Electronic Supplementary Material (ESI) for ChemComm.

Aluminyl Derived Ethene Functionalization with Heteroallenes, Leading to an Intramolecular Ligand Rearrangement

Andrea O'Reilly, Michael G. Gardiner, Claire L. McMullin, J. Robin Fulton and Martyn P. Coles

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General Experimental Procedures

All manipulations were performed under a dry nitrogen atmosphere in a conventional glovebox or under a dry argon atmosphere using standard Schlenk-line techniques. Deuterated solvents were degassed using freeze-pump-thaw method on a Schlenk-line and stored over activated 5 Å sieves for 24 hours prior to use. Hexane, toluene and diethyl ether (Et_2O) were obtained from a PureSolv MD 5 system and stored over activated 5 Å sieves for 24 hours prior to use. NMR spectra were recorded using a Jeol JNM-ECZ500S 500 MHz spectrometer equipped with a ROYAL digital auto tune probe S, operating at 500.1 (^{1}H) and 125.8 (^{13}C{^{1}H}). Spectra were recorded at 294 K (unless stated otherwise) and proton and carbon chemical shifts were referenced internally to residual solvent resonances. Coupling constants are quoted in Hz. IR spectra were recorded on solid samples using a Bruker Alpha FT-IR Spectrometer.

K[Al(NON)(η-C_2H_4)] was prepared according to a modified literature procedures.[S1] All other chemicals were purchased from Sigma-Aldrich and used without further purification.

Synthesis of K[Al(NON)(η-C_2H_4)] (I)

A solution of K[Al(NON)] (300 mg, 0.27 mmol) was sealed in an ampule and degassed on a Schlenk line. The ampule was charged with ethene gas (~1.5 bar) and the reaction mixture was stirred at room temperature for 2 days. The solvent was removed *in vacuo* and the solid was washed with hexane (3 x 10 mL) to afford a white powder that was used without any further purification.

^{1}H NMR (500 MHz, C_6D_6): δ 7.04 (d, J = 7.6, 4H, C_6H_3), 6.92 (t, J = 7.6, 2H, C_6H_3), 4.23 (sept, J = 6.9, 4H, CHMe_2), 1.39 (d, J = 6.9, 12H, CHMe_2), 1.28 (d, J = 6.9, 12H, CHMe_2), 0.47 (s, 12H, SiMe_2), -1.40 (s, 4H, C_2H_4).

IR (solid, cm^{-1}): 2961 (m), 2867 (w), 1463 (w), 1424 (m), 1383 (w), 1361 (w), 1311 (w), 1246 (s), 1188 (m), 1108 (w), 1041 (m), 1014 (s), 963 (w), 942 (s), 933 (s), 841 (s), 824 (s), 792 (vs), 775 (vs), 696 (s), 652 (s), 603 (s), 562 (br s), 449 (m), 433 (m).

Figure S1 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NON)(η-C_2H_4) (**I**)

