Supporting Information for:

Carbon–chalcogen bond formation initiated by [Al(NON^{Dipp})(E)]$^-$ anions containing Al–E (E = S, Se) multiple bonds

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General Experimental Procedures

All manipulations were performed under dry nitrogen using standard Schlenk-line techniques, or in a conventional nitrogen-filled glovebox. Solvents were dried over appropriate drying agents and degassed 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), 125.7 (^{13}C{^{1}H}) and 95.4 (^{77}Se) MHz. Spectra were recorded at 298 K (unless stated otherwise) and proton and carbon chemical shifts were referenced internally to residual solvent resonances. Coupling constants are quoted in Hz. K[Al(NON^{Dipp})] (**K**[**A**]),[S1] K[Al(NON^{Dipp})(S$_4$)] (**K**[**B**]),[S2] and [K(Et$_2$O)][Al(NON^{Dipp})(Se)] ([**K(Et$_2$O)**][**VI**]),[3] were prepared according to the literature procedures. All other chemicals were purchased from Sigma-Aldrich and used without further purification.

Synthesis of K[Al(NON^{Dipp})(S)] (K[1-*S*])

A THF solution of triphenylphosphine (371 mg, 1.42 mmol) was added to a yellow solution of K[Al(NON^{Dipp})(S$_4$)] (**K**[**B**]) (355 mg, 0.52 mmol) in THF. The mixture was stirred for 18 hours to give a pale-yellow solution. The volatiles were removed in vacuo and the product extracted with hexane. Large colourless crystals were grown from a hexane solution *via* slow evaporation at room temperature. Yield 187 mg, 66 %.

^{1}H NMR (C$_6$D$_6$): δ 7.11 – 7.00 (m, 12H*, C$_6$H$_3$ and C$_6$H$_5$), 3.96 (sept, *J* = 6.9, 4H, C*H*Me$_2$), 1.42 (d, *J* = 6.9, 12H, CH*Me$_2$*), 1.38 (br d, 12H, CH*Me$_2$*), 0.34 (s, 12H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (C$_6$D$_6$): δ 147.1, 144.1, 123.7 (C$_6$H$_3$), 28.2 (*C*HMe$_2$), 26.0, 24.2 (CH*Me$_2$*), 2.1 (Si*Me$_2$*).
* overlap with aromatic resonance from residual Ph$_3$P=S. Elemental analysis was not obtained for this compound due to persistent contamination with residual Ph$_3$P=S.

Figure S1 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NON^{Dipp})(S)] **K**[**1-*S***]

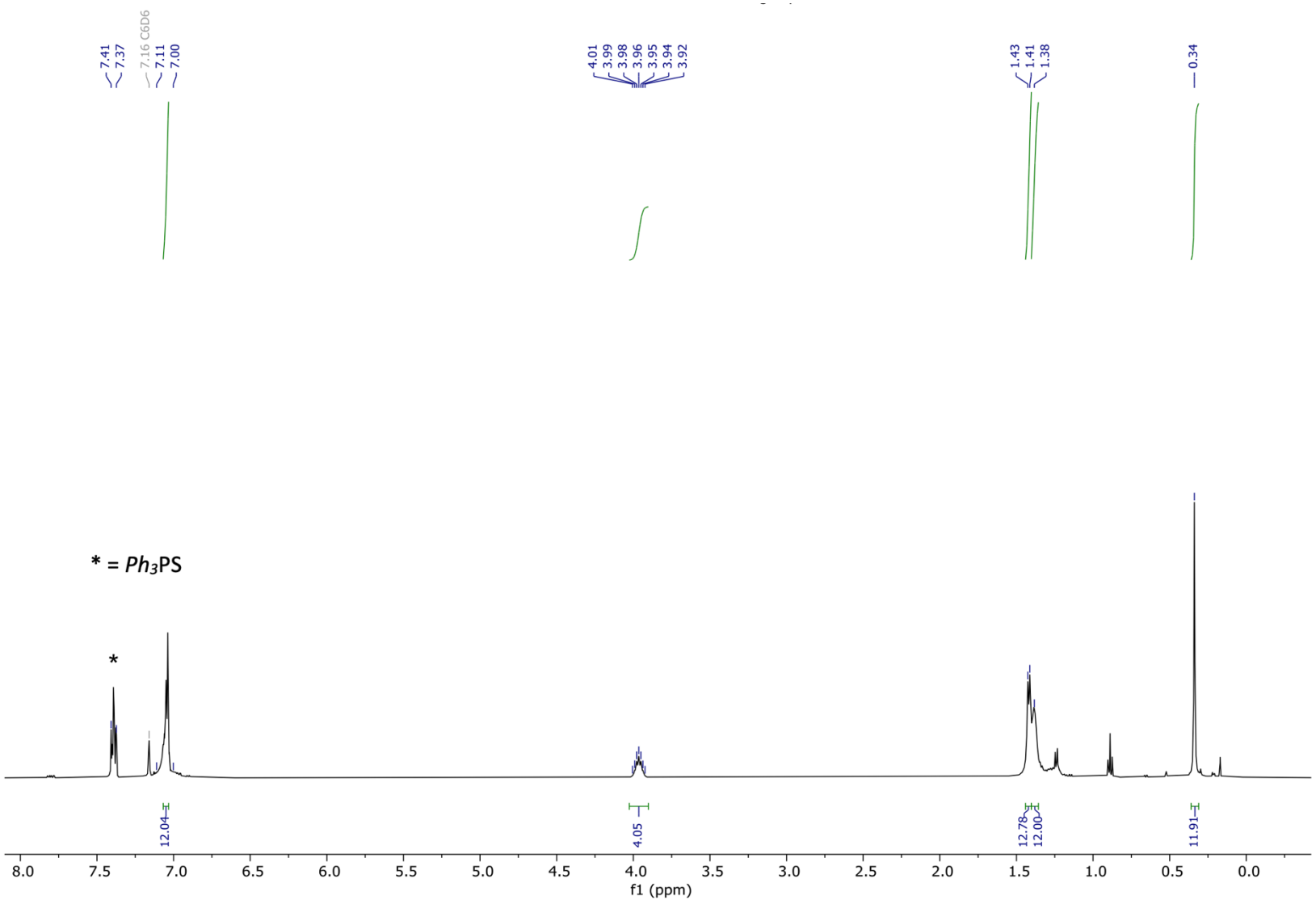


Figure S2 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6) of K[Al(NON^{Dipp})(S)] **K**[**1**-***S***]

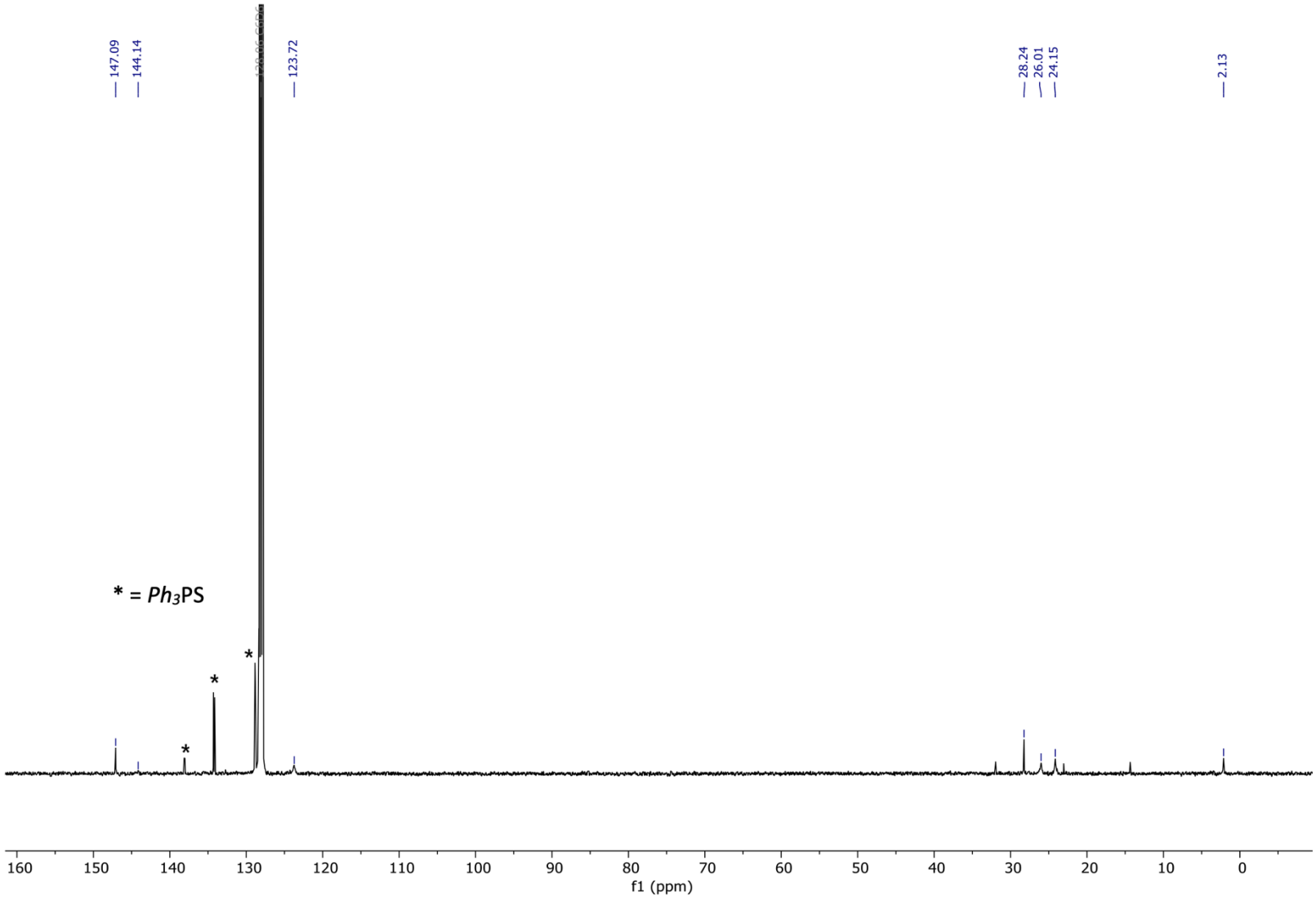


Figure S3 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of [K{Al(NON^{Dipp})(S)}]$_4$ {**K**[**1-*S***]}$_4$ (*asymmetric unit*)

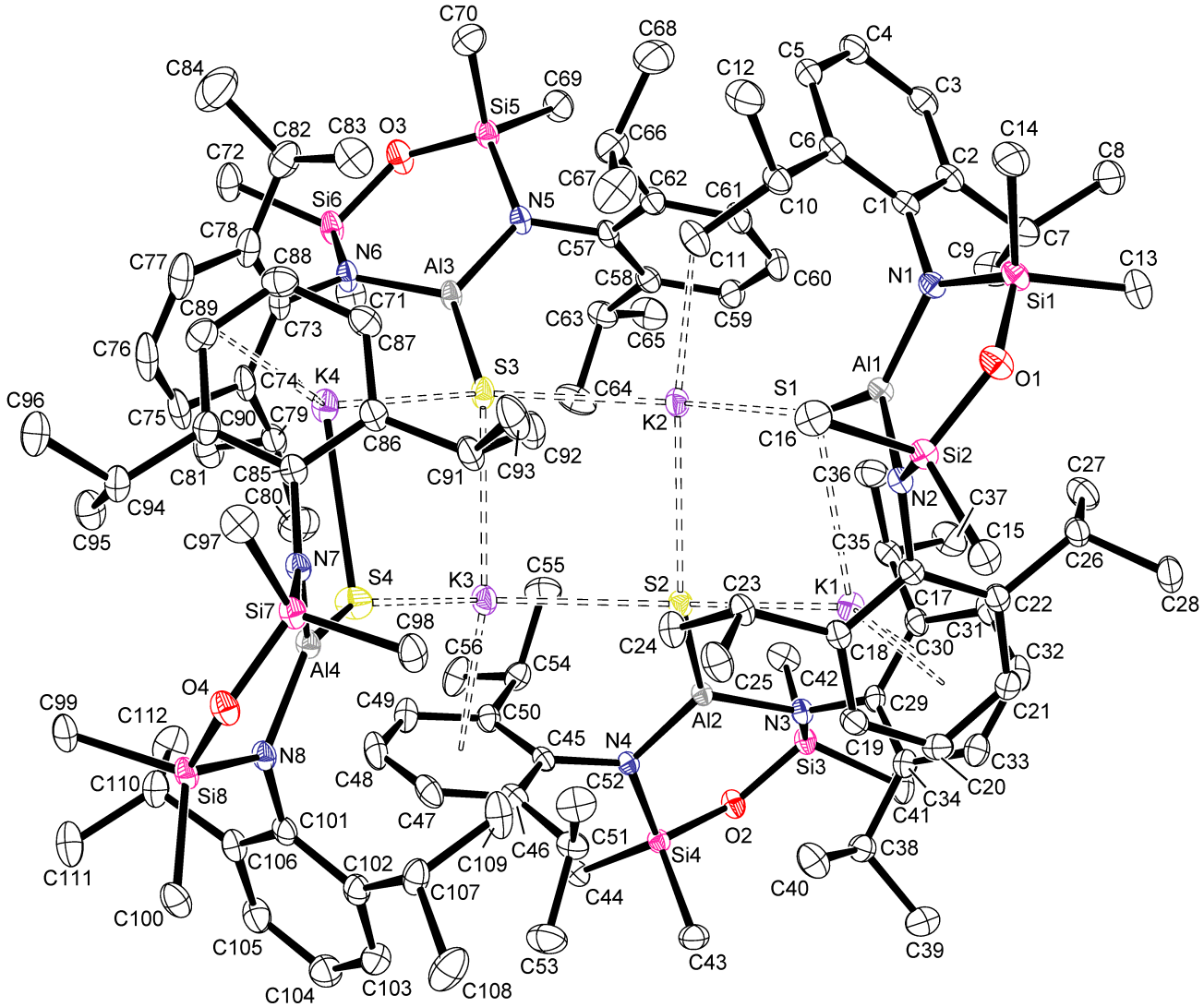
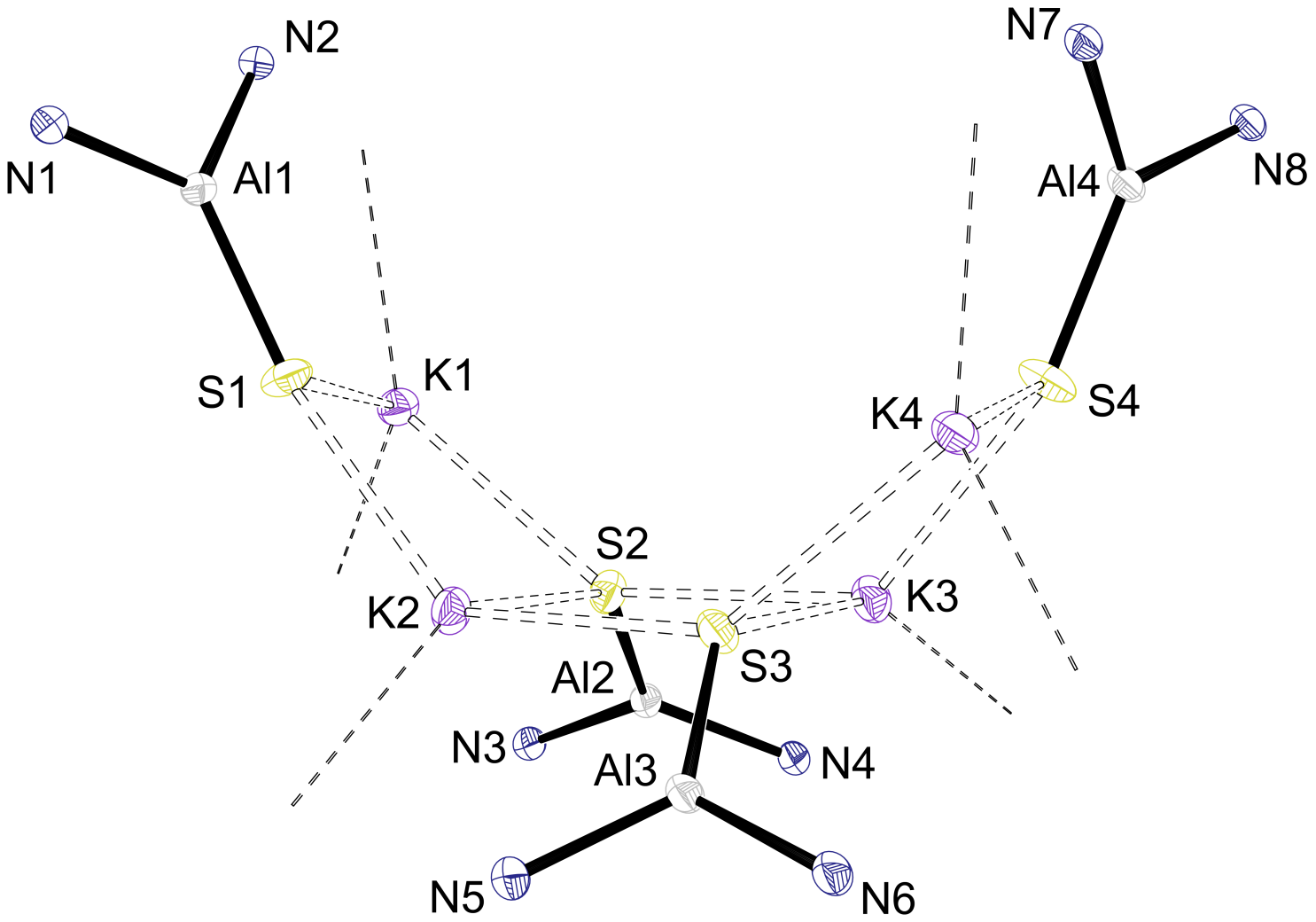


Figure S4 ORTEP (displacement ellipsoids 30 %) of $[K\{Al(NON^{Dipp})(S)\}]_4$ $\{\mathbf{K}[\mathbf{1}\text{-}\boldsymbol{S}]\}_4$ (*core*)



Synthesis of [K(2.2.2-crypt)][Al(NON^{Dipp})(S)] ([K(2.2.2)crypt)][1-*S*])

A solution of **K**[**1**-***S***] was prepared by adding 246 mg of triphenylphosphine (0.94 mmol) to a THF solution of **K**[**B**] (212 mg, 0.31 mmol) and stirring for 2 hours. The volatiles were removed *in vacuo* and the residue dissolved in toluene. A solution of [2.2.2]cryptand (118 mg, 0.31 mmol) in toluene was added at –30 °C to give a white suspension. The suspension was washed three times with cold toluene (–30 °C) and recrystallised from THF at –30 °C to yield large colourless plate-like crystals. Yield 25 mg, 8 %.

Anal. Calc'd for $C_{46}H_{82}AlKN_4O_7SSi_2$ (*957.48*): C, 57.70; H, 8.63; N, 5.85 %. Found: C, 57.37; H, 8.27; N, 5.63 %.

^{1}H NMR (C_6D_6, 343 K): δ 7.13 (d, *J* = 7.6, 4H, C_6H_3), 7.01 (t, *J* = 7.6, 2H, C_6H_3), 4.27 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 3.23 (s, 12H, crypt-CH_2), 3.17 (t, 12H, *J* = 4.7, crypt-CH_2), 2.19 (t, *J* = 4.7, 12H, crypt-CH_2), 1.67 (d, *J* = 6.8, 12H, CHMe_2, 1.50 (d, *J* = 6.8, 12H, CHMe_2), 0.49 (s, 12H, SiMe$_2$).

^{13}C{^{1}H} NMR (C_6D_6, 343 K) δ 146.7, 145.5, 123.0, 122.3 (C_6H_3), 70.8, 68.3, 55.3 (crypt-*C*H$_2$), 28.5 (*C*HMe$_2$), 26.2, 24.7 (CHMe_2), 2.8 (SiMe$_2$).

Figure S5 ^{1}H NMR spectrum (500 MHz, C_6D_6, 343 K) of [K(2.2.2-crypt)][Al(NON^{Dipp})(S)] [**K(2.2.2)crypt)**][**1-*S***]

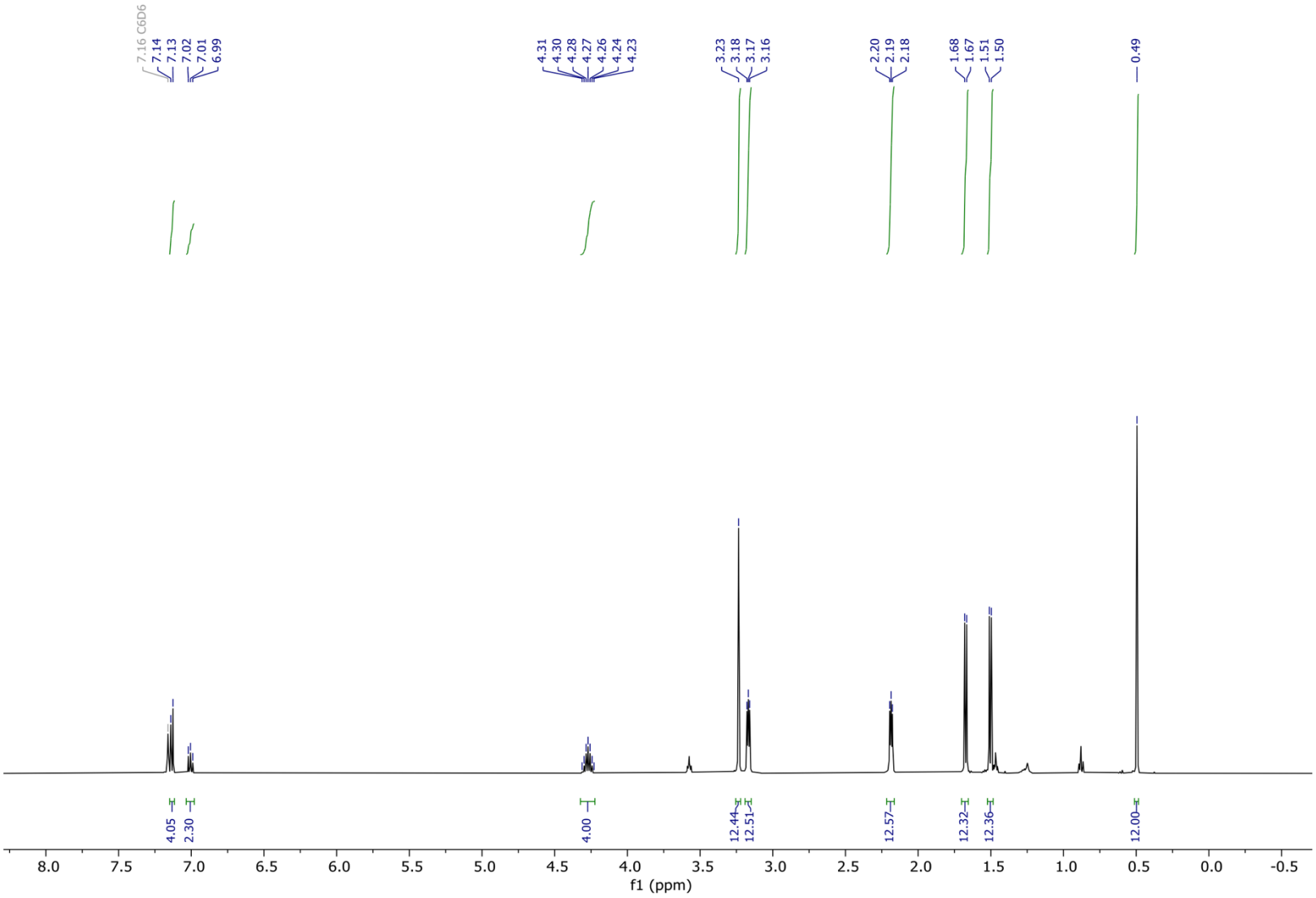


Figure S6 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6, 343 K) of [K(2.2.2-crypt)][Al(NON^{Dipp})(S)] [**K(2.2.2)crypt)**][**1-*S***]

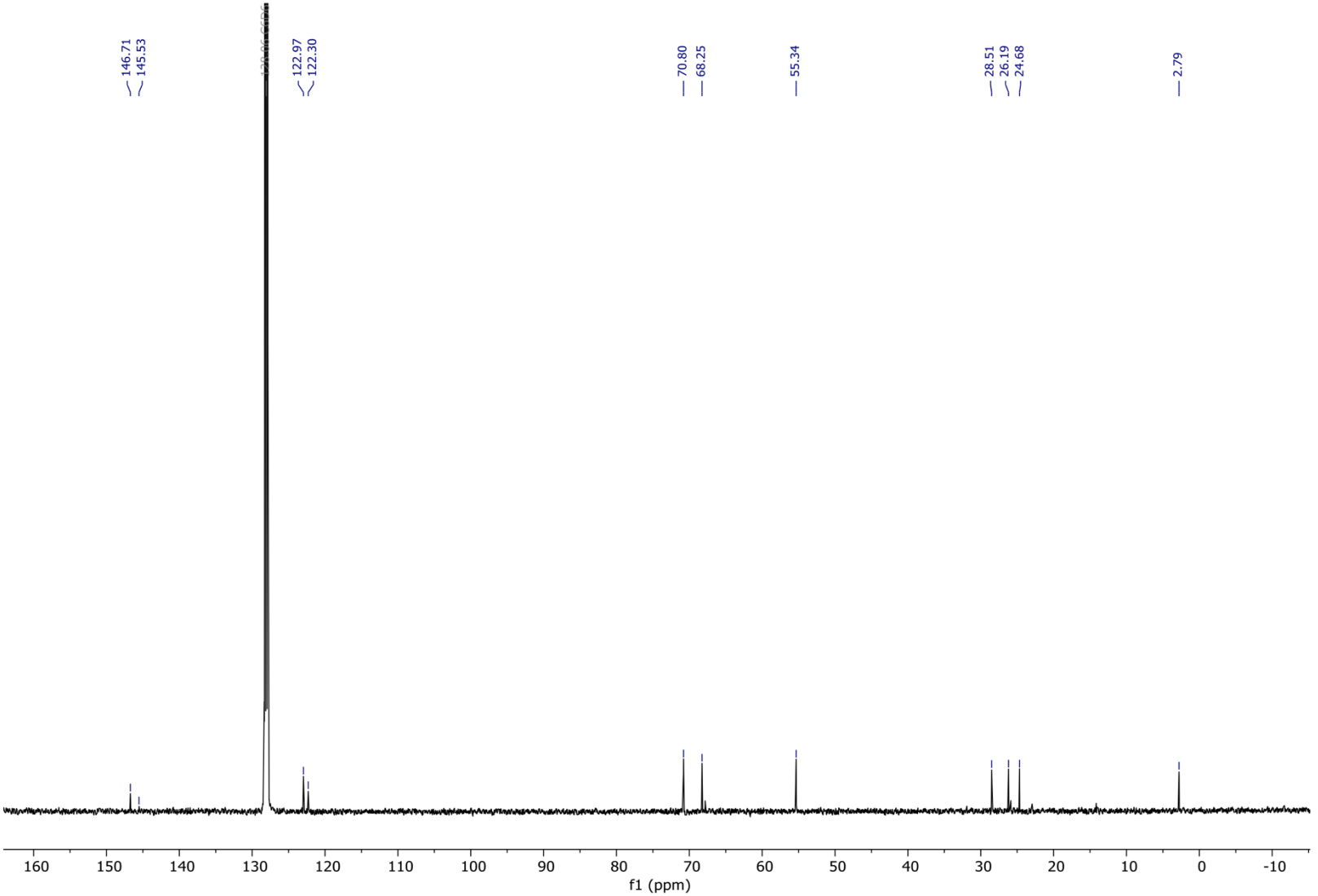
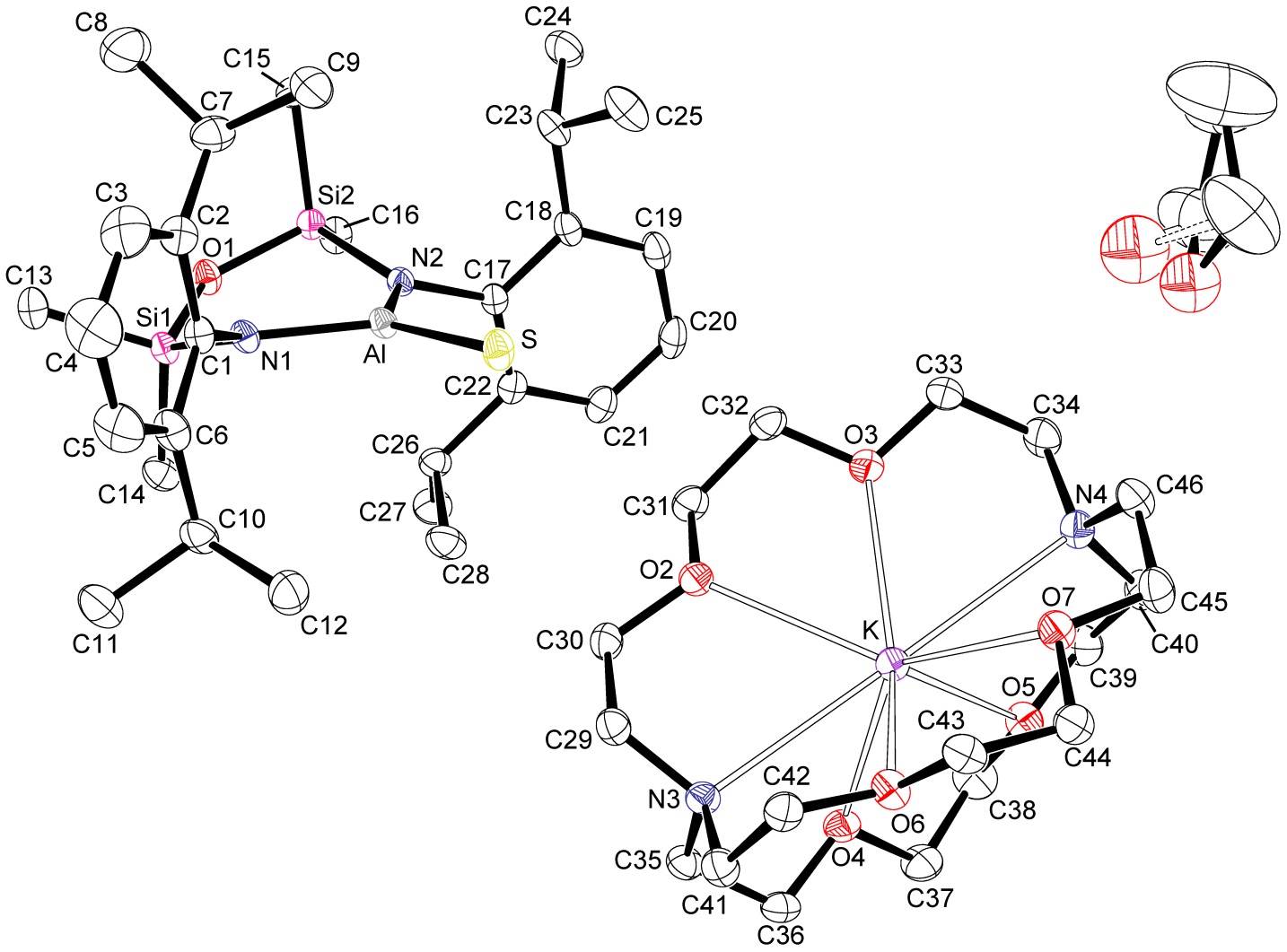


Figure S7 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of [K(2.2.2-crypt)][Al(NON^{Dipp})(S)] [**K(2.2.2)crypt)**][**1-*S***]



Synthesis of [K(Et$_2$O)$_2$][Al(NON^{Dipp})(SC{O}O)] ([K(Et$_2$O)][2-*S*])

A solution of **K**[**1**-***S***] (187 mg, 0.32 mmol) was prepared in toluene-d_8 and added to an NMR tube fitted with a Teflon tap. The toluene solution was degassed and one atmosphere of $^{13}CO_2$ gas was added. Reaction progress was monitored by $^{13}C\{^1H\}$ NMR spectroscopy and shown to be complete after 2 days at room temperature. The solvent was removed *in vacuo* and the white solid dissolved in diethyl ether. Crystals were grown at –30 °C from a diethyl ether solution. Yield 52 mg, 26 %.

