.45907	2.30893
H	-1.37052	4.75395	2.78978
C	-0.27472	4.57260	0.92051
H	-1.10630	4.95304	0.31682
C	0.92556	4.20581	0.27701
C	3.00647	3.13012	3.37724
H	3.90389	3.08089	2.73744
C	3.29897	4.09547	4.54619
H	2.46033	4.14096	5.26399
H	4.18860	3.75848	5.10691
H	3.48891	5.12021	4.18642
C	2.73926	1.70312	3.90429
H	2.60641	0.98988	3.06977
H	3.57929	1.34844	4.52804
H	1.82433	1.67357	4.52431
C	1.01940	4.35725	-1.24219
H	2.05721	4.11536	-1.51983
C	0.72191	5.80340	-1.69655
H	1.36075	6.53306	-1.17078
H	0.89722	5.91237	-2.78139
H	-0.32897	6.08474	-1.50179
C	0.10627	3.35629	-1.98478
H	0.18728	3.49007	-3.07865
H	0.39787	2.31535	-1.75263
H	-0.95453	3.48940	-1.70515
C	-7.82213	4.53985	-1.99077
H	-8.20273	3.50965	-1.85611
H	-8.65456	5.13935	-2.40421
C	-6.62791	4.54383	-2.97527
H	-6.94166	4.11843	-3.94624
C	-7.37383	5.12603	-0.63044
H	-8.22194	5.11809	0.07869
C	-6.23190	4.25983	-0.04636
H	-6.56927	3.21940	0.11221
H	-5.89944	4.65448	0.93114
C	-5.48291	3.67519	-2.40122
H	-4.61942	3.65619	-3.09083
H	-5.81441	2.63106	-2.25609
C	-5.03279	4.26322	-1.03479
C	-4.52819	5.71909	-1.23531
H	-4.18654	6.12370	-0.26505
H	-3.65896	5.71251	-1.91789
C	-6.12463	5.99357	-3.17593
H	-6.92965	6.61660	-3.60844
H	-5.28324	6.01004	-3.89443
C	-6.87092	6.57607	-0.83036
H	-7.68806	7.20802	-1.22558
H	-6.56699	7.01249	0.14007
C	-5.67696	6.57932	-1.81520
H	-5.30927	7.61253	-1.95473
N	-3.96861	3.45556	-0.49828
C	-3.09817	2.77434	-0.06853

C

SCF (BP86) Energy = -3601.60879505
Enthalpy 0K = -3599.805829
Enthalpy 298K = -3599.689167
Free Energy 298K = -3599.972500
Lowest Frequency = 4.4983 cm^{-1}
Second Frequency = 7.5010 cm^{-1}
SCF (BP86-D3BJ) Energy = -3602.20573291
SCF (tol) Energy = -3601.61989371
SCF (BS2) Energy = -6369.12173088

K	-0.94662	0.58102	2.19949
Si	0.86740	-4.79071	1.15733
Si	-0.06102	-4.97728	-1.81006
Al	-0.76526	-2.32259	-0.11774
O	0.04775	-5.44466	-0.18211
N	0.23005	-3.15899	1.38094
N	-0.18708	-3.21578	-1.79822
C	0.33504	-2.45514	2.61209
C	-0.73026	-2.49689	3.58486
C	-0.65092	-1.72660	4.76405
H	-1.47145	-1.78260	5.48964
C	0.45194	-0.90949	5.04118
H	0.50262	-0.33064	5.96964
C	1.49800	-0.86754	4.11115
H	2.37600	-0.24524	4.32181
C	1.46757	-1.61468	2.91395
C	-1.97744	-3.36128	3.39697
H	-1.83567	-3.92689	2.46040
C	-2.16858	-4.36753	4.55473
H	-1.27394	-4.99343	4.69891
H	-3.02344	-5.03635	4.34793
H	-2.37772	-3.85431	5.51067
C	-3.24361	-2.48770	3.24558
H	-3.39468	-1.84584	4.13288
H	-4.14546	-3.11766	3.14074
H	-3.18104	-1.83940	2.35316
C	2.67442	-1.49390	1.98545
H	2.46120	-2.11040	1.09618
C	3.96266	-2.02214	2.65897
H	4.25168	-1.38682	3.51632
H	4.79839	-2.01498	1.93810
H	3.83299	-3.04847	3.04051
C	2.90045	-0.03795	1.51943
H	2.02843	0.34673	0.95901
H	3.78245	0.02287	0.86012
H	3.07733	0.63770	2.37625
C	2.73206	-4.90554	0.79088
H	2.97639	-5.93747	0.48293
H	3.34057	-4.66884	1.67919
H	3.04092	-4.22373	-0.01856
C	0.51268	-5.96013	2.61079
H	-0.56639	-6.15910	2.70854
H	0.87705	-5.53702	3.56258
H	1.02447	-6.92487	2.45117
C	-1.57686	-5.91852	-2.47199
H	-1.41840	-7.00251	-2.33429
H	-1.73433	-5.73514	-3.54822
H	-2.49378	-5.63680	-1.93149
C	1.42874	-5.64268	-2.78776
H	2.39120	-5.34765	-2.34185
H	1.40699	-5.28407	-3.83148
H	1.38746	-6.74559	-2.81142
C	-0.03994	-2.44080	-2.97968
C	-1.18255	-2.05882	-3.77156
C	-1.02006	-1.21417	-4.89012
H	-1.90273	-0.93916	-5.48027
C	0.23942	-0.74065	-5.28028
H	0.34763	-0.10149	-6.16280
C	1.35972	-1.11934	-4.52811
H	2.35226	-0.76306	-4.82861
C	1.25076	-1.95412	-3.39623

C	-2.59241	-2.55806	-3.45537
H	-2.49210	-3.27859	-2.62783
C	-3.22377	-3.28917	-4.66192
H	-3.41738	-2.60032	-5.50377
H	-4.19162	-3.74083	-4.37991
H	-2.56867	-4.09375	-5.03519
C	-3.51412	-1.41400	-2.97430
H	-3.13697	-0.97029	-2.03472
H	-4.53772	-1.78558	-2.78300
H	-3.59490	-0.61586	-3.73584
C	2.52653	-2.27270	-2.61843
H	2.25046	-3.01276	-1.84869
C	3.63808	-2.87051	-3.50874
H	3.29042	-3.76097	-4.05665
H	4.50427	-3.16235	-2.88967
H	4.00249	-2.13853	-4.25206
C	3.05083	-1.01557	-1.89169
H	3.97485	-1.22833	-1.32640
H	2.30157	-0.63362	-1.17587
H	3.28317	-0.20974	-2.61354
K	-0.29576	0.83025	-2.27893
Si	-0.67335	6.71840	-0.89876
Si	-2.95369	6.11774	1.15798
Al	-1.14278	3.59571	0.04278
O	-1.93986	7.05733	0.17680
N	-0.69150	4.98026	-1.24065
N	-2.19653	4.52936	1.38286
C	-0.28419	4.43815	-2.49455
C	1.08447	4.08410	-2.74871
C	1.42364	3.42873	-3.95119
H	2.47289	3.16880	-4.13714
C	0.45733	3.11696	-4.91747
H	0.74336	2.61779	-5.84919
C	-0.87785	3.47626	-4.68242
H	-1.63533	3.25257	-5.44303
C	-1.26696	4.13685	-3.49965
C	2.19922	4.41646	-1.75711
H	1.71940	4.90998	-0.89640
C	3.22121	5.40008	-2.37180
H	2.72908	6.31532	-2.74233
H	3.97670	5.69532	-1.62225
H	3.75804	4.94536	-3.22384
C	2.91169	3.15379	-1.22632
H	3.38664	2.57656	-2.04033
H	3.70552	3.42642	-0.50867
H	2.20255	2.49009	-0.70035
C	-2.73646	4.51436	-3.30844
H	-2.77449	5.18092	-2.42970
C	-3.31712	5.27739	-4.51835
H	-3.37523	4.64180	-5.42021
H	-4.34202	5.62306	-4.29659
H	-2.70478	6.15933	-4.76995
C	-3.59927	3.27473	-2.98041
H	-3.24349	2.77793	-2.05779
H	-4.65634	3.55693	-2.82674
H	-3.56519	2.53627	-3.80308
C	-0.93268	7.74718	-2.47062
H	-0.84660	8.82269	-2.23967
H	-0.17786	7.50106	-3.23686
H	-1.93053	7.57057	-2.90360
C	0.89542	7.32879	-0.01452
H	1.11125	6.71416	0.87600
H	1.78295	7.30857	-0.66866
H	0.74463	8.36942	0.32155
C	-3.18245	7.02722	2.80613
H	-3.72665	7.97345	2.64496
H	-3.76122	6.41808	3.52126
H	-2.21092	7.26760	3.26708
C	-4.62578	6.06910	0.25262
H	-4.55491	5.49436	-0.68631
H	-5.42403	5.62243	0.86853
H	-4.93123	7.09858	-0.00336
C	-2.36768	3.76808	2.57483
C	-1.38406	3.83650	3.62180
C	-1.49109	2.98355	4.73899
H	-0.73442	3.04378	5.53008
C	-2.55020	2.07339	4.87134
H	-2.62351	1.42950	5.75421
C	-3.52466	2.01764	3.86471
H	-4.36623	1.32197	3.96954
C	-3.45829	2.84361	2.72229
C	-0.21096	4.81491	3.54653
H	-0.42277	5.49135	2.70064
C	-0.07004	5.66924	4.82500
H	0.21339	5.05878	5.70121
H	0.71710	6.43170	4.69046
H	-1.01176	6.18815	5.06971
C	1.11486	4.08506	3.23164
H	1.05165	3.54381	2.26882
H	1.95280	4.80167	3.16269
H	1.36369	3.35209	4.02142
C	-4.56738	2.73374	1.67572
H	-4.32166	3.45433	0.87882
C	-5.94187	3.11665	2.27017
H	-5.91863	4.11939	2.72937
H	-6.71940	3.11579	1.48585
H	-6.25758	2.40265	3.05227
C	-4.62840	1.33258	1.02805
H	-5.43201	1.29049	0.27130
H	-3.67960	1.08018	0.52052
H	-4.83718	0.54600	1.77647
C	-7.17741	-6.32522	-0.32717
H	-6.55607	-7.20472	-0.58160
H	-8.23095	-6.66273	-0.32792
C	-6.97879	-5.20853	-1.37968
H	-7.24050	-5.59015	-2.38399
C	-6.79434	-5.78779	1.07243
H	-6.92606	-6.58450	1.82789
C	-5.31046	-5.34929	1.06835
H	-4.64738	-6.19835	0.82242
H	-5.01064	-4.97471	2.06384
C	-5.49590	-4.76624	-1.39029
H	-5.32880	-3.97525	-2.14363
H	-4.83543	-5.61359	-1.64920
C	-5.10679	-4.22317	0.01434
C	-6.01460	-3.01027	0.36505
H	-5.72187	-2.61043	1.35234
H	-5.85008	-2.20838	-0.37737
C	-7.87733	-3.99874	-1.02806
H	-8.94129	-4.30167	-1.04026
H	-7.75999	-3.20236	-1.78745
C	-7.69082	-4.57685	1.42639
H	-8.75212	-4.88780	1.45553
H	-7.43850	-4.19695	2.43473
C	-7.49510	-3.46119	0.37167
H	-8.13014	-2.59192	0.62472
C	-2.57917	-3.50805	-0.00658
N	-3.72861	-3.82246	0.00619
C	6.45983	-1.04975	-0.07538
N	7.63476	-1.00090	0.10088
C	9.05511	-0.94688	0.31948
C	9.54195	0.52475	0.21117
C	9.77820	-1.81146	-0.75011
C	9.38118	-1.49681	1.73590
H	9.28538	0.91964	-0.78879
H	9.00606	1.14025	0.95657

C	11.07026	0.57689	0.44907
H	9.52304	-1.43251	-1.75658
H	9.40978	-2.85151	-0.68586
C	11.30566	-1.75143	-0.50927
H	8.84419	-0.89474	2.49134
H	9.00976	-2.53462	1.81652
C	10.90982	-1.43817	1.96871
H	11.40720	1.62714	0.37018
C	11.78793	-0.28469	-0.61779
C	11.39216	0.02854	1.86026
H	11.81128	-2.36892	-1.27465
C	11.62772	-2.29959	0.90190
H	11.13165	-1.83124	2.97817
H	12.88315	-0.23482	-0.46991
H	11.58093	0.11116	-1.63029
H	10.90011	0.65008	2.63243
H	12.48103	0.08359	2.04789
H	11.30543	-3.35507	0.98378
H	12.72037	-2.28188	1.07415

TS(C-D)

SCF (BP86) Energy = -3601.60921104
Enthalpy 0K = -3599.806183
Enthalpy 298K = -3599.690504
Free Energy 298K = -3599.970371
Lowest Frequency = -21.5680 cm^{-1}
Second Frequency = 3.6627 cm^{-1}
SCF (BP86-D3BJ) Energy = -3602.21342579
SCF (tol) Energy = -3601.62041651
SCF (BS2) Energy = -6369.11923836

K	-1.62898	1.21350	2.05286
Si	-2.51630	-4.50539	2.40706
Si	-1.84998	-5.13861	-0.57123
Al	-1.73198	-2.07070	0.43301
O	-2.78322	-5.12808	0.84668
N	-2.24262	-2.77175	2.22168
N	-0.98861	-3.59755	-0.60059
C	-2.41644	-1.84020	3.28173
C	-3.68108	-1.17972	3.49437
C	-3.81034	-0.19114	4.49207
H	-4.78473	0.29106	4.63624
C	-2.73693	0.18095	5.31034
H	-2.86119	0.94206	6.08805
C	-1.50599	-0.45944	5.12321
H	-0.66075	-0.19249	5.76922
C	-1.32319	-1.45449	4.13956
C	-4.92321	-1.50296	2.66334
H	-4.64802	-2.32648	1.98250
C	-6.11071	-1.96081	3.54074
H	-5.83649	-2.81117	4.18434
H	-6.96096	-2.27204	2.90756
H	-6.47046	-1.14627	4.19499
C	-5.34684	-0.29091	1.80346
H	-5.57137	0.58838	2.43436
H	-6.25935	-0.52133	1.22412
H	-4.55515	-0.01005	1.08697
C	0.05766	-2.10044	4.04371
H	0.01377	-2.82098	3.20995
C	0.41421	-2.86419	5.34023
H	0.53729	-2.17199	6.19287
H	1.36318	-3.41632	5.22013
H	-0.37098	-3.58773	5.61406
C	1.15671	-1.06065	3.72961
H	0.96600	-0.55748	2.76377
H	2.14850	-1.54091	3.66581
H	1.21660	-0.28324	4.51266
C	-1.06533	-5.47179	3.17634
H	-1.25990	-6.55525	3.08921
H	-0.94869	-5.23930	4.24830
H	-0.10609	-5.25403	2.67836
C	-4.06048	-4.95500	3.41663
H	-4.98360	-4.66079	2.89282
H	-4.04912	-4.46622	4.40587
H	-4.09410	-6.04618	3.57924
C	-3.10458	-5.41323	-1.97591
H	-3.64708	-6.35879	-1.80071
H	-2.60464	-5.48775	-2.95659
H	-3.84312	-4.59854	-2.02119
C	-0.72059	-6.67155	-0.59524
H	-0.14254	-6.78770	0.33474
H	-0.01128	-6.62816	-1.43988
H	-1.34062	-7.57573	-0.72437
C	0.12300	-3.36546	-1.45412
C	-0.03650	-2.72761	-2.73528
C	1.09684	-2.40817	-3.51284
H	0.95322	-1.92095	-4.48512
C	2.39495	-2.72070	-3.08735
H	3.26200	-2.47669	-3.71075
C	2.55878	-3.37511	-1.85795
H	3.56855	-3.62684	-1.51680
C	1.45920	-3.70569	-1.04031
C	-1.41444	-2.40525	-3.31171
H	-2.15376	-2.80932	-2.60120
C	-1.63268	-3.09360	-4.67843
H	-0.95639	-2.68919	-5.45295
H	-2.66728	-2.93650	-5.03228
H	-1.45477	-4.18032	-4.61700
C	-1.65030	-0.88316	-3.42579
H	-1.59476	-0.40093	-2.43335
H	-2.64677	-0.66770	-3.85332
H	-0.90240	-0.40936	-4.08823
C	1.72673	-4.38114	0.30275
H	0.74740	-4.71114	0.68505
C	2.65336	-5.61003	0.19206
H	2.27579	-6.34187	-0.54041
H	2.73385	-6.11667	1.17026
H	3.67700	-5.32575	-0.11187
C	2.29331	-3.36611	1.31657
H	2.44653	-3.83585	2.30525
H	1.59212	-2.52488	1.45211
H	3.26202	-2.95659	0.97724
K	1.66908	-0.20298	-0.96819
Si	2.62720	5.98257	-0.80662
Si	-0.34965	6.58053	-0.12378
Al	0.63084	3.44980	0.07290
O	1.31344	6.89037	-0.23694
N	2.11302	4.28698	-0.88000
N	-0.54622	4.94001	0.51414
C	2.83698	3.32328	-1.64697
C	3.92564	2.58143	-1.07570
C	4.52423	1.54078	-1.81651
H	5.34320	0.97006	-1.36582
C	4.08861	1.21032	-3.10740
H	4.57152	0.40207	-3.66757
C	3.04026	1.94573	-3.67821
H	2.70541	1.70473	-4.69420
C	2.41313	2.99784	-2.98151
C	4.45603	2.88134	0.32723
H	3.93407	3.78621	0.67555
C	5.97346	3.17080	0.32007
H	6.23153	3.96710	-0.39858
H	6.31029	3.49033	1.32202
H	6.55823	2.27455	0.04525
C	4.12482	1.74996	1.32667

H	4.55183	0.78346	1.00210
H	4.53135	1.98199	2.32772
H	3.03031	1.63228	1.43107
C	1.27553	3.75920	-3.66239
H	1.05949	4.63056	-3.02114
C	1.66068	4.27508	-5.06564
H	1.83277	3.44732	-5.77692
H	0.84821	4.89707	-5.48116
H	2.57740	4.88673	-5.03386
C	-0.01132	2.90738	-3.72960
H	-0.33338	2.59590	-2.71845
H	-0.83780	3.47545	-4.19323
H	0.14759	1.99335	-4.33101
C	3.16770	6.63976	-2.50549
H	3.57856	7.65887	-2.40300
H	3.95175	6.00001	-2.94607
H	2.32317	6.68238	-3.21193
C	4.01405	6.38162	0.43115
H	3.76247	6.03087	1.44588
H	4.98278	5.94196	0.14166
H	4.14043	7.47768	0.47590
C	-1.08152	7.88897	1.03599
H	-1.02353	8.88614	0.56722
H	-2.14052	7.67856	1.26221
H	-0.52772	7.92791	1.98770
C	-1.07669	6.83580	-1.86425
H	-0.73740	6.05417	-2.56484
H	-2.17971	6.82919	-1.85618
H	-0.74814	7.81279	-2.25963
C	-1.60201	4.60391	1.40530
C	-1.38349	4.61354	2.82729
C	-2.40020	4.16035	3.69281
H	-2.22281	4.17132	4.77475
C	-3.63854	3.71594	3.20593
H	-4.41957	3.38053	3.89635
C	-3.86631	3.72814	1.82216
H	-4.83852	3.39976	1.43477
C	-2.87839	4.16291	0.91362
C	-0.06730	5.11108	3.42776
H	0.50192	5.56858	2.60031
C	-0.28602	6.18478	4.51620
H	-0.78830	5.77136	5.40938
H	0.68351	6.59612	4.84761
H	-0.90275	7.01920	4.14288
C	0.78220	3.94442	3.98136
H	1.02370	3.21848	3.18241
H	1.73447	4.31509	4.40090
H	0.24665	3.40766	4.78664
C	-3.20292	4.16663	-0.58006
H	-2.30442	4.54350	-1.09507
C	-4.37978	5.11634	-0.89882
H	-4.18573	6.13773	-0.52981
H	-4.55141	5.17179	-1.98850
H	-5.31912	4.76928	-0.43148
C	-3.48440	2.74903	-1.12373
H	-3.71244	2.78773	-2.20398
H	-2.61186	2.08427	-0.99164
H	-4.34968	2.28318	-0.61745
C	-8.06519	-2.79422	-3.60826
H	-7.90013	-3.88617	-3.53923
H	-8.96839	-2.64255	-4.22885
C	-6.84612	-2.11077	-4.27226
H	-6.67704	-2.54135	-5.27666
C	-8.28540	-2.19747	-2.19768
H	-9.15089	-2.68816	-1.71495
C	-7.02803	-2.44544	-1.33038
H	-6.82468	-3.52676	-1.22830
H	-7.16842	-2.03883	-0.31246
C	-5.58381	-2.35606	-3.41131
H	-4.69758	-1.88374	-3.87237
H	-5.37332	-3.43723	-3.32272
C	-5.79967	-1.75692	-1.99223
C	-6.06311	-0.22970	-2.11663
H	-6.19416	0.19951	-1.10731
H	-5.17899	0.25512	-2.56860
C	-7.10500	-0.58979	-4.39080
H	-7.99352	-0.40537	-5.02364
H	-6.24805	-0.09396	-4.88510
C	-8.54314	-0.67572	-2.31281
H	-9.45547	-0.49089	-2.91068
H	-8.72145	-0.24202	-1.31036
C	-7.32524	0.00709	-2.98044
H	-7.50299	1.09575	-3.05838
C	-3.66921	-2.24367	-0.53421
N	-4.63127	-1.99431	-1.19248
C	5.14862	-1.54557	-0.20584
N	6.25097	-1.98278	-0.14109
C	7.58706	-2.51100	-0.05711
C	8.61060	-1.34752	-0.17477
C	7.81701	-3.52325	-1.21359
C	7.77340	-3.23062	1.30758
H	8.45710	-0.82349	-1.13577
H	8.42597	-0.61762	0.63427
C	10.04550	-1.92003	-0.08346
H	7.65810	-3.01266	-2.18096
H	7.07048	-4.33501	-1.14049
C	9.25500	-4.08753	-1.11861
H	7.58326	-2.51267	2.12607
H	7.02614	-4.03993	1.39701
C	9.21159	-3.79598	1.39289
H	10.76600	-1.08570	-0.16793
C	10.27315	-2.92764	-1.23592
C	10.22981	-2.63609	1.27610
H	9.40915	-4.80616	-1.94456
C	9.43926	-4.80405	0.24080
H	9.33485	-4.30580	2.36616
H	11.30466	-3.32459	-1.19257
H	10.16385	-2.42077	-2.21354
H	10.08939	-1.91930	2.10736
H	11.26060	-3.02847	1.35970
H	8.72961	-5.64876	0.32654
H	10.45752	-5.23079	0.30779

D

SCF (BP86) Energy = -3601.61027016
Enthalpy 0K = -3599.807049
Enthalpy 298K = -3599.690553
Free Energy 298K = -3599.973212
Lowest Frequency = 3.4084 cm^{-1}
Second Frequency = 7.2272 cm^{-1}
SCF (BP86-D3BJ) Energy = -3602.21848417
SCF (tol) Energy = -3601.62151749
SCF (BS2) Energy = -6369.11921771

K	-1.16803	1.33777	2.07691
Si	-3.24823	-4.09809	2.32709
Si	-2.84395	-4.79953	-0.67962
Al	-1.96485	-1.87188	0.36994
O	-3.70825	-4.59982	0.76867
N	-2.58305	-2.47178	2.15902
N	-1.63451	-3.51393	-0.70528
C	-2.49161	-1.55621	3.24197
C	-3.57036	-0.64738	3.54307
C	-3.42878	0.31180	4.56738
H	-4.26640	0.98682	4.78040

C	-2.25589	0.41914	5.32500
H	-2.17012	1.16320	6.12406
C	-1.20257	-0.46114	5.04844
H	-0.28455	-0.40111	5.64574
C	-1.29365	-1.44024	4.03643
C	-4.89071	-0.66360	2.77179
H	-4.84183	-1.51475	2.07150
C	-6.11236	-0.85224	3.69954
H	-6.01237	-1.75195	4.32648
H	-7.03716	-0.95281	3.10351
H	-6.25002	0.01320	4.37255
C	-5.06116	0.62814	1.94093
H	-5.04450	1.52445	2.58737
H	-6.02846	0.62546	1.40621
H	-4.26141	0.72997	1.18660
C	-0.09453	-2.36657	3.84354
H	-0.34459	-3.03666	3.00392
C	0.16147	-3.22652	5.10298
H	0.48106	-2.60277	5.95746
H	0.95897	-3.96697	4.91451
H	-0.74521	-3.77125	5.41304
C	1.18546	-1.58309	3.47477
H	1.05545	-1.03034	2.52601
H	2.04345	-2.26631	3.34938
H	1.45681	-0.85420	4.25994
C	-2.03222	-5.38628	3.02791
H	-2.47102	-6.39553	2.93771
H	-1.82951	-5.20574	4.09723
H	-1.06638	-5.38205	2.49674
C	-4.81768	-4.20899	3.39049
H	-5.66849	-3.69963	2.91130
H	-4.65971	-3.76335	4.38748
H	-5.09231	-5.26836	3.53413
C	-4.16466	-4.72473	-2.04862
H	-4.91250	-5.51880	-1.87751
H	-3.72213	-4.88698	-3.04616
H	-4.68794	-3.75674	-2.05211
C	-2.13846	-6.56598	-0.77006
H	-1.57641	-6.84907	0.13336
H	-1.47321	-6.68390	-1.64284
H	-2.97323	-7.27887	-0.88725
C	-0.52157	-3.52027	-1.59069
C	-0.55795	-2.80457	-2.83941
C	0.60438	-2.70913	-3.63413
H	0.55671	-2.15606	-4.58049
C	1.80374	-3.33041	-3.26241
H	2.69249	-3.25608	-3.89853
C	1.83223	-4.07569	-2.07573
H	2.75952	-4.58172	-1.78418
C	0.70360	-4.18877	-1.24047
C	-1.84439	-2.17382	-3.37182
H	-2.63861	-2.42504	-2.65014
C	-2.23569	-2.76774	-4.74454
H	-1.50225	-2.50366	-5.52756
H	-3.21802	-2.38105	-5.07005
H	-2.29775	-3.86825	-4.70610
C	-1.75106	-0.63503	-3.45385
H	-1.57794	-0.20019	-2.45318
H	-2.68589	-0.20196	-3.85454
H	-0.93126	-0.31546	-4.12347
C	0.82919	-5.00015	0.04752
H	-0.18962	-5.09289	0.45642
C	1.39871	-6.41582	-0.18505
H	0.81907	-6.97207	-0.93920
H	1.38058	-6.99557	0.75502
H	2.44937	-6.38278	-0.52663
C	1.67346	-4.24909	1.09658
H	1.70775	-4.80680	2.05035
H	1.24633	-3.25376	1.30064
H	2.71099	-4.10532	0.74648
K	1.55738	-0.56532	-1.04652
Si	3.63812	5.52981	-0.90482
Si	0.81433	6.49533	-0.05728
Al	1.36060	3.25887	0.04170
O	2.49971	6.58215	-0.21835
N	2.91994	3.90596	-0.93358
N	0.42308	4.88747	0.57200
C	3.52467	2.86901	-1.71394
C	4.56388	2.04139	-1.17016
C	5.06083	0.96175	-1.92688
H	5.85110	0.33451	-1.49958
C	4.56769	0.66744	-3.20478
H	4.97342	-0.17270	-3.77924
C	3.55980	1.47721	-3.74437
H	3.17930	1.26307	-4.75044
C	3.03527	2.57525	-3.03266
C	5.13539	2.28675	0.22720
H	4.74350	3.25957	0.56164
C	6.67770	2.36122	0.22911
H	7.05178	3.09319	-0.50660
H	7.04800	2.65777	1.22626
H	7.13631	1.38534	-0.01350
C	4.64325	1.23058	1.24187
H	4.94571	0.21196	0.94033
H	5.05969	1.42909	2.24622
H	3.54087	1.24992	1.32044
C	1.94307	3.42094	-3.68924
H	1.79903	4.30156	-3.04027
C	2.33989	3.91667	-5.09688
H	2.44136	3.08192	-5.81351
H	1.56631	4.59635	-5.49622
H	3.29760	4.46204	-5.07886
C	0.59802	2.66289	-3.74365
H	0.26526	2.37399	-2.72922
H	-0.19161	3.28904	-4.19656
H	0.68550	1.74242	-4.35019
C	4.10051	6.13675	-2.64540
H	4.62547	7.10526	-2.57895
H	4.77265	5.41999	-3.14791
H	3.21011	6.27452	-3.27957
C	5.17033	5.76709	0.19603
H	4.97498	5.46676	1.23876
H	6.04934	5.21079	-0.16865
H	5.42838	6.84086	0.19910
C	0.29792	7.86992	1.14052
H	0.47871	8.85884	0.68590
H	-0.77302	7.80065	1.39575
H	0.87773	7.81431	2.07594
C	0.08423	6.86200	-1.77628
H	0.29271	6.04177	-2.48405
H	-1.00772	7.01283	-1.74219
H	0.53977	7.78299	-2.17992
C	-0.60281	4.69234	1.53520
C	-0.27795	4.60213	2.93431
C	-1.28901	4.29188	3.86705
H	-1.03006	4.22605	4.93052
C	-2.61990	4.09080	3.47225
H	-3.39251	3.86596	4.21494
C	-2.94745	4.20399	2.11319
H	-3.98930	4.06789	1.79834
C	-1.97073	4.49876	1.13904
C	1.14250	4.85775	3.44225
H	1.72256	5.22778	2.57920
C	1.18047	5.93685	4.54717
H	0.67370	5.60037	5.46969
H	2.22503	6.17420	4.81460