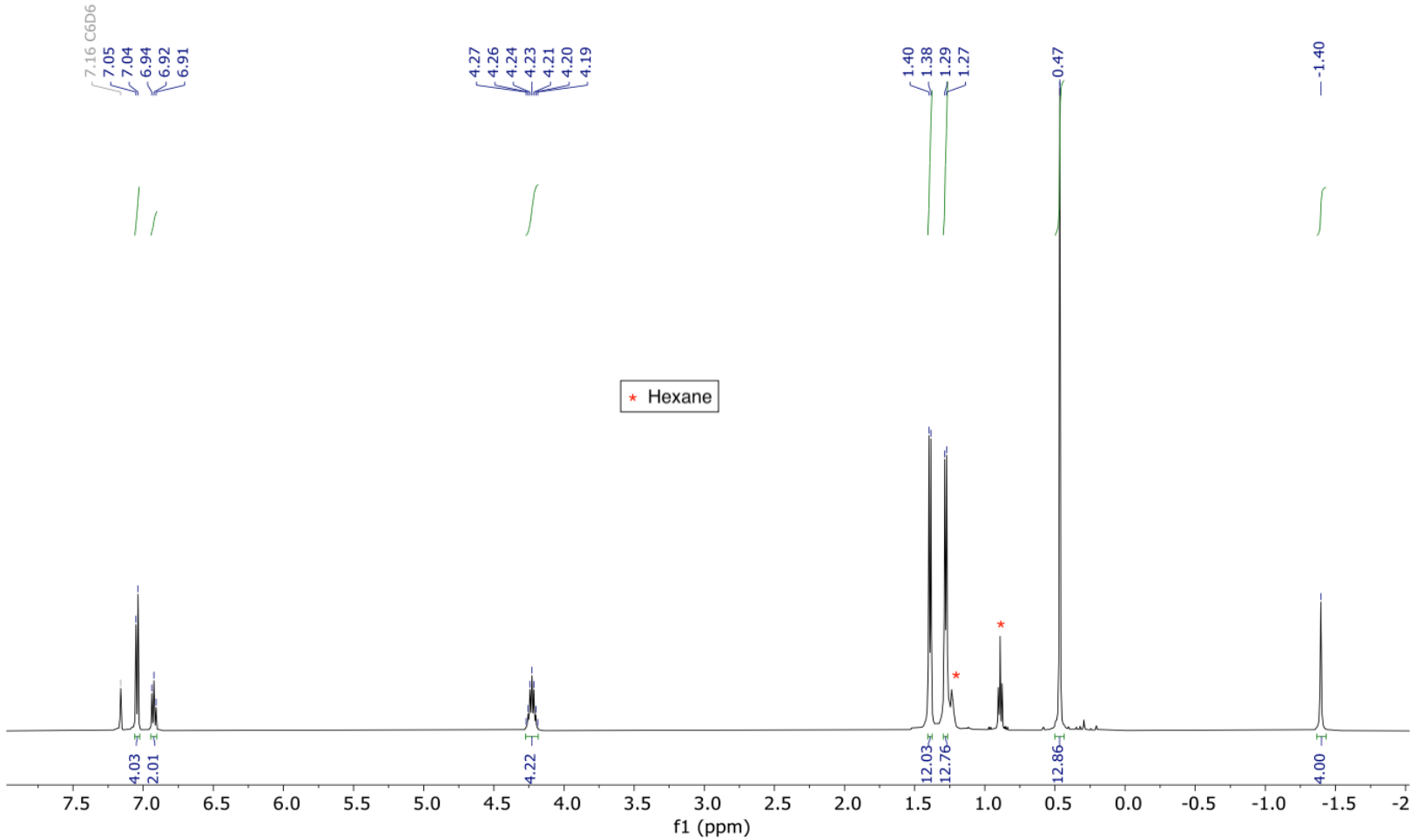
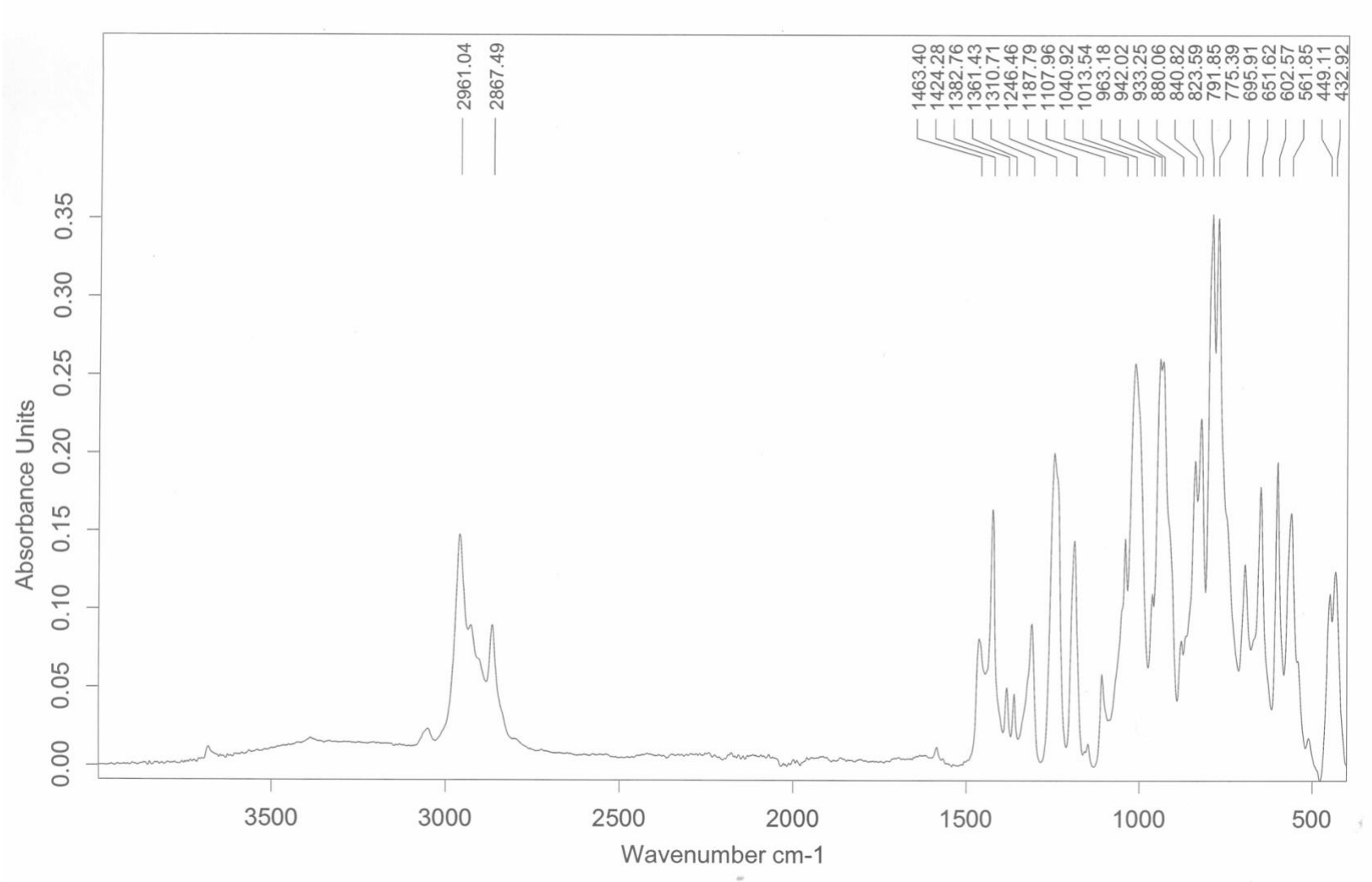