^{1}H NMR (C_6D_6): δ 7.12 (dd, *J* = 7.6, 1.8, 2H, C_6H_3), 7.08 (dd, *J* = 7.6, 1.8, 2H, C_6H_3), 7.00 (t, *J* = 7.6, 2H, C_6H_3), 4.05 (br sept, *J* = 6.8, 4H, C*H*Me$_2$), 3.26 (q, *J* = 7.1, 2H*, OCH_2CH$_3$), 1.39 (d, *J* = 6.8, 6H, C*H*Me$_2$), 1.33 (d, *J* = 6.8, 6H, CHMe_2), 1.23 (br d, 6H, CHMe_2), 1.19 (br d, 6H, CHMe_2), 1.12 (t, *J* = 7.1, 3H*, OCH$_2$CH_3), 0.50 (s, 6H, SiMe_2), 0.39 (s, 6H, SiMe_2).

$^{13}C\{^1H\}$ (C_6D_6): δ 180.1 (S^{13}*C*O$_2$), 147.6, 146.9, 144.1, 124.8, 123.9, 123.5 (C_6H$_3$), 65.9, (O*C*H$_2$CH$_3$), 31.9 (OCH$_2$*C*H$_3$), 28.0, 27.8 (*C*HMe$_2$), 25.7, 25.5, 25.3, 25.0 (CHMe_2), 2.7, 2.0 (SiMe_2). * Sample exposed to vacuum prior to NMR analysis resulting in loss of Et$_2$O, as determined by smaller integrals of the peaks in the ^{1}H NMR spectrum relative to expected value from X-ray diffraction data. Despite repeated attempts we were unable to obtain accurate elemental analysis for [**K(Et$_2$O)**][**2**-***S***].

Figure S8 ^{1}H NMR spectrum (500 MHz, C_6D_6) of $[K(Et_2O)_2][Al(NON^{Dipp})(S^{13}C\{O\}O)]$ [**K(Et$_2$O)**][**2-*S***]

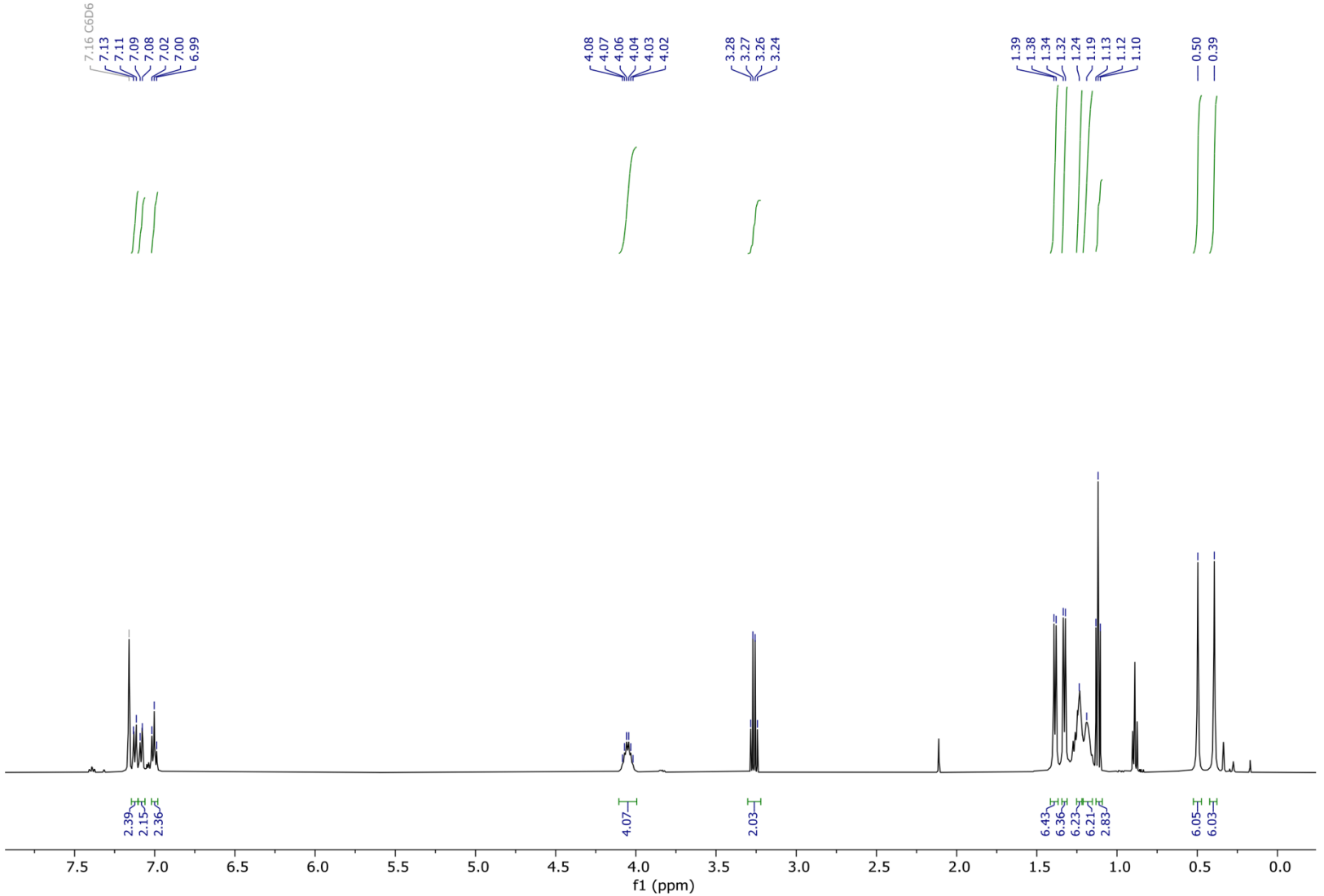


Figure S9 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6) of $[K(Et_2O)_2][Al(NON^{Dipp})(S^{13}C\{O\}O)]$ [**K(Et$_2$O)**][**2-*S***]

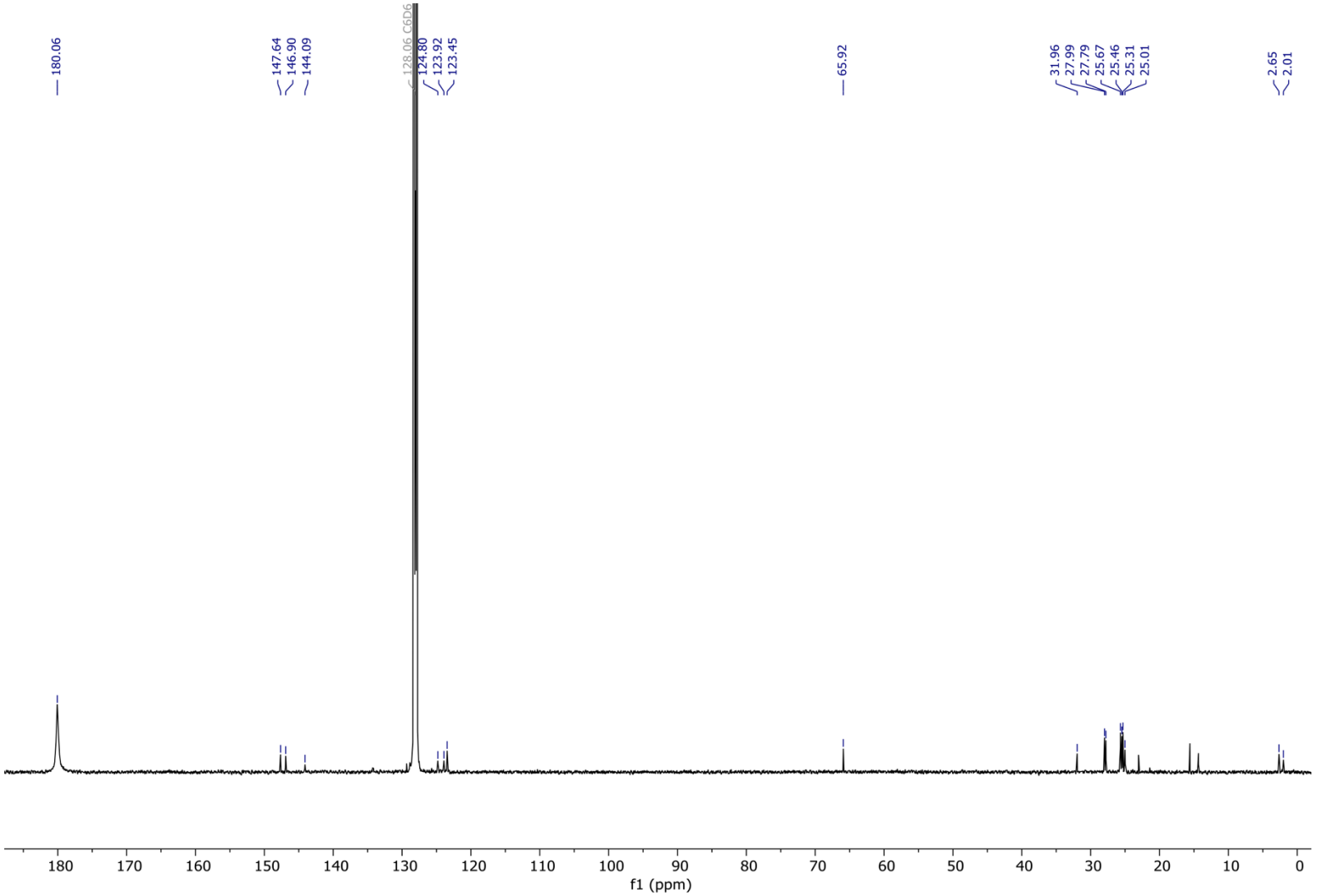
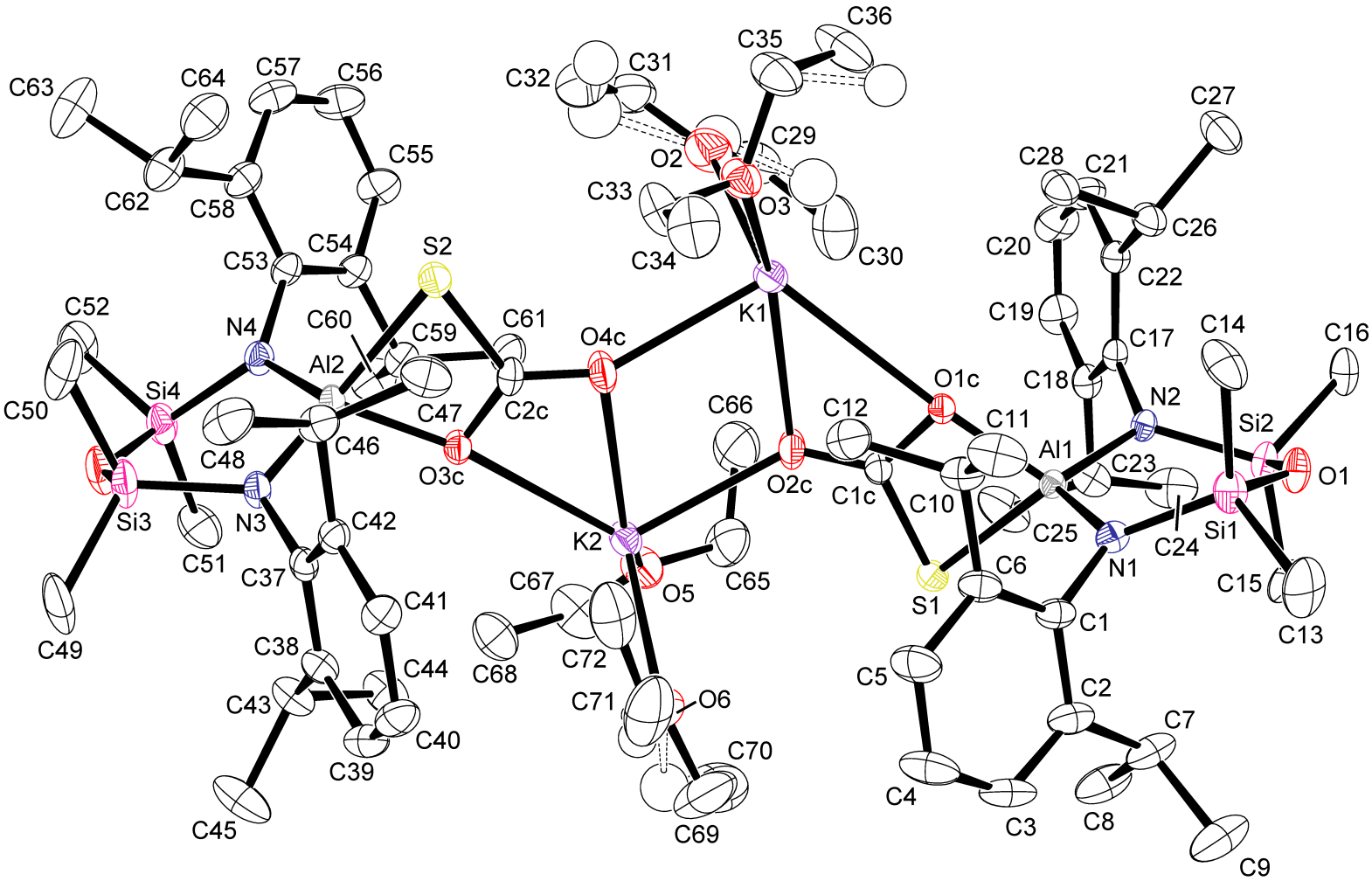


Figure S10 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of $[K(Et_2O)_2][Al(NON^{Dipp})(SC\{O\}O)]$ [**K(Et$_2$O)**][**2-*S***]



Synthesis of [K(THF)$_3$][Al(NON^{Dipp})(SeC{O}O)] ([K(THF)][2-*Se*])

A solution of **K**[**VI**] (150 mg, 0.23 mmol) was prepared in a 50:1 mixture of THF:C_6D_6 and added to an NMR tube fitted with a Teflon tap. The THF/C_6D_6 solution was degassed and one atmosphere of $^{13}CO_2$ gas was added. Reaction progress was monitored by $^{13}C\{^1H\}$ NMR spectroscopy and shown to be complete within 15 minutes at room temperature. The solvent was removed *in vacuo* and the white solid dissolved in THF. Crystals were grown at –30 °C from a THF solution. Yield 50 mg, 31 %.

Anal. Calc'd for $C_{33}H_{54}AlKN_2O_4SeSi_2$ corresponding to loss of 2 × THF, *744.03*): C, 53.27; H, 7.32; N, 3.77 %. Found: C, 53.67; H, 7.34; N, 3.85 %.

^1H NMR (500 MHz, THF-D_8) : δ 6.97 – 6.91 (m, 4H, C_6H_3), 6.84 (t, *J* = 7.6, 2H, C_6H_3), 3.98 (sept, *J* = 6.8, 2H, C*H*Me$_2$), 3.90 (sept, *J* = 6.8, 2H, C*H*Me$_2$), 3.63 – 3.60 (m, 4H, THF-CH_2), 1.79 – 1.76 (m, 4H, THF-CH_2), 1.22 (d, *J* = 6.8, 6H, CHMe_2), 1.19 (d, *J* = 6.8, 6H, CHMe_2), 1.17 (d, *J* = 6.8, 6H, HCMe_2), 1.16 (d, *J* = 6.8, 6H, HCMe_2), 0.12 (s, 6H, SiMe_2), 0.08 (s, 6H, SiMe_2)

$^{13}C\{^1H\}$ (THF-D_8): δ 166.0 ($J_{Se\text{-}C}$ = 128.1, Se$^{13}CO_2$), 147.5, 147.2, 145.0, 123.9, 123.8, 123.0 (C_6H_3), 28.4, 28.3 (*C*HMe$_2$), 26.6, 26.4, 26.2, 26.1 (CHMe_2), 2.9, 2.8 (SiMe_2). ^{77}Se NMR (THF-d_8): δ 150 (d, *J* = 128, *Se*CO_2).

Figure S11 ^{1}H NMR spectrum (500 MHz, THF-d_8) of [K(THF)$_3$][Al(NON^{Dipp})(Se^{13}C{O}O)] [**K(THF)**][**2-*Se***]

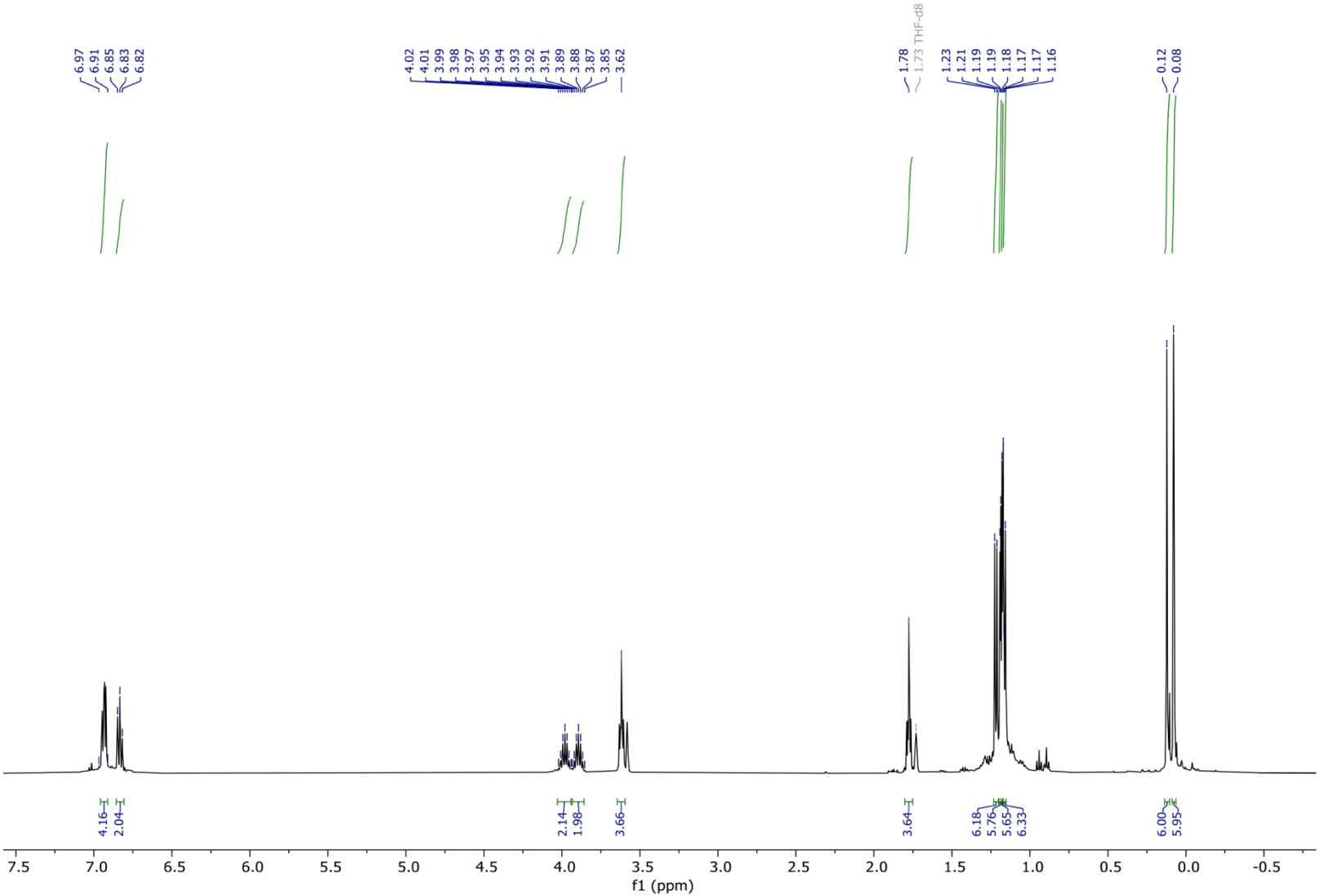


Figure S12 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, THF-d_8) of $[K(THF)_3][Al(NON^{Dipp})(Se^{13}C\{O\}O)]$ [**K(THF)**][**2-*Se***]

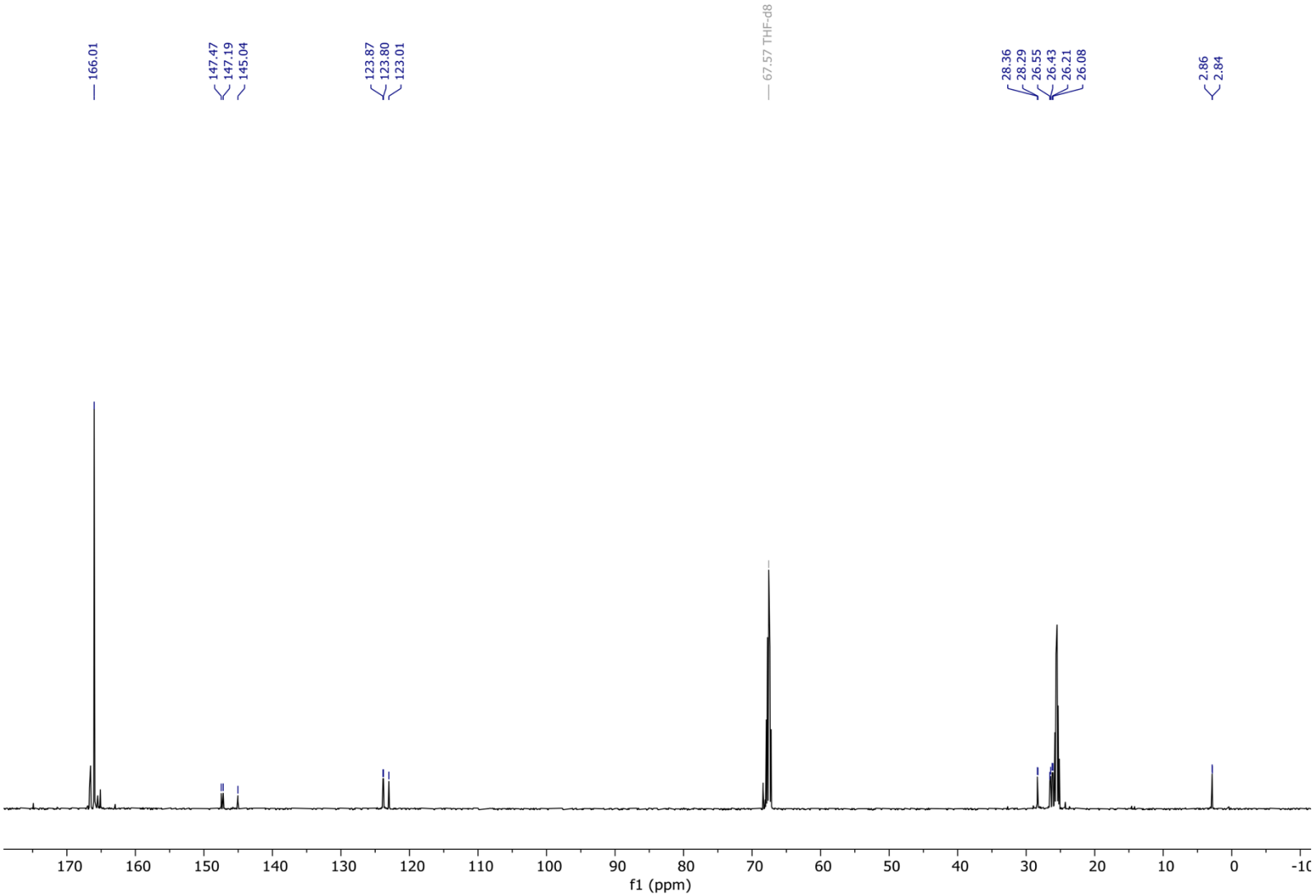


Figure S13 Expansion of $^{13}C\{^{1}H\}$ [Se*^{13}C*{O}O] resonance from [K(THF)$_3$][Al(NON^{Dipp})(Se^{13}C{O}O)] [**K(THF)**][**2-*Se***] showing $^{1}J_{SeC}$ coupling

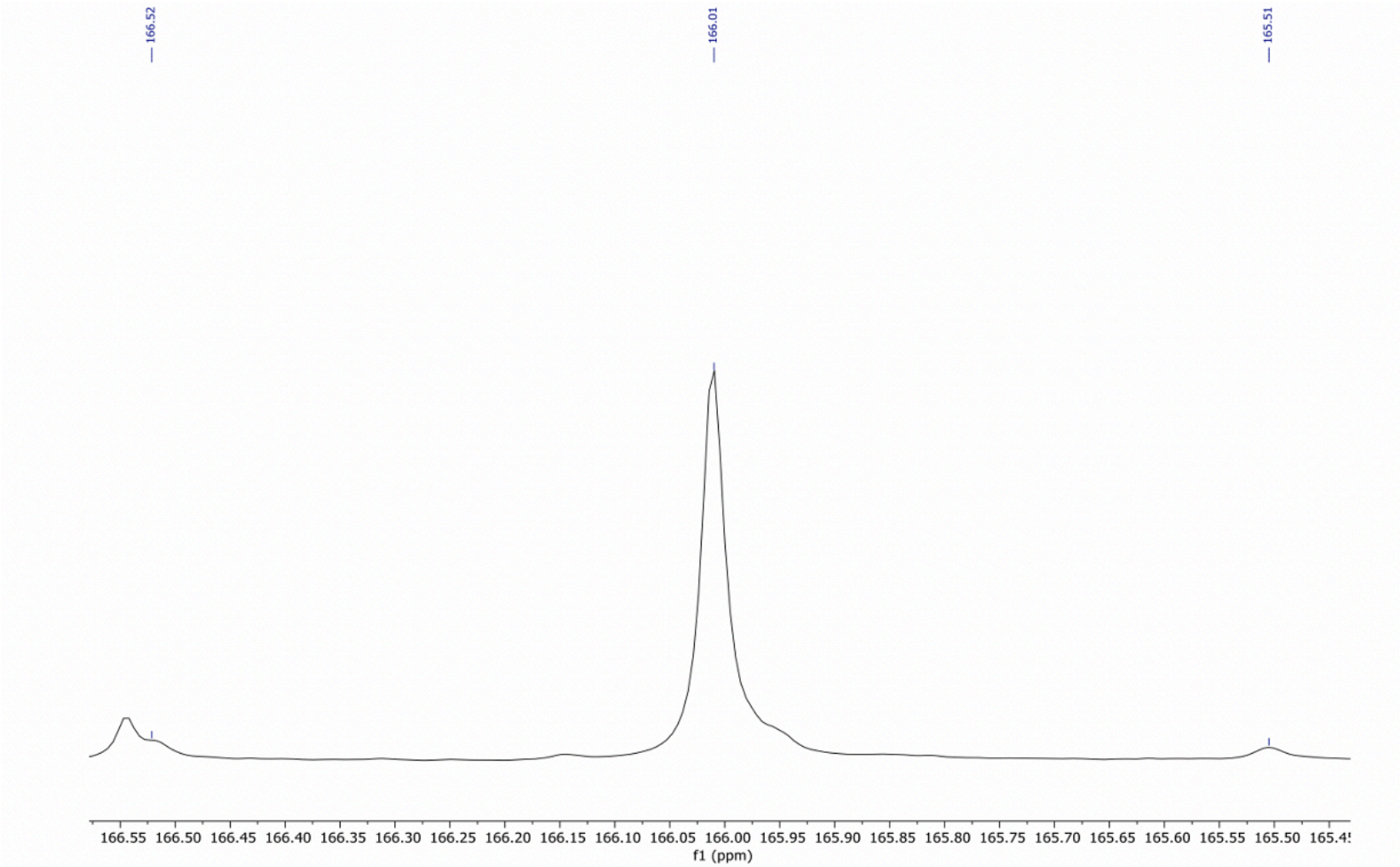


Figure S14 ^{77}Se NMR spectrum (95 MHz, THF-d_8) of [K(THF)$_3$][Al(NON^{Dipp})(Se^{13}C{O}O)] [**K(THF)**][**2-*Se***]