H	0.69062	6.86874	4.21902
C	1.82014	3.55819	3.93331
H	1.89134	2.81612	3.11623
H	2.84379	3.76166	4.29509
H	1.25419	3.10226	4.76714
C	-2.40213	4.62427	-0.32170
H	-1.48841	4.83265	-0.90140
C	-3.38339	5.80211	-0.51865
H	-2.95548	6.75008	-0.15091
H	-3.63115	5.92945	-1.58755
H	-4.33059	5.63423	0.02534
C	-3.00733	3.31523	-0.87203
H	-3.29676	3.43926	-1.93093
H	-2.28417	2.48186	-0.82092
H	-3.91303	3.01764	-0.31281
C	-8.46691	-1.18180	-3.37524
H	-8.49831	-2.28726	-3.33949
H	-9.35850	-0.85138	-3.94073
C	-7.18028	-0.70693	-4.09202
H	-7.14414	-1.12875	-5.11357
C	-8.50314	-0.60010	-1.94181
H	-9.41715	-0.94255	-1.42205
C	-7.26854	-1.09728	-1.15268
H	-7.25926	-2.20015	-1.08536
H	-7.27930	-0.70405	-0.11995
C	-5.93990	-1.20205	-3.31011
H	-5.00791	-0.88099	-3.80972
H	-5.92413	-2.30563	-3.25890
C	-5.97155	-0.62028	-1.86787
C	-5.95986	0.93218	-1.94327
H	-5.95863	1.34579	-0.91909
H	-5.02733	1.26480	-2.43378
C	-7.16562	0.83864	-4.16238
H	-8.03782	1.19955	-4.73939
H	-6.26006	1.18822	-4.69372
C	-8.48664	0.94600	-2.00918
H	-9.37971	1.31039	-2.55101
H	-8.53221	1.37293	-0.98915
C	-7.20100	1.41979	-2.72887
H	-7.18201	2.52456	-2.77214
C	-3.91995	-1.56473	-0.52815
N	-4.82752	-1.09017	-1.13752
C	4.15925	-2.04292	-0.45137
N	5.17111	-2.64217	-0.29467
C	6.39710	-3.36854	-0.09076
C	7.58818	-2.37160	-0.04838
C	6.60335	-4.37460	-1.25693
C	6.31873	-4.14168	1.25517
H	7.62549	-1.80813	-0.99870
H	7.42314	-1.64150	0.76466
C	8.90260	-3.15768	0.17452
H	6.63213	-3.82219	-2.21382
H	5.74181	-5.06579	-1.29811
C	7.92190	-5.15284	-1.03029
H	6.14693	-3.42332	2.07728
H	5.45392	-4.82934	1.23011
C	7.63790	-4.92142	1.47162
H	9.74329	-2.44031	0.20359
C	9.10755	-4.15874	-0.98782
C	8.82325	-3.92720	1.51493
H	8.06017	-5.86536	-1.86427
C	7.84256	-5.92309	0.30974
H	7.57245	-5.46829	2.43022
H	10.05687	-4.70923	-0.84955
H	9.18659	-3.61663	-1.94930
H	8.69704	-3.21854	2.35531
H	9.76838	-4.47343	1.69320
H	7.01057	-6.65212	0.28280
H	8.77216	-6.50102	0.46854

E

SCF (BP86) Energy = -4084.54520627
Enthalpy 0K = -4082.506943
Enthalpy 298K = -4082.379040
Free Energy 298K = -4082.687366
Lowest Frequency = 4.7482 cm^{-1}
Second Frequency = 6.2239 cm^{-1}
SCF (BP86-D3BJ) Energy = -4085.20765592
SCF (tol) Energy = -4084.56011632
SCF (BS2) Energy = -6852.16204623

K	1.91026	2.14452	-0.96144
Si	4.81965	-1.73492	-3.99179
Si	3.34831	-4.27002	-2.96704
Al	2.59781	-1.40477	-1.66407
O	4.68744	-3.27821	-3.29132
N	3.91111	-0.63316	-2.95040
N	2.09171	-3.19695	-2.34188
C	4.16064	0.76650	-2.93262
C	5.04355	1.35327	-1.95321
C	5.19448	2.75354	-1.87673
H	5.86928	3.17209	-1.12045
C	4.52154	3.62002	-2.74661
H	4.66148	4.70448	-2.67932
C	3.68637	3.06350	-3.72327
H	3.17097	3.72734	-4.42750
C	3.49436	1.67010	-3.83807
C	5.86097	0.50714	-0.97663
H	5.65644	-0.54896	-1.22141
C	7.37904	0.75918	-1.12700
H	7.71487	0.60617	-2.16475
H	7.95074	0.07129	-0.47809
H	7.65125	1.78938	-0.83414
C	5.42839	0.75721	0.48504
H	5.54418	1.82070	0.76083
H	6.04801	0.16593	1.18371
H	4.37274	0.47636	0.64574
C	2.57730	1.18039	-4.95746
H	2.51195	0.08375	-4.86255
C	3.15986	1.53005	-6.34732
H	3.16022	2.62229	-6.51544
H	2.55829	1.06988	-7.15076
H	4.20037	1.18179	-6.45361
C	1.15269	1.76204	-4.83118
H	0.67214	1.46527	-3.88278
H	0.50793	1.40222	-5.65128
H	1.15884	2.86572	-4.87639
C	4.20524	-1.88802	-5.78870
H	4.71602	-2.74191	-6.26757
H	4.43115	-0.98806	-6.38353
H	3.11859	-2.06670	-5.84479
C	6.67659	-1.34592	-4.07051
H	7.16238	-1.52894	-3.09887
H	6.85403	-0.29502	-4.35638
H	7.16505	-1.98904	-4.82269
C	4.03859	-5.58120	-1.77142
H	4.87058	-6.11087	-2.26796
H	3.27975	-6.33140	-1.49317
H	4.43077	-5.12080	-0.85113
C	2.82077	-5.21948	-4.52823
H	2.62439	-4.55016	-5.38007
H	1.90791	-5.80988	-4.33688
H	3.61989	-5.92183	-4.82241
C	0.74817	-3.64834	-2.20588

C	0.29149	-4.28038	-0.99599
C	-1.06140	-4.65576	-0.86186
H	-1.39210	-5.12769	0.07017
C	-1.99273	-4.43684	-1.88545
H	-3.03936	-4.73490	-1.76390
C	-1.55473	-3.83583	-3.07328
H	-2.27317	-3.66828	-3.88409
C	-0.21193	-3.44683	-3.25844
C	1.23473	-4.55683	0.17527
H	2.25540	-4.35959	-0.18906
C	1.16505	-6.02528	0.64909
H	0.19015	-6.26349	1.11121
H	1.94229	-6.22488	1.40843
H	1.31666	-6.72914	-0.18634
C	0.96585	-3.59256	1.35303
H	1.16334	-2.54611	1.05573
H	1.61807	-3.82739	2.21506
H	-0.08115	-3.66212	1.69890
C	0.17066	-2.79124	-4.58329
H	1.26697	-2.66662	-4.56577
C	-0.21395	-3.65252	-5.80673
H	0.20665	-4.66868	-5.74055
H	0.16016	-3.18696	-6.73588
H	-1.30984	-3.74802	-5.90908
C	-0.45974	-1.38777	-4.70300
H	-0.17214	-0.90712	-5.65445
H	-0.12611	-0.73279	-3.87955
H	-1.56357	-1.44025	-4.67572
K	-1.42219	-1.32610	-0.69584
Si	-6.74931	2.58393	-1.43311
Si	-4.77332	4.65660	-0.28044
Al	-3.72905	1.52590	-0.71633
O	-6.26789	4.11244	-0.86390
N	-5.67254	1.35316	-0.75259
N	-3.51319	3.47851	-0.71297
C	-6.24921	0.13407	-0.27697
C	-6.45391	-0.98948	-1.14325
C	-7.00653	-2.17844	-0.62594
H	-7.16680	-3.02811	-1.30123
C	-7.37428	-2.29231	0.71930
H	-7.83142	-3.21531	1.09467
C	-7.18011	-1.19522	1.57065
H	-7.49094	-1.26814	2.61990
C	-6.62546	0.01044	1.10316
C	-6.12222	-0.92717	-2.63401
H	-5.68349	0.06767	-2.82069
C	-7.39246	-1.06868	-3.50400
H	-8.14897	-0.30977	-3.24177
H	-7.14964	-0.95466	-4.57586
H	-7.86151	-2.06051	-3.37206
C	-5.07323	-1.98244	-3.04433
H	-5.44201	-3.01095	-2.87795
H	-4.82207	-1.88637	-4.11626
H	-4.14367	-1.86045	-2.46293
C	-6.42342	1.17515	2.07184
H	-6.33900	2.08339	1.45052
C	-7.59650	1.37848	3.05237
H	-7.67862	0.55360	3.78357
H	-7.45251	2.30837	3.63016
H	-8.56105	1.45189	2.52183
C	-5.09111	1.02678	2.84122
H	-4.23516	0.96004	2.14352
H	-4.92240	1.88707	3.51511
H	-5.09150	0.10864	3.45635
C	-8.55097	2.32907	-0.89732
H	-9.18774	3.10974	-1.34778
H	-8.93249	1.34551	-1.21858
H	-8.65566	2.39253	0.19791
C	-6.68070	2.69598	-3.33088
H	-5.63865	2.76358	-3.68549
H	-7.14551	1.81859	-3.81077
H	-7.21706	3.59735	-3.67491
C	-4.44809	6.36642	-1.04140
H	-5.22521	7.07221	-0.70034
H	-3.46591	6.76656	-0.73847
H	-4.48085	6.33330	-2.14215
C	-5.00930	4.90224	1.59259
H	-5.12091	3.93928	2.11721
H	-4.16338	5.44428	2.04774
H	-5.92449	5.49397	1.76911
C	-2.21181	3.98754	-0.99015
C	-1.83696	4.32187	-2.33790
C	-0.54415	4.80803	-2.60572
H	-0.27522	5.07080	-3.63506
C	0.39846	4.99314	-1.58263
H	1.38776	5.41055	-1.80652
C	0.04067	4.66591	-0.26612
H	0.76767	4.81820	0.54171
C	-1.23771	4.15905	0.05008
C	-2.82831	4.14381	-3.48718
H	-3.83065	4.10864	-3.02700
C	-2.80866	5.30176	-4.50598
H	-1.86974	5.33004	-5.08821
H	-3.63248	5.18175	-5.23095
H	-2.92750	6.28111	-4.01207
C	-2.60895	2.78947	-4.19875
H	-2.69125	1.94963	-3.48330
H	-3.35732	2.63788	-4.99777
H	-1.60542	2.74346	-4.65813
C	-1.54742	3.80879	1.50571
H	-2.61646	3.54199	1.54410
C	-1.30902	4.99823	2.46153
H	-1.86081	5.89661	2.13738
H	-1.63651	4.74511	3.48556
H	-0.23828	5.26960	2.51391
C	-0.74927	2.57100	1.97448
H	-1.01074	2.30417	3.01460
H	-0.97776	1.69894	1.33530
H	0.34099	2.76014	1.94361
C	7.07287	-4.84657	3.39421
H	7.45162	-5.47503	2.56611
H	7.57783	-5.18943	4.31695
C	5.54125	-5.01469	3.53461
H	5.29634	-6.07831	3.71185
C	7.40500	-3.35864	3.12994
H	8.49810	-3.23332	3.01928
C	6.71866	-2.90034	1.82096
H	7.06832	-3.49892	0.96053
H	6.95577	-1.84299	1.60494
C	4.84955	-4.55937	2.22742
H	3.75425	-4.68332	2.30018
H	5.19357	-5.16575	1.37005
C	5.17773	-3.06275	1.96093
C	4.66828	-2.20366	3.15294
H	4.88198	-1.13879	2.94989
H	3.57114	-2.31057	3.23248
C	5.03162	-4.15580	4.71666
H	5.50513	-4.49011	5.65905
H	3.93960	-4.28586	4.84010
C	6.89615	-2.49663	4.31043
H	7.40104	-2.80179	5.24639
H	7.14683	-1.43199	4.14090
C	5.36458	-2.66738	4.45487
H	4.99689	-2.04889	5.29495
C	4.00670	-2.28039	-0.25642
N	4.54029	-2.64010	0.74600

C	3.09040	3.59795	1.42246
N	3.51321	4.25841	2.31116
C	4.01175	5.07127	3.38930
C	5.47382	4.65866	3.71579
C	3.11939	4.86490	4.64479
C	3.97489	6.56571	2.96388
H	5.49713	3.58863	3.99159
H	6.09799	4.78255	2.81212
C	6.00212	5.53834	4.87460
H	3.12928	3.79613	4.92650
H	2.07606	5.13274	4.39820
C	3.65753	5.74415	5.79928
H	4.58979	6.70086	2.05539
H	2.93709	6.84557	2.70723
C	4.50960	7.43711	4.12573
H	7.04204	5.23845	5.10048
C	5.11365	5.33308	6.12515
C	5.96597	7.02644	4.45074
H	3.01735	5.59154	6.68754
C	3.62053	7.23231	5.37585
H	4.47991	8.49747	3.81464
H	5.49868	5.94039	6.96550
H	5.14874	4.27555	6.44942
H	6.61470	7.18848	3.56904
H	6.36464	7.66047	5.26455
H	2.58064	7.54241	5.16018
H	3.98153	7.86979	6.20442
C	-2.64024	-2.65029	1.70359
N	-3.24219	-3.24896	2.53048
C	-3.98941	-3.97013	3.52528
C	-3.00963	-4.78314	4.41575
C	-4.98328	-4.93678	2.82325
C	-4.78094	-2.96387	4.40481
H	-2.43146	-5.47927	3.78080
H	-2.29007	-4.09145	4.89111
C	-3.81774	-5.55675	5.48501
H	-4.41775	-5.63437	2.17836
H	-5.65559	-4.34936	2.17216
C	-5.78207	-5.71091	3.89971
H	-4.07276	-2.25990	4.87907
H	-5.45353	-2.37501	3.75582
C	-5.58074	-3.74421	5.47518
H	-3.11388	-6.13290	6.11407
C	-4.80595	-6.52150	4.78625
C	-4.60501	-4.55393	6.36270
H	-6.48529	-6.39756	3.39322
C	-6.56958	-4.70919	4.77820
H	-6.13966	-3.02079	6.09706
H	-5.37117	-7.09637	5.54381
H	-4.25165	-7.25614	4.17144
H	-3.90590	-3.87138	6.88266
H	-5.16689	-5.09761	7.14538
H	-7.28480	-4.13816	4.15705
H	-7.16274	-5.25549	5.53563

TS(E-F)

SCF (BP86) Energy = -4084.51981865
Enthalpy 0K = -4082.482133
Enthalpy 298K = -4082.355533
Free Energy 298K = -4082.658789
Lowest Frequency = -58.1460 cm^{-1}
Second Frequency = 5.0524 cm^{-1}
SCF (BP86-D3BJ) Energy = -4085.19432419
SCF (tol) Energy = -4084.53403873
SCF (BS2) Energy = -6852.13943289

K	1.62862	1.35067	-1.93175
Si	5.54210	-2.76000	-2.50092
Si	4.48659	-4.65585	-0.27565
Al	2.99649	-1.82900	-0.74693
O	5.62390	-3.68110	-1.07492
N	4.29232	-1.53918	-2.22908
N	2.96047	-3.76621	-0.34750
C	4.23945	-0.32982	-2.97532
C	4.85771	0.87716	-2.48129
C	4.70482	2.09384	-3.17891
H	5.18375	2.99616	-2.78037
C	3.97233	2.17802	-4.36930
H	3.87442	3.12994	-4.90252
C	3.39198	1.00867	-4.87628
H	2.83743	1.05357	-5.82114
C	3.51118	-0.23294	-4.21644
C	5.70072	0.90300	-1.20566
H	5.75621	-0.13592	-0.83864
C	7.13791	1.40691	-1.47148
H	7.63264	0.82231	-2.26295
H	7.75008	1.32765	-0.55507
H	7.14694	2.46747	-1.78147
C	5.03454	1.76668	-0.11128
H	4.87535	2.80321	-0.45908
H	5.66951	1.81568	0.79185
H	4.05612	1.35113	0.18848
C	2.86606	-1.44623	-4.88394
H	3.01394	-2.30232	-4.20466
C	3.54355	-1.75797	-6.23952
H	3.34335	-0.95932	-6.97656
H	3.16013	-2.70382	-6.66078
H	4.63779	-1.84442	-6.13913
C	1.34942	-1.25209	-5.09606
H	0.82264	-1.08274	-4.14084
H	0.90296	-2.14271	-5.57062
H	1.14002	-0.38975	-5.75387
C	5.22252	-3.97374	-3.93343
H	5.95010	-4.80177	-3.86840
H	5.34928	-3.49553	-4.91830
H	4.20926	-4.40680	-3.89547
C	7.27529	-2.03168	-2.76404
H	7.64977	-1.55167	-1.84595
H	7.27662	-1.28284	-3.57449
H	7.98130	-2.83296	-3.04227
C	5.24802	-4.91909	1.44824
H	6.23602	-5.39781	1.33053
H	4.62832	-5.57632	2.08053
H	5.39474	-3.96313	1.97475
C	4.39738	-6.37868	-1.07407
H	4.18923	-6.33209	-2.15415
H	3.61237	-6.99108	-0.59747
H	5.36025	-6.89992	-0.93405
C	1.72936	-4.38770	0.00660
C	1.24267	-4.36308	1.36150
C	-0.01161	-4.92885	1.67294
H	-0.36465	-4.90310	2.71071
C	-0.80891	-5.53790	0.69495
H	-1.77259	-5.98398	0.95954
C	-0.34036	-5.57552	-0.62530
H	-0.95161	-6.05893	-1.39679
C	0.90587	-5.02358	-0.98820
C	2.04715	-3.73497	2.49944
H	3.03977	-3.49317	2.08772
C	2.23575	-4.70699	3.68546
H	1.28172	-4.91745	4.20102
H	2.92211	-4.27471	4.43526
H	2.65522	-5.67233	3.35659
C	1.40435	-2.41485	2.98100
H	1.38168	-1.66373	2.17026

H	1.97243	-1.98123	3.82476
H	0.37010	-2.57791	3.33442
C	1.32999	-5.10901	-2.45298
H	2.36316	-4.72540	-2.50345
C	1.30825	-6.55551	-2.99514
H	1.91187	-7.23462	-2.37229
H	1.71060	-6.58543	-4.02325
H	0.28108	-6.96015	-3.03577
C	0.44892	-4.19985	-3.33577
H	0.76368	-4.25367	-4.39274
H	0.52273	-3.14520	-3.01767
H	-0.61315	-4.50371	-3.28974
K	-0.93506	-2.20175	-0.07108
Si	-7.12824	-0.63135	-1.81994
Si	-5.68783	1.99592	-2.47203
Al	-4.14464	-0.33789	-0.71382
O	-6.95931	0.87878	-2.58703
N	-6.03779	-0.67348	-0.41852
N	-4.19804	1.13689	-1.99586
C	-6.53076	-1.29240	0.77915
C	-6.29601	-2.67704	1.05925
C	-6.77366	-3.23961	2.26035
H	-6.58179	-4.30058	2.46303
C	-7.49330	-2.48284	3.18945
H	-7.86165	-2.93864	4.11510
C	-7.74851	-1.13411	2.90872
H	-8.32583	-0.53792	3.62497
C	-7.28905	-0.52503	1.72667
C	-5.53496	-3.58026	0.09087
H	-5.29202	-2.96936	-0.79662
C	-6.37991	-4.78604	-0.37579
H	-7.32693	-4.45879	-0.83752
H	-5.82663	-5.38807	-1.11912
H	-6.63700	-5.45305	0.46667
C	-4.19839	-4.05322	0.70120
H	-4.36375	-4.71944	1.56798
H	-3.60420	-4.61394	-0.04368
H	-3.60937	-3.18875	1.05612
C	-7.58568	0.95652	1.49322
H	-7.42049	1.14909	0.41997
C	-9.03616	1.35768	1.83449
H	-9.23640	1.30376	2.91987
H	-9.22725	2.39954	1.52205
H	-9.77023	0.70792	1.32903
C	-6.58902	1.84219	2.27357
H	-5.54774	1.58945	2.01126
H	-6.75733	2.91432	2.06273
H	-6.70877	1.69321	3.36281
C	-8.95210	-0.84318	-1.35220
H	-9.55281	-0.93114	-2.27396
H	-9.11079	-1.75284	-0.74997
H	-9.32998	0.01865	-0.78086
C	-6.70688	-1.94825	-3.12777
H	-5.63566	-1.93025	-3.38865
H	-6.94730	-2.96140	-2.76217
H	-7.28722	-1.77261	-4.05028
C	-5.52611	2.81632	-4.17654
H	-6.45810	3.36377	-4.40083
H	-4.69074	3.53547	-4.20805
H	-5.37137	2.07312	-4.97461
C	-6.21658	3.33909	-1.23665
H	-6.18373	2.97060	-0.19980
H	-5.56311	4.22533	-1.30535
H	-7.24911	3.66194	-1.45583
C	-2.99471	1.56268	-2.63105
C	-2.56402	0.96338	-3.86601
C	-1.38518	1.41442	-4.48819
H	-1.07753	0.96301	-5.43762
C	-0.61375	2.45112	-3.94170
H	0.27414	2.82049	-4.47041
C	-1.02023	3.02956	-2.72964
H	-0.43058	3.84910	-2.29876
C	-2.18636	2.60246	-2.06097
C	-3.37032	-0.15823	-4.52076
H	-4.38874	-0.09798	-4.10017
C	-3.47762	-0.03042	-6.05467
H	-2.51035	-0.21068	-6.55761
H	-4.18839	-0.77835	-6.44664
H	-3.83213	0.96944	-6.35730
C	-2.80068	-1.54283	-4.13496
H	-2.83354	-1.67906	-3.03576
H	-3.38849	-2.35578	-4.59884
H	-1.75157	-1.64596	-4.46681
C	-2.56171	3.27909	-0.74293
H	-3.54157	2.86990	-0.44564
C	-2.70165	4.81047	-0.88974
H	-3.40734	5.07957	-1.69359
H	-3.06699	5.25820	0.05146
H	-1.73226	5.28585	-1.12940
C	-1.55331	2.93285	0.37565
H	-1.84482	3.41587	1.32561
H	-1.51507	1.84501	0.55549
H	-0.53662	3.28816	0.12053
C	7.38105	-0.90966	5.35658
H	7.96341	-1.77955	4.99837
H	7.83530	-0.58863	6.31278
C	5.90376	-1.31125	5.58068
H	5.84788	-2.14124	6.30900
C	7.45061	0.24082	4.32433
H	8.50498	0.52656	4.15287
C	6.84160	-0.23189	2.98273
H	7.39399	-1.10088	2.58191
H	6.89474	0.57068	2.22510
C	5.28863	-1.78680	4.24269
H	4.23556	-2.09039	4.38206
H	5.83554	-2.66276	3.84946
C	5.35450	-0.63181	3.20339
C	4.55870	0.59098	3.74169
H	4.58688	1.40185	2.99158
H	3.50038	0.30287	3.87734
C	5.10986	-0.09377	6.11174
H	5.52993	0.23869	7.07961
H	4.05620	-0.37615	6.29739
C	6.65662	1.46018	4.85216
H	7.10136	1.81952	5.79918
H	6.71712	2.29644	4.12961
C	5.17963	1.05776	5.08038
H	4.60777	1.92812	5.45259
C	4.33396	-1.44283	0.92302
N	4.79075	-1.07332	1.95816
C	2.06648	4.17452	-0.98345
N	2.19904	5.31358	-0.68552
C	2.34429	6.70041	-0.32720
C	3.72979	6.91869	0.34175
C	1.21721	7.09582	0.66698
C	2.24061	7.57435	-1.60826
H	3.80752	6.27463	1.23662
H	4.52623	6.61094	-0.36014
C	3.87846	8.41159	0.72260
H	1.28114	6.45342	1.56403
H	0.23444	6.91068	0.19700
C	1.37675	8.58811	1.04531
H	3.02823	7.26996	-2.32155
H	1.26440	7.39401	-2.09382
C	2.39581	9.06429	-1.21908
H	4.86594	8.55830	1.19764

C	2.75612	8.80619	1.71260
C	3.77571	9.28225	-0.55275
H	0.57143	8.86089	1.75167
C	1.27284	9.45875	-0.22990
H	2.32097	9.67815	-2.13536
H	2.86950	9.86576	2.00852
H	2.83279	8.20350	2.63752
H	4.58678	9.02240	-1.25932
H	3.90513	10.34934	-0.29264
H	0.28196	9.32566	-0.70367
H	1.36195	10.52875	0.03516
C	-2.60572	-0.59191	1.51380
N	-3.28105	0.00858	2.35356
C	-3.08158	0.19967	3.80510
C	-1.73533	-0.38570	4.30538
C	-4.24398	-0.50290	4.55346
C	-3.11559	1.71766	4.11850
H	-1.70304	-1.46558	4.06758
H	-0.90173	0.09179	3.75635
C	-1.59050	-0.15911	5.82927
H	-4.22522	-1.58248	4.31670
H	-5.20843	-0.11656	4.18113
C	-4.10226	-0.27369	6.07736
H	-2.29292	2.21763	3.57298
H	-4.06350	2.14480	3.74612
C	-2.97441	1.94608	5.64278
H	-0.62572	-0.58248	6.17027
C	-2.75660	-0.85982	6.56731
C	-1.62878	1.35826	6.13076
H	-4.93961	-0.77768	6.59569
C	-4.14131	1.24388	6.37797
H	-3.00376	3.03300	5.84960
H	-2.65339	-0.71903	7.66073
H	-2.72567	-1.94989	6.37732
H	-0.78571	1.86802	5.62490
H	-1.50789	1.53341	7.21735
H	-5.10799	1.67128	6.05019
H	-4.06309	1.41891	7.46844

F

SCF (BP86) Energy = -4084.54901522
Enthalpy 0K = -4082.509629
Enthalpy 298K = -4082.383383
Free Energy 298K = -4082.684081
Lowest Frequency = 3.2482 cm^{-1}
Second Frequency = 5.8851 cm^{-1}
SCF (BP86-D3BJ) Energy = -4085.24473313
SCF (tol) Energy = -4084.56081159
SCF (BS2) Energy = -6852.17032528

K	-0.00040	0.50262	-1.41383
Si	5.78884	-2.31320	-2.23870
Si	5.41377	-3.76123	0.48476
Al	3.15083	-1.65242	-0.51697
O	6.19040	-2.76749	-0.64713
N	4.24784	-1.45504	-2.14573
N	3.69456	-3.36571	0.37490
C	3.85991	-0.53253	-3.16836
C	4.12369	0.87603	-3.03333
C	3.67341	1.78175	-4.01448
H	3.88725	2.85019	-3.88691
C	2.98438	1.35420	-5.15406
H	2.65717	2.07151	-5.91500
C	2.74854	-0.01526	-5.31188
H	2.23044	-0.36846	-6.21186
C	3.16801	-0.96050	-4.35400
C	4.90643	1.45297	-1.85378
H	5.25361	0.59707	-1.25003
C	6.14471	2.25819	-2.31021
H	6.79901	1.65996	-2.96393
H	6.73946	2.58260	-1.43670
H	5.85742	3.16848	-2.86696
C	4.00313	2.33455	-0.96454
H	3.56735	3.16739	-1.54539
H	4.57835	2.77560	-0.12939
H	3.17122	1.74852	-0.53667
C	2.87291	-2.43035	-4.64720
H	3.25017	-3.01193	-3.78944
C	3.59046	-2.90680	-5.93197
H	3.17425	-2.41073	-6.82740
H	3.47025	-3.99612	-6.06980
H	4.66891	-2.68013	-5.90559
C	1.35700	-2.69174	-4.77500
H	0.82857	-2.40090	-3.85109
H	1.15145	-3.75956	-4.96559
H	0.92145	-2.11666	-5.61230
C	5.80545	-3.91232	-3.27610
H	6.74370	-4.45762	-3.07179
H	5.76815	-3.70625	-4.35797
H	4.96284	-4.58014	-3.03080
C	7.22328	-1.23446	-2.85790
H	7.48173	-0.45947	-2.11880
H	6.96620	-0.73650	-3.80819
H	8.11911	-1.85562	-3.02961
C	6.29888	-3.34951	2.11937
H	7.37804	-3.54661	1.99345
H	5.93960	-3.96668	2.95937
H	6.17773	-2.28792	2.38590
C	5.77769	-5.59726	0.14526
H	5.52413	-5.89102	-0.88508
H	5.21024	-6.24341	0.83766
H	6.85151	-5.79850	0.30279
C	2.70243	-4.18401	0.97415
C	2.28146	-3.98255	2.33865
C	1.22033	-4.74337	2.87472
H	0.91873	-4.57529	3.91582
C	0.54985	-5.71340	2.11629
H	-0.26327	-6.30247	2.55414
C	0.96664	-5.93594	0.79620
H	0.46667	-6.70866	0.19965
C	2.02831	-5.20965	0.21781
C	2.94513	-2.94506	3.24455
H	3.79988	-2.53674	2.68233
C	3.47197	-3.57269	4.55423
H	2.64816	-3.92587	5.20024
H	4.04912	-2.83158	5.13520
H	4.12860	-4.43551	4.35380
C	1.98919	-1.77120	3.55697
H	1.71779	-1.22310	2.63634
H	2.46145	-1.04679	4.24535
H	1.06210	-2.12504	4.04559
C	2.42561	-5.53891	-1.21925
H	3.31555	-4.92680	-1.44439
C	2.78596	-7.03049	-1.40054
H	3.56625	-7.35090	-0.69188
H	3.15748	-7.21314	-2.42441
H	1.90687	-7.68293	-1.25082
C	1.31735	-5.13526	-2.21343
H	1.61564	-5.37133	-3.24963
H	1.11645	-4.05089	-2.16221
H	0.37472	-5.67549	-2.00704
K	-0.20062	-2.70607	0.73442
Si	-6.75305	-2.37869	-0.44550
Si	-6.32645	-0.04603	-2.46648
Al	-4.18217	-0.57197	-0.13259