Figure S2 IR spectrum (solid, cm^{-1}) of K[Al(NON)(η-C_2H_4) (**I**)



Synthesis of K[Al(NON){$CH_2CH_2{}^{13}C(=O)O$}] (1)

A C_6D_6 solution of K[Al(NON)(C_2H_4)] (**I**, 30.3 mg, 0.05 mmol) in an NMR tube fitted with a J. Young's Teflon tap was degassed, and the tube was charged with ~1 bar of isotopically labelled $^{13}CO_2$ gas. The reaction was analysed by ^{1}H NMR spectroscopy showing complete conversion to K[Al(NON){$CH_2CH_2{}^{13}C(=O)O$}] (**1**) after ~15 mins. The solvent was removed *in vacuo* and colourless crystals of [**1·(Et$_2$O)$_2$**]$_2$ suitable for X-ray diffraction were obtained by recrystallisation from Et_2O. Yield 32.7 mg, 81 %.

Accurate elemental analysis could not be obtained for **1**.

^{1}H NMR* (500 MHz, C_6D_6): δ 7.05 (d, *J* = 7.5, 2H, C_6H_3), 6.93 (d, *J* = 7.5, 2H, C_6H_3), 6.85 (t, *J* = 7.5, 2H, C_6H_3), 4.16 (m, 4H, C*H*Me$_2$), 1.79 (m, 2H, AlCH$_2$C*H*$_2$), 1.34 (d, *J* = 6.8, 6H, CH*Me*$_2$), 1.30 (dd‡, *J* = 7.1, 12H, CH*Me*$_2$), 1.14 (d, *J* = 6.8, 6H, CH*Me*$_2$), 0.53 (s, 6H, Si*Me*$_2$), 0.37 (s, 6H, Si*Me*$_2$), 0.17 (m, 2H, AlC*H*$_2$CH$_2$). ‡ overlapping peaks.

$^{13}C\{^1H\}$ NMR* (126 MHz, C_6D_6): δ 188.8 (O^{13}*C*{=O}), 148.0, 146.7, 124.3, 123.0, 122.4 (*C*$_6$H$_3$), 34.8 (d, $^1J_{CC}$ = 49, *C*H$_2{}^{13}$C), 27.7, 27.4 (*C*HMe$_2$), 26.0, 25.5, 25.4, 25.1 (CH*Me*$_2$), 3.0 (Si*Me*$_2$), 2.8 (d, $^2J_{CC}$ = 6, Al*C*H$_2$CH$_2{}^{13}$C), 2.5 (Si*Me*$_2$).

* NMR spectra were recorded under an atmosphere of $^{13}CO_2$.

IR (solid, cm^{-1}): 2963 (m), 2867 (w), 1578 (br m, υ_{CO}), 1461 (w), 1428 (m), 1381 (w), 1360 (w), 1312 (w), 1249 (s), 1182 (m), 1105 (w), 1042 (m), 998 (s), 932 (s), 882 (m), 857 (s), 823 (s), 794 (vs), 776 (vs), 747 (m), 703 (m), 675 (s), 629 (m), 603 (m), 576 (m), 450 (m).

Figure S3 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NON){$CH_2CH_2C(=O)O$}] (**1**) (recorded under atmosphere of $^{13}CO_2$).