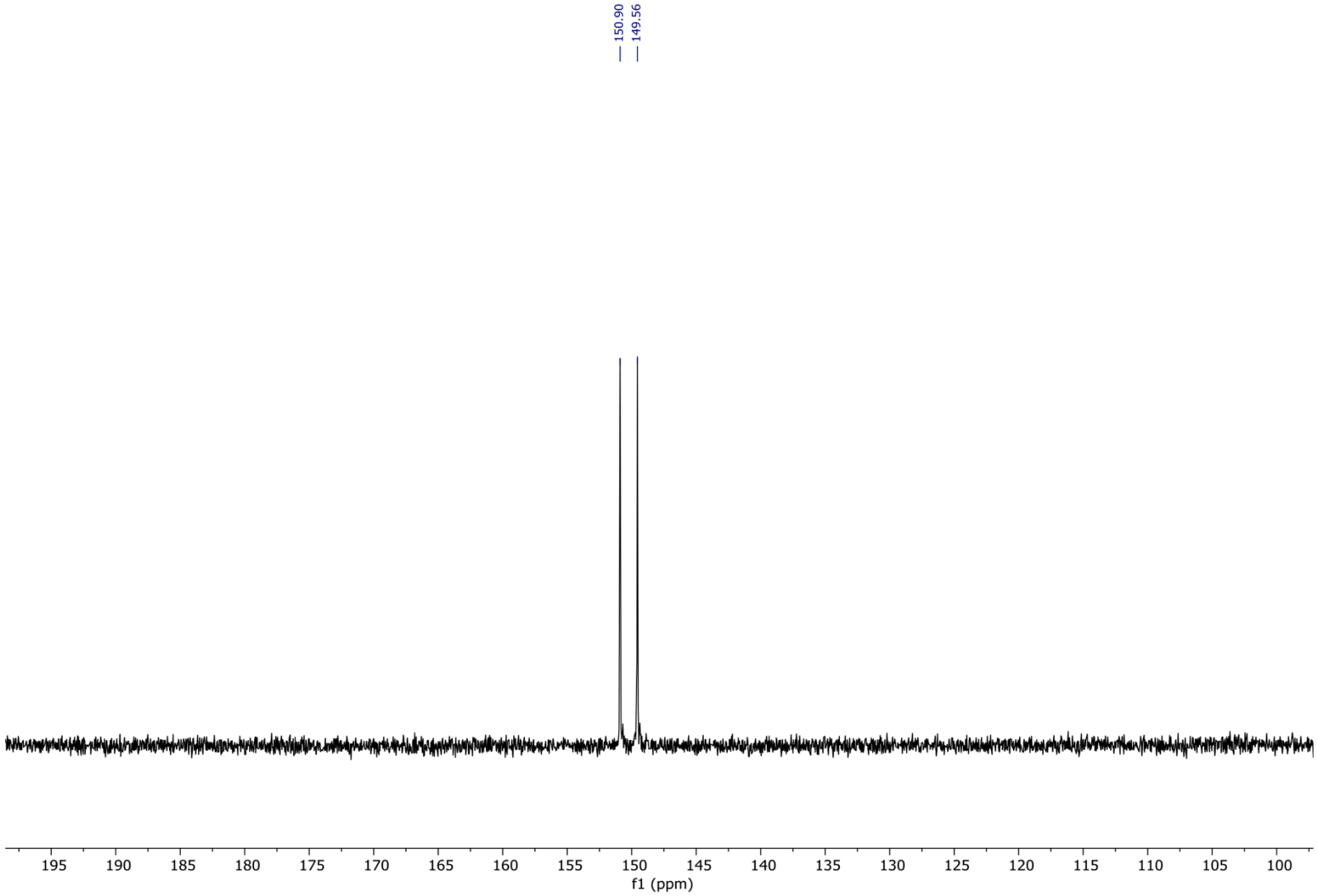
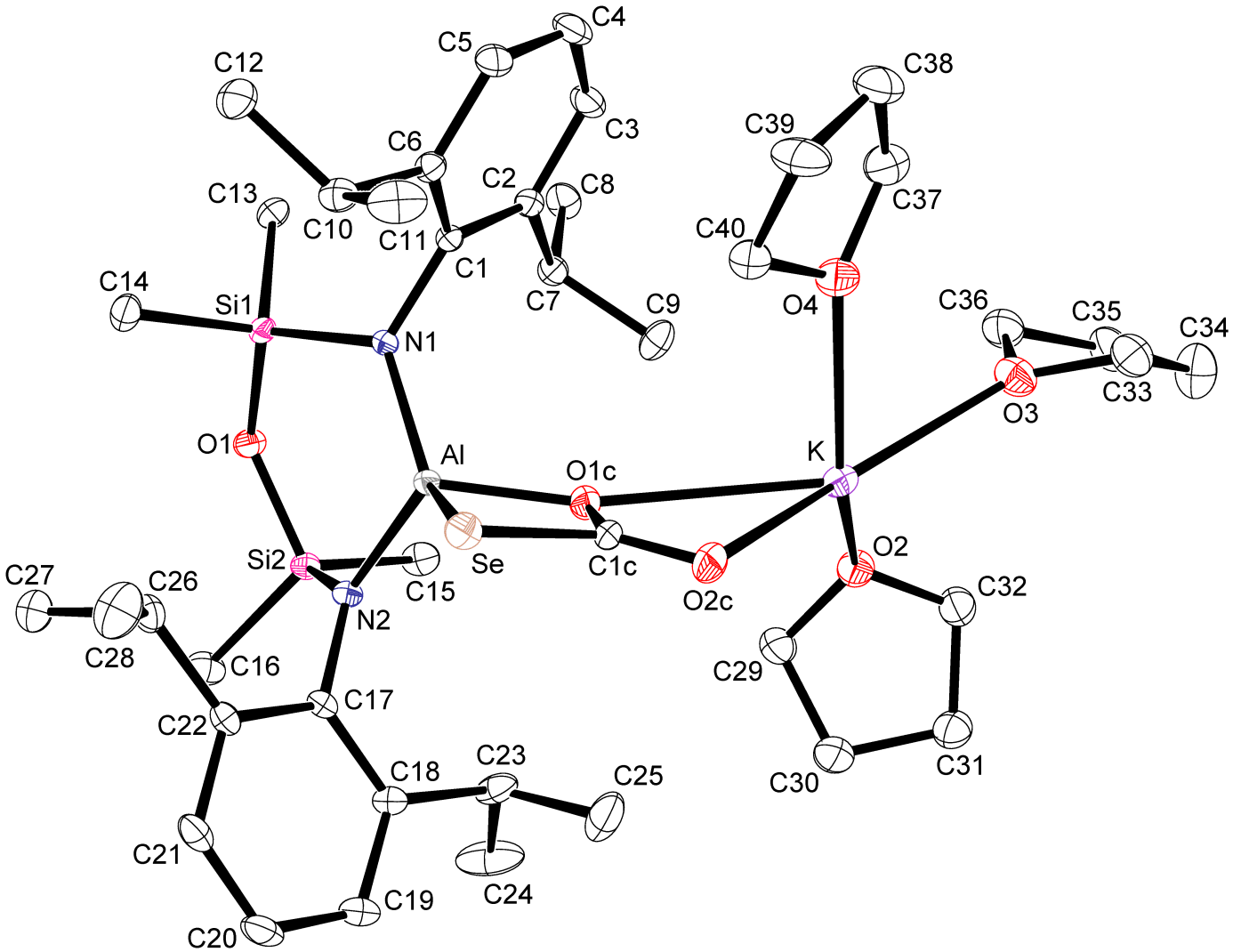


Figure S15 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of [K(THF)][Al(NON^{Dipp})(SeC{O}O)] [**K(Et$_2$O)**][**2-*Se***]



Synthesis of K[Al(NON^{Dipp})(SC{O}Ph$_2$)] ([K][3-*S*])

A solution of **K**[**1-*S***] (50 mg, 0.09 mmol) in Et_2O was added to a stirred solution of benzophenone (16 mg, 0.09 mmol) in Et_2O to give a colourless solution. Crystals were obtained *via.* slow evaporation of the diethyl ether solution at room temperature. Yield 60 mg, 91 %.

Anal. Calc'd for $C_{41}H_{56}AlKN_2O_2SSi_2$ (*763.21*): C, 64.52; H, 7.40; N, 3.67 %. Found: C, 63.92; H, 7.39; N, 3.14 %.

^1H and $^{13}C\{^1H\}$ NMR spectra recorded in THF-D_8 indicated rapid decomposition with release of benzophenone. See Figs. S16 and S17 for representative spectra.

Figure S16 ^{1}H NMR spectrum (500 MHz, THF-d_8) of K[Al(NON^{Dipp})(SC{O}Ph$_2$)] **K**[**3-*S***]

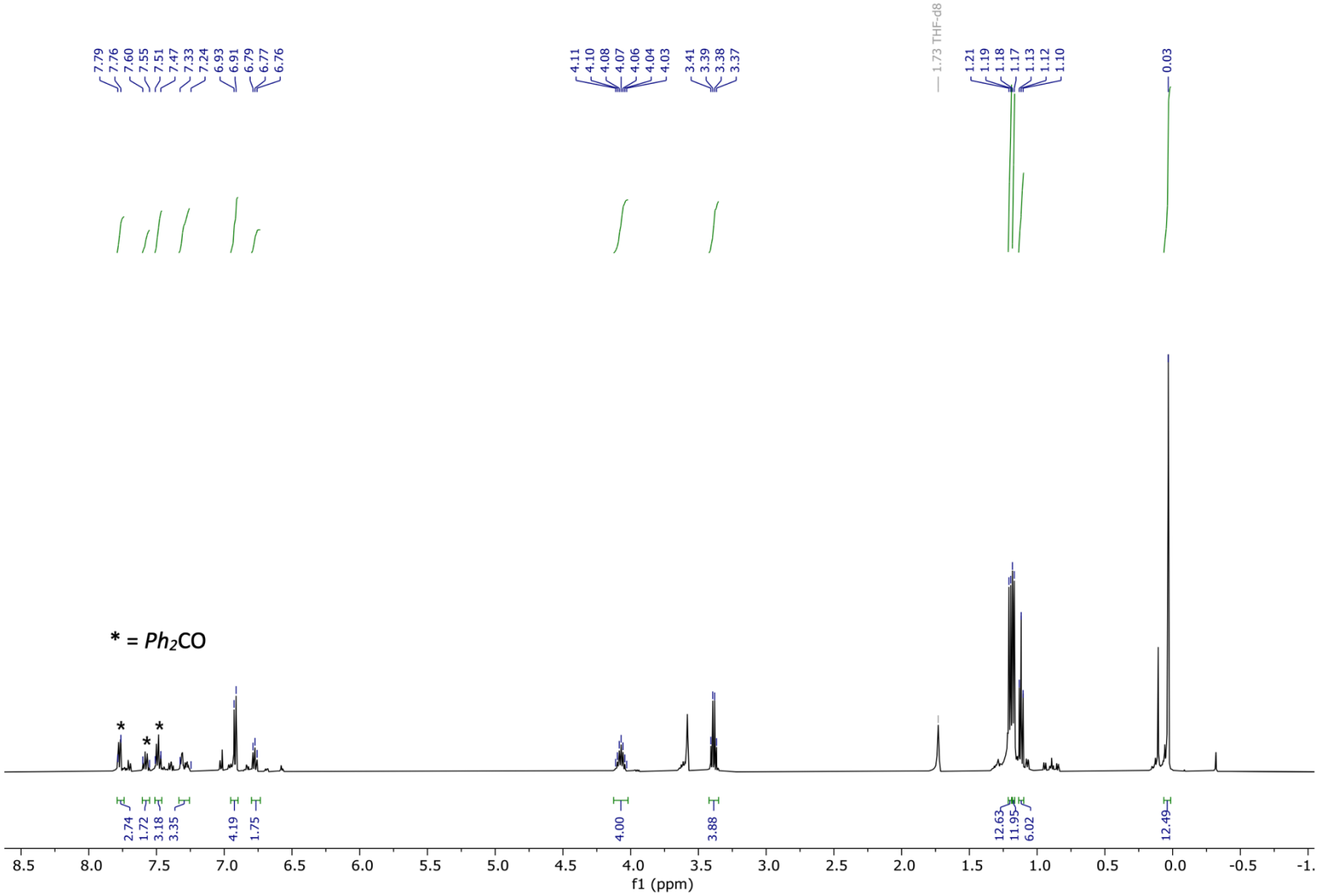


Figure S17 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, THF-d_8) of K[Al(NON^{Dipp})(SC{O}Ph$_2$)] **K[3-*S*]**

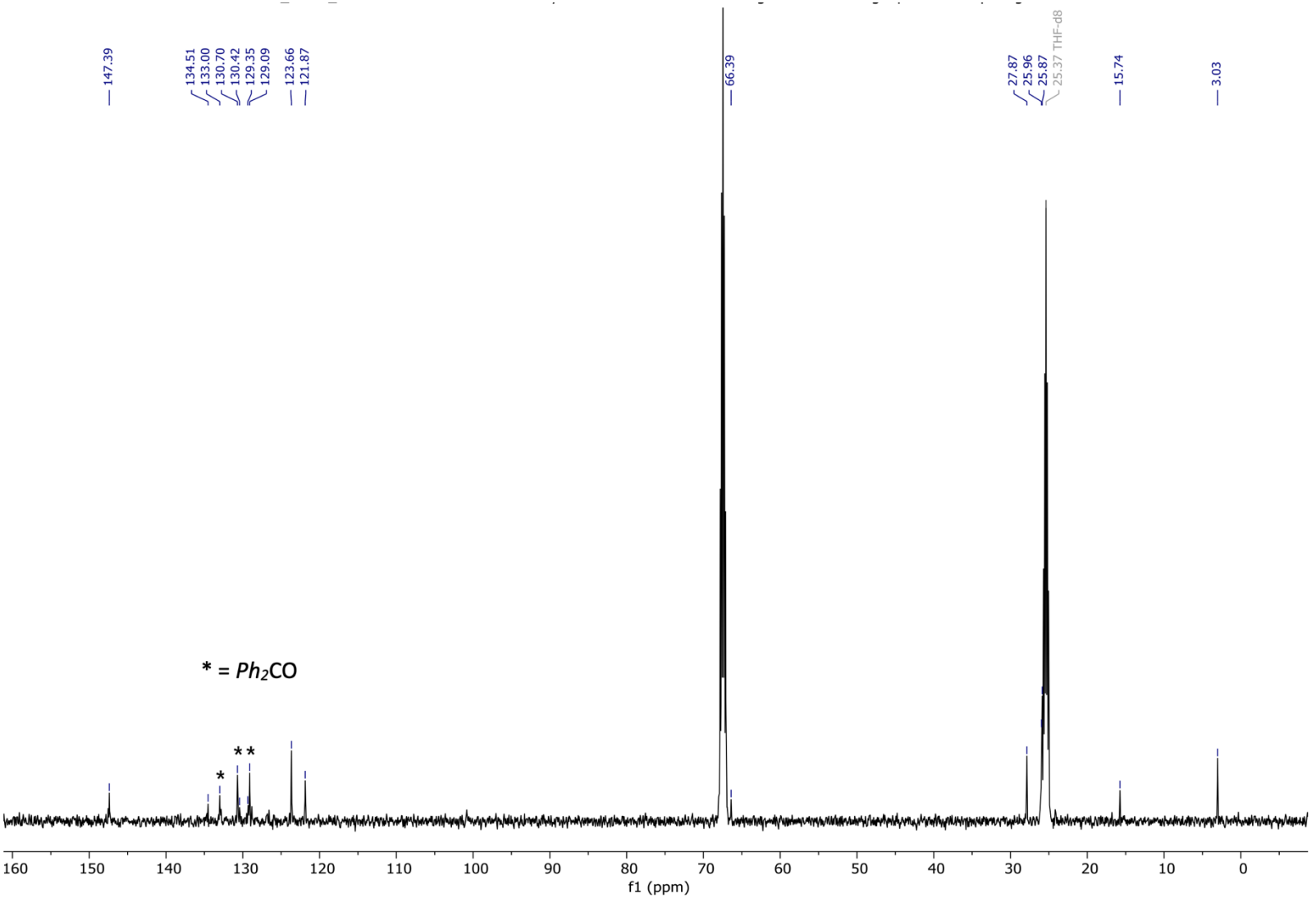
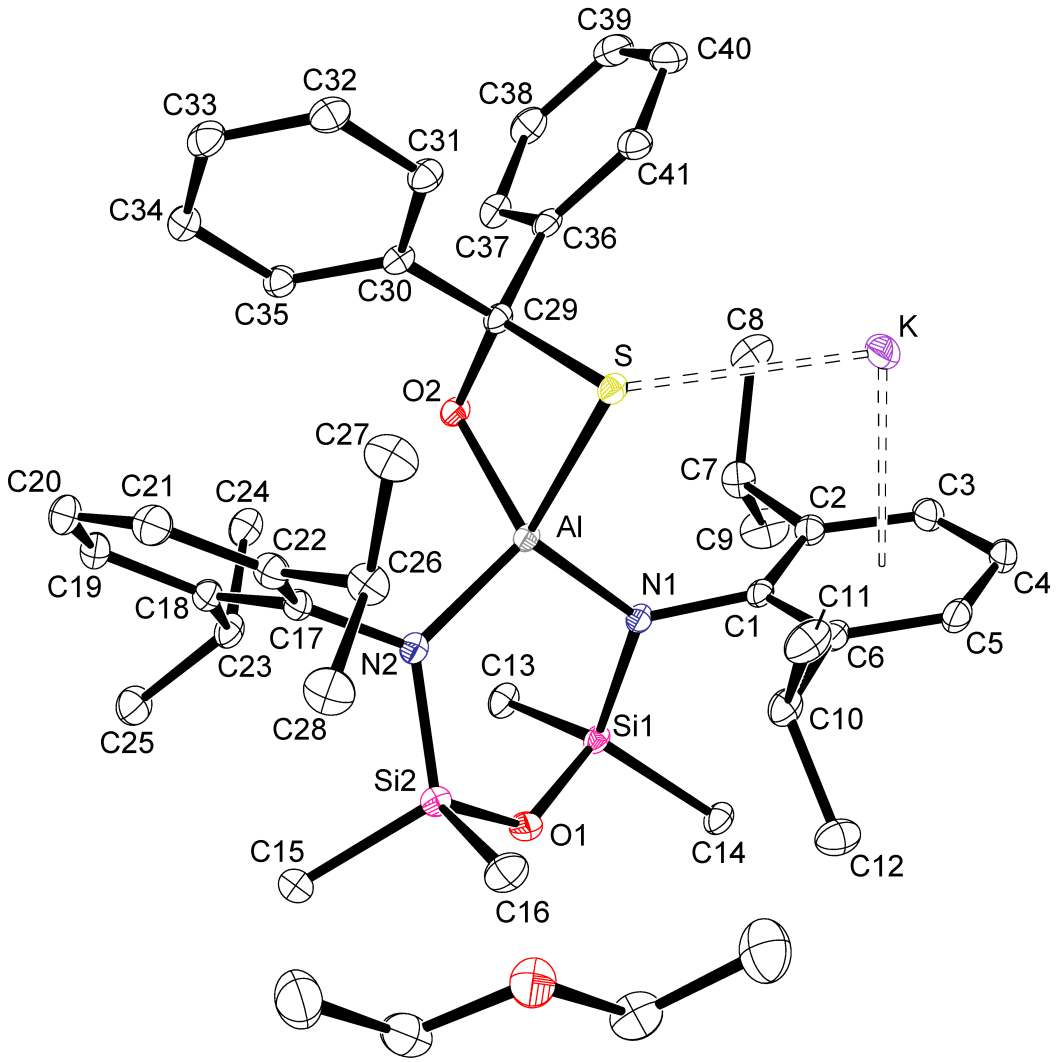


Figure S18 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of K[Al(NON^{Dipp})(SC{O}Ph$_2$)] **K**[**3-*S***]



Synthesis of K[Al(NON^{Dipp})(SeC{O}Ph$_2$)] ([K][3-*Se*])

A solution of **K**[**VI**] (133 mg, 0.22 mmol) in THF was added to a stirred solution of benzophenone (39 mg, 0.22 mmol) in THF to give a colourless solution. Crystals were obtained by storage of the solution at –30 °C for 18 hours. Yield 152 mg, 88 %.

Anal. Calc'd for $C_{41}H_{56}AlKN_2O_2SeSi_2$ corresponding to loss of 3 × THF, (*810.11*): C, 60.79; H, 6.97; N, 3.46 %. Found: C, 60.05; H, 6.99; N, 3.18 %.

^{1}H and ^{13}C{^{1}H} and ^{77}Se NMR spectra recorded in THF-D_8 indicated rapid decomposition with release of benzophenone. See Figs. S19 - S21 for representative spectra.

Figure S19 ^{1}H NMR spectrum (500 MHz, THF-d_8) of [K(THF)$_3$][Al(NON^{Dipp})(SeC{O}Ph$_2$)] [**K(THF)**][**3-*Se***]

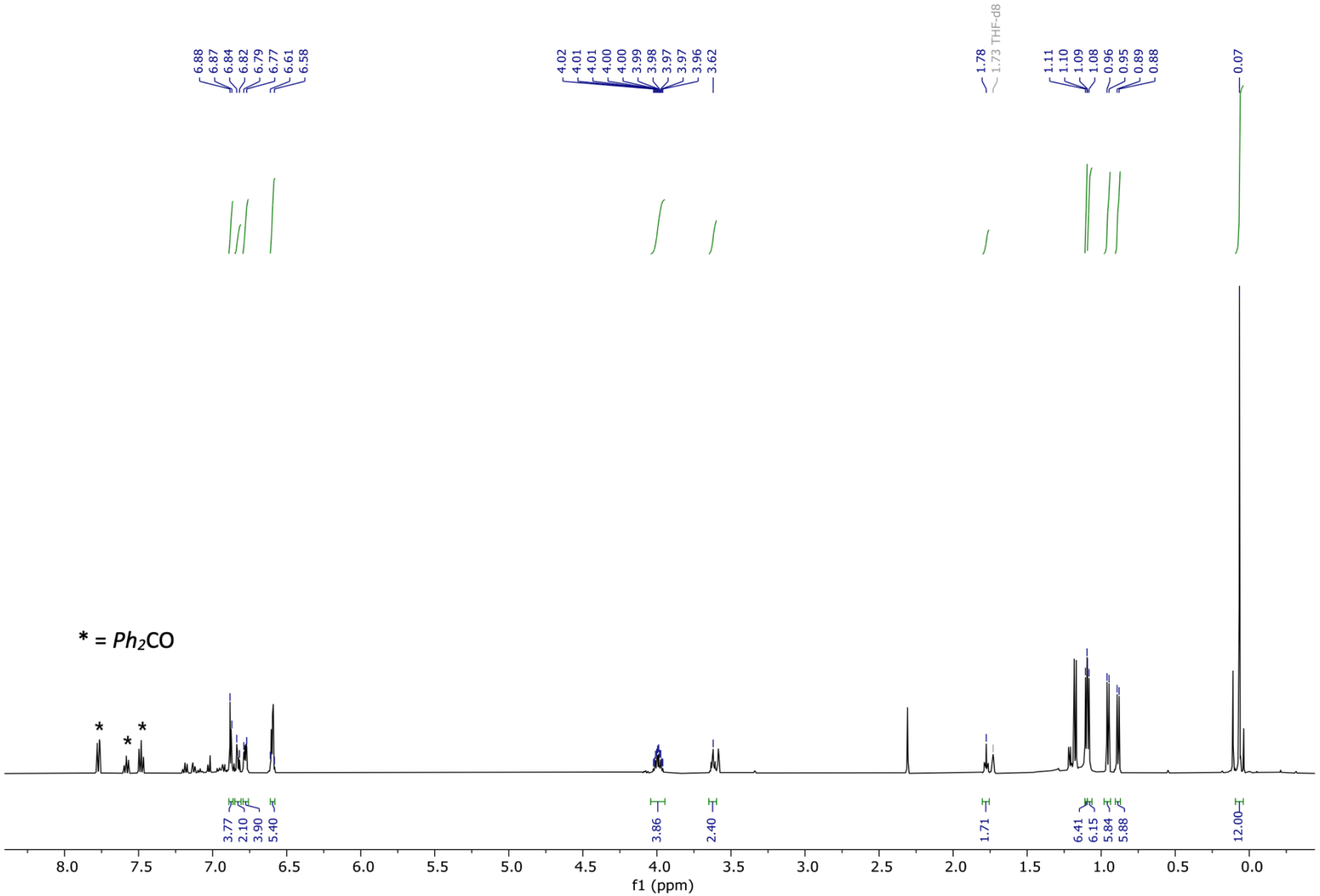


Figure S20 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, THF-d_8) of $[K(THF)_3][Al(NON^{Dipp})(SeC\{O\}Ph_2)]$ [**K(THF)**][[**3-*Se***]

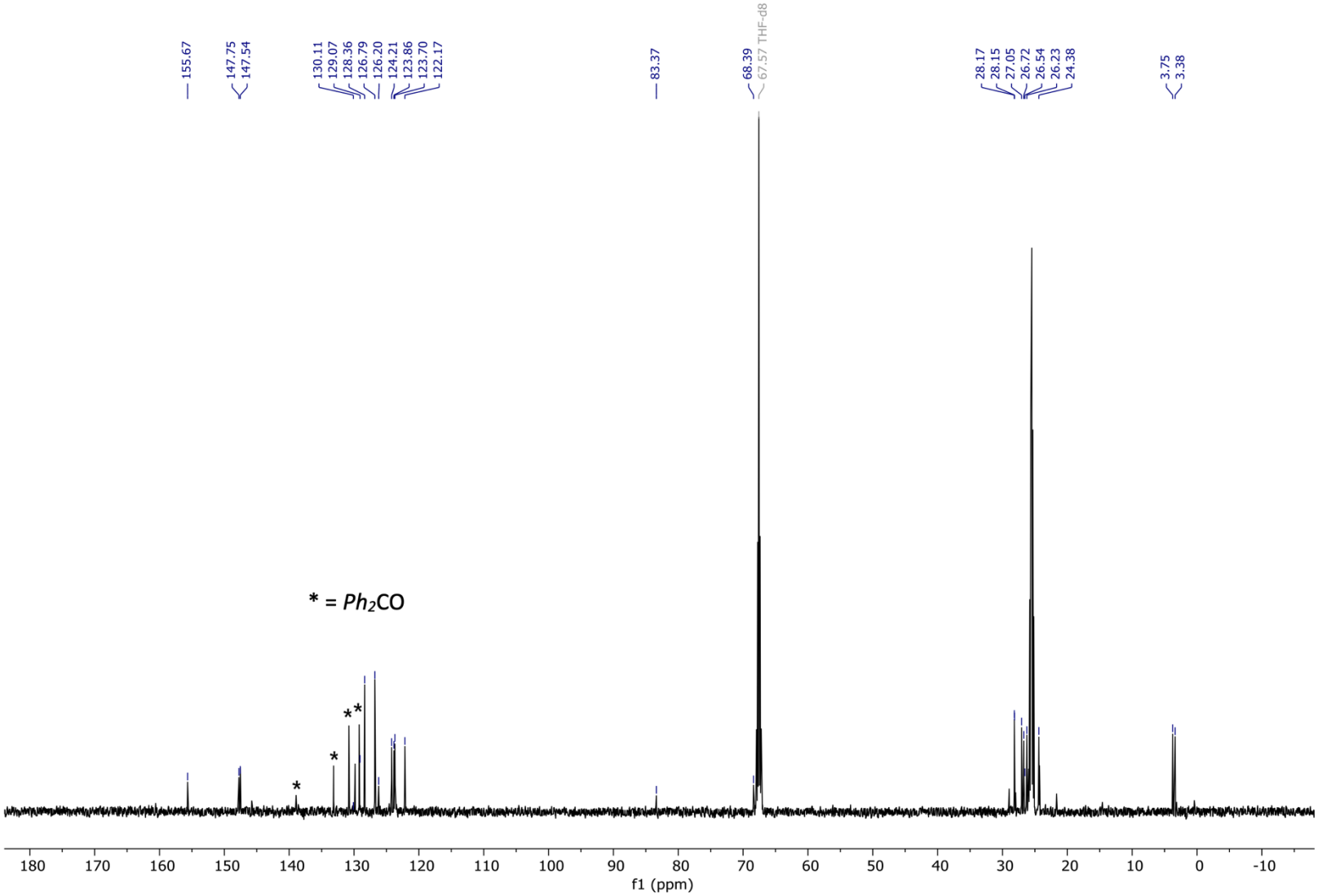


Figure S21 ^{77}Se NMR spectrum (95 MHz, THF-d_8) of [K(THF)$_3$][Al(NON^{Dipp})(SeC{O}Ph$_2$)] [**K(THF)**][**3-*Se***]