O	-7.03736	-1.45892	-1.84541
N	-5.67691	-1.44520	0.61565
N	-4.66136	0.08230	-1.84841
C	-5.89619	-1.47726	2.03672
C	-5.25452	-2.45347	2.86234
C	-5.45834	-2.43079	4.25678
H	-4.95982	-3.18273	4.88068
C	-6.28556	-1.47866	4.86014
H	-6.43030	-1.47442	5.94591
C	-6.94103	-0.54215	4.05174
H	-7.60604	0.19470	4.51662
C	-6.77553	-0.52753	2.65378
C	-4.35764	-3.54502	2.27804
H	-4.32214	-3.38219	1.18699
C	-4.93286	-4.95550	2.53812
H	-5.96105	-5.04955	2.14993
H	-4.31155	-5.73015	2.05305
H	-4.96727	-5.18304	3.61857
C	-2.91344	-3.44348	2.81600
H	-2.87726	-3.58134	3.91156
H	-2.27481	-4.23171	2.37182
H	-2.48632	-2.45018	2.58892
C	-7.53505	0.51375	1.83114
H	-7.49333	0.17788	0.78150
C	-9.02043	0.63819	2.23336
H	-9.14148	1.08271	3.23741
H	-9.55408	1.29330	1.52250
H	-9.52445	-0.34277	2.24135
C	-6.84637	1.89555	1.89798
H	-5.81130	1.84004	1.51964
H	-7.39412	2.64214	1.29443
H	-6.80863	2.26661	2.93842
C	-8.41262	-2.75496	0.38267
H	-9.00532	-3.41620	-0.27225
H	-8.27359	-3.26479	1.35041
H	-8.99557	-1.83747	0.55822
C	-5.99616	-4.01406	-1.05250
H	-4.98075	-3.86422	-1.45622
H	-5.93154	-4.75555	-0.23836
H	-6.62025	-4.44312	-1.85536
C	-6.34433	-0.22010	-4.35372
H	-7.38077	-0.13128	-4.72164
H	-5.73586	0.55186	-4.85299
H	-5.96184	-1.20748	-4.65777
C	-7.45190	1.39822	-1.96313
H	-7.34527	1.64447	-0.89494
H	-7.22672	2.30709	-2.54534
H	-8.50555	1.12761	-2.14904
C	-3.58364	0.41305	-2.73206
C	-2.82041	-0.61717	-3.38059
C	-1.69495	-0.26650	-4.15536
H	-1.11438	-1.05887	-4.64034
C	-1.31930	1.07170	-4.34793
H	-0.44082	1.31928	-4.95408
C	-2.10627	2.08150	-3.77637
H	-1.84884	3.13088	-3.96138
C	-3.23338	1.78254	-2.98306
C	-3.22211	-2.09170	-3.30281
H	-4.21509	-2.12213	-2.82179
C	-3.35060	-2.73531	-4.70166
H	-2.37126	-2.82045	-5.20512
H	-3.76495	-3.75498	-4.61491
H	-4.01436	-2.15000	-5.35935
C	-2.25494	-2.91337	-2.42048
H	-2.22647	-2.47860	-1.40528
H	-2.58751	-3.96537	-2.35218
H	-1.23524	-2.91505	-2.84796
C	-4.10156	2.93377	-2.47447
H	-4.80602	2.50048	-1.74384
C	-4.91689	3.54784	-3.63840
H	-5.52820	2.79161	-4.15724
H	-5.59271	4.34001	-3.26898
H	-4.24539	4.00142	-4.38986
C	-3.30087	4.04523	-1.76557
H	-3.98815	4.80463	-1.35196
H	-2.69600	3.64443	-0.93765
H	-2.61911	4.56475	-2.46359
C	7.34209	1.92390	4.67864
H	8.12633	1.16956	4.47837
H	7.73291	2.59458	5.46691
C	6.04732	1.23148	5.16670
H	6.25899	0.64186	6.07783
C	7.04067	2.73374	3.39511
H	7.96471	3.22403	3.03657
C	6.52566	1.77975	2.29100
H	7.27908	1.00783	2.05165
H	6.31600	2.33564	1.35923
C	5.52881	0.27329	4.06737
H	4.61010	-0.24277	4.39971
H	6.28020	-0.50427	3.83965
C	5.22129	1.08390	2.77642
C	4.14257	2.15891	3.08969
H	3.90712	2.71647	2.16551
H	3.21412	1.65587	3.41688
C	4.97138	2.30065	5.47270
H	5.32678	2.97626	6.27344
H	4.04763	1.81790	5.84443
C	5.96381	3.80334	3.69772
H	6.33402	4.50521	4.46865
H	5.75535	4.40128	2.78999
C	4.66974	3.11140	4.18982
H	3.89572	3.87224	4.40210
C	4.37981	-0.52591	0.87944
N	4.74693	0.19857	1.75057
C	0.41940	3.44714	-0.99282
N	0.60083	4.61804	-0.98053
C	0.81422	6.04134	-0.99153
C	2.13508	6.37352	-0.24375
C	-0.37553	6.74834	-0.28510
C	0.91172	6.53153	-2.46320
H	2.06749	6.00106	0.79465
H	2.97344	5.84469	-0.73242
C	2.35917	7.90502	-0.26558
H	-0.45536	6.37655	0.75260
H	-1.31506	6.48567	-0.80389
C	-0.14126	8.27817	-0.30609
H	1.74192	6.00493	-2.96799
H	-0.02056	6.26900	-2.99557
C	1.14020	8.06205	-2.47497
H	3.30066	8.13245	0.26768
C	1.17451	8.60970	0.43831
C	2.45658	8.39231	-1.73124
H	-0.99165	8.77286	0.19818
C	-0.04505	8.76614	-1.77166
H	1.20808	8.40137	-3.52495
H	1.33777	9.70360	0.44840
H	1.10864	8.28397	1.49386
H	3.31344	7.90957	-2.23836
H	2.64070	9.48264	-1.75515
H	-0.98896	8.55259	-2.30803
H	0.09847	9.86256	-1.79618
C	-2.26323	-0.64368	0.45876
N	-2.97053	0.28988	1.09978
C	-2.45954	1.17499	2.21786
C	-0.96993	0.94587	2.53584
C	-3.29600	0.87034	3.48503

C	-2.66278	2.65357	1.81820
H	-0.80670	-0.11645	2.79936
H	-0.35437	1.13800	1.63559
C	-0.52741	1.87059	3.69563
H	-3.16225	-0.19112	3.76503
H	-4.36880	1.00097	3.26069
C	-2.86417	1.79604	4.64645
H	-2.05617	2.86876	0.91713
H	-3.72219	2.82100	1.54772
C	-2.23590	3.58631	2.97706
H	0.54524	1.69545	3.91118
C	-1.36737	1.56228	4.95825
C	-0.73901	3.34917	3.28954
H	-3.47365	1.56510	5.54048
C	-3.08073	3.27199	4.23486
H	-2.39300	4.64054	2.67617
H	-1.04313	2.20822	5.79743
H	-1.20561	0.51409	5.27573
H	-0.12415	3.58946	2.40022
H	-0.40783	4.01910	4.10705
H	-4.15237	3.45438	4.02769
H	-2.79187	3.94691	5.06396

G

SCF (BP86) Energy = -2283.73993319
Enthalpy 0K = -2282.603044
Enthalpy 298K = -2282.535053
Free Energy 298K = -2282.709227
Lowest Frequency = 7.3255 cm^{-1}
Second Frequency = 8.0790 cm^{-1}
SCF (BP86-D3BJ) Energy = -2284.09478616
SCF (tol) Energy = -2283.74921651
SCF (BS2) Energy = -3667.61187611

K	-2.03970	-1.15189	0.52449
Si	3.70639	-2.78152	0.86733
Si	4.24543	-1.55615	-1.93409
Al	1.87651	-0.39100	-0.13234
O	4.35652	-2.72847	-0.70433
N	2.11417	-2.00103	0.84888
N	3.35096	-0.16240	-1.28784
N	-6.06431	-0.54096	-0.13993
N	1.03217	1.18996	0.58625
C	0.93537	-2.67789	1.27891
C	0.19050	-3.52637	0.38617
C	-0.99012	-4.15539	0.83703
H	-1.53686	-4.81246	0.14972
C	-1.46527	-3.98143	2.14563
H	-2.37060	-4.49781	2.48418
C	-0.74123	-3.15982	3.02137
H	-1.09369	-3.03393	4.05173
C	0.44385	-2.50791	2.61892
C	0.62498	-3.75479	-1.06166
H	1.64786	-3.35387	-1.15352
C	0.66501	-5.24740	-1.45381
H	-0.34393	-5.69768	-1.47801
H	1.27647	-5.83659	-0.75034
H	1.09911	-5.36235	-2.46194
C	-0.27687	-2.96185	-2.03847
H	-0.22763	-1.87729	-1.82730
H	-1.32881	-3.30125	-1.96714
H	0.04149	-3.11439	-3.08498
C	1.20528	-1.66386	3.64005
H	1.92792	-1.05562	3.06862
C	2.00005	-2.56651	4.61361
H	2.69906	-3.22783	4.07604
H	1.31911	-3.20878	5.20131
H	2.58524	-1.95568	5.32379
C	0.28966	-0.71024	4.43604
H	-0.40829	-1.25735	5.09573
H	-0.30627	-0.06821	3.76495
H	0.89434	-0.05149	5.08316
C	3.58621	-4.61231	1.33859
H	4.59854	-5.04952	1.37367
H	2.99932	-5.17731	0.59695
H	3.11717	-4.75639	2.32606
C	4.90848	-1.88323	2.02598
H	4.93402	-0.80341	1.80615
H	5.93142	-2.28048	1.90993
H	4.60946	-2.00626	3.08079
C	3.40314	-2.42360	-3.40263
H	2.33972	-2.63901	-3.21304
H	3.91564	-3.37935	-3.60952
H	3.46372	-1.80350	-4.31298
C	5.99773	-1.11254	-2.50611
H	6.39923	-1.94306	-3.11187
H	6.67970	-0.95020	-1.65750
H	5.99723	-0.20388	-3.13102
C	3.59164	1.15122	-1.83298
C	2.77125	1.67660	-2.88223
C	2.98348	2.99519	-3.33298
H	2.34208	3.39305	-4.12851
C	3.99264	3.80086	-2.79805
H	4.13981	4.82409	-3.16082
C	4.82289	3.27434	-1.80154
H	5.62657	3.89517	-1.38912
C	4.65097	1.96540	-1.31176
C	1.68208	0.84882	-3.56914
H	1.69382	-0.15283	-3.10589
C	1.98099	0.67954	-5.07734
H	2.99003	0.26793	-5.24977
H	1.92522	1.64638	-5.60910
H	1.24699	0.00011	-5.54666
C	0.26990	1.44140	-3.36502
H	0.20206	2.46587	-3.77425
H	-0.00376	1.47421	-2.29613
H	-0.48359	0.82509	-3.88991
C	5.59356	1.46515	-0.21503
H	5.45475	0.37339	-0.14750
C	7.08091	1.74380	-0.52302
H	7.72464	1.25878	0.23228
H	7.31047	2.82401	-0.49676
H	7.37164	1.36453	-1.51628
C	5.21690	2.05547	1.16096
H	4.17966	1.79273	1.42547
H	5.29510	3.15786	1.15446
H	5.88500	1.67286	1.95392
C	-4.95182	-0.86222	0.10895
C	-7.41671	-0.15043	-0.44247
C	-7.76699	-0.59535	-1.89000
H	-7.05516	-0.13027	-2.59610
H	-7.64972	-1.69128	-1.97306
C	-8.38773	-0.83010	0.56209
H	-8.11679	-0.53054	1.59098
H	-8.27366	-1.92744	0.49413
C	-7.54180	1.39456	-0.32680
H	-6.82895	1.87128	-1.02382
H	-7.26497	1.70680	0.69665
C	-9.22012	-0.17064	-2.21201
H	-9.46095	-0.49033	-3.24253
C	-10.18848	-0.84795	-1.21257
H	-11.23196	-0.56917	-1.45008
H	-10.12132	-1.94898	-1.30147
C	-9.83859	-0.40519	0.22865
H	-10.52291	-0.89270	0.94721

C	-9.96489	1.13309	0.34464
H	-11.00474	1.44342	0.13147
H	-9.73719	1.45866	1.37744
C	-8.99631	1.80956	-0.65531
H	-9.07715	2.90873	-0.57017
C	-9.34595	1.36769	-2.09686
H	-10.37590	1.68191	-2.34872
H	-8.67211	1.86176	-2.82225
C	0.07892	0.46832	-0.00074
C	0.79158	2.52375	1.26405
C	1.40557	3.62272	0.36189
H	2.47374	3.40227	0.18381
H	0.90805	3.59644	-0.62552
C	1.49328	2.54291	2.63953
H	2.56553	2.30730	2.51279
H	1.06213	1.75336	3.28274
C	-0.70843	2.81701	1.46300
H	-1.22458	2.75677	0.48723
H	-1.15740	2.02529	2.09709
C	1.23149	5.01087	1.02202
H	1.67747	5.78498	0.36860
C	-0.27633	5.29733	1.21783
H	-0.78948	5.31203	0.23700
H	-0.42182	6.29578	1.67497
C	-0.89414	4.20395	2.12309
H	-1.97568	4.40402	2.25980
C	-0.18714	4.22012	3.49993
H	-0.63744	3.45923	4.16707
H	-0.32724	5.20329	3.99035
C	1.32072	3.93012	3.30618
H	1.83002	3.93131	4.28936
C	1.94001	5.01971	2.39790
H	1.83717	6.01406	2.87461
H	3.02322	4.83381	2.26728

TS(G-H)

SCF (BP86) Energy = -2283.71332952
Enthalpy 0K = -2282.577277
Enthalpy 298K = -2282.510246
Free Energy 298K = -2282.679901
Lowest Frequency = -39.3457 cm^{-1}
Second Frequency = 7.9820 cm^{-1}
SCF (BP86-D3BJ) Energy = -2284.07819768
SCF (tol) Energy = -2283.72258117
SCF (BS2) Energy = -3667.58704751

K	-2.28696	-1.33691	1.27266
Si	3.38006	-2.83323	0.24649
Si	3.36874	-1.28639	-2.44701
Al	1.36372	-0.39854	-0.16193
O	3.75937	-2.56104	-1.38592
N	1.80262	-2.08183	0.59539
N	2.63092	0.01114	-1.48216
N	-3.89015	0.46808	-0.17496
N	0.54484	1.09046	0.78960
C	0.76607	-2.81327	1.24579
C	-0.16176	-3.61888	0.49533
C	-1.21100	-4.28511	1.16564
H	-1.89975	-4.91079	0.58479
C	-1.37717	-4.18789	2.55637
H	-2.18452	-4.73110	3.06092
C	-0.46133	-3.42327	3.29433
H	-0.56117	-3.37155	4.38507
C	0.61042	-2.74737	2.67291
C	-0.05470	-3.76981	-1.02263
H	0.92507	-3.35461	-1.31263
C	-0.10581	-5.24231	-1.48476
H	-1.10119	-5.69365	-1.32123
H	0.63319	-5.86361	-0.95234
H	0.10758	-5.30706	-2.56550
C	-1.14317	-2.94153	-1.74693
H	-1.05974	-1.86764	-1.50201
H	-2.15587	-3.29785	-1.47292
H	-1.05152	-3.04407	-2.84271
C	1.62170	-2.00752	3.54796
H	2.27594	-1.44191	2.86273
C	2.49752	-3.01351	4.33251
H	3.00652	-3.72281	3.65882
H	1.88739	-3.60563	5.03836
H	3.26933	-2.48337	4.91791
C	0.96418	-1.00464	4.51827
H	0.31428	-1.50739	5.25765
H	0.35713	-0.26084	3.97560
H	1.73701	-0.45683	5.08491
C	3.31743	-4.70986	0.49411
H	4.32900	-5.12886	0.35818
H	2.65229	-5.18982	-0.24099
H	2.96818	-4.98269	1.50392
C	4.77464	-2.10531	1.30392
H	4.76577	-1.00410	1.27932
H	5.75492	-2.44846	0.93107
H	4.68052	-2.42228	2.35650
C	2.20941	-2.03953	-3.75183
H	1.22238	-2.29312	-3.33211
H	2.65600	-2.96341	-4.15876
H	2.04818	-1.34120	-4.59031
C	4.94473	-0.72761	-3.33384
H	5.22477	-1.48199	-4.08877
H	5.78779	-0.61493	-2.63530
H	4.79155	0.23394	-3.85170
C	2.82677	1.39864	-1.82819
C	1.89543	2.08163	-2.67281
C	2.05355	3.46388	-2.89825
H	1.32871	3.98341	-3.53611
C	3.11057	4.18326	-2.33145
H	3.20997	5.25953	-2.50960
C	4.05522	3.50198	-1.55452
H	4.90502	4.05392	-1.13606
C	3.94895	2.12008	-1.30494
C	0.75787	1.35419	-3.39281
H	0.78716	0.30066	-3.06598
C	0.98233	1.38237	-4.92378
H	1.97304	0.98127	-5.19888
H	0.92553	2.41351	-5.31640
H	0.21156	0.78496	-5.44317
C	-0.63896	1.91168	-3.04420
H	-0.72671	2.98086	-3.30865
H	-0.86789	1.80428	-1.97173
H	-1.41698	1.36833	-3.61074
C	5.06055	1.43449	-0.50587
H	4.89302	0.34786	-0.59430
C	6.46362	1.75158	-1.07243
H	7.22971	1.13963	-0.56366
H	6.73666	2.81035	-0.91604
H	6.52366	1.54941	-2.15422
C	5.01349	1.78500	0.99708
H	4.06769	1.45636	1.45713
H	5.10325	2.87510	1.15409
H	5.84519	1.29926	1.53911
C	-3.06207	1.37428	-0.16305
C	-5.30579	0.29892	-0.54419
C	-6.05719	-0.41515	0.60952
H	-5.57442	-1.39318	0.81429
H	-5.97945	0.19461	1.52982
C	-5.98517	1.66628	-0.82048

H	-5.43363	2.18250	-1.62715
H	-5.90411	2.29925	0.08247
C	-5.39098	-0.57964	-1.81980
H	-4.89251	-1.55043	-1.63214
H	-4.83642	-0.08286	-2.63640
C	-7.54044	-0.63212	0.22214
H	-8.06070	-1.14024	1.05571
C	-8.20507	0.73873	-0.05193
H	-9.27130	0.59469	-0.31009
H	-8.17586	1.36557	0.85973
C	-7.46619	1.44916	-1.21128
H	-7.93676	2.43110	-1.40617
C	-7.53944	0.57343	-2.48528
H	-8.59405	0.42746	-2.78694
H	-7.03068	1.08191	-3.32603
C	-6.87307	-0.79639	-2.21073
H	-6.91660	-1.42264	-3.12131
C	-7.61324	-1.50707	-1.05231
H	-8.66964	-1.68484	-1.32863
H	-7.16026	-2.49936	-0.86095
C	-0.43625	0.34414	0.30751
C	0.32599	2.36114	1.58509
C	0.06981	3.51580	0.58238
H	0.92271	3.59241	-0.11678
H	-0.83051	3.26971	-0.00863
C	1.58274	2.67840	2.41615
H	2.44903	2.76612	1.73734
H	1.79180	1.84412	3.11448
C	-0.90067	2.23747	2.51770
H	-1.78424	1.99499	1.89996
H	-0.73923	1.40265	3.23098
C	-0.12826	4.84393	1.35224
H	-0.30195	5.66161	0.62674
C	-1.35066	4.71299	2.29145
H	-2.26275	4.51085	1.69904
H	-1.51730	5.66158	2.83836
C	-1.10590	3.56042	3.29525
H	-1.98217	3.45952	3.96542
C	0.15751	3.86759	4.13505
H	0.33031	3.05938	4.87245
H	0.01489	4.80329	4.70986
C	1.38072	4.00088	3.19638
H	2.28739	4.21511	3.79417
C	1.13541	5.15188	2.19043
H	1.01077	6.10943	2.73275
H	2.01218	5.26631	1.52509

H

SCF (BP86) Energy = -2283.80631075
Enthalpy 0K = -2282.666755
Enthalpy 298K = -2282.600451
Free Energy 298K = -2282.766139
Lowest Frequency = 18.6330 cm^{-1}
Second Frequency = 19.4366 cm^{-1}
SCF (BP86-D3BJ) Energy = -2284.17952190
SCF (tol) Energy = -2283.81480132
SCF (BS2) Energy = -3667.67820374

K	1.53634	2.46995	1.89833
Si	-3.77220	1.95409	-0.61077
Si	-2.92133	-0.04972	-2.81629
Al	-1.15874	0.14964	-0.20090
O	-3.84399	1.20751	-2.12904
N	-2.11378	1.76982	0.03880
N	-2.04890	-0.86202	-1.49754
N	3.17059	1.01438	0.35571
N	-0.06142	-0.63284	1.09273
C	-1.49768	2.89060	0.67400
C	-0.69866	3.82248	-0.07961
C	-0.06624	4.89582	0.58423
H	0.53346	5.60130	-0.00278
C	-0.21415	5.10336	1.96496
H	0.26140	5.96126	2.45398
C	-1.02038	4.21917	2.69751
H	-1.17592	4.39430	3.76913
C	-1.66945	3.12560	2.08229
C	-0.52506	3.69962	-1.59363
H	-1.23927	2.92884	-1.92907
C	-0.85325	5.01649	-2.33293
H	-0.10364	5.80130	-2.12539
H	-1.84076	5.41546	-2.04872
H	-0.85228	4.84671	-3.42332
C	0.89599	3.22188	-1.97073
H	1.13437	2.24832	-1.51291
H	1.65717	3.95660	-1.64724
H	0.98922	3.11528	-3.06601
C	-2.57770	2.24484	2.94045
H	-2.97583	1.46018	2.27630
C	-3.76706	3.05350	3.50778
H	-4.33426	3.55803	2.70772
H	-3.42672	3.83236	4.21375
H	-4.46017	2.39000	4.05384
C	-1.80707	1.54415	4.07936
H	-1.34962	2.27226	4.77497
H	-1.01294	0.89582	3.67164
H	-2.48490	0.90579	4.67248
C	-4.21200	3.77981	-0.85251
H	-5.27739	3.85789	-1.12903
H	-3.61990	4.23403	-1.66196
H	-4.05495	4.36930	0.06616
C	-5.10786	1.16571	0.48313
H	-4.82785	0.15549	0.81958
H	-6.04963	1.08718	-0.08695
H	-5.30536	1.78043	1.37752
C	-1.78544	0.78501	-4.08996
H	-0.99068	1.37538	-3.60418
H	-2.37570	1.46609	-4.72711
H	-1.29967	0.04145	-4.74349
C	-4.10040	-1.22394	-3.71463
H	-4.48806	-0.73312	-4.62347
H	-4.95863	-1.49121	-3.07876
H	-3.59175	-2.15436	-4.01677
C	-1.91061	-2.29923	-1.47589
C	-0.80806	-2.94213	-2.12273
C	-0.64540	-4.33560	-1.98709
H	0.20604	-4.82071	-2.47865
C	-1.54375	-5.11125	-1.24656
H	-1.39185	-6.19101	-1.14202
C	-2.65882	-4.49156	-0.67104
H	-3.39086	-5.09987	-0.12686
C	-2.87717	-3.10493	-0.79071
C	0.16634	-2.17971	-3.02235
H	-0.06358	-1.10610	-2.91674
C	-0.05135	-2.57578	-4.50287
H	-1.09791	-2.42416	-4.81841
H	0.18983	-3.64128	-4.66751
H	0.59844	-1.97876	-5.16783
C	1.64487	-2.37566	-2.62812
H	1.94298	-3.43895	-2.65990
H	1.83738	-1.98522	-1.61601
H	2.29940	-1.83024	-3.33186
C	-4.17516	-2.52098	-0.22751
H	-4.23135	-1.47667	-0.57801
C	-5.41917	-3.26921	-0.76053
H	-6.34239	-2.74716	-0.45225

H	-5.47679	-4.29840	-0.36379
H	-5.41325	-3.33885	-1.86071
C	-4.20261	-2.49779	1.31648
H	-3.39910	-1.86610	1.72858
H	-4.07409	-3.51370	1.73154
H	-5.16882	-2.10763	1.68481
C	2.10519	0.32266	0.14135
C	4.43655	0.69574	-0.36251
C	5.53739	1.63787	0.18083
H	5.22217	2.68934	0.02787
H	5.63998	1.48420	1.27351
C	4.87798	-0.77057	-0.12688
H	4.08533	-1.44518	-0.50176
H	4.97352	-0.95079	0.96206
C	4.28689	0.93336	-1.88658
H	3.96201	1.97757	-2.06126
H	3.48588	0.27409	-2.27041
C	6.88318	1.36780	-0.53307
H	7.65681	2.05054	-0.13240
C	7.30765	-0.10058	-0.28816
H	8.27836	-0.30243	-0.78081
H	7.45247	-0.27882	0.79503
C	6.22050	-1.05259	-0.84279
H	6.51969	-2.10321	-0.66404
C	6.05183	-0.81107	-2.36232
H	7.00161	-1.02604	-2.88917
H	5.29040	-1.50087	-2.77351
C	5.62699	0.65653	-2.60952
H	5.50191	0.82978	-3.69569
C	6.71473	1.60703	-2.05328
H	7.67620	1.43252	-2.57370
H	6.43197	2.66067	-2.24317
C	0.78952	0.17195	0.28769
C	0.45193	-1.64836	2.02975
C	1.26212	-2.74788	1.28840
H	0.61568	-3.20470	0.51735
H	2.11715	-2.28117	0.76490
C	-0.74317	-2.32564	2.73647
H	-1.38708	-2.78888	1.96783
H	-1.34751	-1.55654	3.25608
C	1.37704	-1.01177	3.11033
H	2.24228	-0.53333	2.61172
H	0.81053	-0.22616	3.65271
C	1.76477	-3.82226	2.28297
H	2.33813	-4.59086	1.73027
C	2.67391	-3.16372	3.34732
H	3.55877	-2.70760	2.86297
H	3.04997	-3.92740	4.05538
C	1.87259	-2.08409	4.11222
H	2.52147	-1.60617	4.87192
C	0.65331	-2.73763	4.80514
H	0.08339	-1.97516	5.37140
H	0.99475	-3.49416	5.53779
C	-0.25304	-3.39800	3.73906
H	-1.12894	-3.86103	4.23227
C	0.55006	-4.48054	2.97927
H	0.88974	-5.26622	3.68203
H	-0.09514	-4.97159	2.22667

G·Et$_2$O

SCF (BP86) Energy = -2517.40625032
Enthalpy 0K = -2516.135929
Enthalpy 298K = -2516.058701
Free Energy 298K = -2516.258254
Lowest Frequency = 4.0838 cm^{-1}
Second Frequency = 6.6383 cm^{-1}
SCF (BP86-D3BJ) Energy = -2517.79355149
SCF (tol) Energy = -2517.41426954
SCF (BS2) Energy = -3901.33928076

K	1.51818	2.41472	0.08900
Si	-4.02142	1.09475	-2.26899
Si	-3.03289	-1.78974	-2.85752
Al	-1.71691	-0.13241	-0.46147
O	-3.84456	-0.33067	-3.18308
O	2.88081	4.66277	1.24592
N	-2.54799	1.34403	-1.31747
N	-2.42889	-1.72681	-1.18686
N	5.00662	0.27148	-0.47097
N	-1.17922	-0.15166	1.39307
C	-1.79242	2.55203	-1.39587
C	-0.77713	2.73435	-2.39768
C	-0.02724	3.92959	-2.42591
H	0.73102	4.06234	-3.20756
C	-0.25447	4.96316	-1.50546
H	0.31580	5.89721	-1.56270
C	-1.24804	4.79378	-0.53219
H	-1.44541	5.60449	0.17890
C	-2.01702	3.61430	-0.45625
C	-0.47594	1.66286	-3.44557
H	-1.28693	0.91872	-3.37813
C	-0.46275	2.21641	-4.88691
H	0.38601	2.90282	-5.05967
H	-1.38933	2.76700	-5.11986
H	-0.36672	1.38843	-5.61054
C	0.85361	0.93581	-3.13360
H	0.81357	0.45022	-2.14127
H	1.70522	1.64294	-3.15709
H	1.06182	0.15252	-3.88443
C	-3.10643	3.51291	0.61021
H	-3.42257	2.45562	0.63700
C	-4.33383	4.37500	0.23145
H	-4.74675	4.08631	-0.74916
H	-4.06322	5.44515	0.17628
H	-5.13514	4.26795	0.98422
C	-2.60113	3.90243	2.01539
H	-2.33519	4.97361	2.07773
H	-1.71359	3.31110	2.29848
H	-3.38519	3.71958	2.77086
C	-4.30319	2.49916	-3.50881
H	-5.25587	2.33667	-4.04095
H	-3.49760	2.53314	-4.25964
H	-4.35007	3.48371	-3.01446
C	-5.54688	0.88217	-1.16255
H	-5.36654	0.12021	-0.38668
H	-6.41919	0.56388	-1.75873
H	-5.80427	1.82715	-0.65450
C	-1.67135	-1.94063	-4.17800
H	-0.86289	-1.20629	-4.03503
H	-2.10765	-1.78020	-5.17939
H	-1.21938	-2.94706	-4.16316
C	-4.23384	-3.22594	-3.15925
H	-4.36657	-3.36035	-4.24659
H	-5.22355	-3.03346	-2.71772
H	-3.84487	-4.17048	-2.74374
C	-2.27046	-2.95234	-0.44584
C	-1.01059	-3.63130	-0.40324
C	-0.86939	-4.78331	0.39637
H	0.10335	-5.28885	0.43168
C	-1.93778	-5.29935	1.13543
H	-1.80747	-6.19461	1.75324
C	-3.18231	-4.66264	1.06063
H	-4.02891	-5.07214	1.62374
C	-3.37607	-3.50637	0.28075
C	0.19589	-3.17247	-1.22531