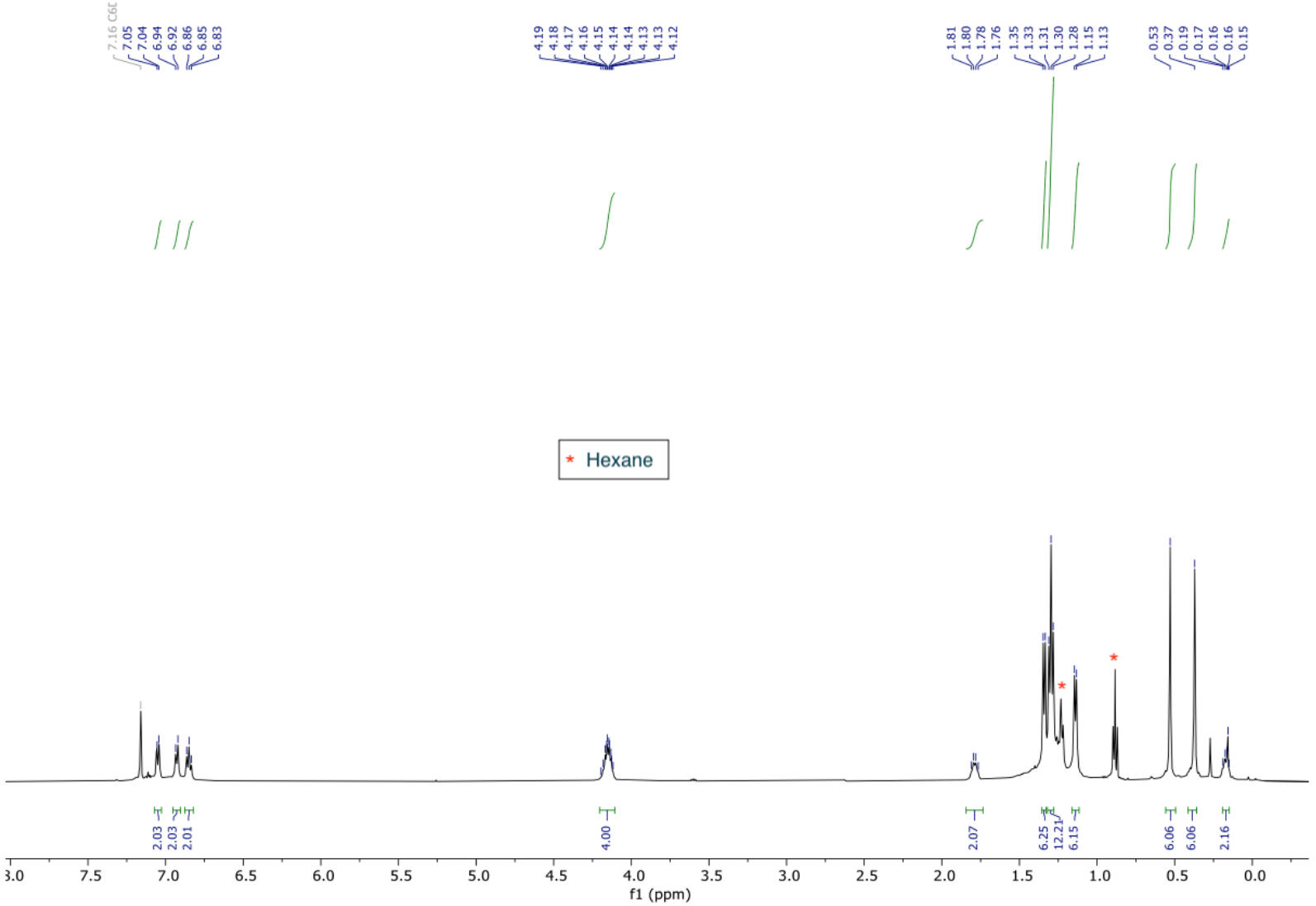


Figure S4 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of K[Al(NON){$CH_2CH_2C(=O)O$}] (**1**) (recorded under atmosphere of $^{13}CO_2$).