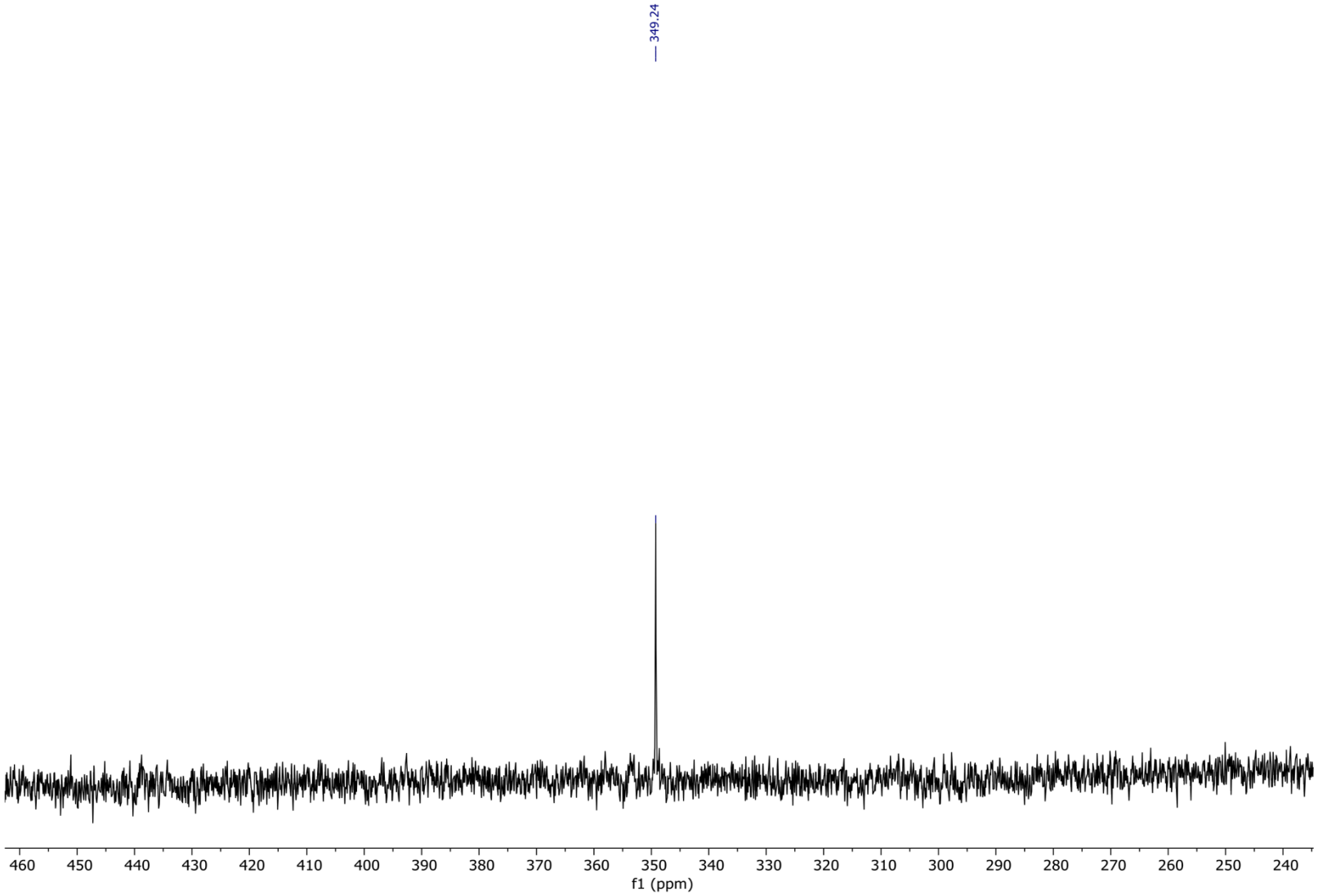
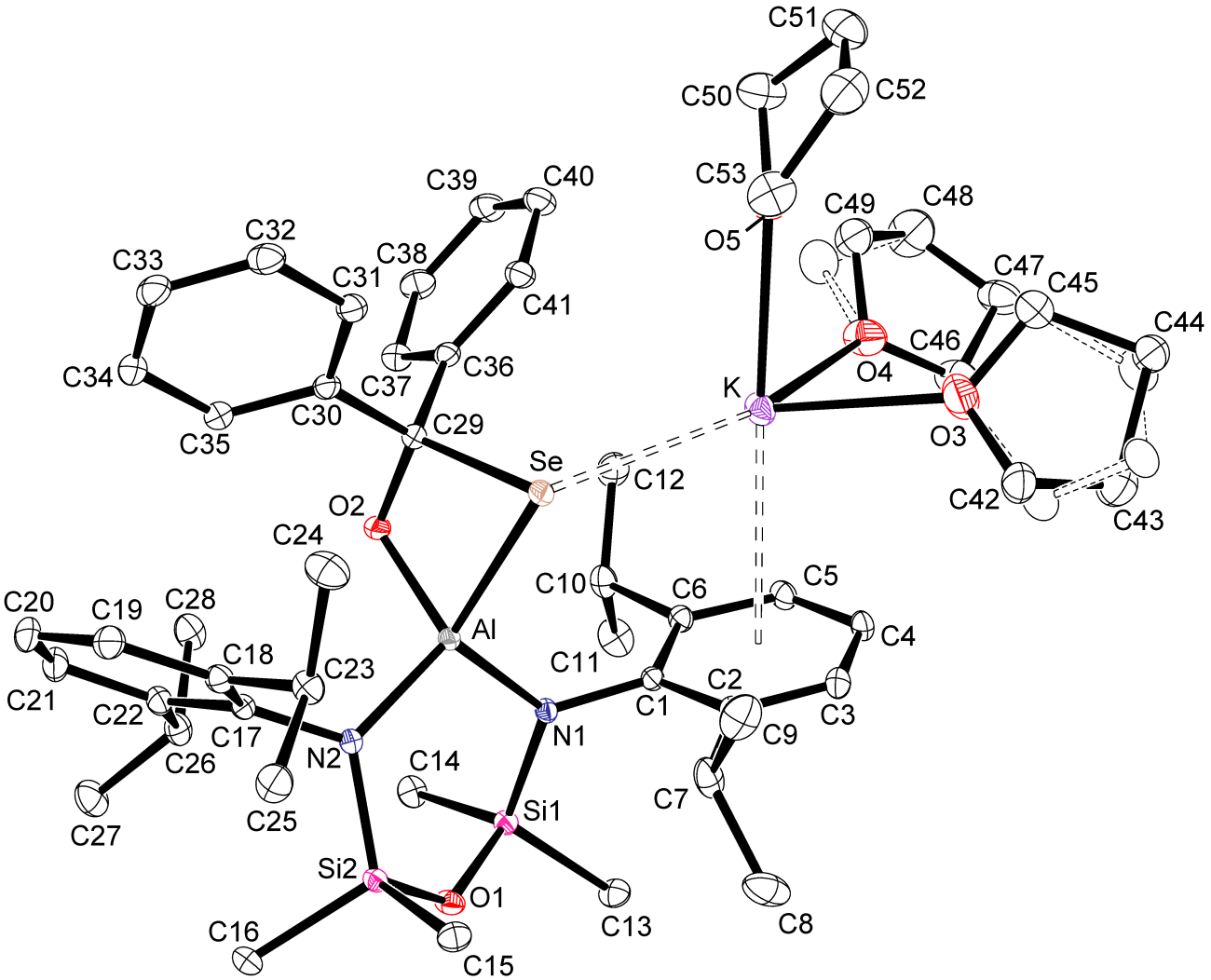


Figure S22 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of $[K(THF)_3][Al(NON^{Dipp})(SeC\{O\}Ph_2)]$ [**K(THF)**][**3-*Se***]



Synthesis of K[Al(NON^{Dipp})({OC(H)Ph}$_2$S)] ([K][4-*S*])

A solution of benzaldehyde (34 mg, 0.32 mmol) in C_6D_6 was added to K[Al(NON^{Dipp})(S)] (96 mg, 0.16 mmol) in an NMR tube fitted with a Teflon tap. The reaction was instantaneous, and the solvent was removed *in vacuo* and replaced with toluene. Slow evaporation at room temperature yielded colourless crystals. Yield 47 mg, 36 %.

^{1}H NMR (500 MHz, C_6D_6): δ 7.64 (d, *J* = 8.3, 4H, C_6H_5), 7.20 – 7.08 (m, 9H, C_6H_5, C_6H_3)*, 6.77 (d, *J* = 7.6, 2H, C_6H_3), 6.52 (t, *J* = 7.6, 1H, C_6H_3), 6.38 (s, 2H, PhC*H*O), 4.52 (sept, *J* = 6.8, 2H, C*H*Me$_2$), 4.31 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 1.36 – 1.31 (m, 18H, CHMe_2)‡, 1.29 (d, *J* = 6.8, 6H, CHMe_2), 0.63 (s, 6H, SiMe_2), 0.58 (s, 6H, SiMe_2). * overlapping with solvent peak; ‡ overlapping doublets from isopropyl substituents.

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 149.4, 149.3, 147.5, 146.0, 145.0, 127.4, 126.5, 123.8, 123.7, 123.0, 122.1 (C_6H$_5$, C_6H$_3$), 84.8 (Ph*C*HO), 27.9, 27.8 (*C*HMe$_2$), 27.2, 26.2, 25.6, 24.7 (CHMe_2), 3.6, 2.7 (SiMe_2). Despite repeated attempts we were unable to obtain accurate elemental analysis for **K**[**4-*S***].

Figure S23 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NON^{Dipp})({OC(H)Ph}$_2$S)] **K**[**4-*S***]

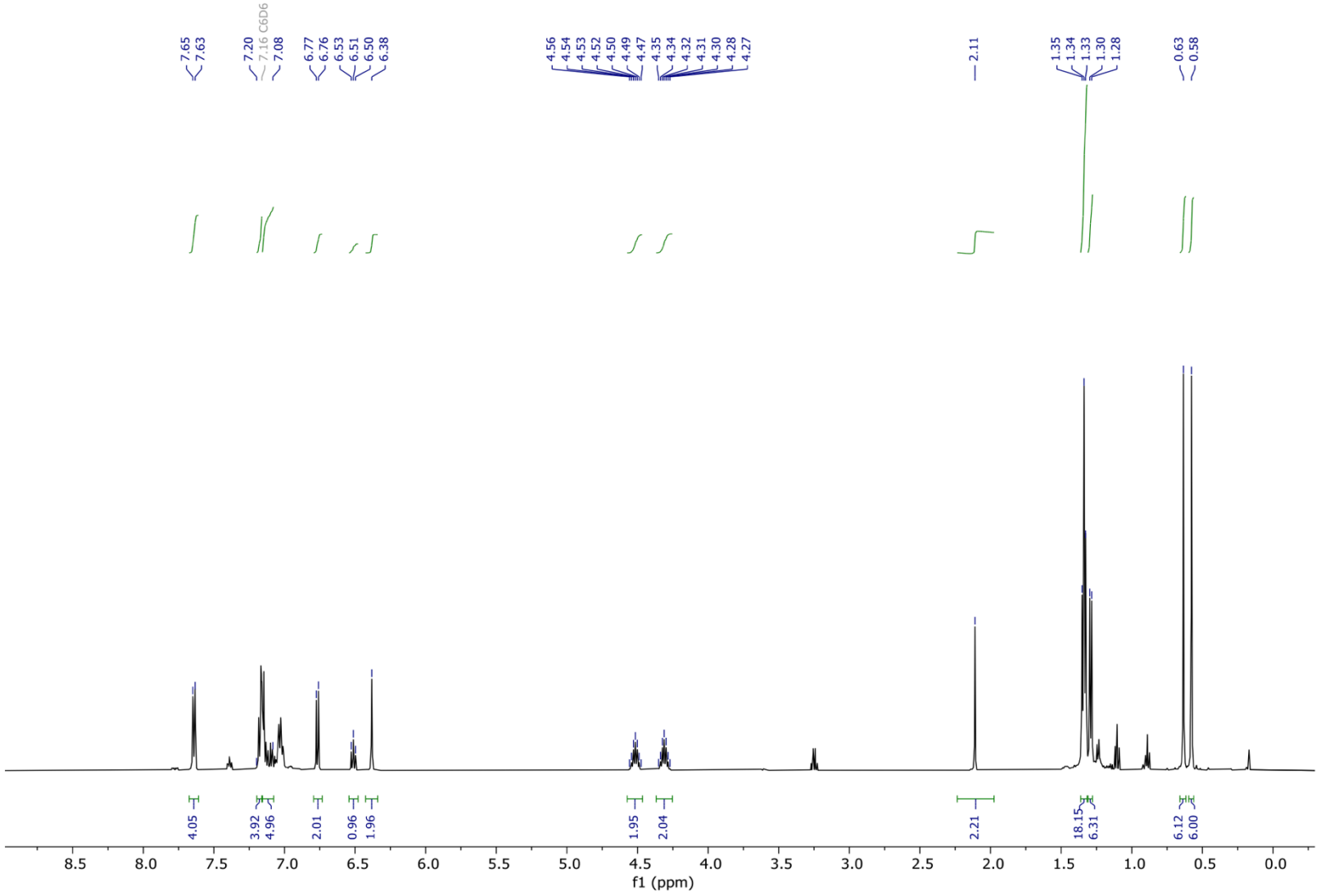


Figure S24 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6) of K[Al(NON^{Dipp})({OC(H)Ph}$_2$S)] **K**[**4-*S***]

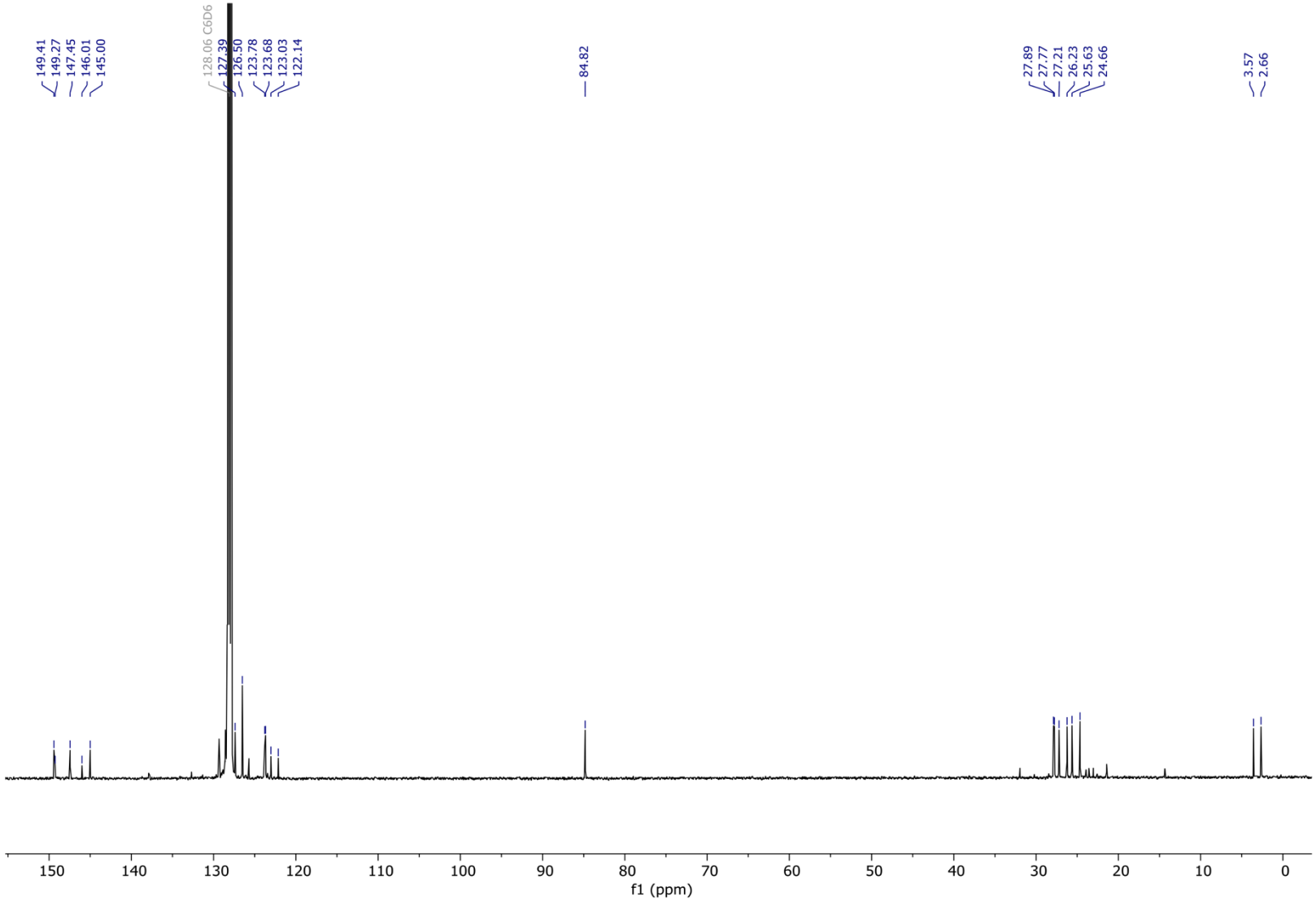
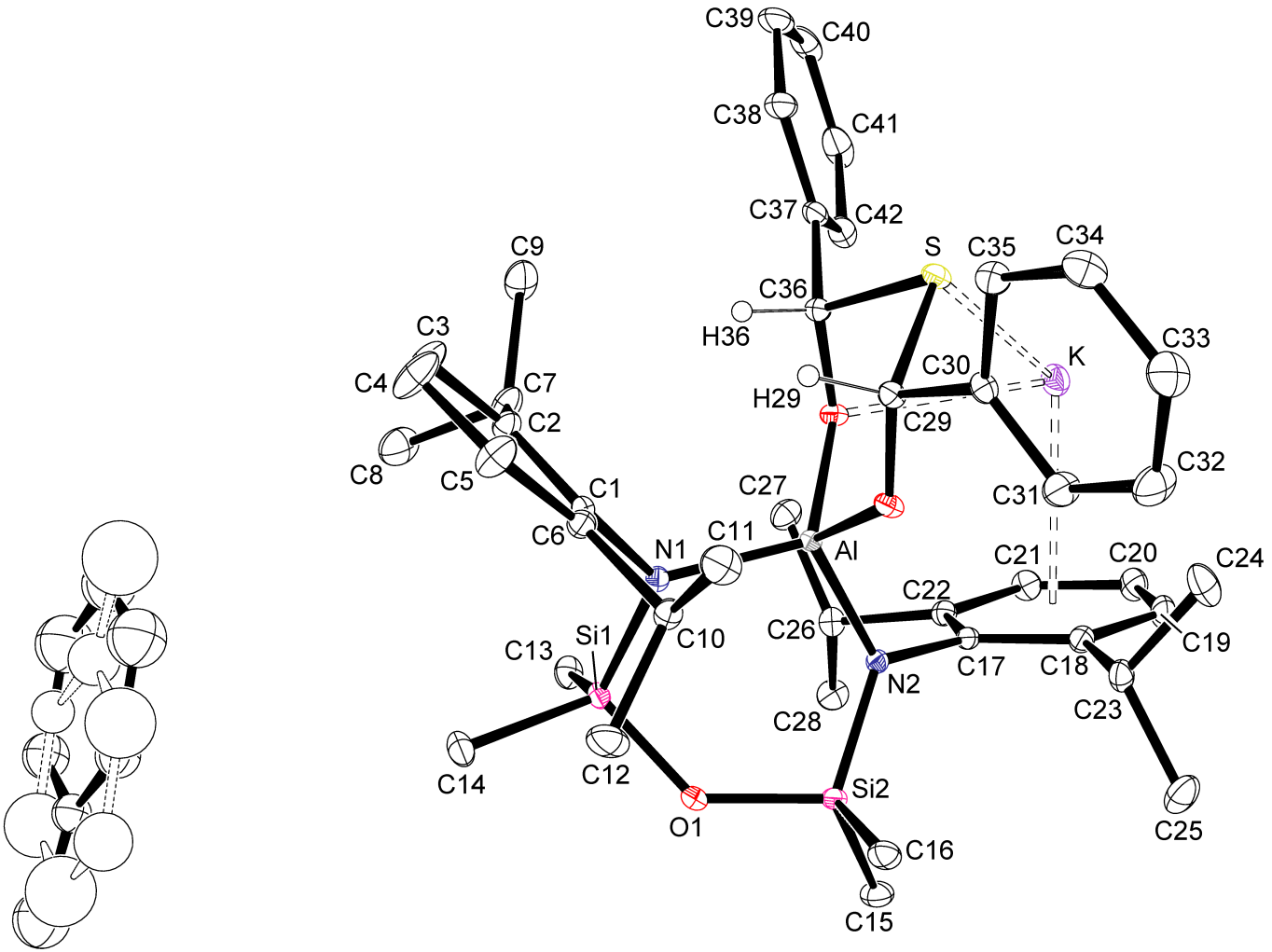


Figure S25 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of K[Al(NON^{Dipp})({OC(H)Ph}$_2$S)] **K**[**4-*S***]



Synthesis of K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] ([K][4-*Se*])

The reaction was performed as outlined for [**K**][**4-*S***], using 16 mg of benzaldehyde (0.15 mmol) and 47 mg of K[Al(NON^{Dipp})(Se)] (0.07 mmol). Slow evaporation from a toluene solution at room temperature yielded colourless crystals. Yield 35 mg, 56 %.

Anal. Calc'd for $C_{42}H_{58}AlKN_2O_3SeSi_2$ (*840.13*): C, 60.04; H, 6.96; N, 3.33 %. Found: C, 59.12; H, 6.79; N, 3.25 %.

^{1}H NMR (500 MHz, C_6D_6): δ 7.61 (d, *J* = 8.4, 2H, C_6H_5), 7.16 – 7.08 (m, 7H, C_6H_5, C_6H_3), 7.00 (t, *J* = 7.6, 2H, C_6H_5), 6.93 (s, 2H, PhC*H*O), 6.81 (d, *J* = 7.6, 2H, C_6H_3), 6.56 (t, *J* = 7.6, 1H, C_6H_3), 4.50 (sept, *J* = 7.2, 4H, C*H*Me$_2$), 4.24 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 1.38 (d, *J* = 6.8, 6H, CH*Me$_2$*), 1.35 (d, *J* = 6.8, 6H, CH*Me$_2$*), 1.30 (d, *J* = 6.8, 6H, CH*Me$_2$*), 1.25 (d, *J* = 6.8, 6H, CH*Me$_2$*), 0.61 (s, 6H, Si*Me$_2$*), 0.56 (s, 6H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 149.4, 149.1, 147.4, 146.3, 146.0, 144.6, 127.1, 126.0, 123.8, 123.7, 123.1, 122.3 (C_6H_5, C_6H_3), 83.2 (Ph*C*HO), 27.9, 27.8 (*C*HMe$_2$), 27.2, 26.2, 25.7, 24.7 (CH*Me$_2$*), 3.5, 2.7 (Si*Me$_2$*).

Figure S26 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] **K**[**4-*Se***]

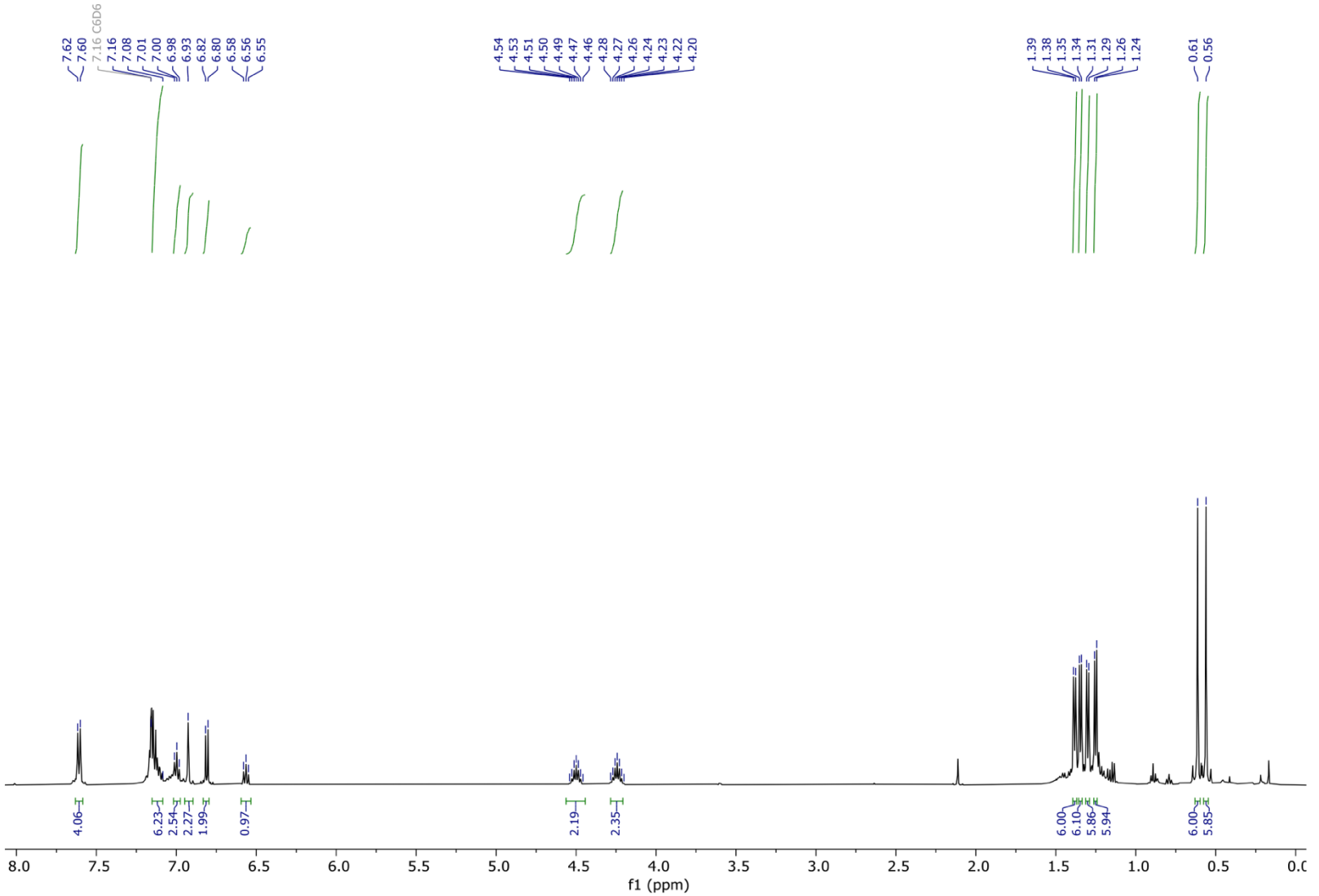


Figure S27 Expansion of ^{1}H OC(*H*)Ph resonance from K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] **K**[**4-*Se***] showing $^{2}J_{SeH}$ coupling

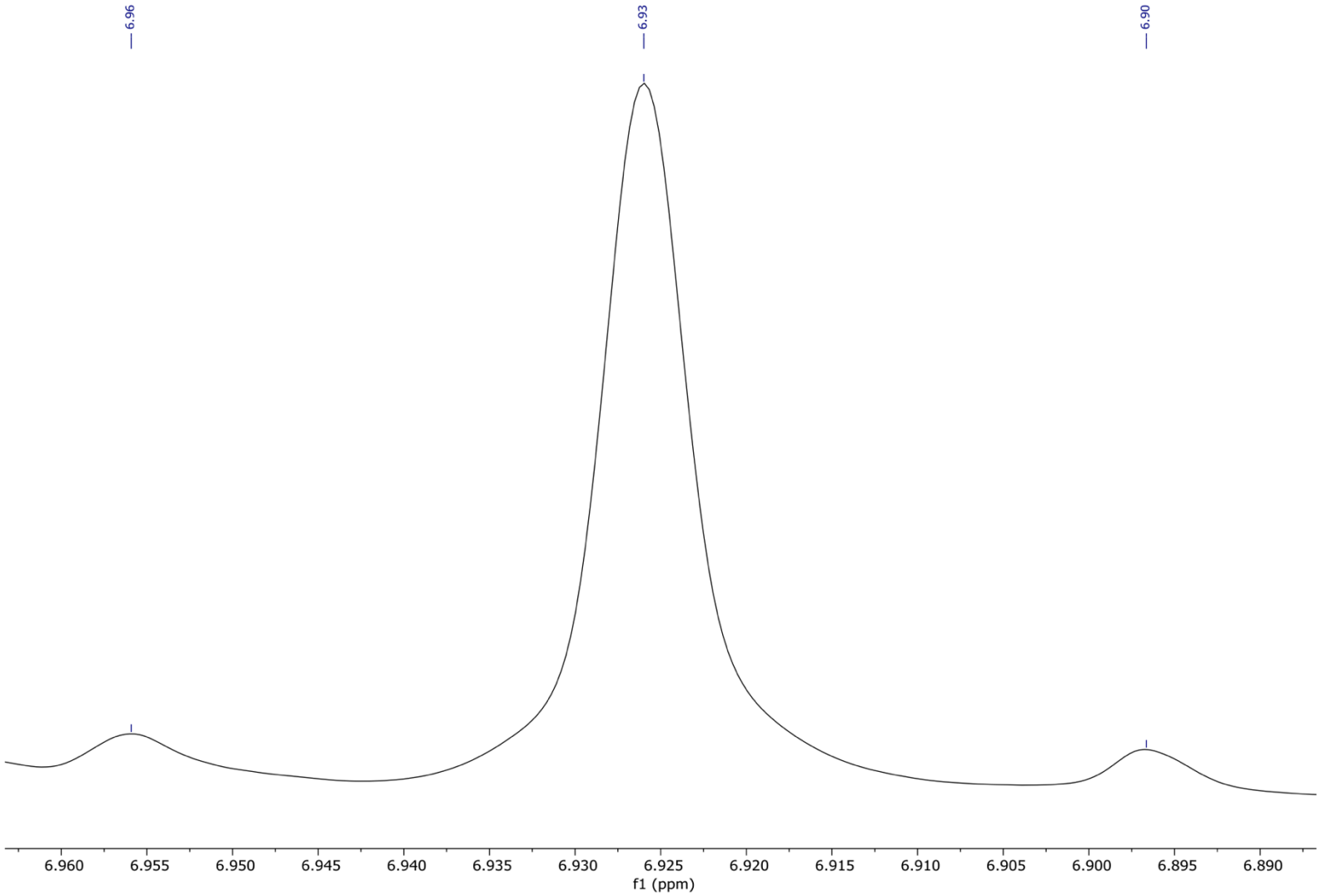


Figure S28 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6) of K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] **K**[**4-*Se***]

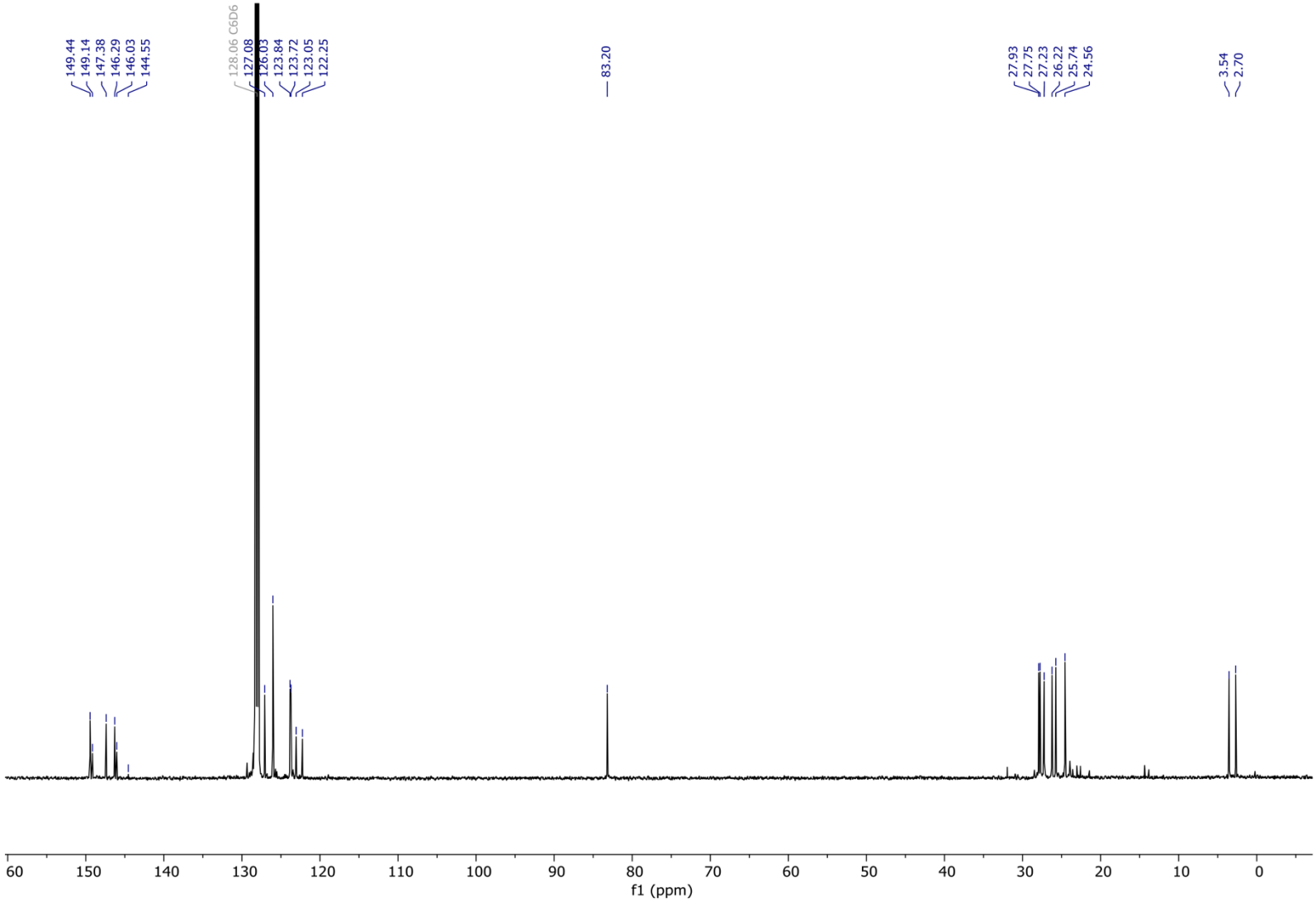


Figure S29 ^{77}Se NMR spectrum (95 MHz, C_6D_6) of K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] **K**[**4-*Se***]