H	-0.12434	-2.29219	-1.80842
C	0.64175	-4.26797	-2.22159
H	-0.19342	-4.60067	-2.86107
H	1.02728	-5.15958	-1.69484
H	1.44855	-3.89431	-2.87782
C	1.38190	-2.73526	-0.33708
H	1.72654	-3.56550	0.30671
H	1.11045	-1.88124	0.30757
H	2.23567	-2.42332	-0.96835
C	-4.76557	-2.86604	0.25442
H	-4.77020	-2.14609	-0.58073
C	-5.89754	-3.88900	0.01546
H	-6.86117	-3.36649	-0.12035
H	-6.01998	-4.57408	0.87334
H	-5.71157	-4.50432	-0.87997
C	-5.03892	-2.06375	1.54471
H	-4.28114	-1.27470	1.67866
H	-5.00612	-2.71935	2.43383
H	-6.03519	-1.58639	1.51193
C	4.18405	1.12326	-0.42380
C	5.97287	-0.79393	-0.51680
C	5.90085	-1.49310	-1.90286
H	4.87864	-1.88218	-2.05982
H	6.09987	-0.75026	-2.69692
C	7.39676	-0.21068	-0.30066
H	7.43355	0.30767	0.67501
H	7.60662	0.54027	-1.08432
C	5.65521	-1.82382	0.60323
H	4.63097	-2.21222	0.46012
H	5.68257	-1.31453	1.58388
C	6.94013	-2.63880	-1.94704
H	6.88261	-3.13022	-2.93568
C	8.35858	-2.05806	-1.73203
H	9.11036	-2.86757	-1.78564
H	8.60286	-1.33778	-2.53601
C	8.42968	-1.36213	-0.35136
H	9.43950	-0.93906	-0.19670
C	8.11426	-2.38826	0.76374
H	8.86233	-3.20288	0.74914
H	8.18268	-1.90573	1.75733
C	6.69563	-2.96820	0.54780
H	6.46271	-3.69581	1.34676
C	6.62424	-3.66495	-0.83232
H	7.34835	-4.50014	-0.87189
H	5.61965	-4.10091	-0.98816
C	-0.13153	0.26963	0.68501
C	-1.16799	-0.34029	2.89757
C	-1.17086	-1.86419	3.17533
H	-2.04126	-2.32962	2.67861
H	-0.26876	-2.31359	2.71976
C	-2.43382	0.29183	3.51588
H	-3.33365	-0.13080	3.03333
H	-2.43855	1.37888	3.31306
C	0.07618	0.28750	3.55529
H	0.98570	-0.12560	3.08108
H	0.08898	1.37665	3.34806
C	-1.19974	-2.12804	4.69917
H	-1.20501	-3.21980	4.88163
C	0.05251	-1.49496	5.35053
H	0.96937	-1.95644	4.93554
H	0.05774	-1.68721	6.44144
C	0.05763	0.02929	5.08040
H	0.95736	0.48319	5.54211
C	-1.21428	0.66152	5.69616
H	-1.21097	1.75703	5.53313
H	-1.23118	0.49778	6.79154
C	-2.46789	0.03225	5.04255
H	-3.38088	0.48801	5.47246
C	-2.47310	-1.49266	5.30750
H	-2.51523	-1.68809	6.39691
H	-3.37559	-1.95207	4.86113
C	2.78775	5.09315	2.61186
H	2.48995	6.16379	2.64532
H	3.78601	5.01505	3.09538
C	1.76860	4.23133	3.34499
H	2.06414	3.16860	3.33685
H	0.76831	4.32481	2.88976
H	1.69055	4.54995	4.39758
C	3.82398	5.45275	0.50750
H	4.82491	5.38291	0.98673
H	3.51914	6.52159	0.53860
C	3.88416	4.95213	-0.93024
H	2.89657	5.03611	-1.41544
H	4.21219	3.89935	-0.96595
H	4.60025	5.55600	-1.51204

TS(G·Et_2O-3·Et_2O)

SCF (BP86) Energy = -2517.38320301
Enthalpy 0K = -2516.113147
Enthalpy 298K = -2516.037128
Free Energy 298K = -2516.228873
Lowest Frequency = -58.3867 cm-1
Second Frequency = 9.9053 cm-1
SCF (BP86-D3BJ) Energy = -2517.78224754
SCF (tol) Energy = -2517.39060952
SCF (BS2) Energy = -3901.3157921

K	2.21251	1.42051	0.89821
Si	-3.38817	2.95620	-0.85089
Si	-3.44861	0.59935	-2.86786
Al	-1.59644	0.36118	-0.31973
O	-3.75960	2.18043	-2.31510
O	4.72910	1.80253	2.15097
N	-1.90523	2.22726	-0.18331
N	-2.88352	-0.35997	-1.48283
N	3.12966	-1.07038	-0.45223
N	-0.94208	-0.80281	1.09444
C	-0.83707	3.05686	0.27214
C	0.18777	3.51169	-0.62993
C	1.25041	4.29961	-0.13742
H	2.01387	4.65949	-0.83789
C	1.33567	4.65928	1.21655
H	2.15261	5.29635	1.57444
C	0.32992	4.23288	2.09493
H	0.37151	4.53658	3.14769
C	-0.75753	3.45257	1.65041
C	0.16175	3.17090	-2.12092
H	-0.83657	2.75144	-2.33120
C	0.36056	4.40862	-3.02308
H	1.38518	4.81567	-2.94617
H	-0.33995	5.22010	-2.76561
H	0.19689	4.13690	-4.08012
C	1.20605	2.08397	-2.47156
H	1.02862	1.15323	-1.90433
H	2.23263	2.44421	-2.26071
H	1.16696	1.83533	-3.54718
C	-1.86357	3.10182	2.64498
H	-2.54451	2.40559	2.12655
C	-2.66716	4.36545	3.03431
H	-3.07842	4.87645	2.14771
H	-2.03055	5.09263	3.57012
H	-3.50867	4.10227	3.69924
C	-1.33248	2.39720	3.91044
H	-0.65782	3.04975	4.49435
H	-0.78267	1.47678	3.65333

H	-2.16886	2.11585	4.57385
C	-3.13643	4.79253	-1.24153
H	-4.09801	5.23146	-1.55802
H	-2.41428	4.93555	-2.06050
H	-2.77745	5.35447	-0.36313
C	-4.88115	2.77668	0.30401
H	-4.98147	1.74718	0.68126
H	-5.80933	3.03786	-0.23274
H	-4.79034	3.44937	1.17369
C	-2.15979	0.77851	-4.25396
H	-1.16804	1.05518	-3.86025
H	-2.47760	1.56189	-4.96368
H	-2.04688	-0.16470	-4.81471
C	-5.03523	-0.09503	-3.63083
H	-5.21737	0.39518	-4.60242
H	-5.90870	0.08981	-2.98711
H	-4.95564	-1.18111	-3.80449
C	-3.26005	-1.74524	-1.34127
C	-2.43633	-2.78621	-1.87510
C	-2.77386	-4.13198	-1.62758
H	-2.13059	-4.92322	-2.03064
C	-3.90760	-4.47877	-0.88558
H	-4.14718	-5.53024	-0.69327
C	-4.74772	-3.46155	-0.41749
H	-5.65832	-3.72769	0.13201
C	-4.46231	-2.10155	-0.64705
C	-1.22299	-2.49246	-2.75866
H	-1.10377	-1.39616	-2.79344
C	-1.47038	-2.99022	-4.20271
H	-2.39674	-2.56619	-4.62707
H	-1.56859	-4.09025	-4.23429
H	-0.62940	-2.71094	-4.86276
C	0.08826	-3.08521	-2.20155
H	0.03085	-4.18480	-2.10923
H	0.33048	-2.66883	-1.21115
H	0.92868	-2.85311	-2.88006
C	-5.47651	-1.05563	-0.17683
H	-5.16720	-0.09199	-0.61533
C	-6.90605	-1.37137	-0.67458
H	-7.58691	-0.53333	-0.44164
H	-7.31825	-2.27172	-0.18514
H	-6.93192	-1.54461	-1.76279
C	-5.48635	-0.88285	1.35763
H	-4.50965	-0.53551	1.73098
H	-5.71923	-1.83730	1.86343
H	-6.25227	-0.14724	1.66373
C	2.48832	-1.59093	0.45667
C	4.39299	-1.33524	-1.15466
C	5.20757	-0.01862	-1.24077
H	4.59549	0.74808	-1.75601
H	5.40906	0.34827	-0.21546
C	5.24368	-2.41122	-0.42887
H	4.65261	-3.34177	-0.34868
H	5.45268	-2.07215	0.60346
C	4.07675	-1.82271	-2.59290
H	3.45321	-1.06610	-3.10418
H	3.47983	-2.75088	-2.53391
C	6.52850	-0.25880	-2.01016
H	7.09819	0.68870	-2.05982
C	7.36516	-1.33424	-1.27584
H	8.32104	-1.49863	-1.80879
H	7.62040	-0.98715	-0.25570
C	6.56133	-2.65476	-1.20206
H	7.15667	-3.42373	-0.67409
C	6.23442	-3.14089	-2.63467
H	7.16997	-3.33740	-3.19247
H	5.67639	-4.09552	-2.59346
C	5.39549	-2.06563	-3.36652
H	5.15375	-2.41284	-4.38853
C	6.20174	-0.74690	-3.44211
H	7.13778	-0.90534	-4.01075
H	5.62154	0.02435	-3.98419
C	0.12119	-0.31938	0.47088
C	-0.88286	-1.76791	2.25728
C	-0.66265	-3.19527	1.69209
H	-1.47218	-3.43857	0.97960
H	0.29282	-3.20440	1.13741
C	-2.21399	-1.73043	3.03120
H	-3.03821	-1.97819	2.33924
H	-2.39695	-0.70663	3.41299
C	0.28968	-1.43019	3.20701
H	1.22557	-1.45443	2.62168
H	0.15655	-0.40408	3.60634
C	-0.62829	-4.21992	2.85181
H	-0.47884	-5.23456	2.43530
C	0.53763	-3.87205	3.80735
H	1.50016	-3.92516	3.26470
H	0.58578	-4.60597	4.63562
C	0.32838	-2.44701	4.37413
H	1.16477	-2.19226	5.05433
C	-1.00774	-2.39380	5.15361
H	-1.15824	-1.38378	5.58258
H	-0.98278	-3.10445	6.00265
C	-2.17518	-2.74511	4.20024
H	-3.13328	-2.70298	4.75308
C	-1.96498	-4.16879	3.62978
H	-1.95707	-4.91023	4.45249
H	-2.80361	-4.43489	2.95874
C	5.16838	0.92151	3.20340
H	5.47016	1.52665	4.08494
H	6.06668	0.36395	2.86162
C	4.04545	-0.03924	3.56852
H	3.74042	-0.65831	2.70637
H	3.16448	0.50379	3.95204
H	4.38341	-0.72269	4.36496
C	5.73238	2.78181	1.83672
H	6.68137	2.26867	1.57037
H	5.93502	3.40532	2.73396
C	5.25142	3.64640	0.67877
H	4.30173	4.14859	0.92865
H	5.10554	3.04194	-0.23238
H	5.99829	4.42493	0.45166

3·Et_2O

SCF (BP86) Energy = -2517.47722829
Enthalpy 0K = -2516.204046
Enthalpy 298K = -2516.128606
Free Energy 298K = -2516.317747
Lowest Frequency = 12.8768 cm^{-1}
Second Frequency = 17.2252 cm^{-1}
SCF (BP86-D3BJ) Energy = -2517.8793527
SCF (tol) Energy = -2517.48364423
SCF (BS2) Energy = -3901.40941287

K	2.35656	1.94054	0.42898
Si	-3.37868	2.66502	-1.21849
Si	-3.77411	-0.16755	-2.40329
Al	-1.47203	0.26472	-0.27886
O	-4.05769	1.50532	-2.25021
O	4.70951	3.00327	1.48550
N	-1.76942	2.08970	-0.68995
N	-2.92765	-0.71285	-0.93812
N	2.90339	-0.55255	-0.53559
N	-0.41657	-0.34555	1.13539
C	-0.69320	3.02906	-0.64252
C	0.15910	3.23661	-1.78365

C	1.22916	4.15250	-1.69670
H	1.86327	4.30962	-2.57716
C	1.47671	4.89313	-0.53062
H	2.29431	5.62186	-0.49527
C	0.63323	4.71335	0.57509
H	0.79652	5.31188	1.47961
C	-0.44734	3.80532	0.54165
C	-0.07061	2.50939	-3.10880
H	-1.05184	2.01222	-3.02753
C	-0.11885	3.47563	-4.31399
H	0.87047	3.92170	-4.52222
H	-0.82984	4.30259	-4.15325
H	-0.42628	2.93004	-5.22275
C	0.99334	1.41477	-3.35177
H	1.00748	0.67336	-2.53697
H	2.00242	1.86025	-3.43655
H	0.79014	0.88102	-4.29720
C	-1.35445	3.71135	1.76872
H	-2.13081	2.96528	1.53213
C	-2.04820	5.06146	2.06111
H	-2.59800	5.43509	1.18099
H	-1.31711	5.83859	2.34849
H	-2.76505	4.95578	2.89414
C	-0.59501	3.21047	3.01522
H	0.22529	3.89706	3.29697
H	-0.17344	2.20724	2.83462
H	-1.27420	3.13685	3.88272
C	-3.24234	4.28259	-2.19359
H	-4.25683	4.67183	-2.38585
H	-2.75142	4.12579	-3.16646
H	-2.68047	5.05363	-1.64061
C	-4.59905	2.94299	0.20902
H	-4.59301	2.11130	0.93037
H	-5.62148	3.03693	-0.19592
H	-4.36684	3.87147	0.75740
C	-2.76115	-0.37593	-3.99704
H	-1.72612	-0.01664	-3.87199
H	-3.22677	0.20128	-4.81448
H	-2.71500	-1.43280	-4.30858
C	-5.44480	-1.02821	-2.61642
H	-5.86106	-0.78344	-3.60842
H	-6.16500	-0.69584	-1.85279
H	-5.34761	-2.12419	-2.54524
C	-3.27815	-1.96474	-0.31124
C	-2.65120	-3.18778	-0.70935
C	-2.93649	-4.37288	-0.00182
H	-2.44526	-5.30438	-0.30699
C	-3.83070	-4.38855	1.07396
H	-4.02825	-5.31733	1.62013
C	-4.49632	-3.20642	1.41802
H	-5.23276	-3.22088	2.23018
C	-4.26046	-1.99896	0.73154
C	-1.72968	-3.27084	-1.92725
H	-1.56238	-2.23933	-2.27994
C	-2.41428	-4.06465	-3.06598
H	-3.39503	-3.63478	-3.33282
H	-2.58579	-5.11523	-2.77024
H	-1.78344	-4.07101	-3.97310
C	-0.34823	-3.87684	-1.60597
H	-0.43134	-4.89706	-1.19033
H	0.19774	-3.24638	-0.88610
H	0.25911	-3.94517	-2.52665
C	-5.11212	-0.77879	1.09046
H	-4.89943	-0.00939	0.32922
C	-6.62404	-1.09922	1.03396
H	-7.21700	-0.17550	1.15657
H	-6.92437	-1.79100	1.84102
H	-6.90707	-1.56625	0.07630
C	-4.75800	-0.18237	2.47026
H	-3.71647	0.17586	2.50389
H	-4.87828	-0.93445	3.27079
H	-5.42131	0.66836	2.71060
C	1.64955	-0.74100	-0.31555
C	3.72299	-1.63057	-1.16103
C	5.19299	-1.14964	-1.19853
H	5.24785	-0.20225	-1.77127
H	5.52885	-0.92709	-0.16642
C	3.65590	-2.94822	-0.34861
H	2.60397	-3.28766	-0.30808
H	3.97569	-2.74855	0.69321
C	3.25779	-1.91364	-2.61186
H	3.29665	-0.97309	-3.19527
H	2.20084	-2.23836	-2.58762
C	6.10065	-2.22186	-1.84730
H	7.14634	-1.85874	-1.86521
C	6.01839	-3.53000	-1.02378
H	6.67617	-4.30116	-1.46935
H	6.38081	-3.35345	0.00756
C	4.55402	-4.03011	-0.99415
H	4.49155	-4.96297	-0.40149
C	4.07299	-4.29958	-2.44033
H	4.69756	-5.08479	-2.90875
H	3.03286	-4.67714	-2.42919
C	4.15434	-2.99268	-3.26564
H	3.80721	-3.18338	-4.29940
C	5.61946	-2.49391	-3.29325
H	6.27081	-3.24903	-3.77433
H	5.69497	-1.57001	-3.89910
C	0.43678	-0.29445	-0.00425
C	-0.06830	-1.09041	2.35813
C	0.10238	-2.60853	2.07238
H	-0.83141	-2.99167	1.62276
H	0.90762	-2.75017	1.32795
C	-1.20708	-0.92195	3.38870
H	-2.14056	-1.31127	2.94488
H	-1.36120	0.15530	3.59412
C	1.25588	-0.56498	2.98853
H	2.07989	-0.68841	2.25932
H	1.14584	0.51791	3.20468
C	0.43448	-3.37914	3.37270
H	0.55108	-4.45499	3.14008
C	1.74938	-2.83514	3.97893
H	2.58613	-2.98533	3.26971
H	2.00411	-3.38953	4.90308
C	1.58585	-1.32944	4.29462
H	2.52756	-0.93525	4.72495
C	0.43076	-1.13509	5.30544
H	0.31827	-0.06131	5.55309
H	0.66192	-1.66179	6.25156
C	-0.88272	-1.68194	4.69739
H	-1.71208	-1.53781	5.41603
C	-0.71795	-3.18893	4.38717
H	-0.50605	-3.74912	5.31888
H	-1.65849	-3.59369	3.96847
C	5.05666	3.15015	2.87177
H	5.35485	4.20228	3.06981
H	5.93362	2.50895	3.10471
C	3.86474	2.75971	3.73568
H	3.57988	1.70657	3.57160
H	2.99322	3.40305	3.52612
H	4.11740	2.87476	4.80253
C	5.80667	3.35522	0.62588
H	6.68515	2.71929	0.86642
H	6.10000	4.41052	0.81384
C	5.39089	3.16205	-0.82687
H	4.52496	3.79813	-1.07994

H 5.13764 2.10702 -1.02921
H 6.22003 3.44195 -1.49739

I
SCF (BP86) Energy = -2686.88830900
Enthalpy 0K = -2685.597203
Enthalpy 298K = -2685.520367
Free Energy 298K = -2685.706205
Lowest Frequency = 15.1340 cm^{-1}
Second Frequency = 22.1038 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.32843993
SCF (tol) Energy = -2686.89721173
SCF (BS2) Energy = -4070.85312648

K 2.09444 -1.24804 -2.86457
Si -2.74172 -2.89128 -0.03456
Si -2.06777 -1.74016 2.75110
Al -0.74059 -0.39477 0.23128
O -3.10688 -2.15066 1.44893
N -1.25801 -2.09071 -0.60522
N -1.04211 -0.43978 2.13329
N 3.69770 -0.17118 -1.05343
N 0.21334 0.91915 -0.71829
C -0.54367 -2.72847 -1.66437
C 0.51804 -3.66828 -1.39518
C 1.20316 -4.28441 -2.46479
H 1.99965 -5.00186 -2.23525
C 0.87662 -4.02730 -3.80444
H 1.40197 -4.54071 -4.61777
C -0.16022 -3.12425 -4.07783
H -0.44151 -2.92885 -5.11967
C -0.87461 -2.47667 -3.04502
C 0.94473 -4.03618 0.02435
H 0.21518 -3.55894 0.69908
C 0.93445 -5.56304 0.26858
H 1.73714 -6.06874 -0.29801
H -0.02201 -6.02760 -0.01796
H 1.11274 -5.77542 1.33736
C 2.33892 -3.46541 0.36205
H 2.35447 -2.36821 0.27732
H 3.11292 -3.88673 -0.30682
H 2.62109 -3.73052 1.39591
C -1.97841 -1.50073 -3.45390
H -2.50805 -1.21587 -2.53032
C -2.99320 -2.12660 -4.43608
H -3.39262 -3.08252 -4.06009
H -2.54028 -2.32199 -5.42473
H -3.84355 -1.44156 -4.59801
C -1.37291 -0.21409 -4.05726
H -0.76674 -0.43985 -4.95569
H -0.74218 0.30131 -3.31281
H -2.16465 0.48960 -4.37177
C -2.55355 -4.76951 0.16530
H -3.53750 -5.20082 0.41895
H -1.84654 -5.04044 0.96311
H -2.21458 -5.23794 -0.77452
C -4.31826 -2.67356 -1.07815
H -4.54571 -1.62887 -1.33900
H -5.17043 -3.07200 -0.49943
H -4.25839 -3.25525 -2.01297
C -1.21961 -3.34984 3.31717
H -0.45821 -3.72198 2.61418
H -1.99183 -4.13044 3.43600
H -0.73182 -3.21327 4.29582
C -3.17332 -1.22850 4.20196
H -3.65348 -2.12505 4.63018
H -3.96448 -0.52803 3.89587
H -2.57793 -0.74992 4.99754
C -0.45972 0.51147 3.05324
C 0.79402 0.24849 3.69801
C 1.38525 1.23405 4.51313
H 2.35150 1.01886 4.98426
C 0.77276 2.46836 4.74150
H 1.25568 3.22644 5.36762
C -0.48446 2.70228 4.17860
H -0.99714 3.64931 4.38554
C -1.12374 1.74792 3.36218
C 1.50844 -1.09857 3.60078
H 0.93405 -1.72371 2.89741
C 1.54113 -1.79763 4.98155
H 0.53840 -1.86321 5.43691
H 2.18256 -1.24222 5.68919
H 1.94972 -2.82055 4.89521
C 2.93983 -0.96494 3.04609
H 3.57119 -0.33733 3.70113
H 2.91757 -0.51196 2.04177
H 3.42346 -1.95611 2.97608
C -2.53921 2.08045 2.88607
H -2.90388 1.20113 2.32877
C -3.49511 2.34386 4.07457
H -4.53057 2.49449 3.71647
H -3.20752 3.25900 4.62182
H -3.49737 1.51317 4.79727
C -2.56675 3.29800 1.93861
H -1.89712 3.14642 1.07879
H -2.23529 4.21395 2.46008
H -3.58772 3.48305 1.55790
C 2.58966 0.12028 -0.45418
C 5.02809 0.16004 -0.48197
C 5.95398 0.54532 -1.66587
H 5.96140 -0.28469 -2.40076
H 5.53231 1.43071 -2.18098
C 5.01077 1.33361 0.52662
H 4.33608 1.08903 1.36625
H 4.58862 2.22897 0.02952
C 5.62530 -1.09478 0.21047
H 5.63406 -1.93491 -0.51197
H 4.96729 -1.39279 1.04653
C 7.38857 0.84091 -1.16806
H 8.02838 1.11506 -2.02902
C 7.34796 2.01084 -0.15542
H 8.37119 2.24189 0.19940
H 6.96249 2.92521 -0.64664
C 6.44150 1.62772 1.03872
H 6.40781 2.46456 1.76257
C 7.01195 0.36643 1.73159
H 8.02809 0.57288 2.12039
H 6.38235 0.09328 2.59969
C 7.05726 -0.80483 0.72081
H 7.46159 -1.70868 1.21618
C 7.96091 -0.41860 -0.47429
H 8.99343 -0.22385 -0.12497
H 8.01722 -1.25755 -1.19514
C 1.26490 0.03490 -0.37099
C 0.48126 2.29277 -1.19911
C 1.11576 3.15535 -0.07149
H 0.43717 3.15485 0.80094
H 2.05692 2.67901 0.25810
C -0.84013 2.95669 -1.65011
H -1.55877 2.94644 -0.81194
H -1.28721 2.35543 -2.46427
C 1.44882 2.30470 -2.42300
H 2.40630 1.83163 -2.14297
H 0.99550 1.70868 -3.24395
C 1.37212 4.60065 -0.55964

H	1.82124	5.19190	0.26115
C	2.33533	4.57766	-1.76953
H	3.30617	4.13575	-1.47401
H	2.54109	5.60905	-2.11637
C	1.70450	3.75147	-2.91553
H	2.39630	3.72628	-3.78000
C	0.36518	4.39622	-3.34026
H	-0.08273	3.82768	-4.17894
H	0.53586	5.42796	-3.70409
C	-0.59788	4.40931	-2.13025
H	-1.56380	4.86095	-2.43078
C	0.02916	5.24090	-0.98545
H	0.18895	6.28440	-1.32050
H	-0.66146	5.28071	-0.12182
C	-2.75125	0.44930	-0.20161
N	-3.85106	0.84504	-0.41372
C	-5.16878	1.23113	-0.62677
C	-5.47465	2.00980	-1.77659
C	-6.16041	0.81466	0.30436
C	-6.81738	2.36725	-1.97948
C	-7.48742	1.19998	0.04363
C	-7.81776	1.96745	-1.08145
H	-7.07546	2.96606	-2.85935
H	-8.26945	0.88789	0.74390
H	-8.85898	2.25384	-1.26102
C	-4.39597	2.43494	-2.74066
H	-3.66397	3.10552	-2.25839
H	-3.82637	1.56789	-3.11756
H	-4.83003	2.96403	-3.60303
C	-5.80514	0.01767	1.53321
H	-5.08188	-0.78934	1.32593
H	-5.33746	0.67009	2.29343
H	-6.70902	-0.42128	1.98388

J

SCF (BP86) Energy = -2686.90477079
Enthalpy 0K = -2685.615210
Enthalpy 298K = -2685.536929
Free Energy 298K = -2685.732722
Lowest Frequency = 7.7229 cm^{-1}
Second Frequency = 9.8385 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.32230264
SCF (tol) Energy = -2686.91256738
SCF (BS2) Energy = -4070.87107112

K	-1.91452	-0.34326	-2.06907
Si	3.65258	-2.39683	-1.98172
Si	4.93930	0.10414	-0.68899
Al	1.84913	-0.42463	-0.18522
O	4.89801	-1.29289	-1.66551
N	2.08136	-1.61279	-1.64348
N	3.55920	0.02866	0.43177
N	0.34046	-0.28717	0.90868
C	1.01185	-1.87051	-2.55923
C	0.82713	-1.03372	-3.71490
C	-0.23754	-1.29705	-4.60511
H	-0.34503	-0.67418	-5.50045
C	-1.12417	-2.36550	-4.39658
H	-1.92861	-2.56963	-5.11222
C	-0.93282	-3.19579	-3.28410
H	-1.60469	-4.04687	-3.12510
C	0.12040	-2.97919	-2.36923
C	1.77801	0.12300	-4.01160
H	2.68034	-0.05363	-3.40277
C	2.20695	0.19312	-5.49264
H	1.37377	0.49653	-6.15249
H	2.58857	-0.77521	-5.85827
H	3.00511	0.94495	-5.61727
C	1.18179	1.47375	-3.56087
H	0.94061	1.48583	-2.48719
H	0.25703	1.69628	-4.12664
H	1.89392	2.29341	-3.76317
C	0.30273	-3.97239	-1.22019
H	1.22668	-3.67994	-0.69431
C	0.47881	-5.41734	-1.73750
H	1.29737	-5.48982	-2.47329
H	-0.43912	-5.79259	-2.22505
H	0.70876	-6.09927	-0.90002
C	-0.85388	-3.89257	-0.20118
H	-1.82782	-4.11397	-0.67369
H	-0.90600	-2.88654	0.24844
H	-0.70157	-4.61990	0.61645
C	3.78333	-2.89909	-3.80391
H	4.73181	-3.44430	-3.95008
H	3.79065	-2.02357	-4.47206
H	2.95839	-3.56313	-4.11044
C	3.98587	-3.94153	-0.93017
H	3.84245	-3.74912	0.14426
H	5.02921	-4.26932	-1.08216
H	3.32500	-4.77605	-1.21922
C	4.88715	1.57480	-1.89149
H	3.88214	1.71105	-2.32425
H	5.59514	1.39828	-2.71983
H	5.17051	2.51699	-1.39346
C	6.58759	0.11521	0.23791
H	7.41800	0.27026	-0.47298
H	6.75612	-0.83952	0.76124
H	6.61782	0.92686	0.98456
C	3.73110	0.41906	1.81027
C	3.55205	1.78010	2.21915
C	3.61946	2.10428	3.58841
H	3.47141	3.14666	3.89491
C	3.87157	1.13099	4.56199
H	3.90352	1.40076	5.62323
C	4.11843	-0.18498	4.15510
H	4.36238	-0.94412	4.90774
C	4.08400	-0.55787	2.79611
C	3.35072	2.91301	1.21062
H	3.24837	2.44695	0.21612
C	4.58880	3.84171	1.18486
H	5.51775	3.28182	0.98048
H	4.72207	4.35615	2.15369
H	4.47830	4.61851	0.40678
C	2.06909	3.73355	1.46399
H	2.05636	4.17994	2.47466
H	1.17351	3.10283	1.34376
H	2.00003	4.56252	0.73607
C	4.48843	-1.98732	2.42121
H	4.55536	-2.02056	1.32028
C	5.87836	-2.35331	2.99655
H	6.22286	-3.31897	2.58562
H	5.84736	-2.45727	4.09571
H	6.63655	-1.58763	2.76004
C	3.45166	-3.04428	2.85898
H	2.49061	-2.90965	2.33649
H	3.25377	-2.98086	3.94416
H	3.81702	-4.06466	2.64539
C	-0.67173	1.66093	-0.40217
C	-1.89063	3.64971	-1.00292
C	-3.15879	3.94332	-1.83919
H	-3.00487	3.57340	-2.87256
H	-4.01140	3.37663	-1.41505
C	-2.12575	4.15132	0.44452
H	-1.22412	3.93280	1.04722
H	-2.96468	3.58429	0.89391