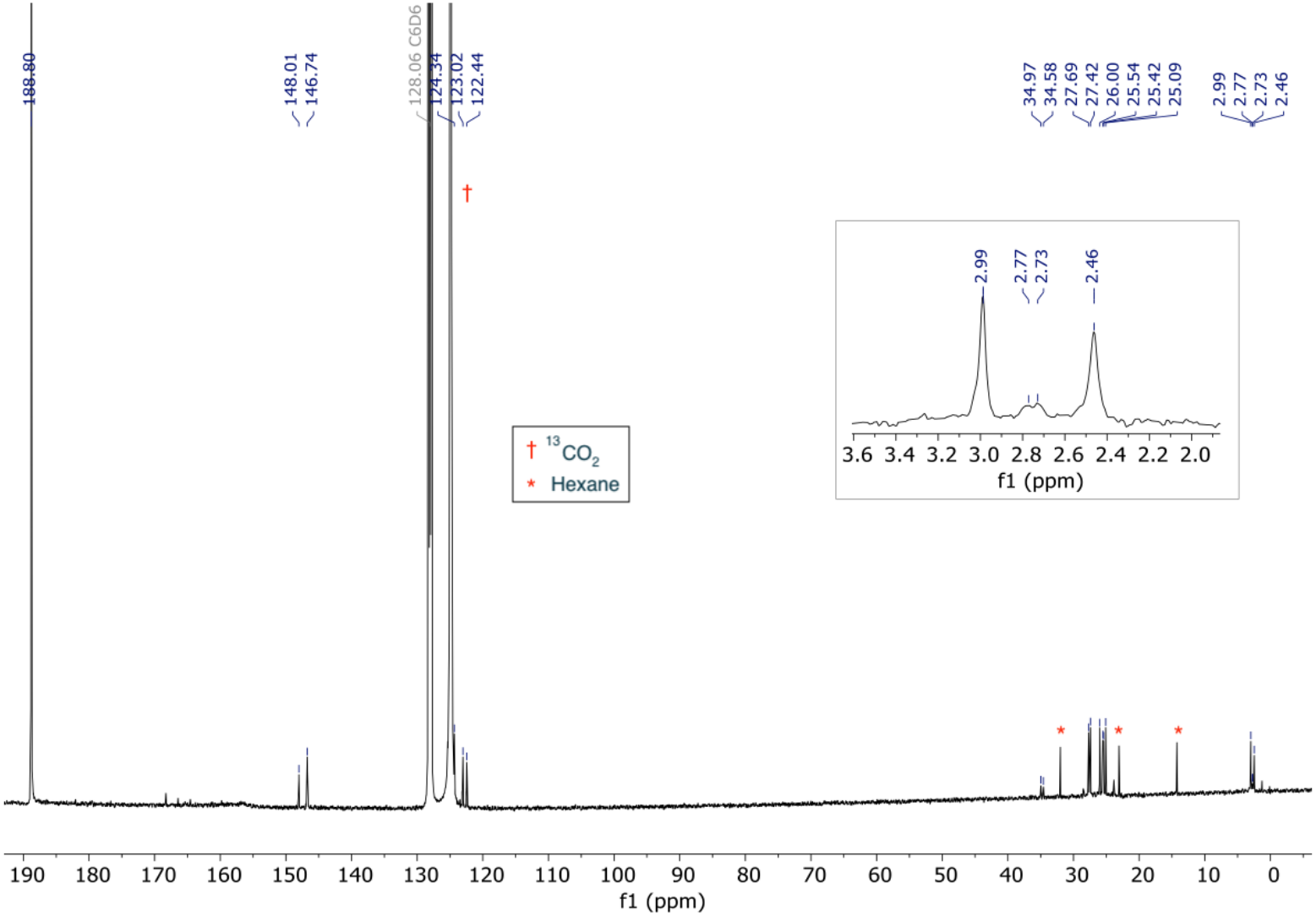


Figure S5 IR spectrum (solid, cm^{-1}) of K[Al(NON){$CH_2CH_2C(=O)O$}] (**1**).

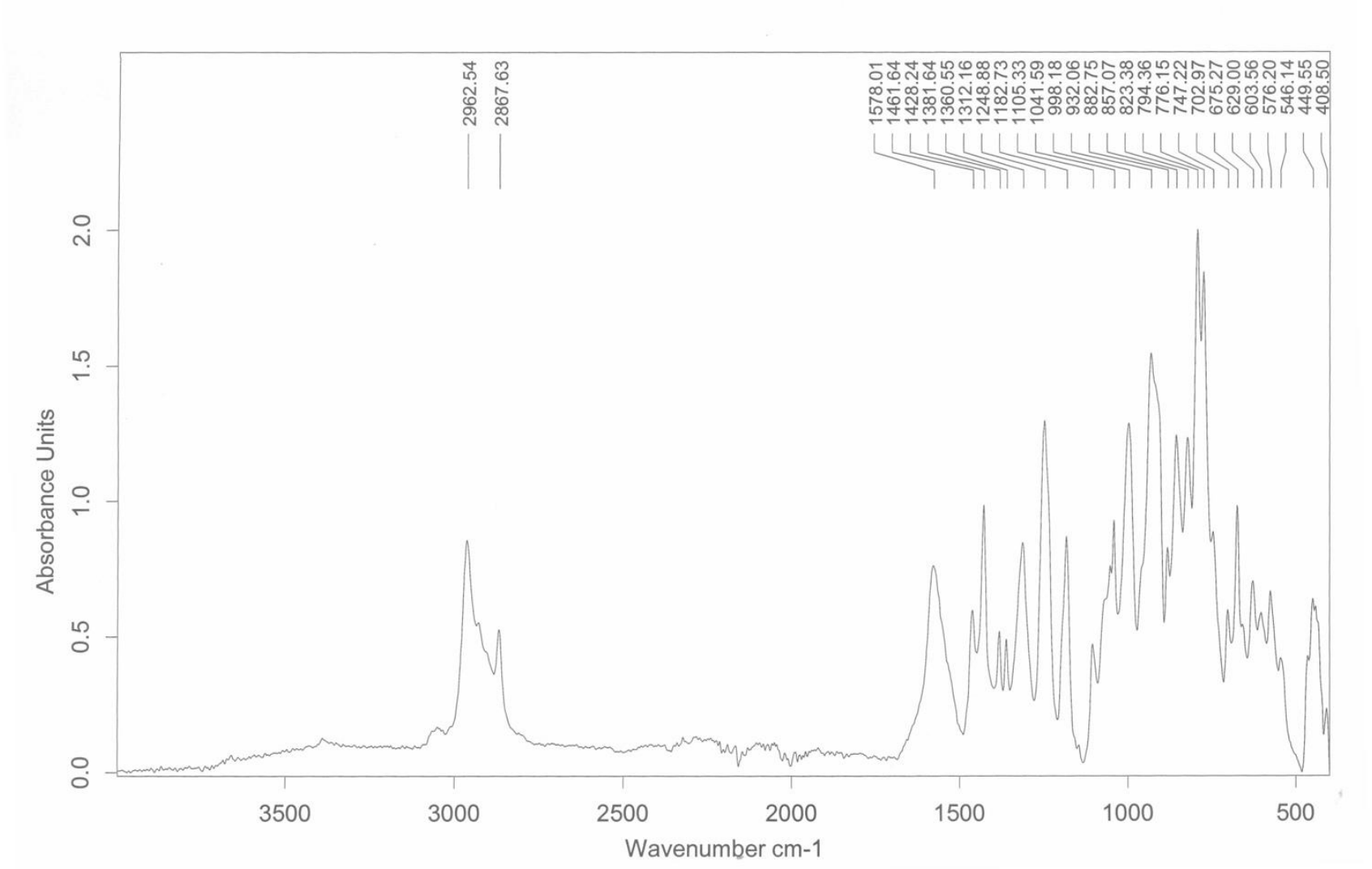
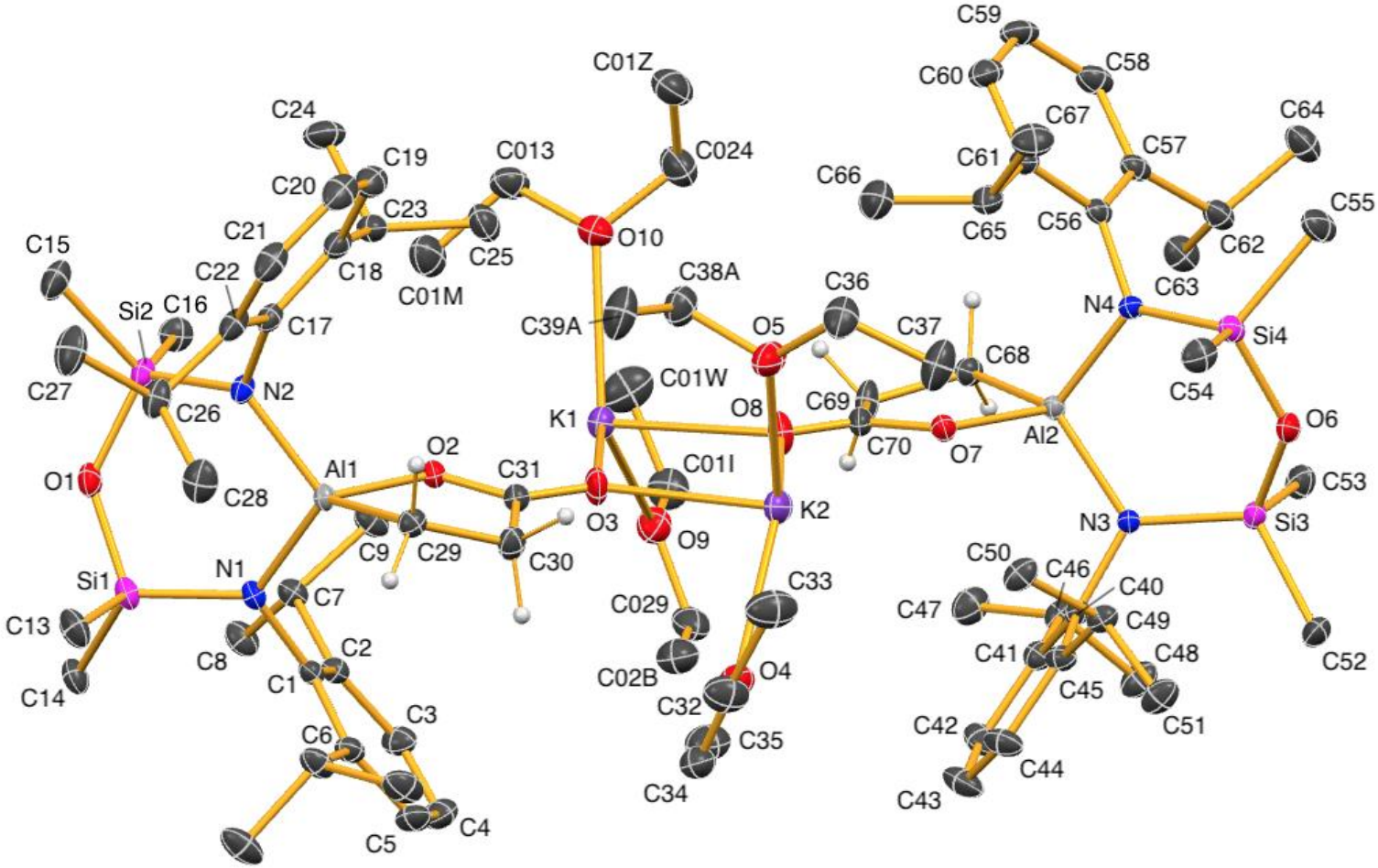