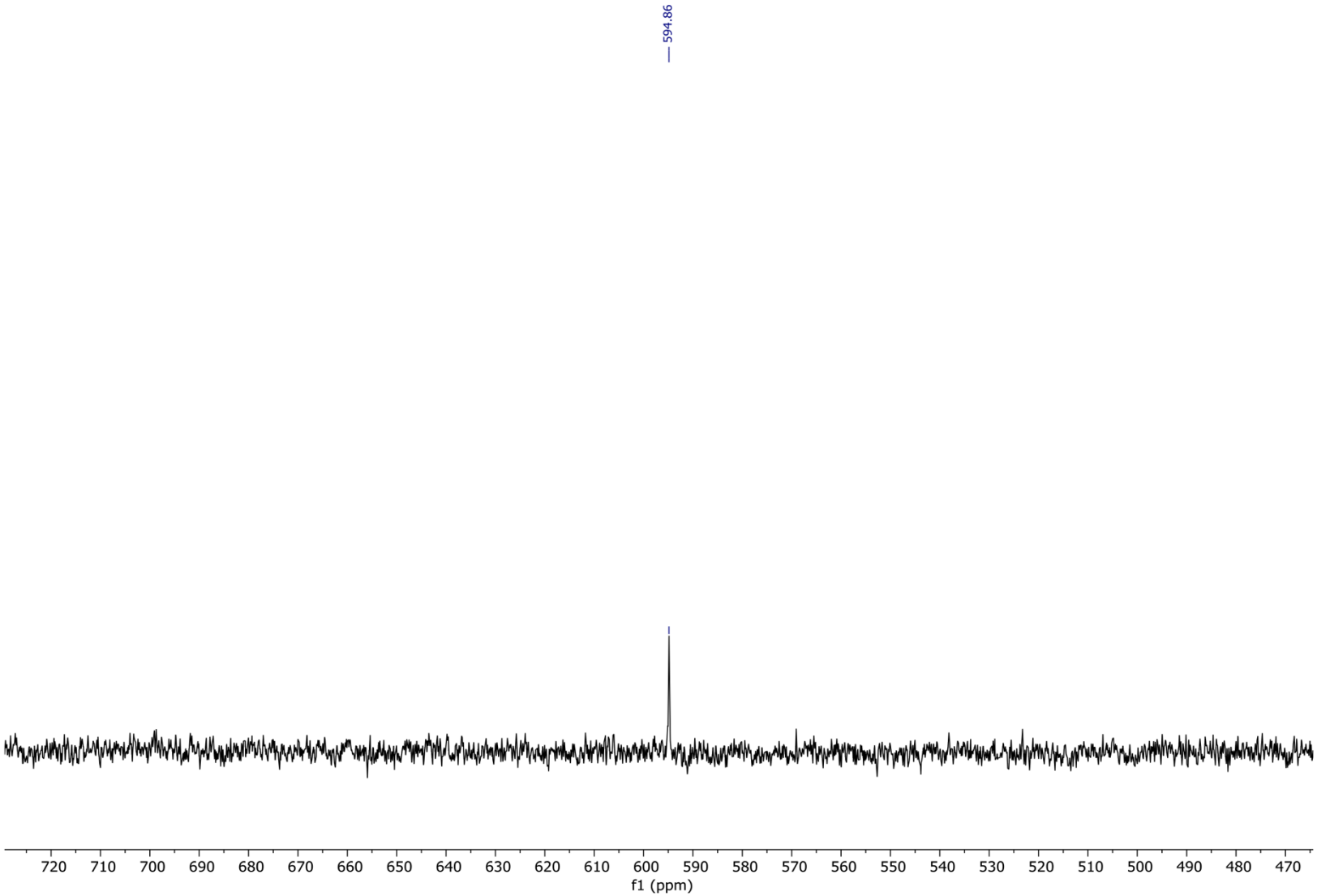


Figure S30 ORTEP (displacement ellipsoids 30 %) of the asymmetric unit of K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] **K**[**4-*Se***]

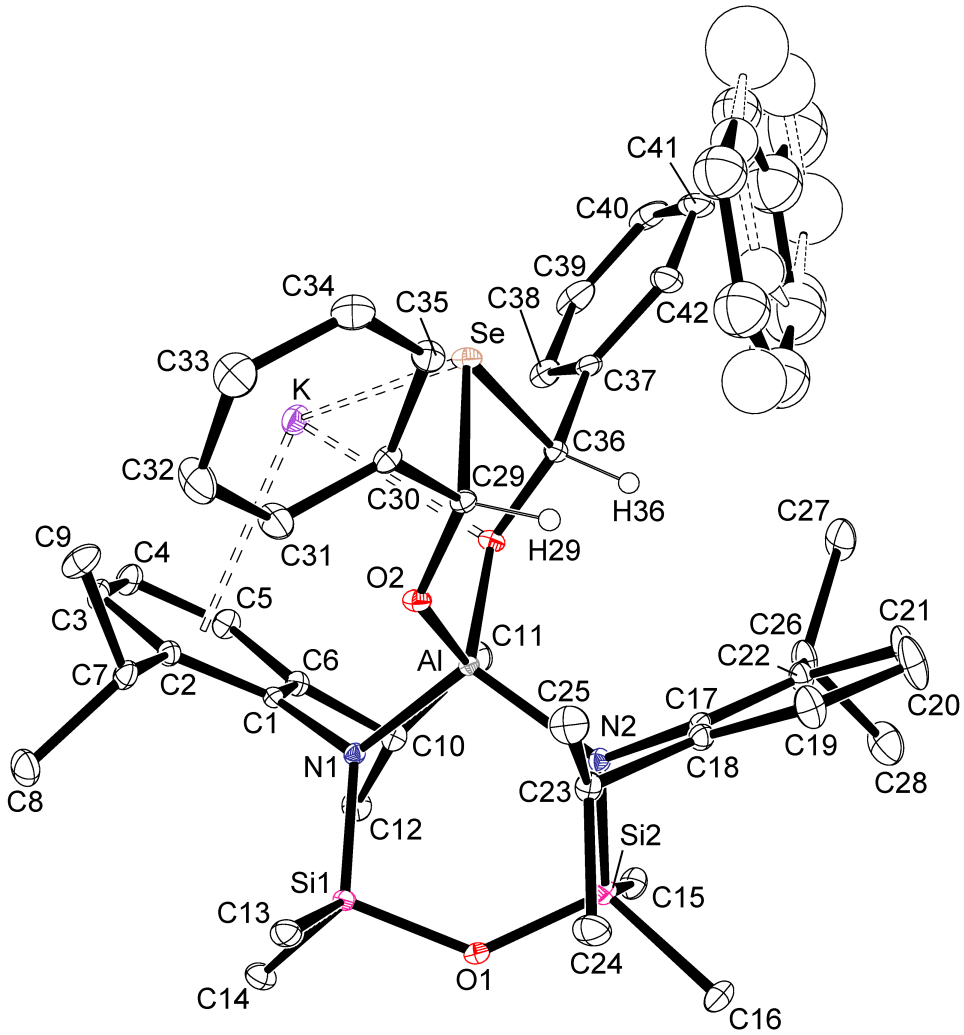
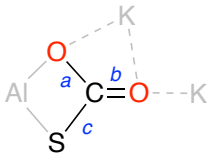


Figure S31 Comparison of bond lengths in thio- and selenocarbonate ligands from **[K(Et$_2$O)][2-*S*]** and **[K(THF)][2-*Se*]** with examples of $[SC\{O\}O]^{2-}$ and $[SeC\{O\}O]^{2-}$ ligands from uranium compounds, $[((^{Ad}ArO)_3N)U]_2(\mu-\eta^1:\kappa^2\text{-EC}\{O\}O)$ (where $[(^{Ad}ArO)_3N]^{3-}$ = the trianion of tris(2-hydroxy-3-adamantyl-5-methylbenzyl)amine).[S4]

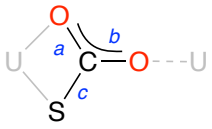
(a)

[K(Et$_2$O)][2-S]



	Al1	Al2
a	1.317(4) Å	1.290(4) Å
b	1.229(4) Å	1.236(4) Å
c	1.766(3) Å	1.783(3) Å

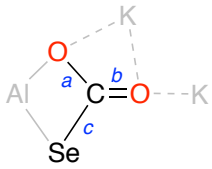
(b)



a = 1.283(5) Å
b = 1.262(5) Å
c = 1.742(5) Å

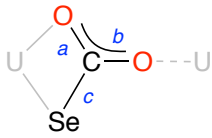
(c)

[K(THF)][2-Se]



a = 1.318(3) Å
b = 1.227(3) Å
c = 1.929(2) Å

(d)



a = 1.285(8) Å
b = 1.252(8) Å
c = 1.925(7) Å

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.[S5] Space groups were determined from systematic absences and checked for higher symmetry. All structures were solved using direct methods with SHELXS,[S6] refined on F^2 using all data by full matrix least-squares procedures with SHELXL-97,[S7] within the WinGX[S8] 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 $\Sigma w(F2o\text{-}F2c)$, with $w = [\sigma 2(F2o) + aP2 + bP]\text{-}1$, 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^{Dipp})(S)}]$_4$ ***{K[1-S]}$_4$***: Several poorly defined solvent molecules are present in the unit cell, with electron density patterns indicative of linear and cyclic arrangements of carbon atoms. From the experimental procedure, the crystals have been exposed to both hexane and toluene and the formula was therefore approximated as containing 3 x hexane and 3 x toluene. This solvents were treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON.

[K(2.2.2-crypt)][Al(NON^{Dipp})(S)] ***[K(2.2.2)crypt)][1-S]***: Data was collected at 150 K. The THF solvate is poorly defined. The oxygen atoms was modelled over two positions with each atom isotropic.

[K(Et$_2$O)$_2$][Al(NON^{Dipp})(SC{O}O)] ***[K(Et$_2$O)][2-S]***: Data was collected at 150 K. The ether molecules are highly disordered. A model was used that treated two separate molecules as disorder over two positions and a third ether molecule as disordered over three positions. Several SIMU and DELU restraints and EADP/EXYZ commands were used to obtain satisfactory models.

[K(THF)$_3$][Al(NON^{Dipp})(SeC{O}Ph$_2$)] ***[K(THF)][3-Se]***: Two of the coordinated THF molecules are disordered and were modelled with two positions for the affected methylene groups (three on one molecule and one on the second molecule).

K[Al(NON^{Dipp})({OC(H)Ph}$_2$S)] ***[K][4-S]*** and *K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)]* ***[K][4-Se]***: Each crystal structure contains a poorly resolved, rotationally disordered toluene solvate. They were modelled over 2 positions with fixed geometry for the aromatic ring (AFIX66) and all carbon atoms refined isotropically. The maximum residual electron density is located in this region and may correspond to a third (not modelled) orientation of the molecule.

Table S1 Crystal structure and refinement data for [K{Al(NON^{Dipp})(S)}]$_4$ {**K**[**1-*S***]}$_4$, [K(2.2.2-crypt)][Al(NON^{Dipp})(S)] [**K(2.2.2)crypt)**][**1-*S***], [K(Et$_2$O)$_2$][Al(NON^{Dipp})(SC{O}O)] [**K(Et$_2$O)**][**2-*S***] and [K(THF)$_3$][Al(NON^{Dipp})(SeC{O}O)] [**K(THF)**][**2-*Se***]

	{**K**[**1-*S***]}$_4$	[**K(2.2.2)crypt)**][**1-*S***]	[**K(Et$_2$O)**][**2-*S***]	[**K(THF)**][**2-*Se***]
Empirical formula	$C_{151}H_{250}Al_4K_4N_8O_4S_4Si_8$	$C_{50}H_{90}AlKN_4O_8SSi_2$	$C_{74}H_{132}Al_2K_2N_4O_{10}S_2Si_4$	$C_{82}H_{140}Al_2K_2N_4O_{12}Se_2Si_4$
CCDC Number	2038726	2038727	2038728	2038729
M_r	2858.85	1029.57	1546.48	1776.42
T [K]	120.0(1)	150.0(2)	150.0(1)	120.0(1)
Crystal size [mm]	0.28 × 0.21 × 0.12	0.15 × 0.12 × 0.11	0.34 × 0.25 × 0.17	0.22 × 0.09 × 0.07
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$ (No.14)	P-1 (No.2)	$P2_1$ (No.4)	$P2_1/n$ (alternative No.14)
a [Å]	25.01159(15)	10.0626(4)	12.27766(9)	15.4374(2)
b [Å]	19.41543(12)	17.1004(6)	24.87997(17)	13.47603(18)
c [Å]	33.7313(2)	17.2361(6)	14.90060(11)	22.5971(3)
α [°]	90	88.851(3)	90	90
β [°]	100.8841(6)	83.037(3)	94.3187(6)	93.2318(13)
γ [°]	90	84.293(3)	90	90
V [Å^3]	16085.64(18)	2929.34(17)	4538.73	4693.51(12)
Z	4	2	2	2
$D_{calc.}$ [mg m^{-3}]	1.181	1.167	1.132	1.257
Absorption coefficient [mm^{-1}]	2.647	2.062	2.447	2.894
θ range for data collection [°]	3.489 to 73.471	3.649 to 73.337	3.553 to 73.5958	3.8207 to 73.4183
Reflections collected	116133	40119	63075	36167
Independent reflections	32116 [R_{int} 0.031]	11663 [R_{int} 0.049]	17697 [R_{int} 0.049]	9384 [R_{int} 0.035]
Reflections with $I > 2\sigma(I)$	26321	8652	17308	8048
Data/restraints/parameters	32116 / 0 / 1345	11663 / 0 / 616	17697 / 19 / 944	9384 / 0 / 499
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.039, wR_2 = 0.112	R_1 = 0.061, wR_2 = 0.138	R_1 = 0.036, wR_2 = 0.096	R_1 = 0.035, wR_2 = 0.087
Final R indices (all data)	R_1 = 0.049, wR_2 = 0.106	R_1 = 0.088, wR_2 = 0.151	R_1 = 0.037, wR_2 = 0.097	R_1 = 0.044, wR_2 = 0.092
GOOF on F^2	1.024	1.083	1.022	1.006
Largest diff. peak/hole [e.Å^{-3}]	0.36 and –0.37	0.57 and –0.34	0.66 and –0.29	0.57 and –0.64

Table S2 Crystal structure and refinement data for K[Al(NON^{Dipp})(SC{O}Ph$_2$)] [**K**][**3-*S***], [K(THF)$_3$][Al(NON^{Dipp})(SeC{O}Ph$_2$)] [**K(THF)**][**3-*Se***], K[Al(NON^{Dipp})({OC(H)Ph}$_2$S)] [**K**][**4-*S***] and K[Al(NON^{Dipp})({OC(H)Ph}$_2$Se)] [**K**][**4-*Se***]

	[**K**][**3-*S***]	[**K(THF)**][**3-*Se***]	[**K**][**4-*S***]	[**K**][**4-*Se***]
Empirical formula	$C_{45}H_{66}AlKN_2O_3SSi_2$	$C_{53}H_{80}AlKN_2O_5SeSi_2$	$C_{49}H_{66}AlKN_2O_3SSi_2$	$C_{49}H_{66}AlKN_2O_3SeSi_2$
CCDC Number	2097188	2097189	2097190	2097191
M_r	837.31	1026.41	885.35	932.25
T [K]	122(2)	120.0(1)	120.0(1)	120.0(1)
Crystal size [mm]	0.18 × 0.13 × 0.05	0.14 × 0.08 × 0.06	0.34 × 0.25 × 0.17	0.45 × 0.31 × 0.11
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$ (No.14)	$P2_1/n$ (alternative No.14)	$P2_1/n$ (alternative No.14)	$P2_1/n$ (alternative No.14)
a [Å]	15.45971(16)	9.75833(9)	14.78551(10)	14.84213(8)
b [Å]	12.38750(13)	31.8983(3)	13.04163(7)	13.02613(7)
c [Å]	24.7548(3)	17.54162(15)	25.96015(16)	26.00620(15)
α [°]	90	90	90	90
β [°]	90.4615(10)	92.6949(8)	104.1317(6)	103.7250(5)
γ [°]	90	90	90	90
V [Å^3]	4740.57(9)	5454.21(8)	4854.33(5)	4884.35(4)
Z	4	4	4	4
$D_{calc.}$ [mg m^{-3}]	1.173	1.25	1.211	1.268
Absorption coefficient [mm^{-1}]	2.351	2.548	2.327	2.765
θ range for data collection [°]	3.568 to 73.5249	3.7476 to 73.5402	3.3889 to 73.4985	3.3929 to 73.5902
Reflections collected	36321	40652	66239	62964
Independent reflections	9498 [R_{int} 0.026]	10877 [R_{int} 0.027]	9751 [R_{int} 0.028]	9821 [R_{int} 0.030]
Reflections with $I > 2\sigma(I)$	8559	9743	8999	9387
Data/restraints/parameters	9498 / 0 / 510	10877 / 0 / 632	9751 / 0 / 514	9821 / 0 / 514
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.031, wR_2 = 0.078	R_1 = 0.031, wR_2 = 0.076	R_1 = 0.048, wR_2 = 0.131	R_1 = 0.044, wR_2 = 0.113
Final R indices (all data)	R_1 = 0.036, wR_2 = 0.081	R_1 = 0.036, wR_2 = 0.079	R_1 = 0.051, wR_2 = 0.134	R_1 = 0.045, wR_2 = 0.114
GOOF on F^2	1.027	1.023	1.057	1.025
Largest diff. peak/hole [e.Å^{-3}]	0.33 and –0.34	0.91 and –0.47	1.52 and –0.76	2.14 and –0.79

Computational Methods

DFT calculations were run with Gaussian 16 (A.03).[S9] The Al, Si, and S centres were described with the Stuttgart RECPs and associated basis sets,[S10] and 6-31G** basis sets were used for all other atoms (BS1).[S11] A polarization function was also added to Al (ζ_d = 0.190) and Si (ζ_d = 0.284) and S (ζ_d = 0.503). Initial BP86[S12] optimizations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as either minima (all positive eigenvalues). The Quantum Theory of Atoms in Molecules (QTAIM, AIMALL program[S13]) and Natural Bonding Orbital (NBO3[S14]) analyses were performed on the BP86-optmised geometries of the [Al(NON^{Dipp})(E)]$^-$ anions. All energies were recomputed with a larger basis set featuring 6-311++G** on all atoms. Corrections for the effect of toluene (ε = 2.2706) solvent were run using the polarizable continuum model and BS1.[S15] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[S16]

Figure S32 Frontier orbitals (LUMO, HOMO, HOMO–1) for the anions [Al(NON^{Dipp})(E)]$^{-}$ (E = O, S, Se, Te).

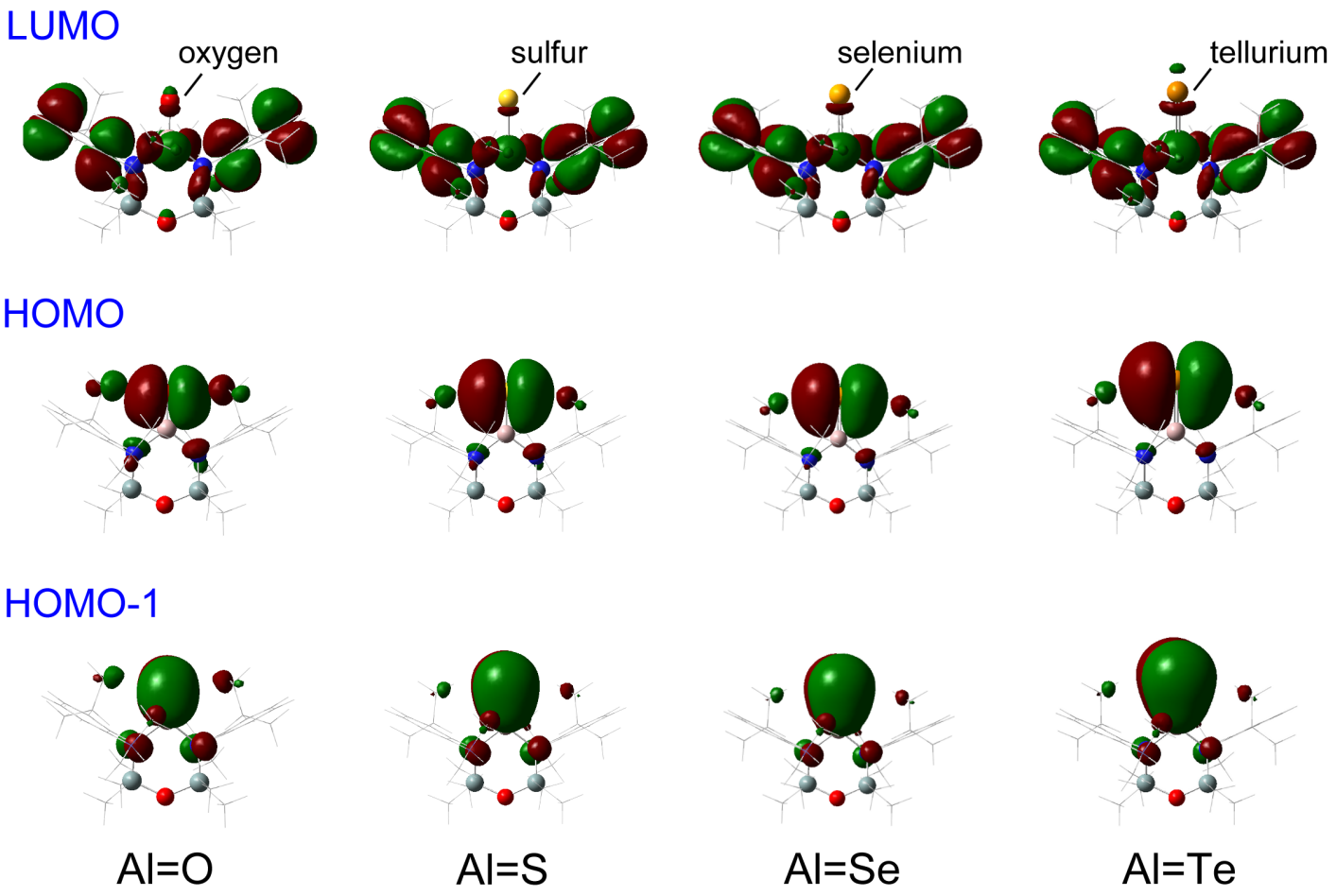


Table S3 Molecular Orbital Coefficients for HOMO / HOMO–1 of K[Al(NON^{Dipp})(**E**)] (**E** = O, S, Se, Te)

Complex	Atom	Atomic Orbital	HOMO-1	HOMO
K[Al(NON^{Dipp})(O)]	O	2p_x	**-0.32153**	**0.43893**
		2p_y	**0.35718**	**0.33719**
		2p_z	**-0.24282**	0.04177
		3p_x	**-0.23005**	**0.31385**
		3p_y	**0.26297**	**0.24063**
		3p_z	**-0.16609**	0.02241
	Al	4p_x	**-0.12337**	**0.10408**
		4p_y	0.00758	0.01487
		4p_z	**-0.09904**	0.03581
K[Al(NON^{Dipp})(S)]	S	3p_x	**0.48992**	**0.33318**
		3p_y	**-0.25812**	**0.48481**
		4p_x	**0.29209**	**0.20249**
		4p_y	**-0.15919**	**0.29243**
	Al	3p_y	0.06323	**-0.07262**
		4p_x	0.02145	0.00201
K[Al(NON^{Dipp})(Se)]	Se	3p_x	**0.46389**	**0.29125**
		3p_y	**-0.19724**	**0.42146**
		3p_z	**0.20287**	**-0.19510**
		4p_x	**-0.33246**	**-0.20979**
		4p_y	**-0.14881**	**-0.29935**
		4p_z	**-0.13505**	**0.14318**
	Al	3p_x	**0.07791**	0.02196
		3p_y	-0.06168	**0.07524**
		4p_z	**0.07005**	0.00638
K[Al(NON^{Dipp})(Te)]	Te	3p_x	-0.05363	**0.45839**
		3p_y	**0.43911**	0.05422
		4p_x	-0.05107	**0.45873**
		4p_y	**0.44517**	0.05602
		5p_x	-0.01903	**0.11185**
		5p_y	**0.10200**	0.00560
	Al	4p_x	0.02520	**-0.07428**
		4p_y	**-0.15097**	0.00216

NOTE: NBO Molecular Orbital Coefficients greater than ±0.07 are emphasised (in bold font).

Table S4 Wiberg Bond Indices (WBIs) of selected compounds and ions

Complex (Species)	Atom Pair	WBI[a]
K[Al(NON^{Dipp})(O)]	Al–O	**0.906** (1.112)
K[Al(NON^{Dipp})(S)] (I_K)	Al–S	**1.145** (1.297)
C (**K**[**3-*S***])	Al–S	**0.5350**
H$_{cis}$ (**K**[**4-*S***])	Al–S	**0.059**
K[Al(NON^{Dipp})(Se)]	Al–Se	**1.236** (1.377)
K[Al(NON^{Dipp})(Te)]	Al–Te	**1.441** (1.534)

a value in parentheses corresponds to the WBI for the anion calculated without the potassium counter-ion.

Table S5 Relative energies (kcal mol^{-1}) for computed structures. Data in **bold** are those used in the manuscript. Values are quoted relative to **A** (**K**[**1**-***S***]).

Ph_2CO	ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/Et_2O}$	$\Delta G_{BSI/Et_2O+D3BJ}$	$\Delta E_{6-311++G**}$	ΔG_{Et_2O}
A	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
TS(A-B)	5.5	5.9	21.1	27.6	4.6	9.5	**8.6**
B	4.9	5.8	20.9	26.7	1.1	9.0	**5.3**
TS(B-C)	6.0	6.4	23.2	29.0	2.3	10.6	**6.9**
C	-13.9	-13.2	4.1	11.3	-15.7	-10.0	**-11.9**
TS(C-D)	17.9	18.9	52.4	61.4	1.0	25.4	**8.5**
D	-3.1	-1.5	32.9	43.4	-17.9	3.7	**-11.1**
PhHCO	ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/C_6H_6}$	$\Delta G_{BSI/C_6H_6+D3BJ}$	$\Delta E_{6-311++G**}$	$\Delta G_{C_6H_6}$
A	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
TS(A-E)	-0.5	0.1	13.9	18.5	4.9	2.9	**8.3**
E	-23.6	-22.2	-7.5	-2.5	-18.5	-19.4	**-14.2**
TS(E-F)	-21.4	-19.2	10.4	17.1	-13.1	-13.9	**-5.6**
F	-21.8	-19.1	10.2	17.0	-15.3	-13.5	**-7.0**
TS(F-H)$_{cis}$	-17.9	-15.7	15.2	21.4	-10.4	-10.1	**-2.6**
INT(F-H)$_{cis}$	-39.5	-36.4	-6.7	0.1	-31.6	-32.3	**-24.4**
H$_{cis}$	-41.9	-38.8	-8.5	-1.9	-34.3	-34.9	**-27.3**
TS(H)$_{cis\text{-}trans}$	-19.0	-16.8	12.9	18.4	-10.8	-12.2	**-3.9**
H$_{trans}$	-32.9	-29.7	0.0	5.9	-28.1	-26.1	**-21.3**

References

S1. R. J. Schwamm, M. D. Anker, M. Lein and M. P. Coles, *Angew. Chem. Int. Ed.*, 2019, **58**, 1489-1493.

S2. M. D. Anker, C. L. McMullin, N. A. Rajabi and M. P. Coles, *Angew. Chem. Int. Ed.*, 2020, **59**, 12806-12810.

S3. M. D. Anker and M. P. Coles, *Angew. Chem. Int. Ed.*, 2019, **58**, 13452-13455.

S4. O. P. Lam, S. M. Franke, F. W. Heinemann and K. Meyer, *J. Am. Chem. Soc.*, 2012, **134**, 16877-16881.

S5. R. Blessing, *Acta Cryst.*, 1995, **A51**, 33-38.

S6. G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112-122.

S7. SHELXL-97, G. M. Sheldrick, University of Gottingen, Germany (1997).

S8. L. J. Farrugia, *J. Appl. Cryst.*, 1999, **32**, 837-838.

S9. Gaussian 16 Rev. C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Wallingford, CT (2016).

S10. D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor. Chim. Acta*, 1990, **77**, 123-141.

S11. (a) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213-222; (b) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.

S12. (a) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100; (b) J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822-8824.

S13. AIMAll (Version 19.10.12), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2019 (aim.tkgristmill.com).

S14. E. D. Glendening, A. E. Reed, J. E. Carpenter and F. Weinhold, "The NBO3.0 Program," University of Wisconsin, Copyright 1996-2001.

S15. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999-3094.