C -0.70127 4.43443 -1.61564
H -0.52242 4.07589 -2.64802
H 0.20923 4.20955 -1.02965
C -3.46856 5.45811 -1.84788
H -4.37676 5.64620 -2.45247
C -3.70117 5.93957 -0.39529
H -3.94113 7.02054 -0.38742
H -4.57023 5.41304 0.04505
C -2.43241 5.66810 0.44915
H -2.59836 6.00796 1.48958
C -1.23506 6.43445 -0.16340
H -1.43461 7.52365 -0.15167
H -0.32647 6.26500 0.44499
C -0.99955 5.95283 -1.61550
H -0.14048 6.49721 -2.05301
C -2.26942 6.22422 -2.45797
H -2.48586 7.30987 -2.48311
H -2.10680 5.90261 -3.50499
C 0.14544 0.64835 -0.13969
C -0.46928 -0.29564 2.13964
C -0.26323 1.00712 2.96388
H 0.81217 1.11531 3.19350
H -0.55697 1.87744 2.34782
C -0.03674 -1.49062 3.01912
H 1.03782 -1.38478 3.25446
H -0.16137 -2.42991 2.44607
C -1.98770 -0.43314 1.82384
H -2.30902 0.42455 1.20253
H -2.15652 -1.35517 1.23257
C -1.09366 0.96938 4.26937
H -0.92846 1.90714 4.83431
C -2.59565 0.82707 3.92853
H -2.93457 1.69766 3.33410
H -3.19922 0.81260 4.85696
C -2.82002 -0.47923 3.12903
H -3.89398 -0.58152 2.87654
C -2.36802 -1.68858 3.98187
H -2.54115 -2.63182 3.42675
H -2.96894 -1.74518 4.91033
C -0.86618 -1.54375 4.32480
H -0.53743 -2.41161 4.92844
C -0.64367 -0.23840 5.12608
H -1.21434 -0.27116 6.07483
H 0.42588 -0.13498 5.39001
N -1.65665 2.17590 -1.05319
N -5.07312 -2.19682 -0.54726
C -4.05799 -2.04697 -1.14953
C -6.30702 -2.26777 0.08929
C -6.61892 -3.43352 0.83606
C -7.19137 -1.15732 -0.03373
C -7.87191 -3.47084 1.47411
C -8.42790 -1.25223 0.62812
C -8.76771 -2.39419 1.37239
H -8.14106 -4.35736 2.05964
H -9.13050 -0.41402 0.55616
C -6.80487 0.06649 -0.83664
H -5.88155 0.53152 -0.44537
H -6.60818 -0.18784 -1.89259
H -7.60648 0.82144 -0.81205
C -5.63169 -4.57317 0.93624
H -5.37661 -4.97656 -0.06058
H -4.68323 -4.24466 1.39694
H -6.04139 -5.39505 1.54483
H -9.73807 -2.44369 1.87851

TS(I-K)
SCF (BP86) Energy = -2686.87934290
Enthalpy 0K = -2685.588606
Enthalpy 298K = -2685.513267
Free Energy 298K = -2685.696304
Lowest Frequency = -166.8351 cm^{-1}
Second Frequency = 8.4061 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.32426080
SCF (tol) Energy = -2686.89018664
SCF (BS2) Energy = -4070.84210828

Si -2.63802 1.88657 2.40803
Si -3.40543 2.29057 -0.68475
Al -1.19209 0.71272 0.23657
O -2.46839 2.45049 0.77578
N -1.74243 0.41964 2.09358
N -2.51187 0.88922 -1.22386
N 3.46881 -0.54744 -1.46768
N 0.55249 1.51988 -0.13286
N 0.17223 -2.20225 -0.59680
C -1.47402 -0.54931 3.11913
C -0.29323 -0.45699 3.94405
C -0.08741 -1.38706 4.97151
H 0.82290 -1.29941 5.58907
C -0.99797 -2.41075 5.24526
H -0.81454 -3.11971 6.06045
C -2.13244 -2.51561 4.43849
H -2.85091 -3.31962 4.63637
C -2.39423 -1.61785 3.39357
C 0.76594 0.62287 3.74568
H 0.39700 1.29631 2.95079
C 2.09525 -0.00234 3.25961
H 2.45199 -0.76551 3.96895
H 2.88676 0.77298 3.17621
H 1.98776 -0.46886 2.27220
C 1.00222 1.45222 5.02590
H 0.06483 1.87032 5.42680
H 1.69542 2.29542 4.81122
H 1.46517 0.85230 5.82522
C -3.65686 -1.86155 2.56973
H -3.71421 -1.07204 1.79935
C -3.61031 -3.23288 1.87169
H -2.75053 -3.30861 1.17735
H -4.52969 -3.41848 1.30540
H -3.50096 -4.05077 2.60780
C -4.94039 -1.78230 3.43962
H -4.96873 -2.59591 4.18614
H -5.83933 -1.87815 2.81609
H -5.00706 -0.82988 3.99699
C -1.88347 3.19103 3.55500
H -0.82281 3.39622 3.33849
H -1.95246 2.85595 4.59908
H -2.45328 4.14264 3.46698
C -4.44441 1.73897 2.96997
H -4.95081 2.71764 2.91949
H -4.45886 1.41179 4.02686
H -5.03093 1.00784 2.38772
C -3.23647 3.89719 -1.67798
H -3.65449 4.74354 -1.10313
H -3.82735 3.81788 -2.61545
H -2.20286 4.13152 -1.95455
C -5.25656 2.16346 -0.29044
H -5.54891 1.21401 0.17350
H -5.84294 2.27465 -1.22620
H -5.56229 2.99140 0.37773
C -2.67324 0.27815 -2.50899
C -1.83283 0.63409 -3.62564
C -1.99084 -0.01620 -4.87062
H -1.35430 0.28532 -5.70457
C -2.99560 -0.96513 -5.08542

H	-3.12736	-1.43170	-6.07111
C	-3.84156	-1.28758	-4.02498
H	-4.64994	-2.01160	-4.17600
C	-3.70355	-0.69865	-2.74932
C	-0.81605	1.76963	-3.57850
H	-0.80814	2.16115	-2.54753
C	0.62769	1.30542	-3.90937
H	1.07246	0.78864	-3.04064
H	1.29104	2.16575	-4.12875
H	0.63828	0.65386	-4.80017
C	-1.22405	2.91514	-4.54142
H	-1.15798	2.59433	-5.59572
H	-0.56362	3.79136	-4.41356
H	-2.26374	3.25083	-4.35525
C	-4.70071	-1.14119	-1.67108
H	-4.40761	-0.63651	-0.73419
C	-4.66408	-2.66344	-1.44657
H	-4.95118	-3.20703	-2.35821
H	-5.39119	-2.94640	-0.66243
H	-3.66438	-3.01994	-1.13093
C	-6.14274	-0.71100	-2.04984
H	-6.20642	0.36054	-2.27547
H	-6.84011	-0.93118	-1.21728
H	-6.49637	-1.26359	-2.93973
C	2.55053	0.03256	-0.77221
C	4.72269	-1.01422	-0.81600
C	1.33026	0.45202	-0.50663
C	1.22154	2.85755	-0.02741
C	2.30033	2.84874	1.09422
H	1.79655	2.60019	2.05477
H	3.03506	2.04535	0.90092
C	1.93091	3.25053	-1.36664
H	2.65641	2.46681	-1.63976
H	1.16125	3.28932	-2.15692
C	0.20212	3.96558	0.30080
H	-0.32712	3.71884	1.23739
H	-0.57111	3.99247	-0.48650
C	2.99585	4.21921	1.21421
H	3.76039	4.17697	2.02353
C	3.69507	4.56718	-0.12218
H	4.21601	5.54028	-0.04402
H	4.46005	3.80460	-0.35641
C	2.62686	4.62128	-1.24788
H	3.12287	4.86122	-2.20867
C	1.58087	5.70563	-0.91722
H	2.06357	6.69846	-0.84170
H	0.83208	5.76686	-1.73078
C	0.88196	5.34545	0.42621
H	0.11903	6.09998	0.65975
C	1.94828	5.30258	1.54557
H	1.45860	5.07393	2.52209
H	2.43339	6.29149	1.64928
C	-0.15906	-1.04430	-0.27144
C	-0.35083	-3.51565	-0.50186
C	-0.98586	-4.11680	-1.62515
C	-0.07062	-4.25682	0.68048
C	-1.21877	-3.36865	-2.92200
H	-2.14081	-3.72637	-3.41843
H	-0.40170	-3.54198	-3.65524
H	-1.34746	-2.28553	-2.77866
C	0.64187	-3.62378	1.84709
H	1.55988	-3.10431	1.51371
H	0.90709	-4.37797	2.60034
H	0.01378	-2.86342	2.34587
C	5.18565	-2.31444	-1.53862
H	4.41573	-3.10341	-1.39782
H	5.27004	-2.11348	-2.62192
C	5.81226	0.06663	-1.02325
H	5.47147	0.99825	-0.52743
H	5.89810	0.29008	-2.09956
C	4.57915	-1.31538	0.68976
H	3.79726	-2.08712	0.84929
H	4.23049	-0.40366	1.21516
C	6.53993	-2.80098	-0.96832
H	6.84840	-3.72578	-1.48998
C	6.38592	-3.08379	0.54997
H	7.34500	-3.44503	0.95983
H	5.63994	-3.88839	0.70737
C	5.93206	-1.79442	1.26969
H	5.81699	-1.99720	2.35748
C	7.00118	-0.69201	1.06856
H	7.96896	-1.01275	1.49246
H	6.70399	0.23263	1.59651
C	7.16832	-0.40830	-0.44893
H	7.92810	0.38427	-0.59834
C	7.60815	-1.69804	-1.17960
H	7.74179	-1.50036	-2.25699
H	8.58630	-2.03902	-0.78783
C	-1.37225	-5.47427	-1.52438
H	-1.87568	-5.93427	-2.37610
C	-1.12717	-6.21460	-0.36376
H	-1.43568	-7.26098	-0.30402
C	-0.47915	-5.61211	0.72164
H	-0.27367	-6.17981	1.62816
K	1.64886	-1.74954	-2.95785

TS (J-K)

SCF (BP86) Energy = -2686.84163907
Enthalpy 0K = -2685.551100
Enthalpy 298K = -2685.475156
Free Energy 298K = -2685.659864
Lowest Frequency = -381.6236 cm^{-1}
Second Frequency = 10.6051 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.28088518
SCF (tol) Energy = -2686.84921080
SCF (BS2) Energy = -4070.80452885

K	2.36658	1.61846	-1.40297
Si	-3.20373	2.95598	-0.97536
Si	-3.87878	0.21874	-2.12397
Al	-1.42871	0.47639	-0.05209
O	-4.07199	1.90420	-1.98360
N	-1.56970	2.25610	-0.70382
N	-3.00924	-0.36980	-0.67409
N	-0.38537	-0.24212	1.26552
C	-0.47764	3.16206	-0.91435
C	0.06359	3.35982	-2.23409
C	1.16150	4.23091	-2.41377
H	1.55708	4.39021	-3.42433
C	1.74032	4.91422	-1.33354
H	2.59084	5.58673	-1.49124
C	1.17430	4.76943	-0.05981
H	1.58899	5.33955	0.77902
C	0.05809	3.93832	0.16885
C	-0.51104	2.65262	-3.46654
H	-1.49752	2.25575	-3.17700
C	-0.70534	3.60089	-4.67045
H	0.25800	3.91286	-5.11283
H	-1.25176	4.51498	-4.38779
H	-1.27665	3.09069	-5.46477
C	0.35369	1.44546	-3.90393
H	0.40257	0.66245	-3.12449
H	1.38077	1.76750	-4.16858
H	-0.06633	0.96730	-4.80539
C	-0.61501	3.98429	1.54215

H	-1.39394	3.20356	1.54442
C	-1.30175	5.35832	1.74255
H	-2.00663	5.59663	0.92831
H	-0.55359	6.17044	1.78004
H	-1.85973	5.37395	2.69528
C	0.34097	3.69632	2.71613
H	1.12648	4.46954	2.80389
H	0.82765	2.71559	2.57667
H	-0.22094	3.69155	3.66678
C	-3.12963	4.61770	-1.88060
H	-4.14263	5.05623	-1.87227
H	-2.82682	4.49760	-2.93170
H	-2.44419	5.33408	-1.40004
C	-4.16594	3.21654	0.63779
H	-4.02080	2.39603	1.35614
H	-5.24526	3.29844	0.42297
H	-3.84588	4.15207	1.12613
C	-2.95571	-0.10927	-3.75328
H	-1.86717	0.01387	-3.65142
H	-3.31468	0.58610	-4.53168
H	-3.14483	-1.13732	-4.10430
C	-5.61250	-0.51675	-2.30296
H	-5.97158	-0.31889	-3.32779
H	-6.31890	-0.04745	-1.60223
H	-5.62756	-1.60596	-2.13775
C	-3.53508	-1.58253	-0.07862
C	-3.08223	-2.86828	-0.51776
C	-3.53921	-4.02877	0.13864
H	-3.17557	-5.00681	-0.19724
C	-4.45187	-3.96207	1.19570
H	-4.78670	-4.87369	1.70196
C	-4.96555	-2.71415	1.56371
H	-5.72418	-2.65811	2.35277
C	-4.55311	-1.52356	0.93207
C	-2.19032	-3.04734	-1.74793
H	-1.88922	-2.04104	-2.08488
C	-2.98826	-3.72060	-2.89154
H	-3.91717	-3.17277	-3.12366
H	-3.27567	-4.75175	-2.61913
H	-2.38075	-3.77541	-3.81277
C	-0.90454	-3.84819	-1.46315
H	-1.12537	-4.84969	-1.05312
H	-0.25617	-3.31794	-0.74796
H	-0.33636	-3.99555	-2.39885
C	-5.29050	-0.23191	1.30406
H	-4.96812	0.54136	0.58729
C	-6.82434	-0.39948	1.16877
H	-7.32433	0.58075	1.26272
H	-7.23068	-1.04987	1.96356
H	-7.11072	-0.84286	0.20191
C	-4.97281	0.27818	2.72786
H	-3.91509	0.55929	2.84461
H	-5.19486	-0.49667	3.48344
H	-5.58989	1.16285	2.96562
C	1.59439	-0.94916	-0.20249
C	3.24777	-2.16377	-1.52717
C	4.74657	-1.93343	-1.84484
H	4.86774	-0.95033	-2.34296
H	5.31386	-1.88718	-0.89647
C	3.10346	-3.54672	-0.83627
H	2.03779	-3.71325	-0.59506
H	3.65509	-3.52510	0.12230
C	2.46393	-2.18921	-2.86527
H	2.56880	-1.20614	-3.37098
H	1.38933	-2.33116	-2.64950
C	5.29316	-3.05282	-2.76203
H	6.36289	-2.86246	-2.97187
C	5.13614	-4.41987	-2.05478
H	5.53851	-5.22766	-2.69593
H	5.72136	-4.43076	-1.11545
C	3.64005	-4.67176	-1.75320
H	3.52162	-5.64635	-1.24258
C	2.84321	-4.68011	-3.07994
H	3.21048	-5.48951	-3.73989
H	1.77528	-4.88723	-2.87957
C	2.99878	-3.31235	-3.78801
H	2.42340	-3.31479	-4.73384
C	4.49578	-3.06171	-4.08858
H	4.88521	-3.84869	-4.76253
H	4.62294	-2.09556	-4.61568
C	0.75434	-0.07289	0.43667
C	-0.37635	-1.14835	2.44813
C	-0.27496	-2.64071	2.03705
H	-1.11550	-2.88282	1.36321
H	0.66377	-2.80096	1.47235
C	-1.69556	-0.94567	3.21999
H	-2.54161	-1.17542	2.54864
H	-1.77453	0.11916	3.51554
C	0.79541	-0.82917	3.40781
H	1.75334	-0.97359	2.87650
H	0.74116	0.23483	3.69970
C	-0.31651	-3.56031	3.28350
H	-0.24315	-4.61664	2.96003
C	0.86221	-3.21935	4.22346
H	1.82576	-3.39072	3.70571
H	0.84888	-3.88194	5.11088
C	0.75175	-1.74013	4.65980
H	1.60074	-1.48385	5.32356
C	-0.58015	-1.51754	5.41271
H	-0.65349	-0.46587	5.75142
H	-0.61911	-2.15343	6.31859
C	-1.75643	-1.85788	4.46916
H	-2.71742	-1.69069	4.99251
C	-1.65257	-3.33851	4.03170
H	-1.70754	-4.00018	4.91845
H	-2.50221	-3.59908	3.37353
N	2.78880	-1.08367	-0.62463
N	3.26125	1.03804	1.23633
C	2.03335	1.07024	1.40800
C	4.46958	1.49425	1.79105
C	4.60646	1.67009	3.20282
C	5.57568	1.75325	0.93137
C	5.84617	2.09730	3.70866
C	6.79240	2.18522	1.48849
C	6.93765	2.35844	2.86906
H	5.94737	2.22946	4.79190
H	7.63760	2.37880	0.81800
C	5.46826	1.57079	-0.56313
H	4.87247	0.66952	-0.79278
H	5.00754	2.45366	-1.05358
H	6.46522	1.45484	-1.01865
C	3.46599	1.40441	4.15193
H	2.58130	2.01614	3.90915
H	3.13992	0.35190	4.10545
H	3.76694	1.62569	5.18842
H	7.89277	2.68910	3.28937

K

SCF (BP86) Energy = -2686.92095911
Enthalpy 0K = -2685.627686
Enthalpy 298K = -2685.551828
Free Energy 298K = -2685.736497
Lowest Frequency = 15.5827 cm^{-1}
Second Frequency = 17.5628 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.36667721

SCF (tol) Energy = -2686.93410979
SCF (BS2) Energy = -4070.88321280

Si	-2.60104	1.91408	2.44572
Si	-3.42916	2.32742	-0.55999
Al	-1.18999	0.50875	0.22186
O	-2.57832	2.63570	0.89122
N	-1.76809	0.41155	2.05858
N	-2.57411	0.87713	-1.09332
N	3.54851	-0.53600	-1.31343
N	0.57816	1.35478	-0.13944
N	0.51789	-2.12975	-0.80118
C	-1.53944	-0.55213	3.10768
C	-0.36425	-0.49507	3.93183
C	-0.19939	-1.40986	4.99103
H	0.70542	-1.34568	5.60677
C	-1.15557	-2.38633	5.27830
H	-1.01350	-3.08276	6.11189
C	-2.29463	-2.45772	4.47350
H	-3.04869	-3.22611	4.67999
C	-2.50783	-1.57210	3.39791
C	0.76013	0.51369	3.70905
H	0.43539	1.18509	2.89635
C	2.05275	-0.19903	3.25283
H	2.37556	-0.94585	4.00035
H	2.87504	0.52741	3.12867
H	1.91113	-0.71397	2.28949
C	1.05360	1.36175	4.96800
H	0.14637	1.84676	5.36142
H	1.79176	2.15141	4.73832
H	1.47923	0.74430	5.77916
C	-3.77397	-1.79014	2.56983
H	-3.80899	-0.99611	1.80315
C	-3.71532	-3.15898	1.85660
H	-2.86731	-3.22166	1.15670
H	-4.64417	-3.34736	1.29335
H	-3.60157	-3.97749	2.58950
C	-5.06199	-1.71462	3.42314
H	-5.11498	-2.55224	4.14141
H	-5.95597	-1.78312	2.77759
H	-5.12741	-0.77920	4.00014
C	-1.72630	3.14510	3.59444
H	-0.67119	3.31153	3.32890
H	-1.76746	2.80005	4.64127
H	-2.25230	4.11468	3.54317
C	-4.35951	1.76751	3.14136
H	-4.81799	2.77031	3.19691
H	-4.31705	1.36709	4.16900
H	-5.01589	1.11616	2.54691
C	-3.23792	3.84718	-1.67803
H	-3.75631	4.70871	-1.22227
H	-3.70426	3.65824	-2.66039
H	-2.18621	4.12638	-1.84310
C	-5.29167	2.21844	-0.20570
H	-5.59559	1.29973	0.31666
H	-5.86465	2.28747	-1.14553
H	-5.57986	3.08346	0.41712
C	-2.86036	0.36706	-2.40902
C	-2.09004	0.76763	-3.55659
C	-2.44095	0.31335	-4.84422
H	-1.84269	0.64401	-5.70198
C	-3.53737	-0.52417	-5.05999
H	-3.80649	-0.85026	-6.07059
C	-4.28295	-0.93269	-3.95199
H	-5.14243	-1.59632	-4.10206
C	-3.97036	-0.51928	-2.64091
C	-0.85633	1.66538	-3.46583
H	-0.76060	1.99603	-2.41765
C	0.41389	0.85247	-3.81524
H	0.55593	0.07241	-3.04884
H	1.31521	1.48862	-3.81816
H	0.31576	0.38131	-4.81106
C	-0.94648	2.91056	-4.37620
H	-0.94838	2.63712	-5.44650
H	-0.07848	3.57385	-4.21013
H	-1.86112	3.49124	-4.17953
C	-4.84808	-1.08859	-1.52544
H	-4.49169	-0.66092	-0.57259
C	-4.70681	-2.62606	-1.45752
H	-4.99994	-3.08853	-2.41733
H	-5.36856	-3.04353	-0.67958
H	-3.67474	-2.93754	-1.23384
C	-6.34227	-0.73230	-1.71247
H	-6.50222	0.34712	-1.85472
H	-6.92863	-1.05304	-0.83310
H	-6.76605	-1.24887	-2.59233
C	2.55916	-0.13864	-0.62272
C	4.83148	-0.97552	-0.67928
C	1.24557	0.16592	-0.45179
C	1.31596	2.63511	-0.09066
C	2.37971	2.63859	1.04811
H	1.86929	2.44002	2.00644
H	3.10069	1.81418	0.89019
C	2.04404	2.95540	-1.43257
H	2.75665	2.14723	-1.67860
H	1.29225	2.99038	-2.24062
C	0.32443	3.78932	0.18581
H	-0.22055	3.59342	1.12370
H	-0.43717	3.81044	-0.61407
C	3.12435	3.99331	1.11864
H	3.87074	3.95519	1.93565
C	3.83756	4.26812	-0.22479
H	4.38825	5.22755	-0.17677
H	4.58535	3.47668	-0.42831
C	2.78867	4.31088	-1.35930
H	3.29423	4.49776	-2.32659
C	1.76882	5.43834	-1.07821
H	2.28213	6.41871	-1.03787
H	1.02903	5.49448	-1.90005
C	1.05450	5.15189	0.26262
H	0.30997	5.94494	0.46517
C	2.10189	5.11928	1.39994
H	1.60308	4.94385	2.37238
H	2.61787	6.09647	1.47310
C	0.20595	-0.93762	-0.37866
C	-0.31950	-3.27334	-0.72692
C	-1.03797	-3.73083	-1.86696
C	-0.25288	-4.08075	0.44793
C	-1.09661	-2.92946	-3.15200
H	-2.05992	-3.07422	-3.66610
H	-0.32179	-3.25491	-3.88287
H	-0.99631	-1.84601	-2.98569
C	0.53689	-3.62118	1.65106
H	1.54685	-3.28200	1.35813
H	0.63709	-4.43434	2.38770
H	0.05518	-2.76832	2.16008
C	5.21421	-2.35444	-1.27863
H	4.43808	-3.09942	-1.00708
H	5.24468	-2.27539	-2.38616
C	5.92141	0.05318	-1.07812
H	5.64511	1.04323	-0.66900
H	5.94220	0.15355	-2.18042
C	4.78253	-1.09779	0.85823
H	3.99371	-1.81803	1.14621
H	4.49027	-0.12445	1.29271
C	6.59323	-2.81220	-0.74401

H	6.84572	-3.79693	-1.18137
C	6.52824	-2.92444	0.79821
H	7.50426	-3.26626	1.19212
H	5.77784	-3.68253	1.09393
C	6.16081	-1.54727	1.40099
H	6.10965	-1.62670	2.50301
C	7.23681	-0.50826	1.00286
H	8.22374	-0.81020	1.40265
H	6.99666	0.47642	1.44684
C	7.30092	-0.39397	-0.53931
H	8.06414	0.35314	-0.82799
C	7.66620	-1.77109	-1.14346
H	7.73580	-1.69796	-2.24626
H	8.65942	-2.09576	-0.77953
C	-1.69255	-4.97782	-1.80595
H	-2.26167	-5.31472	-2.68076
C	-1.63430	-5.77663	-0.65823
H	-2.14852	-6.74263	-0.62899
C	-0.91312	-5.32176	0.45583
H	-0.85869	-5.93718	1.36135
K	2.12063	-2.08622	-3.00117

4·THF

SCF (BP86) Energy = -3151.84905112
Enthalpy 0K = -3150.326306
Enthalpy 298K = -3150.236319
Free Energy 298K = -3150.458199
Lowest Frequency = 12.2235 cm^{-1}
Second Frequency = 13.4223 cm^{-1}
SCF (BP86-D3BJ) Energy = -3152.35157957
SCF (tol) Energy = -3151.85720205
SCF (BS2) Energy = -4535.93075430

Si	-4.54525	1.45901	0.87063
Si	-4.43274	-0.41221	-1.64737
Al	-1.97135	0.21660	-0.04500
O	-4.39382	1.06443	-0.78819
N	-3.01227	0.82357	1.46025
N	-2.86030	-1.07976	-1.19307
N	2.87504	1.52497	-0.88271
N	-0.83586	1.55794	-0.97171
N	1.01498	-0.88703	0.82461
C	-2.70291	0.93240	2.86432
C	-2.06161	2.10057	3.40121
C	-1.83053	2.20535	4.78760
H	-1.34100	3.10726	5.17366
C	-2.21093	1.19815	5.67732
H	-2.03078	1.30215	6.75296
C	-2.82104	0.05224	5.16217
H	-3.11452	-0.75197	5.84698
C	-3.07191	-0.10670	3.78439
C	-1.58228	3.25985	2.53072
H	-1.90781	3.04504	1.49912
C	-0.03975	3.34676	2.53508
H	0.34481	3.47736	3.56272
H	0.30206	4.21043	1.93756
H	0.41651	2.43974	2.10781
C	-2.17869	4.61719	2.96875
H	-3.27768	4.58481	3.03466
H	-1.90226	5.40993	2.25027
H	-1.79497	4.92568	3.95774
C	-3.70366	-1.42833	3.34807
H	-3.87436	-1.36895	2.25875
C	-2.73665	-2.59919	3.63052
H	-1.79681	-2.49979	3.06477
H	-3.20038	-3.56359	3.36585
H	-2.47479	-2.64035	4.70277
C	-5.05580	-1.70099	4.04783
H	-4.92028	-1.86086	5.13253
H	-5.52208	-2.61600	3.64035
H	-5.76651	-0.86949	3.92156
C	-4.80859	3.33792	0.91742
H	-3.94958	3.90525	0.52742
H	-5.00996	3.68105	1.94607
H	-5.69288	3.58682	0.30461
C	-6.11641	0.72735	1.64242
H	-7.00387	1.11233	1.11042
H	-6.19561	1.04998	2.69501
H	-6.14465	-0.37143	1.61793
C	-4.63266	-0.00868	-3.48927
H	-5.62914	0.43142	-3.66795
H	-4.56030	-0.93111	-4.09097
H	-3.87276	0.70007	-3.85156
C	-6.01494	-1.36027	-1.18852
H	-5.99455	-1.81822	-0.18889
H	-6.21847	-2.15264	-1.92785
H	-6.86137	-0.65211	-1.22730
C	-2.40984	-2.26122	-1.88333
C	-1.56225	-2.18137	-3.04370
C	-1.20536	-3.35077	-3.74592
H	-0.57334	-3.25638	-4.63738
C	-1.65246	-4.61534	-3.35626
H	-1.38283	-5.50990	-3.92866
C	-2.45692	-4.70774	-2.21859
H	-2.80786	-5.69328	-1.89102
C	-2.83673	-3.57375	-1.47234
C	-0.97978	-0.87019	-3.56959
H	-1.38237	-0.05157	-2.94917
C	0.55901	-0.86794	-3.40765
H	0.82538	-0.98287	-2.34402
H	0.99970	0.07789	-3.76503
H	1.01606	-1.69680	-3.97819
C	-1.34837	-0.60458	-5.04699
H	-0.89924	-1.35646	-5.72071
H	-0.97499	0.38458	-5.36825
H	-2.43798	-0.62486	-5.20513
C	-3.67088	-3.84140	-0.21832
H	-3.91058	-2.86472	0.23539
C	-2.85977	-4.66950	0.80417
H	-2.55215	-5.63682	0.36724
H	-3.47135	-4.89342	1.69541
H	-1.95158	-4.14258	1.13532
C	-4.98730	-4.59139	-0.53269
H	-5.57073	-4.10121	-1.32654
H	-5.62117	-4.65458	0.36968
H	-4.78525	-5.62666	-0.86147
C	1.65442	1.54129	-0.54065
C	3.88801	2.41541	-0.22960
C	0.38616	1.06234	-0.49101
C	-0.87730	2.78654	-1.79118
C	-0.42664	4.03493	-0.97359
H	-1.07632	4.12656	-0.08586
H	0.60577	3.88655	-0.60394
C	0.02361	2.69307	-3.06128
H	1.07255	2.50565	-2.76952
H	-0.30799	1.83112	-3.66606
C	-2.32738	3.03392	-2.26909
H	-3.00105	3.09197	-1.39840
H	-2.66358	2.16414	-2.86142
C	-0.51106	5.32606	-1.82260
H	-0.18164	6.18721	-1.20911
C	0.39800	5.19538	-3.06554
H	0.35560	6.12245	-3.66989
H	1.45256	5.06131	-2.75472
C	-0.06321	3.98555	-3.91006