Figure S6 ORTEP (ellipsoids 30%, H-atoms {except C*H*$_2$ of metallacycle} and disordered atoms omitted), of the asymmetric unit of [{K(Et$_2$O)$_2$}(Al{NON}{CH$_2$CH$_2$C(=O)O}]$_2$ [**1·(Et$_2$O)$_2$**]$_2$.



Synthesis of K[Al(NON){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (2)

Di*iso*propylcarbodiimide (5.0 mg, 0.04 mmol) was added to a solution of K[Al(NON)(C_2H_4)] (**I**) (22.7 mg, 0.04 mmol) in C_6D_6. After 8 h at room temperature a pale golden-brown solution had formed that was analysed by ^{1}H NMR spectroscopy, showing complete conversion to K[Al(NON){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (**2**). The solution was transferred to a vial and the solvent was removed *in vacuo* to afford **2** as a microcrystalline solid. Crystals suitable for X-ray diffraction were obtained by slow evaporation from a toluene/Et_2O solution, affording the solvated compound [(**2**)(**2·Et_2O**)]. Yield 26 mg, 88 %.

Elemental analysis: Anal. Calcd. for $C_{37}H_{64}AlKN_4OSi_2$ (**2**) (*703.20*): C 63.20, H 9.17, N 7.97 %; Found: C 63.12, H 9.05, N 7.03 %.