S16. S. Grimmer, S. Ehrlich and L. Goerigk, *J. Comp. Chem.* 2011, **32**, 1456-1465.

Cartesian Coordinates and Computed Energies (in Hartrees)

[1-*S*]$^-$

SCF (BP86) Energy = -1299.85282777
Enthalpy 0K = -1299.185961
Enthalpy 298K = -1299.140204
Free Energy 298K = -1299.263213
Lowest Frequency = 14.5811 cm^{-1}
Second Frequency = 24.2796 cm^{-1}

S	0.00003	0.00005	-2.94856
Si	-1.40323	-0.65265	1.97693
Si	1.40332	0.65241	1.97713
Al	0.00000	0.00007	-0.84141
O	-0.00012	0.00012	2.68067
N	-1.50819	-0.12728	0.29097
N	1.50816	0.12733	0.29105
C	-2.81119	0.15250	-0.25548
C	-3.31997	1.49109	-0.23352
C	-4.59928	1.75700	-0.75542
H	-4.97858	2.78574	-0.73999
C	-5.39234	0.73991	-1.29981
H	-6.38745	0.96498	-1.70104
C	-4.88892	-0.56407	-1.33879
H	-5.49381	-1.36237	-1.78631
C	-3.61276	-0.88086	-0.83235
C	-2.46981	2.65003	0.28528
H	-1.66125	2.20194	0.88879
C	-3.24533	3.62950	1.19063
H	-3.74261	3.10628	2.02589
H	-2.55804	4.38179	1.61782
H	-4.02314	4.18165	0.63210
C	-1.81058	3.40088	-0.89664
H	-2.58140	3.87440	-1.53225
H	-1.13313	4.19580	-0.53265
H	-1.23282	2.71215	-1.53950
C	-3.11421	-2.31964	-0.96436
H	-2.13967	-2.37037	-0.45059
C	-4.06577	-3.33225	-0.28870
H	-5.04998	-3.36173	-0.79136
H	-3.64332	-4.35255	-0.33475
H	-4.24608	-3.08267	0.77200
C	-2.87385	-2.68889	-2.44622
H	-2.14113	-1.99754	-2.89835
H	-2.48341	-3.72034	-2.52894
H	-3.81446	-2.63670	-3.02576
C	-2.88980	-0.04093	2.98622
H	-2.93796	1.06002	2.99138
H	-3.83772	-0.42153	2.57115
H	-2.80255	-0.38787	4.03045
C	-1.25267	-2.53594	2.21004
H	-1.03238	-2.76638	3.26732
H	-2.18203	-3.05944	1.93003
H	-0.43379	-2.94610	1.59541
C	1.25340	2.53569	2.21076
H	1.03316	2.76587	3.26811
H	2.18291	3.05901	1.93092
H	0.43463	2.94626	1.59625
C	2.88961	0.03991	2.98635
H	2.93728	-1.06106	2.99138
H	3.83770	0.42013	2.57130
H	2.80254	0.38677	4.03062
C	2.81119	-0.15234	-0.25546
C	3.61270	0.88102	-0.83241
C	4.88881	0.56424	-1.33899
H	5.49362	1.36252	-1.78663
C	5.39223	-0.73974	-1.30009
H	6.38729	-0.96481	-1.70147
C	4.59921	-1.75685	-0.75567
H	4.97850	-2.78560	-0.74033
C	3.31996	-1.49094	-0.23363
C	3.11408	2.31976	-0.96465
H	2.13943	2.37047	-0.45110
C	2.87404	2.68886	-2.44660
H	2.14158	1.99733	-2.89890
H	2.48345	3.72024	-2.52951
H	3.81483	2.63677	-3.02587
C	4.06542	3.33252	-0.28890
H	5.04967	3.36215	-0.79145
H	3.64281	4.35275	-0.33501
H	4.24566	3.08299	0.77183
C	2.46985	-2.64992	0.28513
H	1.66146	-2.20188	0.88892
C	1.81027	-3.40048	-0.89679
H	2.58091	-3.87385	-1.53272
H	1.13291	-4.19547	-0.53279
H	1.23234	-2.71157	-1.53928
C	3.24552	-3.62963	1.19008
H	3.74299	-3.10663	2.02536
H	2.55831	-4.38201	1.61723
H	4.02320	-4.18165	0.63124

HPhCO

SCF (BP86) Energy = -345.568700604
Enthalpy 0K = -345.455589
Enthalpy 298K = -345.454644
Free Energy 298K = -345.492725
Lowest Frequency = 122.5891 cm^{-1}
Second Frequency = 208.5129 cm^{-1}
SCF (BP86-D3BJ) Energy = -345.590746037
SCF (C6H6) Energy = -345.571192783
SCF (Et2O) Energy = -345.572491016
SCF (BS2) Energy = -345.662106507

O	-2.86337	-0.39887	-0.00011
C	-1.99941	0.47368	0.00006
H	-2.27637	1.56455	0.00011
C	-0.53708	0.21716	0.00006
C	-0.04798	-1.10752	0.00006
C	0.36461	1.30093	0.00002
C	1.33077	-1.34072	0.00001
C	1.74661	1.06581	-0.00004
C	2.22796	-0.25467	-0.00004
H	-0.77386	-1.92703	0.00010
H	-0.02654	2.32586	0.00003
H	1.71498	-2.36606	0.00000
H	2.44861	1.90589	-0.00009
H	3.30734	-0.44032	-0.00008

Ph_2CO

SCF (BP86) Energy = -576.623309768
Enthalpy 0K = -576.426282
Enthalpy 298K = -576.425337
Free Energy 298K = -576.475233
Lowest Frequency = 42.1740 cm^{-1}
Second Frequency = 64.3121 cm^{-1}
SCF (BP86-D3BJ) Energy = -576.670272545
SCF (C6H6) Energy = -576.626243352
SCF (Et2O) Energy = -576.627839186
SCF (BS2) Energy = -576.769376491

O	-0.00002	2.32329	-0.00021
C	-0.00001	1.08396	-0.00010
C	-1.30632	0.33683	0.02138
C	-2.44568	0.99590	-0.49235
C	-1.45637	-0.94032	0.60606
C	-3.70002	0.37721	-0.45752
C	-2.71925	-1.55027	0.65909
C	-3.83943	-0.89884	0.11856
H	-2.31543	1.99818	-0.91169
H	-0.58963	-1.44233	1.04659
H	-4.57428	0.88953	-0.87267
H	-2.82900	-2.53407	1.12728
H	-4.82243	-1.38050	0.15271
C	1.30630	0.33685	-0.02143
C	1.45650	-0.94020	-0.60635
C	2.44554	0.99584	0.49259
C	2.71937	-1.55011	-0.65925
C	3.69992	0.37717	0.45789
C	3.83945	-0.89875	-0.11836
H	0.58983	-1.44209	-1.04718
H	2.31525	1.99806	0.91208
H	2.82927	-2.53381	-1.12760
H	4.57408	0.88947	0.87330
H	4.82246	-1.38041	-0.15243

A

SCF (BP86) Energy = -1328.17907414
Enthalpy 0K = -1327.463513
Enthalpy 298K = -1327.462569
Free Energy 298K = -1327.590388
Lowest Frequency = 16.2957 cm^{-1}
Second Frequency = 21.6532 cm^{-1}
SCF (BP86-D3BJ) Energy = -1328.40143163
SCF (C6H6) Energy = -1328.19491236
SCF (Et2O) Energy = -1328.20375439
SCF (BS2) Energy = -3099.85174299

S	0.12354	-0.69429	-2.60164
Si	-1.83178	-0.16746	2.14327
Si	0.98462	1.19312	2.12569
Al	-0.13456	-0.13241	-0.55961
O	-0.43554	0.56546	2.78778
N	-1.73670	-0.05934	0.37026
N	1.28848	0.34335	0.57946
C	-2.96827	0.04519	-0.38675
C	-3.46699	1.33831	-0.74137
C	-4.65996	1.43776	-1.48074
H	-5.03721	2.42877	-1.75640
C	-5.37166	0.29831	-1.87375
H	-6.29984	0.39491	-2.44748
C	-4.87849	-0.96397	-1.53138
H	-5.42490	-1.85961	-1.84923
C	-3.68648	-1.11864	-0.79533
C	-2.69855	2.61151	-0.38736
H	-2.00428	2.34782	0.42973
C	-3.59844	3.75917	0.11558
H	-4.23836	3.43612	0.95422
H	-2.98035	4.60635	0.46178
H	-4.25977	4.14616	-0.67980
C	-1.84591	3.07641	-1.59248
H	-2.49512	3.35627	-2.44136
H	-1.23140	3.95698	-1.32906
H	-1.17588	2.27427	-1.95291
C	-3.19614	-2.53591	-0.49881
H	-2.29135	-2.44353	0.12551
C	-4.24045	-3.35808	0.28980
H	-5.15211	-3.53277	-0.30899
H	-3.83179	-4.34765	0.56204
H	-4.55167	-2.84723	1.21755
C	-2.79107	-3.26986	-1.79833
H	-2.01145	-2.70503	-2.33696
H	-2.40267	-4.27893	-1.56702
H	-3.65867	-3.39254	-2.47159
C	-3.35548	0.73277	2.80796
H	-3.32565	1.80615	2.56167
H	-4.28213	0.31060	2.38556
H	-3.39865	0.63140	3.90571
C	-1.79066	-1.93877	2.82348
H	-1.69004	-1.90961	3.92233
H	-2.70737	-2.49907	2.57816
H	-0.93078	-2.49973	2.41940
C	0.73061	3.06304	1.92751
H	0.36593	3.48341	2.88068
H	1.66725	3.58288	1.66522
H	-0.01774	3.29054	1.15017
C	2.39678	0.88157	3.34650
H	2.47095	-0.18514	3.61190
H	3.36836	1.20490	2.93673
H	2.21217	1.44997	4.27384
C	2.62296	0.02187	0.19414
C	3.43582	0.95932	-0.53029
C	4.74454	0.59412	-0.91638
H	5.36161	1.32432	-1.45390
C	5.27827	-0.66811	-0.61254
H	6.30661	-0.92125	-0.89499
C	4.48585	-1.58737	0.09499
H	4.90283	-2.56747	0.35472
C	3.17572	-1.26833	0.51120
C	2.91748	2.34361	-0.92078
H	1.91797	2.44608	-0.46834
C	2.74172	2.47296	-2.45214
H	2.01041	1.73376	-2.82737
H	2.36461	3.47677	-2.71422
H	3.70512	2.33737	-2.98063
C	3.81646	3.47308	-0.37058
H	4.82153	3.45747	-0.82938
H	3.37086	4.45868	-0.59017
H	3.94999	3.39259	0.72160
C	2.36062	-2.31874	1.26723
H	1.49004	-1.79203	1.69432
C	1.81965	-3.40104	0.30157
H	2.65250	-3.95927	-0.16851
H	1.19826	-4.13504	0.84364
H	1.19662	-2.96042	-0.49922
C	3.14343	-2.97021	2.42709
H	3.56335	-2.21347	3.11043
H	2.47664	-3.62703	3.01150
H	3.97915	-3.59591	2.06509
K	3.03016	-1.33487	-2.75782

TS(A-B)

SCF (BP86) Energy = -1904.79360898
Enthalpy 0K = -1903.879397
Enthalpy 298K = -1903.878452
Free Energy 298K = -1904.031997
Lowest Frequency = -56.8502 cm^{-1}
Second Frequency = 6.3777 cm^{-1}
SCF (BP86-D3BJ) Energy = -1905.09957584
SCF (C6H6) Energy = -1904.80538885
SCF (Et2O) Energy = -1904.81240690
SCF (BS2) Energy = -3676.60601997

S	-0.41863	0.75892	-2.25236
Si	-1.72444	-2.58508	1.43179

Si	0.56224	-3.47490	-0.42100
Al	-0.20414	-0.47521	-0.49738
O	-0.73742	-3.71986	0.65331
O	0.74299	1.45649	0.68139
N	-1.76107	-1.08268	0.45167
N	1.11881	-1.79150	-0.21793
C	-3.01481	-0.41692	0.26666
C	-3.52415	0.47907	1.27331
C	-4.70269	1.21944	1.03349
H	-5.07644	1.89182	1.81538
C	-5.42196	1.08733	-0.16352
H	-6.34284	1.65837	-0.32907
C	-4.97466	0.15863	-1.11527
H	-5.56266	0.00089	-2.02717
C	-3.80805	-0.61343	-0.92252
C	-2.85938	0.61395	2.64414
H	-1.92782	0.02742	2.60529
C	-2.47381	2.06577	2.98827
H	-1.78423	2.47452	2.23374
H	-1.96531	2.10871	3.96750
H	-3.35760	2.72738	3.04654
C	-3.76662	0.02983	3.75252
H	-4.70230	0.60984	3.84780
H	-3.25370	0.05972	4.73008
H	-4.04613	-1.01590	3.54412
C	-3.49851	-1.69436	-1.96043
H	-2.55368	-2.17136	-1.65176
C	-3.31284	-1.14154	-3.39077
H	-4.23384	-0.64757	-3.75483
H	-3.09442	-1.96989	-4.08778
H	-2.47134	-0.42857	-3.42729
C	-4.61025	-2.77319	-1.96227
H	-4.80138	-3.17707	-0.95572
H	-4.32439	-3.61072	-2.62209
H	-5.56282	-2.36176	-2.34271
C	-1.05420	-2.36828	3.19947
H	-0.67411	-3.34125	3.55589
H	-1.85037	-2.04609	3.89119
H	-0.23301	-1.63793	3.25809
C	-3.44332	-3.37673	1.56343
H	-3.67551	-3.94455	0.64911
H	-4.24510	-2.63854	1.72880
H	-3.45083	-4.08542	2.40942
C	1.90958	-4.73187	0.00315
H	2.19094	-4.68128	1.06630
H	2.81716	-4.57399	-0.60200
H	1.52934	-5.74716	-0.20294
C	-0.10617	-3.83614	-2.16127
H	-0.73068	-3.00806	-2.53626
H	-0.71524	-4.75639	-2.15362
H	0.71931	-3.97576	-2.87885
C	2.54624	-1.58997	-0.18602
C	3.24538	-1.66083	1.06693
C	4.64504	-1.50281	1.09557
H	5.16680	-1.56462	2.05748
C	5.38126	-1.28191	-0.07457
H	6.47163	-1.17727	-0.03615
C	4.70339	-1.21704	-1.29575
H	5.27306	-1.05614	-2.21840
C	3.30450	-1.37387	-1.38315
C	2.51202	-1.89185	2.38783
H	1.50672	-2.25862	2.12629
C	2.34034	-0.56665	3.16676
H	3.32430	-0.13391	3.42395
H	1.79269	-0.73386	4.11246
H	1.78790	0.17880	2.57108
C	3.18714	-2.94918	3.28789
H	3.37896	-3.89013	2.74545
H	2.54107	-3.17855	4.15349
H	4.15329	-2.59489	3.69015
C	2.67449	-1.35914	-2.77688
H	1.58077	-1.42813	-2.65405
C	2.95681	-0.04389	-3.53458
H	2.54735	0.81612	-2.98171
H	2.46435	-0.06475	-4.52254
H	4.03879	0.11279	-3.69897
C	3.15611	-2.57043	-3.61063
H	4.24119	-2.51318	-3.81285
H	2.63633	-2.60138	-4.58474
H	2.97067	-3.52719	-3.09273
C	1.19534	2.60264	0.45091
C	2.63141	2.94239	0.54753
C	3.04953	4.29838	0.56320
H	2.30484	5.09659	0.49163
C	4.40591	4.61824	0.68493
H	4.71962	5.66689	0.70518
C	5.36239	3.59152	0.77752
H	6.42509	3.84192	0.86515
C	4.95751	2.24515	0.75235
H	5.69488	1.43932	0.80754
C	3.60214	1.91667	0.64382
H	3.28697	0.87055	0.61475
C	0.25760	3.69978	-0.01252
C	0.22384	4.01178	-1.39164
H	0.86648	3.46104	-2.08391
C	-0.65509	5.00258	-1.86468
H	-0.66777	5.24608	-2.93252
C	-1.50363	5.68664	-0.97281
H	-2.17229	6.47170	-1.34271
C	-1.46348	5.38510	0.40056
H	-2.09626	5.93532	1.10486
C	-0.58242	4.39547	0.87870
H	-0.52859	4.18528	1.95106
K	-2.68881	2.43262	-1.16293

B

SCF (BP86) Energy = -1904.79464076
Enthalpy 0K = -1903.879574
Enthalpy 298K = -1903.878630
Free Energy 298K = -1904.032337
Lowest Frequency = 13.4380 cm^{-1}
Second Frequency = 20.1737 cm^{-1}
SCF (BP86-D3BJ) Energy = -1905.10476092
SCF (C6H6) Energy = -1904.80716641
SCF (Et2O) Energy = -1904.81459614
SCF (BS2) Energy = -3676.60673232

S	-0.48891	0.69946	-2.29863
Si	-1.55807	-2.43037	1.58676
Si	0.71078	-3.36959	-0.26544
Al	-0.13375	-0.35054	-0.42649
O	-0.59442	-3.58861	0.80831
O	0.83135	1.27789	0.53600
N	-1.69143	-0.97804	0.54622
N	1.21453	-1.66409	-0.14980
C	-2.99816	-0.47745	0.24945
C	-3.66664	0.42571	1.15529
C	-4.91638	0.98494	0.80649
H	-5.41075	1.66327	1.51161
C	-5.55599	0.66461	-0.39983
H	-6.53346	1.09515	-0.64626
C	-4.94907	-0.26983	-1.25151
H	-5.46800	-0.57685	-2.16720
C	-3.70279	-0.86196	-0.95146
C	-3.10223	0.74534	2.54129

H	-2.03634	0.45772	2.52631
C	-3.20939	2.23635	2.92695
H	-2.82717	2.89585	2.13252
H	-2.63328	2.43595	3.84755
H	-4.25376	2.53245	3.13364
C	-3.82608	-0.09160	3.62527
H	-4.89623	0.18080	3.66813
H	-3.38902	0.09933	4.62166
H	-3.76860	-1.17192	3.42602
C	-3.20902	-1.97048	-1.88203
H	-2.19606	-2.24050	-1.54460
C	-3.12119	-1.54654	-3.36367
H	-4.11139	-1.26586	-3.76979
H	-2.75250	-2.39122	-3.97205
H	-2.41572	-0.70662	-3.48420
C	-4.11106	-3.22263	-1.74996
H	-4.19367	-3.56673	-0.70773
H	-3.69933	-4.05042	-2.35313
H	-5.13255	-3.01600	-2.11837
C	-0.78675	-2.04484	3.28088
H	-0.33953	-2.95905	3.70749
H	-1.55210	-1.68335	3.98756
H	-0.00235	-1.27677	3.21015
C	-3.23409	-3.29315	1.86147
H	-3.27510	-4.19671	1.23196
H	-4.10236	-2.66116	1.61670
H	-3.32974	-3.61599	2.91252
C	2.07986	-4.57342	0.24374
H	2.32013	-4.48868	1.31455
H	3.00431	-4.40943	-0.33361
H	1.73318	-5.60374	0.05244
C	0.09260	-3.87431	-1.99051
H	-0.47974	-3.06749	-2.47632
H	-0.55011	-4.76860	-1.91921
H	0.94269	-4.11721	-2.64980
C	2.63793	-1.43232	-0.17489
C	3.39121	-1.45911	1.04993
C	4.78598	-1.26104	1.02014
H	5.34539	-1.28712	1.96231
C	5.47055	-1.03940	-0.18053
H	6.55757	-0.89927	-0.18630
C	4.74379	-1.02222	-1.37469
H	5.27182	-0.86460	-2.32239
C	3.34794	-1.22481	-1.40452
C	2.72465	-1.67679	2.40786
H	1.71905	-2.07654	2.20292
C	2.55432	-0.33769	3.16272
H	3.53704	0.12849	3.35839
H	2.05803	-0.49488	4.13774
H	1.95258	0.37549	2.57594
C	3.47057	-2.68949	3.30408
H	3.67613	-3.63524	2.77577
H	2.86625	-2.92045	4.19901
H	4.43753	-2.29196	3.66161
C	2.67245	-1.26672	-2.77634
H	1.58667	-1.37307	-2.61628
C	2.88218	0.03782	-3.57522
H	2.45952	0.89804	-3.03279
H	2.35827	-0.02585	-4.54489
H	3.95215	0.22771	-3.77938
C	3.17480	-2.47818	-3.59784
H	4.24669	-2.37732	-3.84810
H	2.61662	-2.55985	-4.54735
H	3.05604	-3.42717	-3.04764
C	1.14137	2.49082	0.36641
C	2.52572	2.97128	0.49082
C	2.79767	4.36271	0.59230
H	1.97146	5.07938	0.57911
C	4.11297	4.81596	0.72720
H	4.31379	5.88853	0.81427
C	5.17508	3.89316	0.74992
H	6.20570	4.25028	0.84910
C	4.91582	2.51518	0.64221
H	5.73536	1.79083	0.64589
C	3.60287	2.05026	0.51925
H	3.39906	0.98087	0.42694
C	0.09474	3.49171	-0.04600
C	0.07178	3.92546	-1.39216
H	0.78717	3.50915	-2.10585
C	-0.87835	4.87739	-1.80200
H	-0.88151	5.22261	-2.84142
C	-1.80792	5.39752	-0.88036
H	-2.52701	6.16129	-1.19697
C	-1.78651	4.96316	0.45769
H	-2.48730	5.38412	1.18625
C	-0.83693	4.00812	0.87192
H	-0.79999	3.68632	1.91671
K	-2.93732	2.22151	-1.43397

TS(B-C)

SCF (BP86) Energy = -1904.79284346
Enthalpy 0K = -1903.878718
Enthalpy 298K = -1903.877774
Free Energy 298K = -1904.028625
Lowest Frequency = -95.8481 cm^{-1}
Second Frequency = 15.4043 cm^{-1}
SCF (BP86-D3BJ) Energy = -1905.10466907
SCF (C6H6) Energy = -1904.80540897
SCF (Et2O) Energy = -1904.81289117
SCF (BS2) Energy = -3676.60419254

S	-0.33583	0.92039	-2.14251
Si	-1.53370	-2.56502	1.42356
Si	0.85721	-3.30272	-0.36428
Al	-0.08130	-0.28866	-0.34224
O	-0.49030	-3.63406	0.62223
O	0.76223	1.28412	0.82027
N	-1.66996	-1.05146	0.47518
N	1.29227	-1.59084	-0.11964
C	-2.97851	-0.58750	0.13160
C	-3.74896	0.21290	1.05403
C	-5.00024	0.73802	0.66141
H	-5.57139	1.34064	1.37700
C	-5.54717	0.47605	-0.60334
H	-6.52858	0.87699	-0.88195
C	-4.84185	-0.36491	-1.47621
H	-5.28668	-0.63064	-2.44250
C	-3.58630	-0.91521	-1.13704
C	-3.29494	0.44995	2.49685
H	-2.21019	0.24468	2.52922
C	-3.54916	1.88573	3.00602
H	-3.20504	2.64629	2.28953
H	-3.02622	2.05001	3.96427
H	-4.62267	2.06835	3.19354
C	-4.01377	-0.52916	3.45890
H	-5.10310	-0.34351	3.44685
H	-3.65862	-0.38639	4.49518
H	-3.85554	-1.58169	3.18382
C	-2.97452	-1.92438	-2.10931
H	-1.97355	-2.17050	-1.72191
C	-2.80868	-1.38290	-3.54538
H	-3.78154	-1.10944	-3.99627
H	-2.36530	-2.16297	-4.18927
H	-2.13213	-0.51076	-3.55401
C	-3.81439	-3.22527	-2.13046

H	-3.94374	-3.65113	-1.12355
H	-3.32100	-3.98360	-2.76292
H	-4.82024	-3.04176	-2.55052
C	-0.85351	-2.26506	3.17341
H	-0.39957	-3.19209	3.56359
H	-1.65816	-1.96654	3.86547
H	-0.08777	-1.47462	3.18507
C	-3.18316	-3.51177	1.54384
H	-3.13804	-4.37668	0.86226
H	-4.06446	-2.90730	1.27748
H	-3.32997	-3.90194	2.56575
C	2.24240	-4.48662	0.14890
H	2.42932	-4.44900	1.23298
H	3.18684	-4.26582	-0.37442
H	1.93858	-5.51597	-0.10925
C	0.34728	-3.73689	-2.14379
H	-0.21995	-2.92351	-2.62392
H	-0.27498	-4.64837	-2.14537
H	1.23647	-3.93077	-2.76631
C	2.71060	-1.32882	-0.08298
C	3.41647	-1.37638	1.16941
C	4.80636	-1.14776	1.20009
H	5.32888	-1.18736	2.16277
C	5.53306	-0.88601	0.03279
H	6.61696	-0.72797	0.07339
C	4.85310	-0.85037	-1.18844
H	5.41427	-0.65784	-2.11032
C	3.46263	-1.07152	-1.27801
C	2.70414	-1.65612	2.49183
H	1.71014	-2.05224	2.23102
C	2.49810	-0.35481	3.30196
H	3.47101	0.09754	3.56790
H	1.95692	-0.56017	4.24375
H	1.92484	0.38722	2.72324
C	3.42594	-2.70557	3.36570
H	3.65115	-3.62731	2.80407
H	2.79548	-2.97632	4.23096
H	4.38013	-2.32114	3.76897
C	2.83918	-1.06134	-2.67489
H	1.75302	-1.21294	-2.56123
C	3.03015	0.29567	-3.38725
H	2.54563	1.10356	-2.81653
H	2.55486	0.26885	-4.38348
H	4.10000	0.53734	-3.52758
C	3.41492	-2.20311	-3.54629
H	4.48799	-2.04497	-3.75885
H	2.88802	-2.25227	-4.51565
H	3.32144	-3.18647	-3.05472
C	1.00204	2.46381	0.42179
C	2.37721	3.00825	0.43371
C	2.61291	4.41008	0.44936
H	1.77031	5.10612	0.44274
C	3.91848	4.90758	0.50896
H	4.08816	5.98876	0.53123
C	5.00750	4.01897	0.54764
H	6.02991	4.40981	0.58803
C	4.78539	2.63092	0.53803
H	5.62436	1.93001	0.56217
C	3.48293	2.12419	0.48858
H	3.30869	1.04628	0.47421
C	-0.10724	3.42305	0.08881
C	-0.09505	4.18931	-1.10222
H	0.67491	3.98938	-1.85179
C	-1.09205	5.14466	-1.33666
H	-1.07997	5.72234	-2.26691
C	-2.10263	5.37063	-0.37535
H	-2.86497	6.13805	-0.54828
C	-2.10466	4.63026	0.81770
H	-2.86523	4.82179	1.58211
C	-1.11184	3.65600	1.04861
H	-1.09994	3.08520	1.98122
K	-2.96332	2.19767	-1.43504

c

SCF (BP86) Energy = -1904.82446111
Enthalpy 0K = -1903.909867
Enthalpy 298K = -1903.908922
Free Energy 298K = -1904.059009
Lowest Frequency = 20.8920 cm^{-1}
Second Frequency = 24.1567 cm^{-1}
SCF (BP86-D3BJ) Energy = -1905.13681009
SCF (C6H6) Energy = -1904.83571571
SCF (Et2O) Energy = -1904.84230352
SCF (BS2) Energy = -3676.63711201

S	-0.14699	1.35051	-1.67692
Si	-1.40595	-2.96711	1.01006
Si	1.35357	-3.24277	-0.37150
Al	0.05253	-0.32936	-0.05091
O	-0.09084	-3.79310	0.34565
O	0.28841	1.19976	0.93964
N	-1.53815	-1.36035	0.21676
N	1.50898	-1.50729	-0.02051
C	-2.81290	-0.93586	-0.25344
C	-3.82660	-0.45467	0.65335
C	-5.08663	-0.05289	0.15492
H	-5.85340	0.28342	0.86334
C	-5.38779	-0.09576	-1.21405
H	-6.37910	0.19659	-1.57844
C	-4.40790	-0.56534	-2.10328
H	-4.64494	-0.63726	-3.17112
C	-3.13813	-0.99122	-1.65918
C	-3.60279	-0.38600	2.16592
H	-2.54146	-0.62724	2.34250
C	-3.86641	1.02207	2.74361
H	-3.23907	1.78920	2.26021
H	-3.63415	1.04094	3.82268
H	-4.92527	1.32016	2.63392
C	-4.47957	-1.41876	2.91326
H	-5.55342	-1.19582	2.77817
H	-4.26839	-1.39369	3.99687
H	-4.30700	-2.44549	2.55440
C	-2.17775	-1.58545	-2.69002
H	-1.19031	-1.66078	-2.20360
C	-2.01823	-0.72577	-3.96212
H	-2.95619	-0.66722	-4.54402
H	-1.25706	-1.17312	-4.62403
H	-1.68846	0.30002	-3.72354
C	-2.62331	-3.01751	-3.07147
H	-2.69331	-3.66817	-2.18631
H	-1.90344	-3.47218	-3.77385
H	-3.61380	-3.00276	-3.56119
C	-1.10353	-2.87002	2.88352
H	-0.69811	-3.83676	3.22874
H	-2.03286	-2.67535	3.44355
H	-0.37599	-2.08506	3.14505
C	-2.93457	-4.04370	0.66453
H	-2.74343	-4.68054	-0.21441
H	-3.84914	-3.45999	0.47450
H	-3.12470	-4.71188	1.52201
C	2.78543	-4.23393	0.36726
H	2.76284	-4.20089	1.46789
H	3.76245	-3.84857	0.03276
H	2.70377	-5.28867	0.05369
C	1.17548	-3.70360	-2.20751