H	0.59163	3.87956	-4.79670
C	-1.52478	4.20193	-4.36462
H	-1.60226	5.11513	-4.98644
H	-1.85638	3.35327	-4.99362
C	-2.42952	4.32463	-3.11712
H	-3.48141	4.46320	-3.43158
C	-1.97447	5.53960	-2.27520
H	-2.63102	5.65820	-1.39186
H	-2.06044	6.47050	-2.86918
C	0.05211	-0.15166	0.34827
C	0.85351	-2.00783	1.67290
C	0.79573	-3.33220	1.14959
C	0.96294	-1.80070	3.08205
C	0.73145	-3.59662	-0.34015
H	0.26089	-4.57176	-0.54313
H	1.74006	-3.63686	-0.80214
H	0.14243	-2.83999	-0.87937
C	1.03540	-0.39939	3.64073
H	1.77077	0.21187	3.08699
H	1.31095	-0.41337	4.70785
H	0.06746	0.12478	3.55395
O	3.91790	-3.36130	-2.39760
C	3.21429	-3.99202	-3.50997
H	2.13384	-3.94278	-3.28751
H	3.40854	-3.41987	-4.43618
C	3.73613	-5.44562	-3.60018
H	4.47272	-5.54335	-4.41624
H	2.92609	-6.16696	-3.79116
C	4.42429	-5.65886	-2.23418
H	5.21333	-6.42771	-2.26380
H	3.68761	-5.94466	-1.46338
C	4.96517	-4.25578	-1.95002
H	5.14799	-4.02962	-0.88636
H	5.89968	-4.06896	-2.52189
C	5.18311	1.59209	-0.01188
H	4.97692	0.76290	0.69598
H	5.49624	1.14572	-0.97793
C	4.20035	3.56478	-1.22354
H	3.27509	4.14608	-1.39602
H	4.49755	3.13237	-2.19793
C	3.44576	3.01766	1.12111
H	3.20709	2.19990	1.82815
H	2.51134	3.58956	0.97806
C	6.30783	2.49270	0.55508
H	7.22237	1.88677	0.70528
C	5.84803	3.09023	1.90671
H	6.64960	3.72363	2.33250
H	5.65587	2.27946	2.63642
C	4.56297	3.92539	1.69158
H	4.23061	4.35008	2.65749
C	4.85805	5.07100	0.69332
H	5.64205	5.73800	1.10047
H	3.95215	5.68926	0.54744
C	5.31703	4.47429	-0.65885
H	5.52105	5.29010	-1.37792
C	6.60049	3.63708	-0.44414
H	6.95047	3.22108	-1.40870
H	7.41418	4.27858	-0.05531
C	0.83091	-4.41984	2.04720
H	0.76282	-5.43578	1.63970
C	0.93985	-4.22644	3.43053
H	0.96264	-5.08473	4.10992
C	1.00810	-2.91839	3.93429
H	1.08574	-2.75029	5.01497
K	3.26750	-1.24673	-0.79919
O	5.01329	-2.35031	1.05730
C	4.52616	-3.15544	2.16295
H	4.93023	-4.18546	2.06721
H	3.42802	-3.19211	2.10106
C	5.06515	-2.46369	3.43073
H	5.27888	-3.19168	4.22942
H	4.32170	-1.75029	3.81887
C	6.34487	-1.72302	2.93388
H	6.26778	-0.63971	3.11974
H	7.26197	-2.08095	3.42915
C	6.37320	-2.02099	1.41643
H	6.68689	-1.16708	0.79442
H	7.03511	-2.88477	1.19380

L

SCF (BP86) Energy = -2686.87719838
Enthalpy 0K = -2685.587316
Enthalpy 298K = -2685.509311
Free Energy 298K = -2685.707463
Lowest Frequency = 2.6922 cm^{-1}
Second Frequency = 4.8979 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.30910900
SCF (tol) Energy = -2686.88842451
SCF (BS2) Energy = -4070.84104751

K	-3.62622	-0.77744	-0.13145
Si	2.68738	2.59649	-1.53107
Si	2.89345	2.37462	1.64335
Al	1.26545	0.59814	0.02633
O	2.21080	2.80299	0.11458
N	2.22050	0.91111	-1.64197
N	2.23551	0.74818	1.70141
N	-7.66101	-1.18954	1.20567
N	0.35743	-1.19191	-0.06958
N	-1.96748	1.35625	-0.01823
C	2.30487	0.04849	-2.78178
C	1.17883	-0.14508	-3.65285
C	1.25877	-1.07968	-4.70445
H	0.38902	-1.21602	-5.35832
C	2.41913	-1.82132	-4.94682
H	2.45872	-2.54657	-5.76680
C	3.53773	-1.59567	-4.13883
H	4.46585	-2.14251	-4.34304
C	3.51256	-0.67464	-3.07287
C	-0.09602	0.69436	-3.54855
H	-0.02543	1.28534	-2.61900
C	-1.38427	-0.15315	-3.46706
H	-2.26228	0.51067	-3.35778
H	-1.35517	-0.83591	-2.60114
H	-1.53454	-0.75533	-4.38167
C	-0.19417	1.67240	-4.74402
H	0.71051	2.29442	-4.83655
H	-1.06381	2.34558	-4.63325
H	-0.31484	1.12103	-5.69398
C	4.82106	-0.43340	-2.31684
H	4.58719	0.24136	-1.47587
C	5.44534	-1.71976	-1.73467
H	4.76292	-2.22556	-1.03533
H	6.37531	-1.48086	-1.18878
H	5.70960	-2.43947	-2.52997
C	5.85377	0.25660	-3.24146
H	6.16267	-0.42417	-4.05493
H	6.76238	0.53896	-2.67952
H	5.44392	1.16462	-3.71152
C	1.67199	3.85294	-2.52608
H	0.58901	3.68207	-2.42759
H	1.92964	3.80953	-3.59806
H	1.89798	4.87393	-2.17108
C	4.49275	3.11524	-1.80987
H	4.62599	4.14188	-1.42498

H	4.71109	3.14383	-2.89101
H	5.23597	2.46481	-1.32789
C	2.24058	3.59974	2.93222
H	2.65432	4.60509	2.74035
H	2.55400	3.29850	3.94689
H	1.14222	3.66602	2.91608
C	4.77326	2.64555	1.57645
H	5.29804	1.92097	0.93541
H	5.21228	2.58726	2.58549
H	4.97269	3.65999	1.18920
C	2.20394	-0.14124	2.82580
C	3.34212	-0.94870	3.17363
C	3.25172	-1.87358	4.23276
H	4.13050	-2.48015	4.48060
C	2.08214	-2.02832	4.98216
H	2.03214	-2.75681	5.79864
C	0.98704	-1.21395	4.68175
H	0.07570	-1.29789	5.28567
C	1.02168	-0.27264	3.63349
C	4.70474	-0.79061	2.49736
H	4.55540	-0.14917	1.61246
C	5.32462	-2.12415	2.02529
H	5.55261	-2.79077	2.87591
H	6.27478	-1.93810	1.49464
H	4.65672	-2.67116	1.34177
C	5.69473	-0.09327	3.46339
H	5.27736	0.83822	3.87887
H	6.64542	0.14877	2.95532
H	5.92791	-0.75392	4.31778
C	-0.20536	0.62496	3.46395
H	-0.05568	1.22099	2.54727
C	-1.51735	-0.17335	3.29770
H	-1.45412	-0.86625	2.44173
H	-2.36112	0.51966	3.12237
H	-1.75265	-0.76063	4.20386
C	-0.34037	1.59859	4.65918
H	-0.53362	1.04780	5.59735
H	-1.18196	2.29814	4.50282
H	0.57547	2.19257	4.80647
C	-8.26868	-0.60713	2.05515
C	-0.90160	-0.77641	-0.09216
C	0.66486	-2.64685	-0.09903
C	2.19307	-2.83240	-0.16994
H	2.65103	-2.32547	0.69968
H	2.56866	-2.33893	-1.08507
C	0.02381	-3.33119	-1.33494
H	0.38852	-2.83667	-2.25466
H	-1.07134	-3.18100	-1.29138
C	0.13249	-3.33189	1.18811
H	-0.96332	-3.18193	1.23425
H	0.56933	-2.83718	2.07533
C	2.55556	-4.33633	-0.17997
H	3.65599	-4.44809	-0.22813
C	1.91314	-5.00620	-1.41806
H	2.17768	-6.08114	-1.45158
H	2.30332	-4.54327	-2.34399
C	0.37585	-4.83778	-1.35090
H	-0.08808	-5.31070	-2.23841
C	-0.15873	-5.50893	-0.06309
H	0.07168	-6.59208	-0.07337
H	-1.26220	-5.41456	-0.01535
C	0.48402	-4.83809	1.17431
H	0.09811	-5.31046	2.09837
C	2.02155	-5.00414	1.10962
H	2.48715	-4.53949	1.99912
H	2.29012	-6.07850	1.12234
C	-0.81067	0.75275	-0.01178
C	-2.15801	2.81437	0.07214
C	-3.40790	3.05030	0.96967
H	-4.25773	2.46423	0.56206
H	-3.20172	2.66032	1.98534
C	-2.49090	3.34644	-1.35165
H	-3.33182	2.75807	-1.77081
H	-1.61997	3.17494	-2.01141
C	-0.98292	3.63216	0.65289
H	-0.06925	3.47325	0.05788
H	-0.75970	3.25850	1.67054
C	-3.77671	4.55051	1.02983
H	-4.66492	4.68399	1.67675
C	-4.09147	5.05464	-0.39871
H	-4.36971	6.12567	-0.37177
H	-4.96066	4.50681	-0.81329
C	-2.85183	4.85023	-1.30155
H	-3.07470	5.20467	-2.32632
C	-1.65840	5.64605	-0.72102
H	-0.77110	5.52840	-1.37078
H	-1.90054	6.72627	-0.69664
C	-1.34382	5.13767	0.70630
H	-0.48517	5.70106	1.11800
C	-2.58281	5.34678	1.60793
H	-2.36488	5.00818	2.63912
H	-2.83750	6.42263	1.66848
C	-6.94301	-1.85579	0.22173
C	-6.96813	-1.34238	-1.10422
C	-6.21482	-3.02274	0.58225
C	-6.22037	-2.03052	-2.07955
C	-5.48523	-3.67029	-0.43384
C	-5.48596	-3.18281	-1.75180
H	-6.22900	-1.66166	-3.11076
H	-4.92023	-4.57480	-0.18547
C	-7.78386	-0.11703	-1.44036
H	-8.85731	-0.29406	-1.25201
H	-7.49834	0.74900	-0.81805
H	-7.66078	0.15921	-2.49855
C	-6.24326	-3.54185	1.99981
H	-5.90096	-2.78003	2.72207
H	-7.27015	-3.81485	2.29976
H	-5.60440	-4.43158	2.10553
H	-4.91834	-3.70704	-2.52700

TS(L-M)

SCF (BP86) Energy = -2686.85510104
Enthalpy 0K = -2685.564478
Enthalpy 298K = -2685.488468
Free Energy 298K = -2685.674019
Lowest Frequency = -177.2247 cm^{-1}
Second Frequency = 12.5955 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.29851294
SCF (tol) Energy = -2686.86541468
SCF (BS2) Energy = -4070.81653880

K	-3.68776	-0.67450	-1.46475
Si	2.30682	2.61120	-1.66898
Si	2.59387	2.58257	1.46599
Al	0.97281	0.57191	0.03063
O	1.87428	2.96823	-0.05081
N	1.95252	0.88703	-1.63719
N	1.92707	0.96483	1.66376
N	-3.64967	-2.21303	0.93836
N	0.12141	-1.26086	-0.00277
N	-2.28021	1.23804	-0.19539
C	2.21071	0.00887	-2.74422
C	1.19512	-0.28654	-3.71639
C	1.44660	-1.21655	-4.74465
H	0.65649	-1.42865	-5.47522

C	2.68143	-1.85728	-4.87248
H	2.85719	-2.58168	-5.67485
C	3.69680	-1.52838	-3.97049
H	4.68200	-1.99620	-4.08125
C	3.49913	-0.60629	-2.92355
C	-0.15351	0.43283	-3.74212
H	-0.20921	1.06213	-2.83720
C	-1.34363	-0.54959	-3.71171
H	-2.29439	0.01871	-3.76847
H	-1.31334	-1.16235	-2.79310
H	-1.33253	-1.23483	-4.57759
C	-0.27075	1.34058	-4.98937
H	0.57818	2.03759	-5.06344
H	-1.20095	1.93729	-4.96000
H	-0.28568	0.73872	-5.91559
C	4.71463	-0.27690	-2.05443
H	4.37802	0.43315	-1.27980
C	5.30134	-1.51581	-1.34490
H	4.56095	-2.00524	-0.69657
H	6.16507	-1.22706	-0.72033
H	5.66012	-2.26393	-2.07424
C	5.83114	0.38598	-2.89851
H	6.26044	-0.33745	-3.61448
H	6.65491	0.73694	-2.25114
H	5.46131	1.24431	-3.47987
C	1.19516	3.70988	-2.74858
H	0.12948	3.44678	-2.67224
H	1.48923	3.65062	-3.81002
H	1.31592	4.76053	-2.43054
C	4.05822	3.21390	-2.08331
H	4.10326	4.29439	-1.85734
H	4.25212	3.10111	-3.16356
H	4.86492	2.71232	-1.53235
C	2.02872	3.91212	2.68912
H	2.45787	4.88383	2.38798
H	2.38555	3.69238	3.70959
H	0.93306	4.01021	2.71866
C	4.47880	2.78378	1.31707
H	4.95200	2.00075	0.70429
H	4.95464	2.76872	2.31071
H	4.69989	3.76443	0.86098
C	1.91031	0.21030	2.89291
C	3.02662	-0.60817	3.28070
C	2.93664	-1.42044	4.42882
H	3.79540	-2.04294	4.70493
C	1.79305	-1.44116	5.23145
H	1.73891	-2.08971	6.11253
C	0.73505	-0.59086	4.90348
H	-0.14989	-0.56119	5.54945
C	0.77298	0.24540	3.77001
C	4.37811	-0.56048	2.56625
H	4.23036	-0.01285	1.61970
C	4.96148	-1.95074	2.23739
H	5.16781	-2.53291	3.15286
H	5.91780	-1.84924	1.69588
H	4.27943	-2.54639	1.61082
C	5.39995	0.21120	3.43934
H	5.00809	1.18791	3.76594
H	6.34519	0.38060	2.89304
H	5.63586	-0.36471	4.35218
C	-0.39290	1.21853	3.59106
H	-0.24696	1.72900	2.62369
C	-1.76723	0.51870	3.56347
H	-1.81994	-0.27206	2.79729
H	-2.56573	1.25560	3.36006
H	-1.99865	0.05480	4.53984
C	-0.38848	2.28100	4.71811
H	-0.59901	1.81130	5.69570
H	-1.17044	3.04212	4.54073
H	0.58040	2.79719	4.80135
C	-2.51660	-1.84899	1.22451
C	-1.15169	-0.87917	-0.12515
C	0.52203	-2.68860	0.02433
C	2.00107	-2.81359	-0.39846
H	2.61118	-2.18804	0.28060
H	2.13413	-2.41476	-1.42018
C	-0.33825	-3.54609	-0.93953
H	-0.22855	-3.14820	-1.96713
H	-1.40056	-3.44951	-0.65380
C	0.38226	-3.23781	1.47476
H	-0.66163	-3.11860	1.81267
H	1.01279	-2.63200	2.15072
C	2.45977	-4.29216	-0.33906
H	3.52153	-4.35287	-0.64488
C	1.59267	-5.13007	-1.30885
H	1.91926	-6.18791	-1.29509
H	1.71909	-4.76279	-2.34515
C	0.10810	-5.02625	-0.88487
H	-0.51853	-5.62080	-1.57813
C	-0.06155	-5.55824	0.55826
H	0.22982	-6.62547	0.60574
H	-1.12448	-5.49937	0.86244
C	0.81362	-4.72354	1.52240
H	0.69007	-5.09837	2.55610
C	2.29486	-4.84237	1.09744
H	2.93260	-4.27863	1.80297
H	2.62371	-5.89928	1.13749
C	-1.12119	0.65382	-0.06868
C	-2.49403	2.69857	-0.17283
C	-3.74928	2.95663	0.71081
H	-4.58760	2.33767	0.33443
H	-3.53755	2.61919	1.74266
C	-2.84163	3.15333	-1.62088
H	-3.68467	2.53959	-2.00418
H	-1.97489	2.96191	-2.28106
C	-1.33477	3.56759	0.36079
H	-0.41772	3.40117	-0.22545
H	-1.10085	3.25241	1.39491
C	-4.14340	4.45158	0.69681
H	-5.03319	4.59882	1.33833
C	-4.47147	4.87793	-0.75372
H	-4.76827	5.94378	-0.78121
H	-5.33180	4.29453	-1.13741
C	-3.22993	4.65145	-1.64818
H	-3.46032	4.94687	-2.68983
C	-2.05097	5.49765	-1.11162
H	-1.16334	5.36688	-1.75768
H	-2.31670	6.57204	-1.14037
C	-1.72445	5.06700	0.33814
H	-0.87450	5.66452	0.71775
C	-2.96487	5.29848	1.23174
H	-2.73887	5.01579	2.27768
H	-3.23943	6.37107	1.23884
C	-4.93006	-2.47964	0.52268
C	-5.95743	-1.52024	0.80866
C	-5.22810	-3.69190	-0.17879
C	-7.25153	-1.77060	0.32275
C	-6.54474	-3.88890	-0.62707
C	-7.55311	-2.93806	-0.39834
H	-8.04090	-1.04140	0.53896
H	-6.77996	-4.81614	-1.16218
C	-5.65082	-0.31880	1.67247
H	-5.45255	-0.63416	2.71361
H	-4.74696	0.22641	1.34977
H	-6.49840	0.38468	1.68558
C	-4.16126	-4.74039	-0.38553

H -3.30214 -4.36515 -0.97028
H -3.74691 -5.07974 0.58068
H -4.57080 -5.61799 -0.91004
H -8.57022 -3.11507 -0.76089

M
SCF (BP86) Energy = -2686.91742438
Enthalpy 0K = -2685.624253
Enthalpy 298K = -2685.548428
Free Energy 298K = -2685.732673
Lowest Frequency = 12.3787 cm^{-1}
Second Frequency = 20.0505 cm^{-1}
SCF (BP86-D3BJ) Energy = -2687.36821733
SCF (tol) Energy = -2686.92874402
SCF (BS2) Energy = -4070.87871909

K   4.26329 0.56605 -1.37158
Si -1.87593 -2.74268 -1.87617
Si -2.38851 -2.80850 1.22270
Al -0.88278 -0.58755 -0.05295
O -1.54139 -3.12830 -0.24087
N -1.68972 -0.99772 -1.76939
N -1.90800 -1.13101 1.48425
N   3.10529 2.24646 0.96276
N -0.25428 1.25700 0.01775
N   2.45686 -1.01427 -0.06312
C -1.94278 -0.04989 -2.81686
C -0.88540 0.41299 -3.67049
C -1.13386 1.42918 -4.61411
H -0.31377 1.77162 -5.25672
C -2.40181 1.99734 -4.76694
H -2.57418 2.79327 -5.49922
C -3.45248 1.50221 -3.98929
H -4.46108 1.90730 -4.13208
C -3.25961 0.48504 -3.03315
C   0.50069 -0.23301 -3.67676
H   0.54348 -0.92771 -2.82060
C   1.64786 0.78811 -3.51752
H   2.61931 0.26136 -3.62359
H   1.60434 1.29958 -2.54000
H   1.62556 1.55784 -4.30904
C   0.70677 -1.04091 -4.98106
H -0.10840 -1.76386 -5.14207
H   1.65987 -1.60116 -4.95655
H   0.73125 -0.37085 -5.85909
C -4.50526 -0.05674 -2.32740
H -4.16030 -0.79494 -1.58329
C -5.31685 1.02520 -1.58397
H -4.72150 1.52174 -0.80446
H -6.20102 0.57367 -1.10023
H -5.68512 1.80275 -2.27680
C -5.43274 -0.76259 -3.34772
H -5.86580 -0.02866 -4.05069
H -6.27217 -1.26552 -2.83450
H -4.89553 -1.51422 -3.94658
C -0.57984 -3.68636 -2.89622
H   0.44619 -3.33630 -2.70713
H -0.77971 -3.59102 -3.97683
H -0.63190 -4.76003 -2.64316
C -3.52450 -3.48356 -2.45748
H -3.49245 -4.57124 -2.26699
H -3.63702 -3.34866 -3.54679
H -4.41679 -3.07366 -1.96542
C -1.76571 -4.03563 2.52308
H -2.12423 -5.05234 2.28660
H -2.14650 -3.76874 3.52395
H -0.66590 -4.05533 2.56781
C -4.21798 -3.23165 0.92015
H -4.72923 -2.50523 0.26923
H -4.77958 -3.29483 1.86498
H -4.26860 -4.22333 0.43758
C -2.04790 -0.41962 2.73153
C -3.30447 0.15494 3.13252
C -3.38632 0.91261 4.31846
H -4.35341 1.34271 4.60280
C -2.27927 1.11969 5.14419
H -2.36409 1.71931 6.05684
C -1.06818 0.52147 4.79000
H -0.19832 0.64242 5.44576
C -0.92922 -0.24938 3.61845
C -4.61575 -0.08279 2.38122
H -4.36419 -0.56054 1.41949
C -5.40256 1.21291 2.08324
H -5.74329 1.70368 3.01197
H -6.30340 0.98611 1.48678
H -4.79900 1.94353 1.52307
C -5.52406 -1.03582 3.19851
H -4.99199 -1.95015 3.50793
H -6.41742 -1.33131 2.61963
H -5.87091 -0.53677 4.12111
C   0.42370 -0.92714 3.40221
H   0.40138 -1.39689 2.40418
C   1.60589 0.06427 3.43779
H   1.48384 0.88609 2.71624
H   2.54868 -0.45667 3.19495
H   1.72769 0.50953 4.44168
C   0.65381 -2.03748 4.45610
H   0.72830 -1.60586 5.47046
H   1.59790 -2.57714 4.25553
H -0.16603 -2.77268 4.46804
C   2.21138 1.80249 0.15461
C   1.09046 0.99389 0.13564
C -0.80985 2.60940 0.17456
C -2.34875 2.49570 0.11523
H -2.68467 1.81572 0.92070
H -2.62841 2.04215 -0.85342
C -0.35885 3.54451 -0.98136
H -0.65402 3.08884 -1.94509
H   0.74251 3.62576 -0.98081
C -0.41332 3.24659 1.53841
H   0.68583 3.33492 1.60928
H -0.74006 2.57627 2.35481
C -3.01022 3.88607 0.26812
H -4.11081 3.77324 0.22215
C -2.53930 4.80730 -0.88168
H -3.01575 5.80299 -0.79210
H -2.84524 4.38359 -1.85697
C -0.99962 4.94567 -0.82415
H -0.65368 5.59912 -1.64840
C -0.59117 5.56094 0.53591
H -1.03613 6.56933 0.64359
H   0.50790 5.69003 0.58411
C -1.06697 4.64234 1.68653
H -0.76981 5.07943 2.65887
C -2.60590 4.50035 1.62875
H -2.95616 3.85508 2.45637
H -3.08660 5.48966 1.75799
C   1.25426 -0.52397 0.03112
C   2.76848 -2.45878 -0.01765
C   3.95212 -2.62355 0.98189
H   4.78080 -1.94952 0.68071
H   3.62269 -2.29228 1.98430
C   3.27416 -2.90864 -1.41924
H   4.11692 -2.25638 -1.73983
H   2.46537 -2.77782 -2.16200

C	1.63001	-3.40334	0.42544
H	0.75948	-3.30819	-0.24155
H	1.28325	-3.09409	1.42879
C	4.44826	-4.08765	1.02529
H	5.28518	-4.16664	1.74502
C	4.93187	-4.50618	-0.38345
H	5.30259	-5.54865	-0.36606
H	5.78211	-3.86941	-0.70047
C	3.76268	-4.37727	-1.38827
H	4.10477	-4.66753	-2.40022
C	2.59977	-5.29581	-0.94426
H	1.76627	-5.23129	-1.66768
H	2.93837	-6.34970	-0.93311
C	2.11875	-4.87255	0.46356
H	1.27954	-5.52111	0.77705
C	3.28684	-5.00888	1.46710
H	2.94952	-4.73224	2.48417
H	3.63282	-6.05940	1.51602
C	4.35320	2.79130	0.56159
C	5.49992	2.23236	1.20867
C	4.51004	3.86192	-0.37054
C	6.78029	2.69900	0.85949
C	5.81376	4.30811	-0.67024
C	6.94624	3.72794	-0.08119
H	7.65487	2.26198	1.35579
H	5.93191	5.13948	-1.37573
C	5.32393	1.16248	2.26411
H	4.63843	1.51368	3.05427
H	4.85923	0.24253	1.86657
H	6.29207	0.89533	2.71867
C	3.32020	4.55888	-0.99314
H	2.79015	3.93066	-1.72918
H	2.57567	4.82865	-0.22519
H	3.63778	5.48265	-1.50412
H	7.94733	4.09482	-0.32975

I'

SCF (BP86) Energy = -2766.73137886
Enthalpy 0K = -2765.355373
Enthalpy 298K = -2765.278907
Free Energy 298K = -2765.465192
Lowest Frequency = 10.0967 cm^{-1}
Second Frequency = 14.5353 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.18704463
SCF (tol) Energy = -2766.74070260
SCF (BS2) Energy = -4150.70999803

K	-2.25668	0.67897	-3.06189
Si	2.15186	3.23981	-0.25937
Si	1.50876	2.38447	2.63163
Al	0.40719	0.59710	0.28591
O	2.53357	2.71745	1.30348
N	0.80533	2.20257	-0.78101
N	0.57852	0.94928	2.17385
N	-3.86280	-0.31978	-1.21301
N	-0.31863	-0.95289	-0.50740
C	0.10527	2.60452	-1.95707
C	-1.06596	3.44453	-1.88691
C	-1.73706	3.81892	-3.07153
H	-2.62039	4.46365	-2.99432
C	-1.29243	3.41466	-4.33894
H	-1.81386	3.74131	-5.24589
C	-0.14425	2.61372	-4.42094
H	0.23013	2.31091	-5.40626
C	0.56305	2.20917	-3.26709
C	-1.62695	3.95954	-0.56238
H	-0.90281	3.66912	0.21728
C	-1.79276	5.49699	-0.54930
H	-2.59705	5.82287	-1.23341
H	-0.86992	6.02131	-0.84268
H	-2.07392	5.83740	0.46272
C	-2.97638	3.29007	-0.22524
H	-2.87369	2.19730	-0.14366
H	-3.73661	3.52066	-0.99524
H	-3.36148	3.66828	0.73761
C	1.80474	1.33831	-3.46071
H	2.30786	1.28928	-2.48208
C	2.78852	1.92250	-4.49783
H	3.03622	2.97500	-4.28324
H	2.37882	1.88018	-5.52312
H	3.72865	1.34344	-4.50227
C	1.41468	-0.10510	-3.84456
H	0.84855	-0.12865	-4.79586
H	0.80433	-0.56139	-3.04708
H	2.31195	-0.73490	-3.98344
C	1.74212	5.09328	-0.30081
H	2.65246	5.66531	-0.05040
H	0.95678	5.37074	0.41737
H	1.41807	5.40444	-1.30876
C	3.79767	3.09737	-1.20732
H	4.14491	2.05706	-1.30063
H	4.56207	3.66499	-0.64757
H	3.73295	3.53394	-2.21743
C	0.52602	3.97591	2.99161
H	-0.25153	4.18938	2.24090
H	1.22916	4.82718	3.01438
H	0.03431	3.92529	3.97629
C	2.65450	2.13822	4.11958
H	3.06399	3.11574	4.42748
H	3.49852	1.47608	3.87206
H	2.11280	1.70957	4.97868
C	0.00924	0.16396	3.24764
C	-1.27999	0.47280	3.79748
C	-1.81587	-0.32400	4.82918
H	-2.80746	-0.07545	5.22517
C	-1.12069	-1.41075	5.36229
H	-1.55731	-2.01898	6.16190
C	0.15125	-1.69544	4.86083
H	0.71755	-2.53419	5.28296
C	0.73496	-0.93204	3.83033
C	-2.12502	1.65973	3.33726
H	-1.55453	2.18502	2.55342
C	-2.40490	2.64134	4.50052
H	-1.48407	2.93042	5.03369
H	-3.08396	2.19002	5.24602
H	-2.89076	3.56067	4.12747
C	-3.45952	1.19301	2.72061
H	-4.05880	0.62267	3.45357
H	-3.27389	0.55118	1.84403
H	-4.06594	2.05977	2.40130
C	2.14266	-1.34043	3.39104
H	2.47828	-0.60130	2.64375
C	3.15231	-1.35237	4.56339
H	4.17336	-1.55720	4.19140
H	2.90966	-2.14460	5.29373
H	3.17210	-0.39515	5.10598
C	2.12565	-2.73448	2.72891
H	1.45758	-2.74999	1.85507
H	1.76672	-3.50264	3.43697
H	3.13637	-3.03753	2.40025
C	-2.77852	-0.39871	-0.51216
C	-5.18963	-0.71318	-0.67299
C	-5.98400	-1.36657	-1.83433
H	-6.02289	-0.65797	-2.68605
H	-5.43827	-2.26465	-2.18483