^{1}H NMR (500 MHz, C_6D_6): δ 7.14 (s, 2H, C_6H_3), 7.02 (d, *J* = 7.5 , 2H, C_6H_3), 6.91 (t, *J* = 7.5 , 2H, C_6H_3), 4.39 (sept, *J* = 6.7 , 2H, C*H*Me_2), 4.31 (sept, *J* = 6.7 , 2H, C*H*Me_2), 3.50 (sept, *J* = 6.0 , 1H, C*H*Me_2), 3.14 (sept, *J* = 6.7, 1H, C*H*Me_2), 2.44 (t, *J* = 7.7 , 2H, CH_2), 1.46 (d, *J* = 6.7, 6H, CHMe_2), 1.36 (m, 12H, CHMe_2), 1.21 (d, *J* = 6.7 , 6H, CHMe_2), 0.91 (d, *J* = 6.7 , 6H, CHMe_2), 0.72 (d, *J* = 6.0, 6H, CHMe_2), 0.55 (s, 6H, SiMe_2), 0.51 (s, 6H, SiMe_2), 0.36 (br t , 2H, CH_2).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 174.2 (*C*=N), 148.3, 148.0, 147.9, 124.0, 123.9, 121.8 (C_6H_3), 47.2 (N*C*HMe_2), 46.8 (N*C*HMe_2), 28.8 (AlCH_2*C*H_2), 27.7, 27.7 (*CH*Me_2), 27.6, 27.2, 26.3, 26.2, 26.0, 23.3 (CHMe_2), 4.7, 4.0 (SiMe_2) 3.3 (Al*C*H_2).

IR (solid, cm^{-1}): 2963 (m), 2869 (br m), 1604 (m, υ_{CN}), 1587 (m, υ_{CN}), 1462 (w), 1427 (m), 1390 (w), 1381 (w), 1247 (m), 1174 (m), 1106 (w), 1040 (w), 1004 (br m), 976 (br m), 929 (s), 911 (s), 880 (m), 846 (s), 822 (s), 792 (vs), 781 (vs), 746 (m), 704 (s), 676 (s), 642 (w), 629 (m), 576 (w), 449 (w), 432 (w).

Figure S7 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NON){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (**2**). DIC = di*iso*propylcarbodiimide.