H	0.43504	-3.06814	-2.72023
H	0.83241	-4.75025	-2.28166
H	2.13009	-3.61803	-2.75043
C	2.83482	-0.98550	0.24509
C	3.29636	-0.85416	1.59503
C	4.56622	-0.29874	1.84122
H	4.90638	-0.19063	2.87793
C	5.40498	0.10513	0.79732
H	6.38987	0.53549	1.00903
C	4.97384	-0.06579	-0.52108
H	5.63436	0.22751	-1.34533
C	3.70891	-0.60838	-0.82339
C	2.46482	-1.32075	2.79070
H	1.61264	-1.88608	2.37730
C	1.89628	-0.13343	3.60154
H	2.71512	0.47683	4.02502
H	1.28291	-0.49491	4.44791
H	1.27391	0.51852	2.96676
C	3.25315	-2.26933	3.72204
H	3.69985	-3.11109	3.16706
H	2.58760	-2.68397	4.50004
H	4.07376	-1.74274	4.24124
C	3.35485	-0.82490	-2.29630
H	2.31685	-1.19587	-2.33154
C	3.40824	0.47439	-3.12746
H	2.71354	1.22662	-2.72413
H	3.12574	0.26809	-4.17605
H	4.42332	0.91022	-3.13723
C	4.28017	-1.89318	-2.92735
H	5.32698	-1.54104	-2.95575
H	3.97510	-2.11306	-3.96654
H	4.27001	-2.83838	-2.35803
C	0.36228	2.21921	-0.02713
C	1.76017	2.85742	-0.11851
C	2.21957	3.51010	-1.28024
H	1.62261	3.46021	-2.19726
C	3.45014	4.18415	-1.28313
H	3.79533	4.67744	-2.19841
C	4.24279	4.21171	-0.12452
H	5.20605	4.73302	-0.12762
C	3.79790	3.55200	1.03149
H	4.41630	3.55012	1.93529
C	2.56446	2.88312	1.03706
H	2.21958	2.35995	1.93176
C	-0.64122	3.35129	0.28420
C	-0.95898	4.36078	-0.65585
H	-0.47344	4.35261	-1.63717
C	-1.88857	5.36683	-0.34605
H	-2.11551	6.14170	-1.08724
C	-2.50829	5.39741	0.91927
H	-3.22377	6.18903	1.16534
C	-2.17386	4.41928	1.86959
H	-2.62937	4.44507	2.86567
C	-1.24849	3.40538	1.55470
H	-0.97793	2.63514	2.28226
K	-3.14671	2.14978	-0.98959

TS(C-D)

SCF (BP86) Energy = -2481.39723918
Enthalpy 0K = -2480.284108
Enthalpy 298K = -2480.283164
Free Energy 298K = -2480.457335
Lowest Frequency = -81.7292 cm^{-1}
Second Frequency = 15.0589 cm^{-1}
SCF (BP86-D3BJ) Energy = -2481.80984268
SCF (C6H6) Energy = -2481.40943262
SCF (Et2O) Energy = -2481.41657199
SCF (BS2) Energy = -4253.35006683

S	0.37287	1.95847	0.76413
Si	0.30357	-3.57046	-1.22784
Si	2.47865	-2.67665	0.73058
Al	0.18075	-0.54798	0.09621
O	1.73473	-3.76845	-0.32501
O	-0.91085	-0.20137	1.52635
O	-0.39346	0.57341	-1.79434
N	-0.61924	-2.19964	-0.56813
N	2.07660	-1.00407	0.21752
C	-2.05974	-2.36502	-0.54527
C	-2.86336	-2.14020	-1.71906
C	-4.26963	-2.18903	-1.62671
H	-4.86503	-2.00191	-2.52779
C	-4.92057	-2.47789	-0.42425
H	-6.01489	-2.49448	-0.36973
C	-4.14412	-2.80510	0.69189
H	-4.64056	-3.11050	1.62077
C	-2.73595	-2.79594	0.64947
C	-2.26226	-1.97716	-3.11955
H	-1.18382	-1.78900	-2.99283
C	-2.45871	-3.28954	-3.92098
H	-2.06280	-4.16896	-3.38883
H	-1.96235	-3.22932	-4.90680
H	-3.53414	-3.47173	-4.09753
C	-2.85254	-0.81592	-3.94791
H	-3.91803	-0.98410	-4.18628
H	-2.31940	-0.73227	-4.91243
H	-2.77876	0.14836	-3.42685
C	-2.00051	-3.38246	1.85728
H	-0.92335	-3.31921	1.63035
C	-2.26567	-2.63039	3.17674
H	-1.93968	-1.58483	3.09514
H	-1.71643	-3.10551	4.00994
H	-3.33860	-2.65358	3.44235
C	-2.37470	-4.87384	2.05078
H	-3.42593	-4.97679	2.37514
H	-1.74209	-5.32934	2.83388
H	-2.25537	-5.45980	1.12690
C	0.89292	-3.43099	-3.04062
H	1.05685	-2.39317	-3.36542
H	0.16408	-3.88591	-3.72981
H	1.84299	-3.98378	-3.14260
C	-0.61579	-5.22494	-1.08246
H	-0.18260	-5.94293	-1.80027
H	-1.69477	-5.14033	-1.28736
H	-0.48444	-5.64055	-0.07142
C	4.33659	-3.04007	0.59647
H	4.52992	-4.02484	1.05599
H	4.97283	-2.29603	1.10029
H	4.64691	-3.09890	-0.45852
C	1.89758	-3.09053	2.48816
H	0.81338	-2.93675	2.60454
H	2.41374	-2.47826	3.24513
H	2.10987	-4.15300	2.69996
C	3.22145	-0.17462	-0.00720
C	3.82205	0.61404	1.04476
C	4.94713	1.42320	0.76483
H	5.39261	2.00005	1.58297
C	5.52695	1.48598	-0.51019
H	6.41104	2.10719	-0.69514
C	4.98620	0.68495	-1.52581
H	5.46179	0.67466	-2.51363
C	3.87602	-0.15798	-1.29517
C	3.34386	0.56300	2.49383
H	2.34646	0.09546	2.48988
C	3.21221	1.95734	3.14161

H	4.19247	2.45889	3.24768
H	2.78568	1.85715	4.15258
H	2.53258	2.60047	2.55850
C	4.29532	-0.30227	3.35671
H	4.41059	-1.32482	2.96423
H	3.90564	-0.37282	4.38721
H	5.30258	0.15053	3.40681
C	3.42849	-1.05765	-2.44529
H	2.74282	-1.80329	-2.01449
C	2.64181	-0.25167	-3.49844
H	1.72126	0.16309	-3.05737
H	2.35162	-0.88923	-4.35253
H	3.25515	0.57789	-3.90028
C	4.59696	-1.81156	-3.11727
H	5.24944	-1.13613	-3.70002
H	4.19875	-2.56440	-3.81905
H	5.22971	-2.33293	-2.38059
C	-0.79459	1.11391	2.00870
C	-0.20095	1.16197	3.43652
C	0.24009	-0.01869	4.06058
H	0.19025	-0.95327	3.49928
C	0.72000	-0.00196	5.38232
H	1.04931	-0.93745	5.84837
C	0.76116	1.19893	6.10626
H	1.12315	1.21230	7.13998
C	0.32218	2.38560	5.49121
H	0.34399	3.33126	6.04434
C	-0.15196	2.36609	4.17291
H	-0.50261	3.29526	3.71288
C	-0.93264	1.69978	-1.99745
C	-0.11249	2.77386	-2.67921
C	-0.00611	4.06600	-2.10972
H	-0.54912	4.27920	-1.18386
C	0.81563	5.03801	-2.70528
H	0.89069	6.03438	-2.25581
C	1.52103	4.74106	-3.88844
H	2.14778	5.50468	-4.36115
C	1.39568	3.46922	-4.47380
H	1.92045	3.23990	-5.40693
C	0.58758	2.48943	-3.87054
H	0.48276	1.50239	-4.32826
C	-2.16775	1.81915	2.07354
C	-3.27918	1.08409	2.53735
C	-2.33677	3.19126	1.80431
C	-4.52013	1.70805	2.73213
C	-3.57921	3.81715	1.99710
C	-4.67678	3.07884	2.46557
H	-3.16516	0.01561	2.73475
H	-1.47876	3.76153	1.43124
H	-5.36982	1.11892	3.09528
H	-3.68818	4.88582	1.78002
H	-5.64524	3.56633	2.62207
C	-2.35280	1.99058	-1.72950
C	-3.00377	3.06468	-2.39633
C	-3.11490	1.13414	-0.89712
C	-4.37704	3.27029	-2.23425
C	-4.48789	1.34767	-0.74079
C	-5.12046	2.41193	-1.40472
H	-2.43722	3.71372	-3.06952
H	-2.62518	0.31139	-0.37195
H	-4.87092	4.09254	-2.76194
H	-5.05928	0.67835	-0.09396
H	-6.19673	2.57142	-1.27947
K	2.70375	2.76461	-0.96901

D

SCF (BP86) Energy = -2481.43056624
Enthalpy 0K = -2480.316593
Enthalpy 298K = -2480.315649
Free Energy 298K = -2480.488452
Lowest Frequency = 21.7869 cm^{-1}
Second Frequency = 28.2110 cm^{-1}
SCF (BP86-D3BJ) Energy = -2481.84461462
SCF (C6H6) Energy = -2481.44114314
SCF (Et2O) Energy = -2481.44748741
SCF (BS2) Energy = -4253.38456608

S	-0.07790	-2.73052	0.14585
Si	-0.19428	3.88566	-0.35595
Si	-2.19039	2.55983	1.54327
Al	-0.14938	0.63313	0.04502
O	-1.52888	3.87223	0.69989
O	0.79434	-0.34084	1.25611
O	-0.07308	-0.47942	-1.42258
N	0.68526	2.34419	-0.17292
N	-1.97102	1.06487	0.57200
C	2.12885	2.45133	-0.26271
C	2.79389	2.41633	-1.53449
C	4.20311	2.39546	-1.58083
H	4.69968	2.35555	-2.55762
C	4.97706	2.43820	-0.41659
H	6.07062	2.40282	-0.47184
C	4.33130	2.58767	0.81569
H	4.93188	2.70046	1.72600
C	2.92675	2.63792	0.91726
C	2.03468	2.53181	-2.86121
H	0.96009	2.47950	-2.62325
C	2.33052	3.90997	-3.50461
H	2.14151	4.74213	-2.80592
H	1.70772	4.06503	-4.40407
H	3.38851	3.97801	-3.81527
C	2.33621	1.41732	-3.88488
H	3.40933	1.37417	-4.14320
H	1.78246	1.60944	-4.82194
H	2.04529	0.42693	-3.50563
C	2.32125	3.01341	2.27494
H	1.24739	3.19431	2.10013
C	2.44043	1.91001	3.34596
H	1.91642	0.99423	3.03444
H	2.00634	2.25237	4.30288
H	3.49793	1.65304	3.53848
C	2.94718	4.31849	2.82562
H	3.99169	4.15905	3.14754
H	2.38421	4.66705	3.70991
H	2.95075	5.12696	2.07760
C	-0.90368	4.26967	-2.08608
H	-1.21555	3.37821	-2.65016
H	-0.16004	4.80745	-2.69643
H	-1.78037	4.92974	-1.96544
C	0.84962	5.39825	0.10861
H	0.33049	6.30222	-0.25472
H	1.85313	5.37449	-0.34652
H	0.96283	5.49026	1.19905
C	-4.01971	3.00748	1.76081
H	-4.07565	3.92594	2.37031
H	-4.61044	2.22560	2.26283
H	-4.49381	3.22045	0.78957
C	-1.35914	2.44960	3.24267
H	-0.31185	2.12198	3.15613
H	-1.88711	1.73593	3.89683
H	-1.36814	3.43791	3.73348
C	-3.21285	0.42615	0.26754
C	-3.81776	-0.52580	1.16965
C	-5.07224	-1.09788	0.85621
H	-5.52295	-1.79860	1.56861

C	-5.76068	-0.78403	-0.32352
H	-6.73812	-1.23048	-0.53824
C	-5.19029	0.15009	-1.20067
H	-5.73411	0.43602	-2.10852
C	-3.95719	0.77724	-0.91997
C	-3.16098	-0.95136	2.48195
H	-2.13923	-0.53734	2.48192
C	-3.05479	-2.48738	2.61147
H	-4.05081	-2.96584	2.65251
H	-2.52134	-2.75271	3.53844
H	-2.48234	-2.92691	1.77658
C	-3.91757	-0.39222	3.70993
H	-3.99230	0.70654	3.69007
H	-3.39519	-0.68341	4.63765
H	-4.94531	-0.79560	3.76178
C	-3.45421	1.83547	-1.89733
H	-2.64586	2.37333	-1.37918
C	-2.85013	1.18016	-3.15803
H	-1.99618	0.53605	-2.89223
H	-2.48814	1.94531	-3.86759
H	-3.60687	0.57199	-3.68989
C	-4.53466	2.86567	-2.28952
H	-5.32985	2.42120	-2.91511
H	-4.07596	3.68000	-2.87589
H	-5.01436	3.31442	-1.40406
C	0.97703	-1.69110	1.43053
C	0.44343	-2.17547	2.80617
C	0.08611	-1.21869	3.77402
H	0.12671	-0.16229	3.50179
C	-0.30394	-1.61057	5.06589
H	-0.56163	-0.84571	5.80676
C	-0.35486	-2.97043	5.40940
H	-0.65394	-3.27746	6.41724
C	-0.00864	-3.93449	4.44720
H	-0.04011	-4.99989	4.70024
C	0.39304	-3.54122	3.16205
H	0.68167	-4.30614	2.43580
C	0.33950	-1.80772	-1.51673
C	-0.49507	-2.52562	-2.61156
C	-0.89700	-3.88060	-2.54348
H	-0.60448	-4.48468	-1.67681
C	-1.66139	-4.46012	-3.57472
H	-1.95681	-5.51276	-3.50180
C	-2.02155	-3.70215	-4.70172
H	-2.60900	-4.15429	-5.50761
C	-1.59710	-2.36460	-4.79494
H	-1.84902	-1.77002	-5.67957
C	-0.84118	-1.78530	-3.76283
H	-0.50383	-0.74833	-3.83340
C	2.47094	-2.10464	1.35576
C	3.44559	-1.14300	1.68279
C	2.89341	-3.42522	1.09934
C	4.80035	-1.49422	1.77851
C	4.24815	-3.77636	1.19236
C	5.20926	-2.81505	1.54354
H	3.13658	-0.10920	1.83506
H	2.16055	-4.17528	0.78828
H	5.53767	-0.72343	2.02774

TS(A-E)

SCF (BP86) Energy = -1673.74863875
Enthalpy 0K = -1672.917974
Enthalpy 298K = -1672.917029
Free Energy 298K = -1673.060994
Lowest Frequency = -84.5337 cm^{-1}
Second Frequency = 9.1472 cm^{-1}
SCF (BP86-D3BJ) Energy = -1674.01484000
SCF (C6H6) Energy = -1673.75954657
SCF (Et2O) Energy = -1673.76580584
SCF (BS2) Energy = -3445.50925254

S	-0.19807	1.37707	-1.76629
Si	-0.57681	-3.04175	0.94212
Si	2.26022	-2.63746	-0.31976
Al	0.19940	-0.29291	-0.43885
O	0.90266	-3.48721	0.25541
O	-0.56872	1.82400	1.37186
N	-1.10334	-1.52259	0.14110
N	1.91771	-0.91040	-0.06567
C	-2.47642	-1.28158	-0.18353
C	-3.41358	-0.85633	0.82274
C	-4.73598	-0.52595	0.45088
H	-5.44468	-0.21947	1.22989
C	-5.16583	-0.59586	-0.88218
H	-6.19722	-0.34045	-1.15042
C	-4.26708	-1.05194	-1.85700
H	-4.60716	-1.15369	-2.89398
C	-2.94337	-1.42081	-1.53887
C	-3.04340	-0.76554	2.30537
H	-1.96241	-0.96154	2.38018
C	-3.29039	0.63622	2.90900
H	-2.63667	1.38922	2.43732
H	-3.04723	0.63251	3.98581
H	-4.34768	0.94702	2.81672
C	-3.80029	-1.83866	3.12312
H	-4.89023	-1.65826	3.10578
H	-3.47650	-1.82248	4.17870
H	-3.62809	-2.85322	2.72685
C	-2.08557	-2.03239	-2.64985
H	-1.07653	-2.19339	-2.23086
C	-1.94876	-1.12538	-3.89201
H	-2.92887	-0.93952	-4.36880
H	-1.30950	-1.61597	-4.64693
H	-1.48880	-0.15826	-3.62709
C	-2.65191	-3.41414	-3.06010
H	-2.75999	-4.08807	-2.19516
H	-1.98491	-3.89852	-3.79428
H	-3.64690	-3.31071	-3.52932
C	-0.29593	-2.91429	2.81634
H	0.33568	-3.76365	3.12961
H	-1.23941	-2.97114	3.38331
H	0.22127	-1.98351	3.09892
C	-1.80090	-4.44239	0.58970
H	-1.67280	-4.81460	-0.43911
H	-2.84867	-4.12263	0.71517
H	-1.61427	-5.28271	1.27978
C	3.80740	-3.19366	0.61305
H	3.63695	-3.19202	1.70098
H	4.66115	-2.52951	0.39705
H	4.08292	-4.21732	0.30803
C	2.37715	-3.16807	-2.13830
H	2.35986	-4.27033	-2.19647
H	3.30004	-2.81348	-2.62390
H	1.51897	-2.78669	-2.71781
C	2.96129	0.06329	0.18338
C	3.28880	0.41602	1.53374
C	4.22544	1.44062	1.77365
H	4.45664	1.71482	2.80964
C	4.87066	2.10403	0.72524
H	5.59475	2.89985	0.93160
C	4.59498	1.71804	-0.59038
H	5.12184	2.20963	-1.41629
C	3.65929	0.70690	-0.88937
C	2.68426	-0.30319	2.74091
H	2.06789	-1.12624	2.34220

C	1.76430	0.61788	3.57362
H	2.32840	1.47841	3.97738
H	1.34306	0.06759	4.43506
H	0.92956	1.00891	2.96968
C	3.77776	-0.91778	3.64529
H	4.46622	-1.56355	3.07582
H	3.31839	-1.52409	4.44635
H	4.38501	-0.13498	4.13380
C	3.49263	0.29619	-2.35334
H	2.63601	-0.39622	-2.40597
C	3.18116	1.48209	-3.29124
H	2.24582	1.97860	-2.98653
H	3.05301	1.11982	-4.32709
H	4.00049	2.22362	-3.30289
C	4.75929	-0.44921	-2.84100
H	5.63455	0.22512	-2.84527
H	4.62144	-0.82494	-3.87085
H	5.01150	-1.30559	-2.19213
C	0.06974	2.64959	0.66737
C	-0.47356	4.00216	0.34199
C	-1.63541	4.47385	0.99508
H	-2.09775	3.84338	1.76440
C	-2.14075	5.75196	0.70831
H	-3.02827	6.12185	1.23373
C	-1.48891	6.56906	-0.23178
H	-1.88097	7.56668	-0.45566
C	-0.31972	6.11223	-0.87003
H	0.19284	6.75276	-1.59511
C	0.18891	4.84023	-0.58120
H	1.08616	4.46711	-1.08663
H	1.14358	2.50235	0.43391
K	-2.92911	1.88467	-0.57022

E

SCF (BP86) Energy = -1673.78543001
Enthalpy 0K = -1672.953567
Enthalpy 298K = -1672.952622
Free Energy 298K = -1673.095059
Lowest Frequency = 9.6952 cm^{-1}
Second Frequency = 20.9610 cm^{-1}
SCF (BP86-D3BJ) Energy = -1674.05523107
SCF (C6H6) Energy = -1673.79583529
SCF (Et2O) Energy = -1673.80176615
SCF (BS2) Energy = -3445.54474318

S	-0.38602	1.44383	-1.83550
Si	-0.07140	-3.04454	0.89326
Si	2.57007	-2.15458	-0.50506
Al	0.24784	-0.04170	-0.12599
O	1.45668	-3.23590	0.20304
O	-0.20674	1.46791	0.82246
N	-0.81937	-1.57438	0.18795
N	2.05580	-0.51054	-0.08911
C	-2.21954	-1.52478	-0.08188
C	-3.16803	-1.22182	0.95876
C	-4.54187	-1.10894	0.64892
H	-5.25185	-0.89418	1.45711
C	-5.01853	-1.28310	-0.65911
H	-6.08962	-1.20714	-0.87848
C	-4.10285	-1.60764	-1.67190
H	-4.47045	-1.78581	-2.68942
C	-2.72291	-1.75221	-1.41370
C	-2.74006	-1.02020	2.41306
H	-1.64655	-1.14506	2.44404
C	-3.04749	0.40620	2.92015
H	-2.48762	1.15707	2.33731
H	-2.73765	0.51615	3.97394
H	-4.12866	0.63596	2.87090
C	-3.38133	-2.07790	3.33975
H	-4.47960	-1.96530	3.38513
H	-2.99485	-1.97490	4.36869
H	-3.16865	-3.10348	2.99431
C	-1.82143	-2.21045	-2.56208
H	-0.79184	-2.23719	-2.16609
C	-1.85019	-1.25655	-3.77726
H	-2.85761	-1.21167	-4.23128
H	-1.15790	-1.61556	-4.55847
H	-1.54872	-0.23196	-3.50308
C	-2.20216	-3.63927	-3.02053
H	-2.21340	-4.35161	-2.18093
H	-1.48169	-4.00400	-3.77303
H	-3.20486	-3.65437	-3.48484
C	0.18795	-2.99241	2.77589
H	0.89283	-3.79704	3.04872
H	-0.74967	-3.16636	3.32946
H	0.61918	-2.03793	3.11822
C	-1.09278	-4.58759	0.48761
H	-0.94413	-4.89158	-0.56028
H	-2.17121	-4.43051	0.65741
H	-0.76535	-5.42237	1.13047
C	4.28820	-2.53755	0.18547
H	4.27259	-2.54209	1.28712
H	5.03064	-1.79117	-0.14212
H	4.62151	-3.53120	-0.15863
C	2.49776	-2.57139	-2.35749
H	2.59827	-3.66205	-2.49405
H	3.29995	-2.07861	-2.92965
H	1.53204	-2.26300	-2.79332
C	3.01950	0.52424	0.21270
C	3.32770	0.83690	1.57681
C	4.22783	1.88032	1.86479
H	4.44707	2.11716	2.91268
C	4.85098	2.61256	0.84919
H	5.55073	3.41953	1.09280
C	4.57380	2.29046	-0.48277
H	5.07048	2.84874	-1.28497
C	3.67136	1.26345	-0.82719
C	2.71413	0.06878	2.74659
H	2.13063	-0.75752	2.30618
C	1.74636	0.95435	3.56471
H	2.28522	1.79794	4.03336
H	1.27507	0.37064	4.37720
H	0.95622	1.36831	2.91699
C	3.79048	-0.55098	3.66583
H	4.49604	-1.18228	3.09997
H	3.31961	-1.17585	4.44564
H	4.38187	0.22745	4.18032
C	3.46866	0.95527	-2.31199
H	2.64284	0.22786	-2.38435
C	3.06239	2.19772	-3.13422
H	2.12573	2.63378	-2.75131
H	2.89469	1.91709	-4.18961
H	3.84718	2.97516	-3.12044
C	4.74346	0.31847	-2.91608
H	5.58967	1.02834	-2.88754
H	4.58006	0.03568	-3.97184
H	5.05572	-0.58400	-2.36356
C	-0.15743	2.43168	-0.20589
C	-1.19193	3.53875	-0.03061
C	-1.74165	3.77936	1.24709
H	-1.39781	3.16352	2.08311
C	-2.69459	4.79667	1.43718
H	-3.10753	4.97335	2.43654
C	-3.10509	5.59339	0.35559
H	-3.84276	6.38901	0.50414

C -2.54838 5.37312 -0.91793
H -2.84994 6.00008 -1.76428
C -1.60084 4.35428 -1.11016
H -1.17291 4.17730 -2.10357
H 0.84907 2.89310 -0.28565
K -3.29804 1.44159 -0.68850

TS(E-F)
SCF (BP86) Energy = -2019.35050520
Enthalpy 0K = -2018.403384
Enthalpy 298K = -2018.402440
Free Energy 298K = -2018.559309
Lowest Frequency = -31.3234 cm^{-1}
Second Frequency = 14.9005 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.66502404
SCF (C6H6) Energy = -2019.36060763
SCF (Et2O) Energy = -2019.36634898
SCF (BS2) Energy = -3791.19813010

S 0.06075 -0.08111 -2.27600
Si -1.78271 1.56894 2.18744
Si -0.48937 -1.17844 2.88150
Al 0.16552 0.15253 0.09869
O -1.73395 -0.05172 2.70469
O 1.90551 0.52948 -0.51353
O -2.42706 -0.55305 -0.27027
N -0.56018 1.70023 0.90976
N 0.28262 -1.34448 1.28060
C -0.07255 2.99345 0.48236
C -0.74584 3.73247 -0.54753
C -0.20513 4.95340 -0.99944
H -0.72714 5.50149 -1.79277
C 0.96989 5.48286 -0.45928
H 1.37698 6.43061 -0.82837
C 1.60704 4.78696 0.57222
H 2.51952 5.20238 1.01603
C 1.11090 3.56306 1.06235
C -2.07230 3.28036 -1.16213
H -2.32990 2.31474 -0.69612
C -3.19662 4.29739 -0.85057
H -3.25990 4.52427 0.22649
H -4.17794 3.91152 -1.18007
H -3.02189 5.25347 -1.37600
C -1.97876 3.06475 -2.68964
H -1.69374 3.99632 -3.21092
H -2.95943 2.75186 -3.09411
H -1.24053 2.28395 -2.93695
C 1.87923 2.90320 2.20872
H 1.31256 1.99989 2.49446
C 3.29056 2.45806 1.76561
H 3.21703 1.77232 0.90733
H 3.81449 1.94734 2.59453
H 3.90544 3.32861 1.47240
C 1.98755 3.82790 3.44371
H 2.61237 4.71265 3.22637
H 2.46265 3.29237 4.28564
H 1.00340 4.19034 3.77995
C -3.60932 1.83864 1.74592
H -3.92990 1.23056 0.88783
H -3.83659 2.89548 1.53420
H -4.21191 1.53658 2.62105
C -1.42837 2.73200 3.64524
H -2.26782 2.69041 4.36066
H -1.32984 3.77563 3.30077
H -0.50643 2.45883 4.18102
C -1.27351 -2.80028 3.46568
H -1.59041 -2.69955 4.51776
H -0.56300 -3.64215 3.40550
H -2.16144 -3.04757 2.86330
C 0.63323 -0.55183 4.28493
H 1.18650 0.35989 4.00572
H 1.36345 -1.30846 4.61453
H -0.00692 -0.30647 5.15071
C 0.98745 -2.53199 0.92023
C 2.37273 -2.72226 1.27560
C 3.07039 -3.86244 0.81864
H 4.12152 -3.98833 1.10514
C 2.45412 -4.83848 0.02337
H 3.01066 -5.72045 -0.31331
C 1.09653 -4.68452 -0.29055
H 0.59059 -5.46115 -0.87649
C 0.34620 -3.57399 0.15345
C 3.14715 -1.72458 2.13705
H 2.45147 -0.90879 2.38871
C 4.33566 -1.10032 1.37207
H 5.05781 -1.87102 1.04263
H 4.88267 -0.39273 2.01845
H 3.97733 -0.53399 0.49652
C 3.64191 -2.38281 3.44580
H 2.82192 -2.87910 3.99102
H 4.09138 -1.62675 4.11274
H 4.41350 -3.14802 3.24491
C -1.14559 -3.55234 -0.18308
H -1.56149 -2.62882 0.25152
C -1.40488 -3.52206 -1.70640
H -0.92786 -2.64878 -2.18322
H -2.48914 -3.47253 -1.90995
H -1.02444 -4.43689 -2.19855
C -1.87660 -4.76652 0.43891
H -1.54333 -5.71615 -0.01777
H -2.96443 -4.68360 0.26832
H -1.70448 -4.83911 1.52413
C 1.62400 0.91137 -1.84250
H 1.32862 1.98038 -1.90834
C 2.79766 0.68793 -2.79467
C 4.11673 0.77748 -2.29594
H 4.26197 1.00412 -1.23529
C 5.21932 0.59579 -3.14901
H 6.23544 0.67438 -2.74665
C 5.02163 0.32807 -4.51414
H 5.88049 0.19089 -5.17960
C 3.71305 0.24976 -5.02204
H 3.54890 0.05174 -6.08698
C 2.61015 0.42574 -4.16954
H 1.58903 0.35691 -4.56131
C -3.08583 -0.45266 -1.31336
H -2.60419 -0.04731 -2.23693
C -4.50665 -0.84176 -1.42958
C -5.16180 -0.70077 -2.67224
H -4.60656 -0.30398 -3.53047
C -6.50884 -1.06468 -2.80080
H -7.01897 -0.95585 -3.76320
C -7.20367 -1.56817 -1.68737
H -8.25708 -1.85114 -1.78621
C -6.55503 -1.70927 -0.44488
H -7.10556 -2.09959 0.41723
C -5.21044 -1.34882 -0.31295
H -4.67918 -1.44257 0.63935
K 2.48358 -2.08102 -1.75656

F
SCF (BP86) Energy = -2019.35129004
Enthalpy 0K = -2018.403296
Enthalpy 298K = -2018.402352
Free Energy 298K = -2018.559557

Lowest Frequency = 17.0054 cm^{-1}
Second Frequency = 24.1036 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.66924640
SCF (C6H6) Energy = -2019.36127558
SCF (Et2O) Energy = -2019.36692158
SCF (BS2) Energy = -3791.19752099