C	-5.12608	-1.71811	0.50209
H	-4.54265	-1.27937	1.33126
H	-4.57995	-2.62357	0.17234
C	-5.95999	0.55400	-0.21303
H	-6.00195	1.27492	-1.05351
H	-5.39747	1.04056	0.60406
C	-7.41320	-1.74492	-1.37881
H	-7.95818	-2.21047	-2.22269
C	-7.32715	-2.74365	-0.19956
H	-8.34449	-3.03333	0.12827
H	-6.81631	-3.67102	-0.52374
C	-6.55272	-2.09303	0.97157
H	-6.48610	-2.80728	1.81471
C	-7.29686	-0.81624	1.43217
H	-8.31207	-1.07579	1.79050
H	-6.76201	-0.35185	2.28239
C	-7.38803	0.18345	0.25410
H	-7.91688	1.09892	0.58300
C	-8.15927	-0.46985	-0.91728
H	-9.18916	-0.72573	-0.60109
H	-8.24850	0.24441	-1.75903
C	-1.47956	-0.15302	-0.36205
C	-0.40552	-2.38893	-0.85318
C	-1.10658	-3.19082	0.28084
H	-0.55158	-3.03699	1.22366
H	-2.11864	-2.77658	0.44019
C	1.01452	-2.96745	-1.06594
H	1.61436	-2.80910	-0.15280
H	1.51730	-2.41226	-1.88094
C	-1.21303	-2.62223	-2.16928
H	-2.23583	-2.22314	-2.04555
H	-0.72001	-2.07008	-2.99657
C	-1.17741	-4.69685	-0.06576
H	-1.67531	-5.24102	0.75956
C	-1.97926	-4.89260	-1.37363
H	-3.01367	-4.52057	-1.24464
H	-2.05054	-5.96931	-1.62285
C	-1.28151	-4.12874	-2.52371
H	-1.85820	-4.25916	-3.46030
C	0.15097	-4.67832	-2.71491
H	0.65113	-4.15497	-3.55347
H	0.11557	-5.75285	-2.98000
C	0.95233	-4.47704	-1.40744
H	1.98197	-4.86297	-1.54190
C	0.25695	-5.24512	-0.25770
H	0.22704	-6.32779	-0.48969
H	0.83436	-5.13121	0.67944
C	2.50235	-0.09062	0.04250
N	3.60832	-0.47363	-0.12472
C	4.97113	-0.90301	-0.30932
C	5.91081	-0.00425	0.54231
C	5.35260	-0.78463	-1.81194
C	5.11645	-2.38176	0.14290
H	5.78386	1.04973	0.23836
H	5.61680	-0.07757	1.60469
C	7.37365	-0.46759	0.34005
H	5.22567	0.26278	-2.14074
H	4.66474	-1.40852	-2.41143
C	6.81914	-1.24221	-2.00227
H	4.82435	-2.46501	1.20451
H	4.42391	-3.01392	-0.44174
C	6.58255	-2.83517	-0.05616
H	8.03446	0.17744	0.94791
C	7.75321	-0.34458	-1.15533
C	7.51810	-1.94052	0.79197
H	7.08096	-1.15065	-3.07266
C	6.96345	-2.71517	-1.55082
H	6.67282	-3.88758	0.27030
H	8.80602	-0.64931	-1.30468
H	7.67218	0.70868	-1.48448
H	7.26813	-2.03667	1.86549
H	8.56693	-2.27171	0.67400
H	6.31429	-3.36842	-2.16436
H	8.00388	-3.05752	-1.70513

J'

SCF (BP86) Energy = -2766.75451006
Enthalpy 0K = -2765.379811
Enthalpy 298K = -2765.301862
Free Energy 298K = -2765.497513
Lowest Frequency = 4.1944 cm^{-1}
Second Frequency = 5.1651 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.18701365
SCF (tol) Energy = -2766.76189153
SCF (BS2) Energy = -4150.73406555

K	1.81032	0.68883	-1.08765
Si	-3.62311	3.24539	-1.50392
Si	-5.27298	0.62936	-1.35636
Al	-2.33754	0.62456	-0.17874
O	-4.95427	2.24109	-1.80683
N	-2.19218	2.22256	-1.18525
N	-4.15756	0.20029	-0.04103
N	-1.08505	0.03073	1.07389
C	-0.94084	2.60005	-1.76621
C	-0.54532	2.10417	-3.05807
C	0.71186	2.46470	-3.58780
H	0.99945	2.08309	-4.57456
C	1.58532	3.32240	-2.90204
H	2.54734	3.60737	-3.34254
C	1.19023	3.83394	-1.65779
H	1.85231	4.52844	-1.12659
C	-0.05297	3.49697	-1.07969
C	-1.45752	1.20826	-3.89642
H	-2.44206	1.20978	-3.39900
C	-1.64456	1.73870	-5.33595
H	-0.71392	1.65827	-5.92629
H	-1.95733	2.79573	-5.35017
H	-2.41389	1.14563	-5.85997
C	-0.94992	-0.25108	-3.93295
H	-0.86768	-0.67776	-2.92069
H	0.04289	-0.30988	-4.41733
H	-1.63897	-0.88578	-4.51826
C	-0.42805	4.13565	0.25779
H	-1.42905	3.75576	0.52049
C	-0.50615	5.67539	0.14541
H	-1.19516	5.99032	-0.65634
H	0.48259	6.11601	-0.07659
H	-0.85998	6.11525	1.09440
C	0.53721	3.72219	1.38901
H	1.57517	4.04063	1.17862
H	0.52494	2.62806	1.52801
H	0.23728	4.18469	2.34590
C	-3.36728	4.32578	-3.03835
H	-4.21362	5.02819	-3.12810
H	-3.33328	3.71918	-3.95650
H	-2.43826	4.91674	-2.97770
C	-4.08757	4.38539	-0.05812
H	-4.07982	3.85707	0.90781
H	-5.10236	4.78838	-0.21940
H	-3.39280	5.23909	0.01513
C	-5.03569	-0.40452	-2.93267
H	-3.97152	-0.48738	-3.20943
H	-5.57168	0.06765	-3.77411
H	-5.43087	-1.42630	-2.80632

C	-7.08177	0.51805	-0.81341
H	-7.73825	0.63116	-1.69292
H	-7.33293	1.31437	-0.09567
H	-7.30300	-0.45382	-0.34194
C	-4.61376	-0.57288	1.08848
C	-4.57739	-2.00314	1.06464
C	-4.92839	-2.72279	2.22452
H	-4.88955	-3.81827	2.20107
C	-5.32640	-2.07466	3.39868
H	-5.58188	-2.65192	4.29397
C	-5.42637	-0.67866	3.40054
H	-5.77973	-0.16578	4.30294
C	-5.10374	0.08650	2.26256
C	-4.23527	-2.78757	-0.20313
H	-3.90131	-2.05648	-0.95839
C	-5.49487	-3.50297	-0.74839
H	-6.32380	-2.79602	-0.92427
H	-5.85864	-4.26469	-0.03552
H	-5.27225	-4.01568	-1.70153
C	-3.08831	-3.79942	-0.00324
H	-3.32164	-4.53747	0.78510
H	-2.15214	-3.28299	0.26272
H	-2.91193	-4.36163	-0.93813
C	-5.34396	1.59740	2.30834
H	-5.20401	1.97121	1.28012
C	-6.78795	1.93590	2.74602
H	-6.97817	3.01850	2.63773
H	-6.96425	1.67644	3.80520
H	-7.53484	1.39260	2.14403
C	-4.33690	2.33795	3.21516
H	-3.30235	2.21993	2.85459
H	-4.37596	1.95252	4.25004
H	-4.56581	3.41857	3.25347
C	0.08079	-1.55287	-0.55922
C	1.35018	-3.38594	-1.47787
C	2.76142	-3.54364	-2.09324
H	2.84518	-2.88430	-2.97969
H	3.51671	-3.19828	-1.35985
C	1.25101	-4.29574	-0.22757
H	0.24765	-4.17380	0.22217
H	1.99037	-3.95867	0.52562
C	0.30083	-3.85125	-2.51874
H	0.36266	-3.19948	-3.41178
H	-0.70887	-3.71764	-2.08763
C	3.02008	-5.01755	-2.48679
H	4.03232	-5.11074	-2.92559
C	2.91547	-5.91083	-1.22679
H	3.11497	-6.96731	-1.49185
H	3.68279	-5.61362	-0.48559
C	1.50191	-5.77352	-0.61120
H	1.42678	-6.40791	0.29302
C	0.44395	-6.21995	-1.64906
H	0.60146	-7.28202	-1.92009
H	-0.57010	-6.14415	-1.21249
C	0.54654	-5.32825	-2.91000
H	-0.21221	-5.64459	-3.65159
C	1.96116	-5.46650	-3.52306
H	2.14580	-6.51587	-3.82461
H	2.04020	-4.84884	-4.43868
C	-0.73583	-0.57974	-0.16393
C	-0.53745	-0.42011	2.36524
C	-0.93862	-1.89043	2.67119
H	-2.04078	-1.96761	2.65606
H	-0.55249	-2.54698	1.86945
C	-1.10260	0.47428	3.49136
H	-2.20416	0.39370	3.48316
H	-0.84581	1.53163	3.28525
C	1.01714	-0.32821	2.38804
H	1.43188	-0.97343	1.59013
H	1.32045	0.71780	2.17699
C	-0.38188	-2.33810	4.04417
H	-0.68081	-3.38666	4.23545
C	1.16117	-2.23208	4.04066
H	1.58641	-2.89874	3.26583
H	1.57040	-2.56409	5.01483
C	1.57541	-0.76725	3.76436
H	2.68027	-0.68774	3.75522
C	0.99637	0.15067	4.86698
H	1.30391	1.19975	4.68860
H	1.40136	-0.14083	5.85563
C	-0.54695	0.04133	4.86980
H	-0.96420	0.70248	5.65341
C	-0.95839	-1.42368	5.15102
H	-0.58506	-1.74066	6.14459
H	-2.06117	-1.50896	5.17323
N	1.16405	-1.94940	-1.12899
N	5.81258	1.13967	-0.17039
C	4.67304	1.08791	-0.48831
C	7.19577	1.18851	0.22555
C	7.53882	2.62006	0.72349
H	7.33931	3.34529	-0.08640
H	6.87889	2.87862	1.57153
C	7.43779	0.16581	1.37067
H	7.16559	-0.84586	1.01891
H	6.77739	0.40988	2.22252
C	8.09278	0.83035	-0.99189
H	7.89652	1.54494	-1.81195
H	7.82483	-0.17748	-1.35777
C	9.02633	2.66487	1.14903
H	9.26218	3.68577	1.50154
C	9.26799	1.64704	2.28964
H	10.32376	1.68988	2.61612
H	8.64811	1.90432	3.16936
C	8.92579	0.22172	1.79296
H	9.08908	-0.50804	2.60703
C	9.81988	-0.13524	0.58119
H	10.88456	-0.12098	0.88010
H	9.59736	-1.16101	0.23105
C	9.57780	0.88317	-0.55876
H	10.20882	0.62765	-1.42975
C	9.92048	2.30873	-0.06304
H	10.98666	2.36173	0.22599
H	9.77084	3.04292	-0.87739

TS(I'-K')

SCF (BP86) Energy = -2766.72222833
Enthalpy 0K = -2765.346594
Enthalpy 298K = -2765.271238
Free Energy 298K = -2765.454523
Lowest Frequency = -90.8213 cm^{-1}
Second Frequency = 8.6688 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.19184354
SCF (tol) Energy = -2766.73383484
SCF (BS2) Energy = -4150.70040786

K	-2.76478	0.69482	-2.69158
Si	2.70554	2.63271	-1.11546
Si	2.58991	2.12258	1.95064
Al	1.14439	0.28654	0.01954
O	2.15526	2.89833	0.47960
N	2.39699	0.90799	-1.31434
N	1.80296	0.54348	1.80294
N	-3.39537	-1.60299	-1.54096
N	0.24123	-1.31311	-0.42962
N	-1.65956	2.02696	-0.49419

C	2.95065	0.11915	-2.38330
C	2.21817	-0.11527	-3.59499
C	2.74748	-0.96084	-4.59019
H	2.17396	-1.12491	-5.51028
C	3.99003	-1.58254	-4.44508
H	4.37959	-2.24469	-5.22544
C	4.73395	-1.31859	-3.29275
H	5.72412	-1.77472	-3.17845
C	4.25575	-0.47447	-2.27078
C	0.89834	0.58990	-3.91412
H	0.60264	1.14583	-3.00591
C	-0.22786	-0.40468	-4.27798
H	-1.10074	0.13443	-4.70365
H	-0.53879	-1.00598	-3.40598
H	0.08678	-1.10684	-5.06789
C	1.09604	1.60313	-5.06777
H	1.92355	2.29873	-4.85623
H	0.18138	2.20239	-5.23759
H	1.33508	1.08448	-6.01298
C	5.20281	-0.20598	-1.10007
H	4.68330	0.48663	-0.41723
C	5.54943	-1.48287	-0.30576
H	4.65253	-1.95397	0.12052
H	6.23748	-1.24401	0.52454
H	6.05234	-2.22908	-0.94658
C	6.51780	0.45450	-1.58230
H	7.11990	-0.25550	-2.17687
H	7.13527	0.76525	-0.72023
H	6.33635	1.33990	-2.21087
C	1.64274	3.77834	-2.20192
H	0.60623	3.41570	-2.27816
H	2.05497	3.84956	-3.22241
H	1.62865	4.79721	-1.77671
C	4.47667	3.25834	-1.37495
H	4.47891	4.35262	-1.22539
H	4.80197	3.06765	-2.41224
H	5.21676	2.81590	-0.69399
C	1.92774	3.17009	3.38267
H	2.52508	4.09201	3.48713
H	2.00206	2.60865	4.32990
H	0.87411	3.45301	3.23620
C	4.48767	2.20503	2.07165
H	4.99842	1.50828	1.38902
H	4.83814	1.99353	3.09377
H	4.80333	3.23175	1.81603
C	1.47073	-0.27598	2.94524
C	2.44300	-1.14474	3.55253
C	2.05936	-2.00707	4.59921
H	2.81419	-2.66522	5.04406
C	0.75327	-2.03867	5.09284
H	0.47435	-2.72668	5.89808
C	-0.17909	-1.14989	4.55522
H	-1.19722	-1.13039	4.96098
C	0.15132	-0.25995	3.51351
C	3.92988	-1.12008	3.19272
H	4.03826	-0.52937	2.26696
C	4.53283	-2.52116	2.94783
H	4.51346	-3.13753	3.86357
H	5.58895	-2.43559	2.63861
H	3.99311	-3.07395	2.16310
C	4.72794	-0.42735	4.32622
H	4.30257	0.55518	4.58868
H	5.78545	-0.28409	4.04030
H	4.70680	-1.04382	5.24274
C	-0.93738	0.72955	3.09543
H	-0.52341	1.35393	2.28480
C	-2.19925	0.01818	2.56159
H	-1.98127	-0.59176	1.67018
H	-2.97187	0.75859	2.28389
H	-2.63985	-0.63760	3.33400
C	-1.32038	1.66015	4.27200
H	-1.79925	1.09135	5.08861
H	-2.04364	2.42869	3.94090
H	-0.44260	2.17380	4.69561
C	-2.26033	-1.45503	-0.92636
C	-4.60533	-1.98830	-0.76305
C	-4.30069	-2.93446	0.42409
H	-3.59021	-2.43806	1.11017
H	-3.79615	-3.84052	0.03688
C	-5.58106	-2.70276	-1.73059
H	-5.08533	-3.60202	-2.14229
H	-5.79412	-2.03445	-2.58901
C	-5.30853	-0.71591	-0.21145
H	-5.53977	-0.03286	-1.05775
H	-4.60993	-0.18627	0.46409
C	-5.60372	-3.31790	1.16444
H	-5.36284	-3.99363	2.00710
C	-6.56162	-4.03174	0.18079
H	-7.49313	-4.32838	0.70062
H	-6.09337	-4.96050	-0.19764
C	-6.88979	-3.08502	-0.99923
H	-7.57111	-3.59551	-1.70650
C	-7.57092	-1.80546	-0.45630
H	-7.83377	-1.12841	-1.29293
H	-8.51749	-2.06514	0.05563
C	-6.61562	-1.08932	0.52827
H	-7.09720	-0.16991	0.91442
C	-6.28324	-2.03686	1.70534
H	-7.20962	-2.29772	2.25252
H	-5.61451	-1.52764	2.42524
C	-1.05521	-0.98649	-0.74571
C	0.61966	-2.74976	-0.38972
C	2.12534	-2.84773	-0.07794
H	2.32316	-2.34406	0.88900
H	2.68936	-2.31150	-0.86467
C	0.35992	-3.44005	-1.75683
H	0.92318	-2.90054	-2.54166
H	-0.71538	-3.36690	-2.00592
C	-0.16306	-3.50680	0.71781
H	-1.24752	-3.42533	0.52055
H	0.03035	-3.01832	1.69124
C	2.57530	-4.32840	-0.01765
H	3.65817	-4.37152	0.20969
C	2.30975	-4.99756	-1.38669
H	2.64510	-6.05281	-1.36455
H	2.89125	-4.48609	-2.17721
C	0.79817	-4.92405	-1.70741
H	0.60266	-5.39651	-2.68945
C	-0.00195	-5.65939	-0.60624
H	0.28865	-6.72769	-0.57326
H	-1.08406	-5.62596	-0.83807
C	0.26886	-4.99260	0.76341
H	-0.30471	-5.51658	1.55210
C	1.77993	-5.06910	1.08373
H	1.97818	-4.61121	2.07157
H	2.10825	-6.12528	1.14214
C	-0.69887	1.27580	-0.30117
C	-2.00117	3.43803	-0.17169
C	-3.34628	3.43044	0.60432
H	-4.11604	2.90601	0.00533
H	-3.22007	2.85733	1.54026
C	-2.20940	4.21388	-1.49934
H	-2.99252	3.70821	-2.10389
H	-1.27409	4.21031	-2.08725
C	-0.92871	4.14656	0.68553
H	0.04941	4.12005	0.17824

H	-0.80532	3.58468	1.62911
C	-3.79051	4.88237	0.90962
H	-4.74596	4.85342	1.46582
C	-3.98174	5.65243	-0.41814
H	-4.31163	6.68816	-0.21258
H	-4.77643	5.17707	-1.02581
C	-2.64744	5.66875	-1.19981
H	-2.77893	6.20657	-2.15759
C	-1.55664	6.36524	-0.35115
H	-0.60198	6.39738	-0.90938
H	-1.85015	7.41337	-0.15251
C	-1.37131	5.60030	0.98075
H	-0.58974	6.09486	1.58670
C	-2.70705	5.58648	1.76053
H	-2.57815	5.06027	2.72517
H	-3.02458	6.61997	1.99628

TS(J′-K′)

SCF (BP86) Energy = -2766.68943910
Enthalpy 0K = -2765.314913
Enthalpy 298K = -2765.239038
Free Energy 298K = -2765.424070
Lowest Frequency = -340.7802 cm^{-1}
Second Frequency = 11.8052 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.14863384
SCF (tol) Energy = -2766.69723897
SCF (BS2) Energy = -4150.66548696

K	-2.20390	-1.18547	-1.90238
Si	3.29300	-3.10730	-0.97428
Si	4.33130	-0.36049	-1.81298
Al	1.65235	-0.53246	-0.02880
O	4.33905	-2.06338	-1.80752
N	1.71182	-2.28387	-0.77327
N	3.35615	0.20486	-0.42801
N	0.60555	0.21743	1.27182
C	0.56165	-3.04428	-1.16102
C	0.12816	-3.06827	-2.53402
C	-1.02257	-3.80706	-2.89028
H	-1.32982	-3.84265	-3.94302
C	-1.75927	-4.52382	-1.93448
H	-2.64322	-5.10007	-2.23074
C	-1.30601	-4.54504	-0.60856
H	-1.84530	-5.14522	0.13315
C	-0.14768	-3.84918	-0.20597
C	0.88552	-2.32196	-3.63804
H	1.87615	-2.06621	-3.22801
C	1.09464	-3.17117	-4.91097
H	0.15001	-3.33612	-5.46056
H	1.51951	-4.16074	-4.67758
H	1.78460	-2.65503	-5.60035
C	0.19783	-0.98910	-4.01891
H	0.13621	-0.29457	-3.16046
H	-0.81797	-1.16912	-4.42595
H	0.76063	-0.46775	-4.81215
C	0.38154	-4.07024	1.21238
H	1.21730	-3.36467	1.35370
C	0.93168	-5.51196	1.34787
H	1.69143	-5.74387	0.58269
H	0.11981	-6.25422	1.24257
H	1.39024	-5.65735	2.34186
C	-0.65749	-3.79719	2.31751
H	-1.50085	-4.51145	2.27009
H	-1.05648	-2.77282	2.22291
H	-0.19004	-3.91359	3.31130
C	3.15310	-4.67263	-2.03261
H	4.12059	-5.20256	-1.99255
H	2.94541	-4.43667	-3.08728
H	2.37246	-5.36084	-1.67025
C	4.08448	-3.59592	0.67839
H	3.96273	-2.82269	1.45122
H	5.16418	-3.77749	0.54006
H	3.63028	-4.52597	1.05924
C	3.65159	0.18267	-3.50391
H	2.55234	0.15369	-3.54154
H	4.04579	-0.47838	-4.29507
H	3.96632	1.21386	-3.73540
C	6.13618	0.20247	-1.72678
H	6.60482	0.03643	-2.71220
H	6.70133	-0.37806	-0.98233
H	6.22845	1.27208	-1.47799
C	3.89667	1.31574	0.32755
C	3.59138	2.66683	-0.03666
C	4.05428	3.72663	0.76888
H	3.80513	4.75624	0.48674
C	4.83079	3.49682	1.90876
H	5.17173	4.33246	2.52933
C	5.20240	2.18386	2.21655
H	5.85502	1.99903	3.07753
C	4.77863	1.08879	1.43708
C	2.85875	3.01988	-1.33263
H	2.51430	2.07322	-1.78250
C	3.83300	3.70146	-2.32461
H	4.73329	3.08928	-2.50283
H	4.17300	4.67801	-1.93589
H	3.34031	3.88162	-3.29710
C	1.62019	3.91210	-1.11485
H	1.87637	4.85298	-0.59606
H	0.85324	3.38760	-0.52293
H	1.17594	4.18727	-2.08848
C	5.35495	-0.29044	1.77563
H	5.07137	-0.96764	0.95305
C	6.90081	-0.25633	1.85486
H	7.30160	-1.28314	1.92413
H	7.24819	0.28976	2.74987
H	7.35047	0.23187	0.97545
C	4.79971	-0.88494	3.08911
H	3.71581	-1.06964	3.03485
H	4.97666	-0.20083	3.93844
H	5.29989	-1.84221	3.32110
C	-1.09505	1.17824	-0.39099
C	-2.59617	2.55537	-1.75086
C	-4.05218	2.35581	-2.24450
H	-4.11789	1.40815	-2.82015
H	-4.71786	2.24417	-1.36791
C	-2.53186	3.88031	-0.94401
H	-1.49829	4.02132	-0.57825
H	-3.18247	3.78768	-0.05415
C	-1.67269	2.67785	-2.99055
H	-1.71896	1.73688	-3.57815
H	-0.62878	2.79368	-2.64867
C	-4.49887	3.54244	-3.13055
H	-5.53873	3.37518	-3.47044
C	-4.42402	4.85095	-2.30710
H	-4.75735	5.70670	-2.92511
H	-5.10849	4.79333	-1.43911
C	-2.97080	5.07359	-1.82508
H	-2.91432	6.00617	-1.23205
C	-2.03207	5.17938	-3.05074
H	-2.32382	6.04092	-3.68168
H	-0.99272	5.36023	-2.71746
C	-2.10652	3.87154	-3.87613
H	-1.43159	3.94401	-4.75052
C	-3.56074	3.65134	-4.35680
H	-3.87916	4.48961	-5.00567

H	-3.62480	2.72984	-4.96869
C	-0.39480	0.18832	0.26526
C	0.46174	1.01710	2.51578
C	0.49652	2.54056	2.22154
H	1.43412	2.77686	1.68829
H	-0.34374	2.80230	1.54960
C	1.64582	0.67617	3.44474
H	2.58914	0.89887	2.91628
H	1.62682	-0.41010	3.66034
C	-0.85503	0.70157	3.27793
H	-1.72102	0.94846	2.63843
H	-0.90537	-0.38284	3.48613
C	0.41014	3.36073	3.53239
H	0.43807	4.44098	3.29054
C	-0.90561	3.02571	4.27162
H	-1.77565	3.29642	3.64236
H	-0.98304	3.61830	5.20434
C	-0.93677	1.51371	4.59514
H	-1.88310	1.26439	5.11402
C	0.26184	1.15387	5.50286
H	0.23236	0.07756	5.76155
H	0.20476	1.71774	6.45454
C	1.57592	1.48770	4.76040
H	2.44277	1.22225	5.39582
C	1.61391	3.00004	4.43516
H	1.57985	3.59098	5.37166
H	2.56029	3.25234	3.92109
N	-2.24265	1.41191	-0.88782
N	-3.04049	-0.68931	0.67441
C	-1.86889	-0.92765	0.97554
C	-4.37244	-1.08799	1.12719
C	-4.31523	-2.16629	2.24097
H	-3.77778	-3.05427	1.86008
H	-3.72496	-1.77294	3.08842
C	-5.10505	0.16787	1.67052
H	-5.12042	0.94139	0.88115
H	-4.52469	0.58004	2.51618
C	-5.17816	-1.65125	-0.07461
H	-4.65870	-2.54736	-0.47231
H	-5.21427	-0.88537	-0.87516
C	-5.74791	-2.54003	2.69072
H	-5.68943	-3.30712	3.48582
C	-6.46509	-1.28019	3.23301
H	-7.48438	-1.54120	3.57654
H	-5.92083	-0.88161	4.11006
C	-6.53722	-0.20709	2.11993
H	-7.04277	0.69794	2.50583
C	-7.32615	-0.76851	0.91281
H	-8.35935	-1.02261	1.21685
H	-7.40287	-0.00231	0.11753
C	-6.61174	-2.02949	0.37057
H	-7.16721	-2.42969	-0.49884
C	-6.53666	-3.10220	1.48367
H	-7.55768	-3.39271	1.79628
H	-6.04494	-4.01672	1.09929

K′

SCF (BP86) Energy = -2766.76419918
Enthalpy 0K = -2765.386136
Enthalpy 298K = -2765.310971
Free Energy 298K = -2765.493301
Lowest Frequency = 10.9403 cm^{-1}
Second Frequency = 17.2415 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.23261919
SCF (tol) Energy = -2766.77622767
SCF (BS2) Energy = -4150.73972154

K	-3.03178	1.44388	-2.72098
Si	3.46884	2.21613	-0.48917
Si	2.86663	1.38970	2.45233
Al	1.22665	0.27350	0.17863
O	2.76795	2.38832	1.05788
N	2.71089	0.71039	-1.00084
N	1.76305	0.08092	2.02076
N	-3.50847	-0.79792	-1.36999
N	0.07468	-1.10364	-0.54518
N	-1.57944	2.02160	-0.49307
C	3.05992	0.01662	-2.20927
C	2.31713	0.21397	-3.42183
C	2.61416	-0.55000	-4.56761
H	2.03355	-0.38531	-5.48355
C	3.64301	-1.49575	-4.57484
H	3.85596	-2.08560	-5.47270
C	4.41378	-1.64868	-3.41915
H	5.24669	-2.36146	-3.42224
C	4.15914	-0.91026	-2.24615
C	1.25241	1.30220	-3.56074
H	1.10883	1.74968	-2.56234
C	-0.10783	0.74602	-4.03346
H	-0.79889	1.59190	-4.22971
H	-0.53560	0.05771	-3.28425
H	-0.01755	0.19398	-4.98517
C	1.72567	2.40502	-4.53752
H	2.71042	2.80409	-4.24868
H	1.01055	3.24829	-4.56252
H	1.81777	2.01062	-5.56534
C	5.12133	-1.11658	-1.07406
H	4.77559	-0.46586	-0.25311
C	5.13468	-2.56950	-0.55319
H	4.14274	-2.88626	-0.20186
H	5.84322	-2.66826	0.28841
H	5.45794	-3.27502	-1.33953
C	6.56439	-0.71408	-1.46535
H	6.97884	-1.41696	-2.21002
H	7.22942	-0.74005	-0.58337
H	6.61252	0.29529	-1.90197
C	2.98344	3.78042	-1.45431
H	1.90611	3.83460	-1.67072
H	3.52827	3.83528	-2.41199
H	3.26363	4.66981	-0.86282
C	5.36306	2.32782	-0.41524
H	5.62094	3.29895	0.04404
H	5.78646	2.32759	-1.43407
H	5.85257	1.53321	0.16364
C	2.34211	2.46123	3.92297
H	3.10365	3.24126	4.09669
H	2.26186	1.85972	4.84434
H	1.37440	2.95517	3.74627
C	4.70322	0.97605	2.73445
H	5.09906	0.24276	2.01401
H	4.87335	0.57927	3.74757
H	5.29067	1.90601	2.64096
C	1.18490	-0.84885	2.96200
C	1.88052	-2.04339	3.36177
C	1.24079	-2.98623	4.19130
H	1.78542	-3.89318	4.47690
C	-0.05544	-2.79046	4.67391
H	-0.53677	-3.54178	5.30930
C	-0.70770	-1.59838	4.35430
H	-1.70613	-1.40681	4.76459
C	-0.11592	-0.62095	3.52932
C	3.35149	-2.30355	3.03118
H	3.64641	-1.58776	2.24465
C	3.64078	-3.73343	2.52440
H	3.43013	-4.49019	3.30059

H	4.70619	-3.83579	2.25533
H	3.04083	-3.99111	1.63772
C	4.21387	-2.04905	4.29417
H	3.99553	-1.07127	4.75270
H	5.29229	-2.09021	4.05778
H	4.00553	-2.81863	5.05908
C	-0.89295	0.68352	3.34894
H	-0.32675	1.30422	2.63380
C	-2.30882	0.45978	2.77707
H	-2.27868	-0.06836	1.81120
H	-2.81962	1.42756	2.62298
H	-2.93121	-0.12914	3.47535
C	-1.00413	1.44855	4.69055
H	-1.62175	0.88523	5.41296
H	-1.48572	2.43225	4.53968
H	-0.02064	1.61621	5.15577
C	-2.39700	-0.72991	-0.75516
C	-4.78112	-1.16324	-0.66648
C	-4.58146	-2.10407	0.54365
H	-3.90275	-1.62729	1.27344
H	-4.08711	-3.03223	0.20032
C	-5.70057	-1.86113	-1.69825
H	-5.20532	-2.78034	-2.06406
H	-5.83385	-1.19757	-2.57650
C	-5.47323	0.13887	-0.18300
H	-5.62481	0.81940	-1.04886
H	-4.80828	0.65753	0.53232
C	-5.94690	-2.43541	1.19315
H	-5.78486	-3.10720	2.05699
C	-6.85530	-3.13398	0.15309
H	-7.83001	-3.39263	0.60944
H	-6.39262	-4.08287	-0.17915
C	-7.06970	-2.19455	-1.05838
H	-7.71241	-2.69301	-1.80851
C	-7.74584	-0.88711	-0.57970
H	-7.92710	-0.21382	-1.44066
H	-8.73399	-1.11095	-0.13459
C	-6.84129	-0.18716	0.46296
H	-7.31793	0.75252	0.80171
C	-6.62106	-1.12762	1.67213
H	-7.59051	-1.35319	2.15610
H	-5.98835	-0.62918	2.43063
C	-1.09859	-0.34986	-0.62538
C	0.07356	-2.54470	-0.82642
C	1.52305	-3.06078	-0.70786
H	1.89080	-2.82787	0.30973
H	2.16004	-2.51448	-1.42700
C	-0.42633	-2.85437	-2.26927
H	0.21204	-2.30527	-2.98718
H	-1.46301	-2.48964	-2.39364
C	-0.79974	-3.32774	0.19654
H	-1.84304	-2.96627	0.15474
H	-0.42770	-3.11747	1.21616
C	1.59538	-4.58278	-0.98001
H	2.64562	-4.91856	-0.88194
C	1.09295	-4.86551	-2.41592
H	1.15380	-5.94949	-2.63451
H	1.73647	-4.34626	-3.15123
C	-0.36806	-4.37530	-2.55081
H	-0.73211	-4.57011	-3.57831
C	-1.26220	-5.12113	-1.53184
H	-1.24904	-6.20908	-1.73858
H	-2.31311	-4.78619	-1.63347
C	-0.75232	-4.84684	-0.09695
H	-1.39200	-5.37924	0.63319
C	0.70671	-5.34184	0.03338
H	1.06861	-5.17211	1.06497
H	0.76124	-6.43196	-0.15529
C	-0.70616	1.08587	-0.25860
C	-1.39316	3.44753	-0.15220
C	-2.73552	3.92448	0.47816
H	-3.56693	3.68609	-0.21668
H	-2.92090	3.34660	1.40223
C	-1.17747	4.26197	-1.46089
H	-2.01091	4.05558	-2.16920
H	-0.24419	3.92946	-1.95269
C	-0.24974	3.78023	0.83253
H	0.72113	3.44221	0.43758
H	-0.41376	3.21539	1.76883
C	-2.70556	5.44049	0.77931
H	-3.67097	5.74239	1.22845
C	-2.47884	6.21907	-0.53836
H	-2.46748	7.30816	-0.34248
H	-3.31360	6.02880	-1.24250
C	-1.13574	5.78190	-1.16879
H	-0.97103	6.32935	-2.11679
C	0.01625	6.08470	-0.18178
H	0.98650	5.80568	-0.63109
H	0.05558	7.17178	0.02401
C	-0.21134	5.29994	1.13172
H	0.61879	5.50592	1.83279
C	-1.55118	5.74261	1.76411
H	-1.71770	5.20691	2.71811
H	-1.52617	6.82387	2.00079

5·toluene

SCF (BP86) Energy = -3038.33476310
Enthalpy 0K = -3036.831504
Enthalpy 298K = -3036.747657
Free Energy 298K = -3036.954491
Lowest Frequency = 7.1556 cm^{-1}
Second Frequency = 9.1801 cm^{-1}
SCF (BP86-D3BJ) Energy = -3038.83828388
SCF (tol) Energy = -3038.34368070
SCF (BS2) Energy = -4422.37300350

K	-3.49225	-0.73813	1.25668
Si	2.95740	-3.16464	0.19225
Si	3.51019	-1.47650	-2.36185
Al	1.64328	-0.44460	-0.21708
O	2.73731	-2.69724	-1.43428
N	2.54032	-1.66081	1.00894
N	2.73425	-0.01279	-1.74918
N	-2.84579	1.80626	0.65379
N	0.76499	1.02351	0.68209
N	-1.60593	-1.20345	-0.71584
C	2.69984	-1.45887	2.42219
C	1.61017	-1.67107	3.33224
C	1.76134	-1.37151	4.70056
H	0.91550	-1.53805	5.37882
C	2.96543	-0.88815	5.21979
H	3.06281	-0.65420	6.28531
C	4.05140	-0.73944	4.35273
H	5.01208	-0.39416	4.75252
C	3.95423	-1.02445	2.97605
C	0.28935	-2.30457	2.89478
H	0.32541	-2.41695	1.79773
C	-0.93484	-1.43194	3.24410
H	-1.86353	-1.99715	3.02779
H	-0.92077	-0.48354	2.68018
H	-0.96592	-1.18327	4.31950
C	0.12342	-3.70567	3.53098
H	0.99706	-4.34607	3.33238
H	-0.77188	-4.21868	3.13279
H	0.01078	-3.63220	4.62768

C	5.23385	-0.88957	2.14769
H	4.97522	-1.15468	1.10866
C	5.79935	0.54654	2.14320
H	5.08082	1.26610	1.72656
H	6.72159	0.59369	1.53705
H	6.05931	0.87853	3.16439
C	6.33052	-1.85575	2.65879
H	6.68943	-1.54848	3.65738
H	7.20263	-1.84963	1.98033
H	5.96828	-2.89187	2.74275
C	1.78198	-4.63374	0.47053
H	0.72055	-4.34542	0.44195
H	1.97985	-5.11515	1.44325
H	1.95756	-5.38970	-0.31505
C	4.67274	-3.92966	0.47457
H	4.76846	-4.79293	-0.20819
H	4.75332	-4.31880	1.50388
H	5.51843	-3.25271	0.29311
C	3.16908	-1.88065	-4.18025
H	3.71111	-2.80055	-4.46040
H	3.52011	-1.06929	-4.84028
H	2.09615	-2.04019	-4.36784
C	5.38683	-1.68674	-2.11937
H	5.73639	-1.35268	-1.12954
H	5.95688	-1.13521	-2.88312
H	5.63407	-2.75691	-2.23083
C	2.74716	1.25838	-2.43445
C	3.84051	2.18233	-2.28498
C	3.77383	3.45622	-2.88427
H	4.61496	4.14599	-2.75171
C	2.67982	3.85763	-3.65417
H	2.64551	4.85634	-4.10286
C	1.64715	2.94208	-3.86319
H	0.80234	3.22383	-4.50262
C	1.66158	1.65489	-3.28957
C	5.15556	1.81926	-1.59243
H	4.99117	0.87774	-1.04076
C	5.65618	2.88879	-0.59682
H	5.90455	3.83522	-1.10880
H	6.57561	2.54338	-0.09348
H	4.90960	3.11741	0.17962
C	6.25613	1.59344	-2.66064
H	5.92818	0.89906	-3.45071
H	7.17959	1.19259	-2.20553
H	6.50986	2.54859	-3.15472
C	0.51881	0.71963	-3.68578
H	0.64576	-0.21330	-3.11111
C	-0.86927	1.30463	-3.35032
H	-0.96701	1.52813	-2.27640
H	-1.66549	0.58905	-3.62450
H	-1.05700	2.23438	-3.91783
C	0.57665	0.38407	-5.19614
H	0.38538	1.28516	-5.80621
H	-0.19473	-0.36315	-5.45904
H	1.55746	-0.01638	-5.49530
C	-1.66919	1.49326	0.28966
C	-3.69586	2.74486	-0.15066
C	-2.89593	3.84536	-0.88538
H	-2.15839	3.37589	-1.56073
H	-2.32662	4.43447	-0.14191
C	-4.69683	3.41716	0.81995
H	-4.13607	3.99161	1.58136
H	-5.26119	2.63187	1.36181
C	-4.49310	1.92004	-1.19538
H	-5.07431	1.12969	-0.67405
H	-3.78189	1.41302	-1.87325
C	-3.85755	4.76791	-1.67393
H	-3.26884	5.54695	-2.19389
C	-4.85100	5.43452	-0.69245
H	-5.53399	6.11144	-1.24082
H	-4.30173	6.05515	0.04104
C	-5.66431	4.34044	0.04087
H	-6.37110	4.81262	0.74947
C	-6.44935	3.50403	-0.99830
H	-7.05540	2.73084	-0.48570
H	-7.15677	4.15110	-1.55122
C	-5.45875	2.83755	-1.98309
H	-6.01662	2.23190	-2.72291
C	-4.64088	3.93016	-2.71247
H	-5.31805	4.58268	-3.29629
H	-3.94077	3.46376	-3.43100
C	-0.54555	0.73234	0.28846
C	1.08116	2.24989	1.42350
C	2.58893	2.23952	1.75225
H	3.14961	2.16447	0.80095
H	2.82056	1.33902	2.34950
C	0.30061	2.33136	2.76934
H	0.53285	1.42808	3.36445
H	-0.78777	2.33300	2.57246
C	0.78333	3.52499	0.58227
H	-0.28703	3.55383	0.30991
H	1.35408	3.46824	-0.36297
C	2.99879	3.51418	2.52860
H	4.08424	3.47456	2.74236
C	2.21044	3.57342	3.85848
H	2.50382	4.47192	4.43585
H	2.45117	2.69073	4.48088
C	0.69467	3.60791	3.55122
H	0.12407	3.64545	4.49963
C	0.36605	4.85551	2.69713
H	0.61992	5.77750	3.25589
H	-0.72066	4.89465	2.48639
C	1.16362	4.80098	1.37214
H	0.92860	5.69289	0.75963
C	2.67758	4.77030	1.68496
H	3.25500	4.75709	0.74125
H	2.97517	5.68430	2.23549
C	-0.47985	-0.60811	-0.45021
C	-1.72149	-2.46036	-1.48455
C	-2.86297	-2.23346	-2.52063
H	-3.77310	-1.89215	-1.98676
H	-2.56868	-1.41313	-3.20076
C	-2.17765	-3.60293	-0.53141
H	-3.10073	-3.29344	0.00531
H	-1.39895	-3.77570	0.23522
C	-0.46185	-2.92551	-2.24834
H	0.38217	-3.07974	-1.55871
H	-0.14803	-2.12189	-2.93959
C	-3.15854	-3.52305	-3.32049
H	-3.96929	-3.32418	-4.04744
C	-3.59739	-4.64013	-2.34496
H	-3.82715	-5.56833	-2.90233
H	-4.52801	-4.34256	-1.82017
C	-2.46708	-4.90280	-1.32177
H	-2.77854	-5.69651	-0.61518
C	-1.18959	-5.34437	-2.07397
H	-0.38093	-5.56464	-1.35361
H	-1.38841	-6.27877	-2.63369
C	-0.75085	-4.22269	-3.04436
H	0.17045	-4.53159	-3.57244
C	-1.87930	-3.96553	-4.06984
H	-1.57091	-3.18099	-4.78691
H	-2.08045	-4.88111	-4.65919
C	-6.59867	-2.27692	1.59821
C	-6.79040	-0.99238	2.15397
H	-7.46776	-0.28879	1.65639

C	-6.14447	-0.61104	3.34449
H	-6.31982	0.38583	3.76243
C	-5.28588	-1.51032	4.00197
H	-4.79145	-1.22052	4.93459
C	-5.07763	-2.79078	3.45603
H	-4.41814	-3.50265	3.96345
C	-5.72448	-3.16577	2.26509
H	-5.56462	-4.16964	1.85497
C	-7.34006	-2.70737	0.35011
H	-7.66750	-1.84208	-0.24854
H	-8.24465	-3.28470	0.61455
H	-6.71937	-3.35545	-0.29083

L′

SCF (BP86) Energy = -2766.73339515
Enthalpy 0K = -2765.357885
Enthalpy 298K = -2765.280697
Free Energy 298K = -2765.474080
Lowest Frequency = 2.3889 cm^{-1}
Second Frequency = 5.8066 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.17816448
SCF (tol) Energy = -2766.74351081
SCF (BS2) Energy = -4150.70853235

K	-2.94268	0.44665	-0.85022
Si	4.23579	1.94178	-1.03775
Si	3.89783	1.44363	2.08205
Al	2.08153	0.31665	0.09068
O	3.61816	2.18674	0.55130
N	3.34928	0.46803	-1.37832
N	2.80396	0.08417	1.87714
N	-7.04189	-0.20077	-0.54860
N	0.74026	-1.11392	-0.31600
N	-0.75915	1.99221	-0.28659
C	3.37511	-0.30618	-2.58346
C	2.39601	-0.10941	-3.61644
C	2.38430	-0.95817	-4.74134
H	1.62754	-0.79585	-5.51820
C	3.31778	-1.98695	-4.90047
H	3.28720	-2.63920	-5.78003
C	4.30863	-2.14707	-3.92705
H	5.06925	-2.92577	-4.05894
C	4.36637	-1.32804	-2.78203
C	1.40066	1.05247	-3.59840
H	1.48359	1.54138	-2.61231
C	-0.06678	0.60670	-3.77806
H	-0.73479	1.48628	-3.72132
H	-0.36455	-0.10581	-2.99051
H	-0.23038	0.12851	-4.76094
C	1.76454	2.08800	-4.68976
H	2.80877	2.42750	-4.59795
H	1.10815	2.97502	-4.62649
H	1.64536	1.65377	-5.69886
C	5.54866	-1.52753	-1.83093
H	5.38076	-0.86437	-0.96513
C	5.67952	-2.97286	-1.30450
H	4.77842	-3.29309	-0.76063
H	6.53903	-3.05342	-0.61545
H	5.85154	-3.69044	-2.12660
C	6.87141	-1.12200	-2.52609
H	7.10417	-1.81627	-3.35348
H	7.71772	-1.15385	-1.81615
H	6.81888	-0.10815	-2.95328
C	3.75755	3.49470	-2.01844
H	2.66653	3.62810	-2.07850
H	4.15420	3.45124	-3.04704
H	4.19189	4.38565	-1.53148
C	6.13522	1.93764	-1.05632
H	6.49113	2.86284	-0.56908
H	6.50041	1.95807	-2.09728
H	6.59619	1.07901	-0.54838
C	3.42903	2.69421	3.42579
H	4.14385	3.53540	3.42707
H	3.46601	2.22212	4.42294
H	2.41640	3.09743	3.27272
C	5.76573	1.14562	2.27545
H	6.14952	0.34514	1.62457
H	6.01935	0.88899	3.31650
H	6.29913	2.07969	2.02668
C	2.35229	-0.82208	2.89331
C	3.15046	-1.94677	3.30260
C	2.64465	-2.86455	4.24444
H	3.26965	-3.71498	4.54068
C	1.37909	-2.71496	4.81800
H	1.00299	-3.44379	5.54416
C	0.61535	-1.60088	4.46058
H	-0.36473	-1.45081	4.92884
C	1.07167	-0.65072	3.52507
C	4.58717	-2.16032	2.82350
H	4.76203	-1.45344	1.99485
C	4.86303	-3.58848	2.30385
H	4.76194	-4.34020	3.10685
H	5.89449	-3.66287	1.91713
H	4.17567	-3.87262	1.49196
C	5.57884	-1.84748	3.97174
H	5.38722	-0.86128	4.42460
H	6.62392	-1.86784	3.61397
H	5.48362	-2.59841	4.77672
C	0.18225	0.57132	3.28874
H	0.63283	1.15609	2.46844
C	-1.25495	0.19549	2.86539
H	-1.25121	-0.43108	1.95775
H	-1.83735	1.11066	2.65115
H	-1.78251	-0.35510	3.66541
C	0.13249	1.46547	4.55088
H	-0.35156	0.93590	5.39138
H	-0.44858	2.38578	4.35679
H	1.14063	1.76101	4.88201
C	-5.89783	0.03248	-0.74418
C	-8.42896	-0.49198	-0.29175
C	-8.52708	-1.75887	0.60332
H	-7.97983	-1.58168	1.54702
H	-8.03844	-2.60676	0.08977
C	-9.16197	-0.74529	-1.63828
H	-8.67682	-1.58715	-2.16495
H	-9.06503	0.14902	-2.28046
C	-9.07986	0.71560	0.43868
H	-8.98226	1.61852	-0.19120
H	-8.53624	0.90732	1.38165
C	-10.01816	-2.06733	0.88016
H	-10.07938	-2.96888	1.51677
C	-10.74977	-2.32050	-0.46003
H	-11.81132	-2.56532	-0.27010
H	-10.30640	-3.19136	-0.97901
C	-10.65038	-1.05899	-1.35123
H	-11.16482	-1.23812	-2.31311
C	-11.30024	0.14298	-0.62432
H	-11.25336	1.04640	-1.26157
H	-12.37039	-0.06333	-0.43690
C	-10.56851	0.39523	0.71596
H	-11.02414	1.25829	1.23506
C	-10.66744	-0.86567	1.60792
H	-11.72751	-1.08768	1.83132
H	-10.16455	-0.68858	2.57748
C	-0.33411	-0.34788	-0.46072

C	0.62839	-2.58966	-0.46136
C	2.03228	-3.21161	-0.33208
H	2.46003	-2.91916	0.64505
H	2.68039	-2.79258	-1.12366
C	0.03994	-2.97369	-1.84440
H	0.67858	-2.54969	-2.64174
H	-0.96011	-2.51127	-1.94155
C	-0.28452	-3.16910	0.65220
H	-1.28525	-2.70603	0.55746
H	0.11769	-2.88352	1.64204
C	1.95505	-4.75166	-0.45679
H	2.97175	-5.17909	-0.35862
C	1.36997	-5.12165	-1.84071
H	1.32460	-6.22250	-1.95434
H	2.02542	-4.73567	-2.64410
C	-0.04680	-4.51289	-1.97682
H	-0.46762	-4.76957	-2.96844
C	-0.95855	-5.07801	-0.86147
H	-1.04245	-6.17814	-0.95840
H	-1.98227	-4.66593	-0.96260
C	-0.37245	-4.70780	0.52199
H	-1.02628	-5.10421	1.32293
C	1.04474	-5.31463	0.66072
H	1.46463	-5.06643	1.65378
H	0.99541	-6.41901	0.59218
C	0.16754	1.07799	-0.19996
C	-0.54319	3.43178	-0.06005
C	-1.78832	3.95794	0.71271
H	-2.70383	3.67321	0.15453
H	-1.83897	3.45589	1.69840
C	-0.51635	4.13549	-1.44777
H	-1.42227	3.84689	-2.01733
H	0.35393	3.76488	-2.02105
C	0.72212	3.83084	0.73129
H	1.62826	3.45441	0.23055
H	0.69078	3.34014	1.72288
C	-1.72726	5.49279	0.88944
H	-2.62256	5.83410	1.44433
C	-1.69085	6.16448	-0.50395
H	-1.65970	7.26576	-0.39501
H	-2.61309	5.92220	-1.06794
C	-0.44631	5.67195	-1.28005
H	-0.41941	6.14607	-2.28006
C	0.83089	6.04458	-0.48996
H	1.72993	5.71940	-1.04604
H	0.89951	7.14427	-0.37853
C	0.79316	5.36892	0.90169
H	1.71045	5.62882	1.46324
C	-0.44913	5.86644	1.67709
H	-0.47716	5.40874	2.68477
H	-0.39885	6.96322	1.82171

TS(L'-K')

SCF (BP86) Energy = -2766.69426403
Enthalpy 0K = -2765.318908
Enthalpy 298K = -2765.243372
Free Energy 298K = -2765.427883
Lowest Frequency = -73.0719 cm^{-1}
Second Frequency = 9.6645 cm^{-1}
SCF (BP86-D3BJ) Energy = -2767.15206688
SCF (tol) Energy = -2766.70527059
SCF (BS2) Energy = -4150.67094316

K	-2.87460	1.30140	-2.15297
Si	3.87717	1.62974	-0.90910
Si	3.43873	1.12431	2.16938
Al	1.48663	0.22250	0.14703
O	3.30092	1.95914	0.67036
N	2.84223	0.25186	-1.26506
N	2.14064	-0.04434	1.94285
N	-4.17150	-0.37190	-0.45486
N	-0.03077	-1.01742	-0.37327
N	-1.02981	2.29483	-0.48397
C	2.92971	-0.52225	-2.47114
C	2.11122	-0.22250	-3.61328
C	2.15760	-1.04893	-4.75363
H	1.52356	-0.80335	-5.61424
C	3.00433	-2.15789	-4.82639
H	3.02283	-2.79172	-5.71942
C	3.84758	-2.42259	-3.74390
H	4.54113	-3.26968	-3.80113
C	3.84086	-1.63030	-2.57886
C	1.22778	1.02330	-3.69043
H	1.24822	1.50634	-2.69851
C	-0.24201	0.68528	-4.02126
H	-0.83195	1.62222	-4.08345
H	-0.66620	0.01628	-3.25112
H	-0.33699	0.18264	-5.00009
C	1.77358	2.01990	-4.74042
H	2.83050	2.26570	-4.55364
H	1.19658	2.96281	-4.73011
H	1.70822	1.59566	-5.75842
C	4.86228	-1.98287	-1.49548
H	4.69492	-1.28965	-0.65315
C	4.70511	-3.42483	-0.96717
H	3.70596	-3.59911	-0.54325
H	5.45139	-3.62830	-0.17898
H	4.86612	-4.16634	-1.77008
C	6.30739	-1.80243	-2.02196
H	6.53517	-2.55274	-2.80016
H	7.04115	-1.93941	-1.20720
H	6.46859	-0.80831	-2.46607
C	3.58120	3.22783	-1.89250
H	2.51262	3.46391	-2.00801
H	4.03215	3.16880	-2.89733
H	4.06489	4.06678	-1.36153
C	5.76387	1.42419	-0.94554
H	6.21198	2.33542	-0.51050
H	6.11723	1.35553	-1.98854
H	6.14479	0.55448	-0.39342
C	3.19864	2.40678	3.54079
H	4.05746	3.10042	3.54903
H	3.15022	1.92234	4.53086
H	2.27877	2.99364	3.39693
C	5.22317	0.49289	2.34952
H	5.45930	-0.34121	1.67059
H	5.41970	0.15621	3.38003
H	5.91857	1.32321	2.13572
C	1.54972	-0.83216	2.99519
C	2.13287	-2.07860	3.41016
C	1.48776	-2.86674	4.38419
H	1.94659	-3.81580	4.68468
C	0.29168	-2.46674	4.98520
H	-0.19807	-3.09926	5.73357
C	-0.25026	-1.22999	4.62881
H	-1.16886	-0.88539	5.11770
C	0.35417	-0.39951	3.66438
C	3.49309	-2.56890	2.91169
H	3.79354	-1.91273	2.07710
C	3.47136	-4.02447	2.39872
H	3.20188	-4.73392	3.20109
H	4.46754	-4.31836	2.02510
H	2.74858	-4.15916	1.57880
C	4.54360	-2.45480	4.04464
H	4.55057	-1.45127	4.49985

H	5.55975	-2.67376	3.67041
H	4.31950	-3.17518	4.85179
C	-0.28479	0.97058	3.43577
H	0.26547	1.45420	2.61049
C	-1.77024	0.87687	3.02990
H	-1.92744	0.25022	2.13829
H	-2.17078	1.88442	2.81445
H	-2.38030	0.45478	3.84975
C	-0.15596	1.85490	4.70013
H	-0.74913	1.43569	5.53275
H	-0.53678	2.87401	4.50323
H	0.88606	1.93907	5.04574
C	-3.17856	-0.61151	0.23739
C	-5.61597	-0.58005	-0.21901
C	-5.88523	-1.30467	1.12590
H	-5.45421	-0.70818	1.95052
H	-5.35800	-2.27618	1.12261
C	-6.19324	-1.43016	-1.38012
H	-5.67147	-2.40430	-1.41046
H	-5.99109	-0.92217	-2.34406
C	-6.32747	0.79811	-0.20236
H	-6.13524	1.32496	-1.15969
H	-5.90172	1.41847	0.60796
C	-7.40675	-1.50238	1.32267
H	-7.58291	-2.02069	2.28375
C	-7.97102	-2.35356	0.15997
H	-9.05618	-2.51887	0.29993
H	-7.49135	-3.35066	0.15059
C	-7.71600	-1.62792	-1.18323
H	-8.11123	-2.23636	-2.01812
C	-8.41553	-0.24756	-1.16560
H	-8.25978	0.27219	-2.13117
H	-9.50749	-0.37708	-1.04392
C	-7.85086	0.60390	-0.00332
H	-8.34161	1.59517	0.00793
C	-8.10527	-0.12170	1.34014
H	-9.19304	-0.24585	1.50050
H	-7.72265	0.48798	2.18060
C	-0.93792	-0.08840	-0.64834
C	-0.30303	-2.46620	-0.54940
C	1.03063	-3.20539	-0.78980
H	1.70558	-2.99300	0.06129
H	1.51892	-2.81244	-1.69988
C	-1.24528	-2.74093	-1.75074
H	-0.77785	-2.33803	-2.67053
H	-2.19848	-2.20738	-1.59583
C	-0.94749	-3.02718	0.75209
H	-1.88466	-2.47971	0.95039
H	-0.26799	-2.83944	1.60362
C	0.78938	-4.72903	-0.92791
H	1.75937	-5.23447	-1.09644
C	-0.14629	-4.98595	-2.13301
H	-0.31479	-6.07310	-2.25955
H	0.32473	-4.61821	-3.06456
C	-1.49272	-4.26135	-1.89662
H	-2.16554	-4.43765	-2.75865
C	-2.15330	-4.79542	-0.60315
H	-2.36490	-5.87795	-0.70279
H	-3.12382	-4.28853	-0.43729
C	-1.21131	-4.54473	0.59812
H	-1.68218	-4.92182	1.52598
C	0.12712	-5.27976	0.35743
H	0.79433	-5.13714	1.22750
H	-0.04457	-6.36940	0.25660
C	-0.28033	1.24638	-0.28466
C	-0.65002	3.68187	-0.16758
C	-1.87356	4.32184	0.55414
H	-2.77728	4.17522	-0.07163
H	-2.05088	3.78398	1.50401
C	-0.44938	4.44144	-1.51171
H	-1.35129	4.30494	-2.14506
H	0.40029	3.99329	-2.06013
C	0.59980	3.88533	0.71651
H	1.48647	3.42576	0.25174
H	0.44733	3.35777	1.67659
C	-1.63830	5.82753	0.81491
H	-2.52107	6.25015	1.33195
C	-1.42827	6.55436	-0.53461
H	-1.27082	7.63676	-0.36507
H	-2.33376	6.45629	-1.16574
C	-0.20357	5.94815	-1.25980
H	-0.05350	6.45866	-2.23056
C	1.05465	6.12208	-0.37611
H	1.94238	5.71360	-0.89395
H	1.24714	7.19863	-0.20331
C	0.84246	5.39388	0.97244
H	1.74508	5.51191	1.60105
C	-0.37977	6.00415	1.69719
H	-0.52928	5.50723	2.67484
H	-0.20784	7.07833	1.90363