S	0.30050	0.03068	-2.44509
Si	-1.97291	1.57211	1.99391
Si	-0.86831	-1.25703	2.68398
Al	0.01020	0.11976	-0.02601
O	-2.05122	-0.07286	2.43390
O	1.84713	0.44147	-0.37509
O	-2.10211	-0.36883	-0.46657
N	-0.64819	1.69855	0.82500
N	0.05130	-1.40587	1.16376
C	-0.06600	2.98163	0.50743
C	-0.59912	3.78876	-0.55320
C	0.03520	4.99900	-0.89897
H	-0.37949	5.59864	-1.71803
C	1.17005	5.45398	-0.22206
H	1.65281	6.39433	-0.50985
C	1.66744	4.69307	0.84000
H	2.54617	5.04996	1.39017
C	1.07281	3.47632	1.22774
C	-1.87480	3.41962	-1.31409
H	-2.21822	2.45143	-0.91180
C	-2.98285	4.47291	-1.07297
H	-3.14885	4.65745	0.00115
H	-3.93951	4.14628	-1.51872
H	-2.71480	5.44054	-1.53375
C	-1.63894	3.25379	-2.83248
H	-1.26817	4.19102	-3.28514
H	-2.58619	2.99812	-3.34306
H	-0.90941	2.45312	-3.03928
C	1.69005	2.73973	2.41744
H	1.05228	1.86059	2.61422
C	3.10964	2.22753	2.09061
H	3.07134	1.56282	1.21363
H	3.52986	1.67204	2.94924
H	3.79335	3.06848	1.87302
C	1.73101	3.61759	3.68996
H	2.42540	4.46791	3.56696
H	2.08902	3.02778	4.55332
H	0.74186	4.03024	3.94381
C	-3.73672	1.97211	1.40899
H	-4.00461	1.48272	0.46088
H	-3.88748	3.05735	1.29056
H	-4.44161	1.62191	2.18406
C	-1.70604	2.64383	3.53801
H	-2.60977	2.60129	4.17044
H	-1.53777	3.69846	3.26078
H	-0.84930	2.30581	4.14044
C	-1.77283	-2.86370	3.12609
H	-2.21422	-2.77825	4.13376
H	-1.08486	-3.72641	3.13050
H	-2.58586	-3.07264	2.41296
C	0.11714	-0.72508	4.22330
H	0.73378	0.17024	4.04014
H	0.77500	-1.52224	4.60480
H	-0.60690	-0.47970	5.02030
C	0.76587	-2.59832	0.84990
C	2.10121	-2.83704	1.34319
C	2.81968	-3.97755	0.92070
H	3.83155	-4.13812	1.31198
C	2.27469	-4.91006	0.02749
H	2.84766	-5.79108	-0.28287
C	0.96042	-4.71480	-0.41895
H	0.50342	-5.45914	-1.08210
C	0.18952	-3.60474	-0.01212
C	2.80225	-1.89157	2.31835
H	2.10877	-1.05867	2.51392
C	4.09158	-1.29068	1.71581
H	4.82270	-2.07736	1.45068
H	4.58126	-0.61880	2.44132
H	3.85799	-0.69107	0.82090
C	3.12386	-2.60577	3.65190
H	2.23345	-3.09302	4.08270
H	3.51518	-1.88630	4.39201
H	3.89123	-3.38881	3.51279
C	-1.26117	-3.54363	-0.49281
H	-1.70584	-2.64082	-0.04401
C	-1.36424	-3.42161	-2.03007
H	-0.82393	-2.53525	-2.40548
H	-2.42062	-3.33947	-2.34206
H	-0.94708	-4.31485	-2.53174
C	-2.06606	-4.77507	-0.01341
H	-1.69933	-5.70673	-0.48083
H	-3.12979	-4.66542	-0.28910
H	-2.00658	-4.90262	1.07903
C	1.79540	0.92525	-1.69759
H	1.54544	2.00760	-1.73187
C	3.10207	0.72493	-2.46692
C	4.32899	0.79319	-1.76882
H	4.31100	0.98825	-0.69230
C	5.54988	0.63193	-2.44620
H	6.49156	0.69349	-1.88939
C	5.56570	0.40505	-3.83292
H	6.51717	0.28332	-4.36141
C	4.35147	0.34825	-4.53861
H	4.35349	0.18331	-5.62177
C	3.12994	0.50497	-3.86146
H	2.18084	0.45468	-4.40710
C	-2.75848	-0.33989	-1.52656
H	-2.25463	-0.03159	-2.47094
C	-4.17790	-0.70107	-1.59568
C	-4.83911	-0.65482	-2.84486
H	-4.28351	-0.34291	-3.73681
C	-6.19187	-1.00503	-2.93446
H	-6.70637	-0.96914	-3.89979
C	-6.88719	-1.40180	-1.77839
H	-7.94549	-1.67478	-1.84797
C	-6.23355	-1.44867	-0.53113
H	-6.78519	-1.75559	0.36314
C	-4.88331	-1.10050	-0.43391
H	-4.35022	-1.11845	0.52190
K	2.55116	-2.06937	-1.62253

TS(F-H)$_{cis}$
SCF (BP86) Energy = -2019.34506483
Enthalpy 0K = -2018.397765
Enthalpy 298K = -2018.396820
Free Energy 298K = -2018.551595
Lowest Frequency = -73.1326 cm^{-1}
Second Frequency = 20.3581 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.66222985
SCF (C6H6) Energy = -2019.35601848
SCF (Et2O) Energy = -2019.36219719
SCF (BS2) Energy = -3791.19203555

S	-0.36477	-0.19625	2.99811
Si	1.99271	1.54575	-2.10354
Si	0.87019	-1.28896	-2.76937
Al	0.08257	0.08591	-0.08191

O	2.06312	-0.11446	-2.48857
O	-1.56161	0.30701	0.64150
O	1.93920	-0.33582	0.54455
N	0.68392	1.67896	-0.91430
N	-0.04359	-1.42654	-1.24579
C	0.11731	2.96444	-0.57818
C	0.65977	3.75176	0.48894
C	0.03803	4.96670	0.84126
H	0.45351	5.55307	1.66920
C	-1.08739	5.44087	0.16160
H	-1.55948	6.38457	0.45543
C	-1.59280	4.69506	-0.90800
H	-2.46654	5.06612	-1.45632
C	-1.01116	3.47396	-1.29932
C	1.92023	3.34831	1.25743
H	2.28074	2.40614	0.81086
C	3.03229	4.41253	1.09942
H	3.22619	4.65126	0.04036
H	3.97646	4.06065	1.55209
H	2.75546	5.35573	1.60319
C	1.64542	3.09605	2.75764
H	1.23121	3.99781	3.24320
H	2.58581	2.84533	3.28293
H	0.93763	2.26335	2.91810
C	-1.63433	2.72397	-2.47582
H	-0.95157	1.89239	-2.71997
C	-2.98976	2.10369	-2.07699
H	-2.85277	1.41981	-1.22400
H	-3.42816	1.53953	-2.92044
H	-3.71230	2.88723	-1.78465
C	-1.79524	3.60755	-3.73249
H	-2.53327	4.41335	-3.57184
H	-2.15625	3.00258	-4.58371
H	-0.84433	4.08001	-4.02782
C	3.74906	1.97299	-1.52534
H	4.02743	1.46857	-0.58761
H	3.86969	3.05883	-1.37880
H	4.46299	1.66096	-2.30818
C	1.69301	2.58888	-3.66029
H	2.58932	2.55183	-4.30328
H	1.51470	3.64385	-3.39047
H	0.83261	2.23589	-4.24881
C	1.76488	-2.89059	-3.23869
H	2.18475	-2.79682	-4.25476
H	1.07616	-3.75250	-3.23566
H	2.59262	-3.10511	-2.54482
C	-0.14082	-0.73695	-4.28185
H	-0.75480	0.15501	-4.07584
H	-0.81013	-1.53412	-4.64423
H	0.55735	-0.48957	-5.10074
C	-0.76421	-2.61113	-0.89809
C	-2.12690	-2.81282	-1.32068
C	-2.83993	-3.95278	-0.88871
H	-3.87338	-4.08935	-1.22891
C	-2.26057	-4.91640	-0.05267
H	-2.82844	-5.79837	0.26408
C	-0.92457	-4.74744	0.33384
H	-0.44733	-5.51001	0.96055
C	-0.16012	-3.63604	-0.08176
C	-2.86150	-1.83282	-2.23486
H	-2.17179	-0.99626	-2.43288
C	-4.12665	-1.25509	-1.56216
H	-4.85349	-2.05052	-1.31375
H	-4.63605	-0.54665	-2.23738
H	-3.87253	-0.70433	-0.64151
C	-3.23836	-2.50078	-3.57815
H	-2.36637	-2.97050	-4.06243
H	-3.66142	-1.75751	-4.27614
H	-3.99770	-3.29036	-3.43301
C	1.30426	-3.59146	0.35912
H	1.74534	-2.68460	-0.08666
C	1.43903	-3.49139	1.89590
H	0.90319	-2.61217	2.29618
H	2.50190	-3.41514	2.18652
H	1.03232	-4.39299	2.39067
C	2.09078	-4.82115	-0.15380
H	1.73092	-5.75473	0.31465
H	3.16129	-4.72009	0.09789
H	2.00460	-4.93989	-1.24536
C	-1.57700	0.79414	1.99281
H	-1.23444	1.84944	2.01260
C	-3.01304	0.77214	2.53769
C	-4.09713	1.04390	1.67248
H	-3.89109	1.27194	0.62328
C	-5.41891	1.03862	2.14925
H	-6.24441	1.25287	1.46112
C	-5.68229	0.77185	3.50338
H	-6.71225	0.77275	3.87644
C	-4.61145	0.51917	4.37704
H	-4.80303	0.32617	5.43867
C	-3.28944	0.51775	3.89886
H	-2.44456	0.31592	4.56718
C	2.57041	-0.35477	1.63174
H	1.99932	-0.14820	2.56397
C	3.99743	-0.64738	1.69246
C	4.64061	-0.60846	2.95341
H	4.05794	-0.35160	3.84507
C	6.00739	-0.89360	3.05020
H	6.50800	-0.86107	4.02278
C	6.73470	-1.22317	1.89240
H	7.80391	-1.44741	1.96854
C	6.09947	-1.26830	0.63528
H	6.67573	-1.52687	-0.25864
C	4.73592	-0.98171	0.52861
H	4.21797	-1.00685	-0.43530
K	-2.45754	-2.12119	1.75934

INT(F-H)*cis*

SCF (BP86) Energy = -2019.37934393
Enthalpy 0K = -2018.430865
Enthalpy 298K = -2018.429921
Free Energy 298K = -2018.586463
Lowest Frequency = 13.1562 cm^{-1}
Second Frequency = 18.5187 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.69628406
SCF (C6H6) Energy = -2019.38938201
SCF (Et2O) Energy = -2019.39509552
SCF (BS2) Energy = -3791.22740967

S	-1.35718	-1.38199	-2.47469
Si	-1.12261	0.58644	3.17802
Si	1.98594	0.11249	2.88331
Al	0.10327	-0.01523	0.44304
O	0.41097	-0.10390	3.46758
O	0.25872	0.54457	-1.30093
O	-0.59914	-1.67332	0.16977
N	-1.09248	1.03747	1.45875
N	1.86046	-0.23028	1.14006
C	-1.89844	2.11112	0.93316
C	-3.31654	1.96830	0.74672
C	-4.06919	3.04405	0.23377
H	-5.15037	2.91637	0.10493
C	-3.47867	4.26134	-0.11313
H	-4.08226	5.08355	-0.51208
C	-2.10078	4.40724	0.06609

H	-1.62467	5.36060	-0.19144
C	-1.30273	3.36874	0.58357
C	-4.08427	0.69327	1.09890
H	-3.34324	-0.06902	1.39333
C	-5.03904	0.92666	2.29378
H	-4.50605	1.32256	3.17426
H	-5.54105	-0.01264	2.58735
H	-5.82429	1.65764	2.03057
C	-4.88906	0.13950	-0.10134
H	-5.71612	0.81650	-0.37924
H	-5.33181	-0.84065	0.14766
H	-4.25770	0.01076	-0.99759
C	0.18293	3.66235	0.77907
H	0.65767	2.72705	1.12437
C	0.86628	4.08532	-0.53789
H	0.75849	3.30217	-1.30500
H	1.94210	4.26950	-0.37289
H	0.43232	5.01815	-0.93946
C	0.40038	4.74217	1.86488
H	-0.04292	5.70618	1.55766
H	1.47772	4.91342	2.04163
H	-0.06511	4.45592	2.82241
C	-2.26231	-0.84156	3.69080
H	-2.18544	-1.67087	2.96818
H	-3.32036	-0.55196	3.77994
H	-1.92620	-1.21621	4.67335
C	-1.42088	2.09632	4.28273
H	-1.58028	1.78312	5.32833
H	-2.31117	2.65748	3.95176
H	-0.55868	2.78202	4.25586
C	3.10976	-1.10800	3.79334
H	3.32221	-0.72937	4.80759
H	4.07390	-1.24149	3.27366
H	2.62501	-2.09146	3.89097
C	2.54658	1.86450	3.35624
H	1.96087	2.64615	2.84885
H	3.61258	2.03508	3.13455
H	2.40868	1.99087	4.44465
C	2.91802	-0.79081	0.36045
C	3.87963	0.05946	-0.29848
C	4.84033	-0.49684	-1.16901
H	5.55980	0.16904	-1.65932
C	4.92255	-1.87760	-1.39416
H	5.68799	-2.29249	-2.05949
C	4.03968	-2.71842	-0.70484
H	4.12735	-3.80387	-0.83141
C	3.04909	-2.21662	0.17034
C	3.95562	1.56159	-0.02749
H	3.05051	1.83432	0.54057
C	3.99635	2.41478	-1.31241
H	4.88079	2.18569	-1.93359
H	4.04921	3.48735	-1.05959
H	3.09366	2.26672	-1.92736
C	5.19950	1.87265	0.84120
H	5.22251	1.26024	1.75759
H	5.21445	2.93651	1.13627
H	6.13038	1.66416	0.28348
C	2.17523	-3.25212	0.88369
H	1.42994	-2.70145	1.48109
C	1.41160	-4.15029	-0.11611
H	0.71107	-3.55927	-0.72737
H	0.80451	-4.89712	0.42252
H	2.10418	-4.70822	-0.77358
C	3.02401	-4.14194	1.82414
H	3.72120	-4.77886	1.25019
H	2.36898	-4.81320	2.40673
H	3.62213	-3.54721	2.53126
C	-0.84263	0.45025	-2.14810
H	-1.75059	0.90350	-1.69897
C	-0.58187	1.05513	-3.52336
C	0.67578	1.60749	-3.83481
H	1.43314	1.65589	-3.04555
C	0.92998	2.14839	-5.10829
H	1.90952	2.58809	-5.32693
C	-0.07549	2.14735	-6.08575
H	0.11727	2.57093	-7.07686
C	-1.34092	1.61570	-5.77697
H	-2.13694	1.62496	-6.52904
C	-1.59272	1.07386	-4.50946
H	-2.57728	0.65417	-4.27675
C	-1.72734	-1.77718	-0.61208
H	-2.47224	-0.98816	-0.37848
C	-2.40816	-3.13836	-0.51969
C	-3.43271	-3.52399	-1.41035
H	-3.70989	-2.85807	-2.23478
C	-4.09131	-4.75228	-1.24902
H	-4.88122	-5.03926	-1.95167
C	-3.74203	-5.61064	-0.19286
H	-4.25742	-6.56898	-0.06815
C	-2.73218	-5.22769	0.70357
H	-2.45894	-5.88568	1.53594
C	-2.07049	-3.99981	0.54212
H	-1.28722	-3.68390	1.23596
K	1.84177	-1.28904	-2.54688

H_{cis}

SCF (BP86) Energy = -2019.38325836
Enthalpy 0K = -2018.434691
Enthalpy 298K = -2018.433746
Free Energy 298K = -2018.589415
Lowest Frequency = 13.5058 cm^{-1}
Second Frequency = 23.3818 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.70130019
SCF (C6H6) Energy = -2019.39360435
SCF (Et2O) Energy = -2019.39942822
SCF (BS2) Energy = -3791.23155250

S	0.67906	3.05256	-0.16460
Si	0.43408	-3.36456	1.13142
Si	-1.26377	-2.94025	-1.43444
Al	-0.00243	-0.42889	-0.04084
O	-0.52691	-3.83311	-0.19819
O	0.91620	0.52822	-1.28392
O	-0.63518	0.93733	1.02917
N	1.05223	-1.73154	0.81956
N	-1.49545	-1.27064	-0.84629
C	2.38462	-1.31146	1.18816
C	2.64060	-0.72184	2.47329
C	3.90279	-0.15255	2.73535
H	4.08669	0.30853	3.71222
C	4.92942	-0.17570	1.78406
H	5.89830	0.28764	1.99985
C	4.71254	-0.83909	0.57211
H	5.52952	-0.91091	-0.15547
C	3.47206	-1.43285	0.26174
C	1.62433	-0.81104	3.61521
H	0.63777	-1.00603	3.16048
C	1.99059	-2.01066	4.52588
H	2.07640	-2.95048	3.95639
H	1.23272	-2.15385	5.31738
H	2.96461	-1.83499	5.01701
C	1.51256	0.45688	4.48770
H	2.44348	0.65307	5.04901
H	0.70926	0.33022	5.23451
H	1.28019	1.35827	3.89942

C	3.36873	-2.24523	-1.03131
H	2.35068	-2.66984	-1.06300
C	3.56467	-1.39159	-2.30154
H	2.80332	-0.60117	-2.36615
H	3.49146	-2.02328	-3.20544
H	4.56025	-0.91262	-2.31473
C	4.38265	-3.41484	-1.02803
H	5.42159	-3.04249	-1.07607
H	4.22430	-4.06285	-1.90863
H	4.29458	-4.03629	-0.12242
C	-0.70925	-3.51248	2.64354
H	-1.42751	-2.67959	2.69776
H	-0.13768	-3.52626	3.58558
H	-1.27974	-4.45518	2.57773
C	1.82359	-4.63904	1.30705
H	1.42954	-5.55645	1.77650
H	2.64917	-4.26135	1.93324
H	2.23424	-4.90942	0.32197
C	-2.92474	-3.75704	-1.83438
H	-2.74505	-4.74631	-2.28844
H	-3.51713	-3.15849	-2.54664
H	-3.52771	-3.90722	-0.92487
C	-0.12451	-3.03130	-2.94798
H	0.79107	-2.43741	-2.79257
H	-0.62513	-2.65282	-3.85510
H	0.17320	-4.07744	-3.13436
C	-2.72426	-0.58411	-1.06401
C	-2.95009	0.19991	-2.25046
C	-4.15006	0.93418	-2.38812
H	-4.31603	1.51163	-3.30552
C	-5.13720	0.93041	-1.39194
H	-6.06234	1.50373	-1.51981
C	-4.94212	0.13226	-0.25410
H	-5.72856	0.08447	0.50830
C	-3.77950	-0.64817	-0.08528
C	-1.94005	0.24811	-3.39794
H	-1.02895	-0.26431	-3.04633
C	-1.54758	1.69274	-3.77838
H	-2.42217	2.29149	-4.09292
H	-0.83776	1.69124	-4.62232
H	-1.04136	2.20746	-2.94289
C	-2.48689	-0.50292	-4.63493
H	-2.76038	-1.54326	-4.39191
H	-1.73144	-0.52657	-5.43983
H	-3.38967	-0.00838	-5.03690
C	-3.68585	-1.56509	1.13373
H	-2.82310	-2.22899	0.95900
C	-3.40193	-0.77295	2.42880
H	-2.43174	-0.25301	2.36141
H	-3.36821	-1.44716	3.30265
H	-4.19639	-0.02650	2.61952
C	-4.94440	-2.44467	1.30387
H	-5.83076	-1.85018	1.58991
H	-4.77929	-3.18802	2.10269
H	-5.19179	-2.98750	0.37647
C	1.68999	1.62936	-1.01842
H	2.47410	1.42933	-0.25639
C	2.32506	2.25802	-2.25086
C	2.01248	1.78662	-3.53817
H	1.30667	0.95725	-3.62977
C	2.61760	2.35549	-4.67116
H	2.37080	1.97405	-5.66818
C	3.54204	3.40159	-4.52889
H	4.01521	3.84401	-5.41201
C	3.86730	3.87039	-3.24371
H	4.59675	4.67845	-3.12213
C	3.26555	3.30099	-2.11300
H	3.52183	3.66617	-1.11174
C	0.20611	2.00198	1.36280
H	1.18726	1.64724	1.74244
C	-0.42179	2.96052	2.37493
C	0.24988	4.14154	2.76642
H	1.22964	4.36800	2.33293
C	-0.33113	5.02112	3.68982
H	0.20603	5.92974	3.98176
C	-1.59563	4.74366	4.24024
H	-2.04718	5.43367	4.96054
C	-2.26312	3.56672	3.87241
H	-3.23455	3.32360	4.31736
C	-1.67765	2.67905	2.95041
H	-2.16913	1.73259	2.70631
K	-2.51434	2.45059	-0.17472

TS(H) ***cis-trans***

SCF (BP86) Energy = -2019.34672441
Enthalpy 0K = -2018.399533
Enthalpy 298K = -2018.398589
Free Energy 298K = -2018.555260
Lowest Frequency = -54.3046 cm^{-1}
Second Frequency = 15.0834 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.65958100
SCF (C6H6) Energy = -2019.35885664
SCF (Et2O) Energy = -2019.36594854
SCF (BS2) Energy = -3791.19534178

S	1.07274	-0.40377	3.39609
Si	1.11364	0.91373	-3.12062
Si	-1.14883	-1.24778	-2.99888
Al	0.07389	-0.12316	-0.44082
O	0.40235	-0.62861	-3.30412
O	-0.51853	0.18134	1.21669
O	1.77381	-1.01903	-0.25196
N	0.65374	1.34264	-1.46538
N	-1.19352	-1.31553	-1.21920
C	0.84295	2.66806	-0.92253
C	2.08441	3.05335	-0.31665
C	2.20608	4.33603	0.25528
H	3.15598	4.61635	0.72529
C	1.15460	5.25654	0.23391
H	1.27049	6.24586	0.68942
C	-0.04415	4.89528	-0.38787
H	-0.87128	5.61410	-0.42072
C	-0.22077	3.62624	-0.97201
C	3.31901	2.14861	-0.29493
H	3.04164	1.20144	-0.78576
C	4.48167	2.78993	-1.09085
H	4.16984	3.09229	-2.10455
H	5.32663	2.08475	-1.18446
H	4.85953	3.69475	-0.58210
C	3.79911	1.81613	1.13672
H	4.06267	2.73251	1.69453
H	4.70209	1.18142	1.09820
H	3.03936	1.27389	1.72483
C	-1.56593	3.32237	-1.63003
H	-1.47457	2.32316	-2.08975
C	-2.69984	3.26072	-0.58480
H	-2.47814	2.51713	0.19650
H	-3.66045	2.99610	-1.06262
H	-2.83247	4.23617	-0.08371
C	-1.92169	4.34010	-2.73739
H	-2.08240	5.34975	-2.31945
H	-2.85619	4.04573	-3.24853
H	-1.12605	4.41704	-3.49578
C	2.94265	0.58226	-3.49143
H	3.01975	0.12494	-4.49340

H	3.37683	-0.11803	-2.76132
H	3.54700	1.50300	-3.49096
C	0.50489	2.15856	-4.41359
H	0.85866	1.86123	-5.41574
H	0.91752	3.15879	-4.19508
H	-0.59191	2.24156	-4.44159
C	-1.26584	-2.94140	-3.83344
H	-1.39975	-2.80641	-4.92040
H	-2.12423	-3.52481	-3.45896
H	-0.34600	-3.52486	-3.67313
C	-2.40013	-0.10391	-3.86074
H	-2.47146	0.88667	-3.38320
H	-3.41064	-0.53997	-3.89942
H	-2.06299	0.04437	-4.90180
C	-2.04100	-2.15688	-0.43159
C	-3.40838	-1.79647	-0.14781
C	-4.18497	-2.58993	0.72327
H	-5.22237	-2.29632	0.92072
C	-3.68047	-3.75619	1.31333
H	-4.30703	-4.36874	1.97135
C	-2.37418	-4.14969	0.99563
H	-1.98363	-5.08769	1.40667
C	-1.54970	-3.38967	0.13656
C	-4.10575	-0.62072	-0.83127
H	-3.32704	-0.03128	-1.34223
C	-4.85242	0.31533	0.14263
H	-5.67572	-0.20396	0.66526
H	-5.30099	1.15834	-0.40980
H	-4.17929	0.74227	0.90297
C	-5.10450	-1.15617	-1.88789
H	-4.62639	-1.86206	-2.58678
H	-5.53789	-0.32723	-2.47447
H	-5.93679	-1.69375	-1.39885
C	-0.17149	-3.96965	-0.19004
H	0.39995	-3.18504	-0.71330
C	0.60962	-4.40865	1.07152
H	0.62823	-3.62976	1.85316
H	1.65436	-4.65173	0.81352
H	0.17039	-5.31767	1.52094
C	-0.30161	-5.18884	-1.13592
H	-0.84578	-6.01140	-0.63772
H	0.69693	-5.56822	-1.41618
H	-0.84537	-4.93893	-2.05837
C	0.17906	0.82614	2.28354
H	0.95005	1.50833	1.87805
C	-0.78152	1.64121	3.14932
C	-2.16529	1.66397	2.88989
H	-2.53171	1.14813	1.99618
C	-3.05089	2.38056	3.71804
H	-4.12297	2.38970	3.48925
C	-2.55711	3.10320	4.81216
H	-3.23922	3.66786	5.45657
C	-1.17151	3.11036	5.06431
H	-0.77346	3.68236	5.90963
C	-0.29534	2.38465	4.24845
H	0.77735	2.36637	4.46598
C	2.27155	-1.61787	0.76377
H	1.63743	-1.83025	1.64045
C	3.67693	-1.99535	0.81500
C	4.20194	-2.50025	2.03185
H	3.56020	-2.51697	2.91920
C	5.53241	-2.92399	2.09874
H	5.93926	-3.30197	3.04196
C	6.35059	-2.85466	0.95503
H	7.39292	-3.18603	1.00943
C	5.83573	-2.35850	-0.25761
H	6.47560	-2.31062	-1.14465
C	4.50813	-1.92592	-0.33093
H	4.08699	-1.54899	-1.26716
K	-1.79521	-1.53127	2.83724

H_{trans}

SCF (BP86) Energy = -2019.36889229
Enthalpy 0K = -2018.420171
Enthalpy 298K = -2018.419227
Free Energy 298K = -2018.575878
Lowest Frequency = 16.1717 cm^{-1}
Second Frequency = 21.8753 cm^{-1}
SCF (BP86-D3BJ) Energy = -2019.68960943
SCF (C6H6) Energy = -2019.38019437
SCF (Et2O) Energy = -2019.38676972
SCF (BS2) Energy = -3791.21753970

S	-0.11947	-2.51744	1.95413
Si	1.22564	1.07120	-3.17974
Si	-1.14861	2.71568	-1.99583
Al	-0.01154	0.21250	-0.43990
O	-0.21202	1.99134	-3.20385
O	0.22372	0.17578	1.38802
O	-0.38153	-1.56083	-0.67405
N	1.48940	0.60110	-1.48936
N	-1.43748	1.43524	-0.77487
C	2.81706	0.33572	-0.97882
C	3.43727	-0.94897	-1.11916
C	4.70990	-1.16957	-0.55171
H	5.17319	-2.15669	-0.66448
C	5.39318	-0.16868	0.14405
H	6.37706	-0.36675	0.58298
C	4.80325	1.09417	0.25760
H	5.33542	1.89229	0.78809
C	3.54078	1.37063	-0.29970
C	2.79943	-2.10230	-1.89540
H	1.78960	-1.77831	-2.19590
C	3.61836	-2.42089	-3.16915
H	3.76429	-1.52629	-3.79826
H	3.11309	-3.19202	-3.77799
H	4.62139	-2.80540	-2.91077
C	2.64358	-3.37618	-1.03574
H	3.62048	-3.74862	-0.67865
H	2.17700	-4.18511	-1.62424
H	2.00140	-3.19635	-0.15789
C	2.97576	2.78028	-0.15464
H	2.09965	2.82454	-0.82095
C	2.48469	3.04522	1.28632
H	1.72606	2.30243	1.58320
H	2.04454	4.05614	1.37374
H	3.32085	2.98046	2.00569
C	3.97054	3.87416	-0.59940
H	4.84322	3.93631	0.07492
H	3.48107	4.86451	-0.59026
H	4.34956	3.68812	-1.61822
C	0.83093	-0.34258	-4.38222
H	0.46379	0.08001	-5.33364
H	0.03767	-0.98807	-3.96922
H	1.70806	-0.97144	-4.60225
C	2.67344	2.09490	-3.84287
H	2.53379	2.29734	-4.91821
H	3.62737	1.55541	-3.71650
H	2.75556	3.05988	-3.31756
C	-2.76025	3.34722	-2.78483
H	-2.65496	4.42123	-3.01519
H	-3.63122	3.22573	-2.11937
H	-2.97417	2.82357	-3.72982
C	-0.21956	4.28327	-1.43245
H	0.59901	4.09692	-0.72175

H	-0.90625	5.01977	-0.98349
H	0.21552	4.74759	-2.33530
C	-2.63212	1.33532	-0.00208
C	-2.91455	2.26032	1.06768
C	-4.06142	2.08583	1.87463
H	-4.26787	2.81487	2.66815
C	-4.94053	1.01379	1.67848
H	-5.82837	0.89322	2.30935
C	-4.69267	0.12695	0.61889
H	-5.40160	-0.68600	0.43477
C	-3.58529	0.27233	-0.24409
C	-2.01749	3.46200	1.36850
H	-1.14197	3.38552	0.70637
C	-1.48533	3.47046	2.81882
H	-2.30142	3.50576	3.56395
H	-0.84780	4.35459	2.99056
H	-0.85741	2.58474	3.01982
C	-2.75292	4.78819	1.06585
H	-3.12908	4.81498	0.02992
H	-2.07885	5.65069	1.21026
H	-3.62051	4.92606	1.73599
C	-3.47463	-0.66322	-1.45593
H	-2.40485	-0.87784	-1.62020
C	-4.21438	-2.00821	-1.29162
H	-3.96670	-2.52962	-0.35174
H	-3.93725	-2.68207	-2.11863
H	-5.31181	-1.88104	-1.33253
C	-4.00566	0.03148	-2.73187
H	-5.06447	0.32223	-2.60891
H	-3.93844	-0.65689	-3.59234
H	-3.42502	0.93029	-2.97235
C	0.95825	-0.92174	1.84738
H	1.77422	-1.19462	1.15085
C	1.51648	-0.73747	3.25198
C	1.24336	0.42928	3.99071
H	0.68869	1.23922	3.50659
C	1.73926	0.58545	5.29731
H	1.53219	1.50822	5.85085
C	2.51655	-0.42563	5.88088
H	2.90588	-0.30577	6.89724
C	2.81088	-1.58581	5.14222
H	3.43245	-2.37269	5.58245
C	2.31834	-1.74098	3.83949
H	2.55042	-2.64688	3.26907
C	-1.04176	-2.36299	0.20911
H	-2.02752	-1.94364	0.51128
C	-1.26825	-3.78079	-0.29389
C	-1.96261	-4.72263	0.49389
H	-2.31046	-4.44467	1.49682
C	-2.20458	-6.01639	0.01104
H	-2.74083	-6.73889	0.63567
C	-1.76219	-6.38376	-1.27178
H	-1.95209	-7.39354	-1.65066
C	-1.08117	-5.44688	-2.06434
H	-0.73965	-5.72341	-3.06786
C	-0.83617	-4.15148	-1.57943
H	-0.31481	-3.40720	-2.18675
K	-2.03343	-0.14032	2.84318