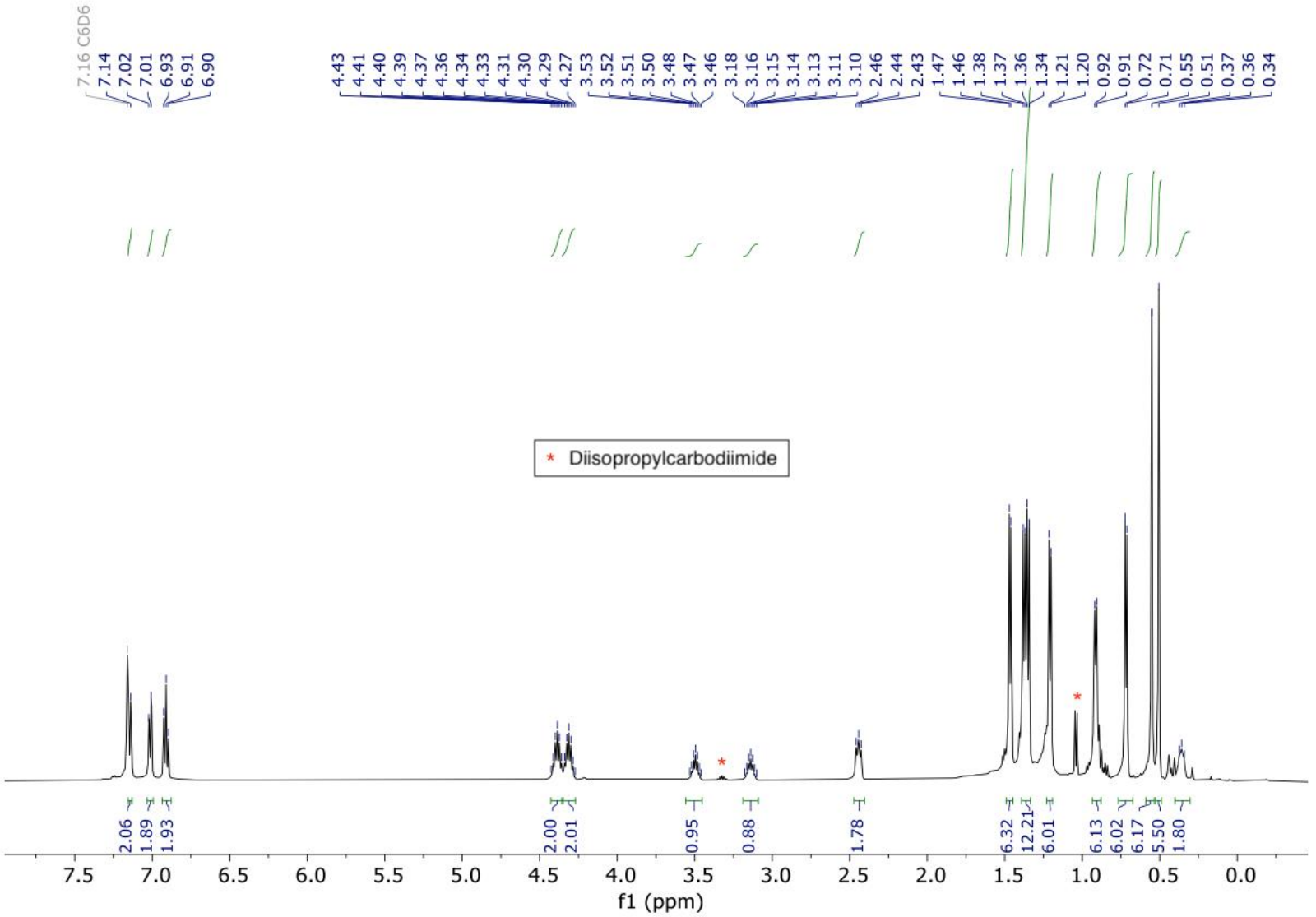


Figure S8 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of K[Al(NON){$CH_2CH_2C(=N$*i*Pr)N*i*Pr}] (**2**).

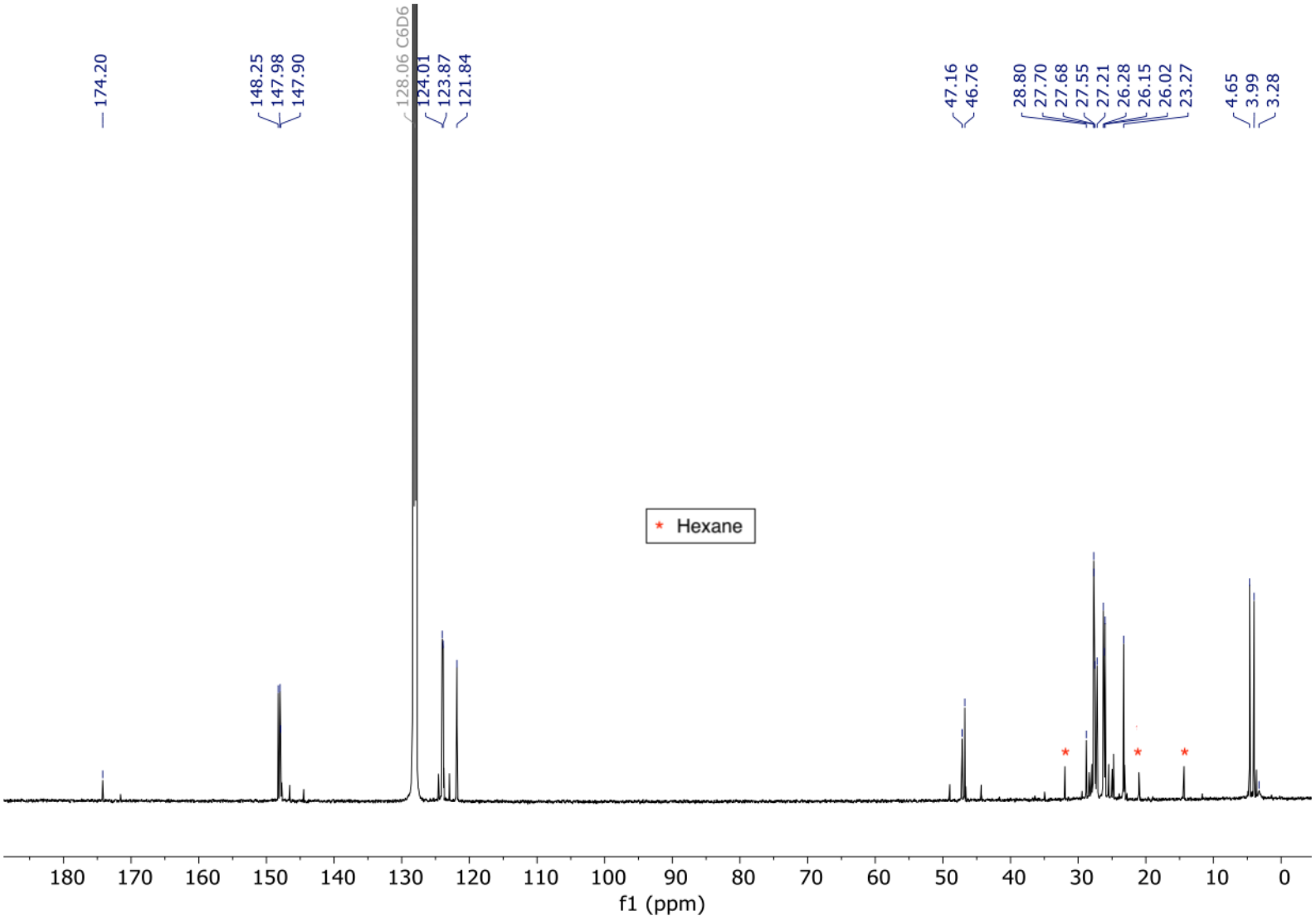


Figure S9 IR spectrum (solid, cm^{-1}) of K[Al(NON){$CH_2CH_2C(=N$*i*Pr)N*i*Pr}] (**2**).

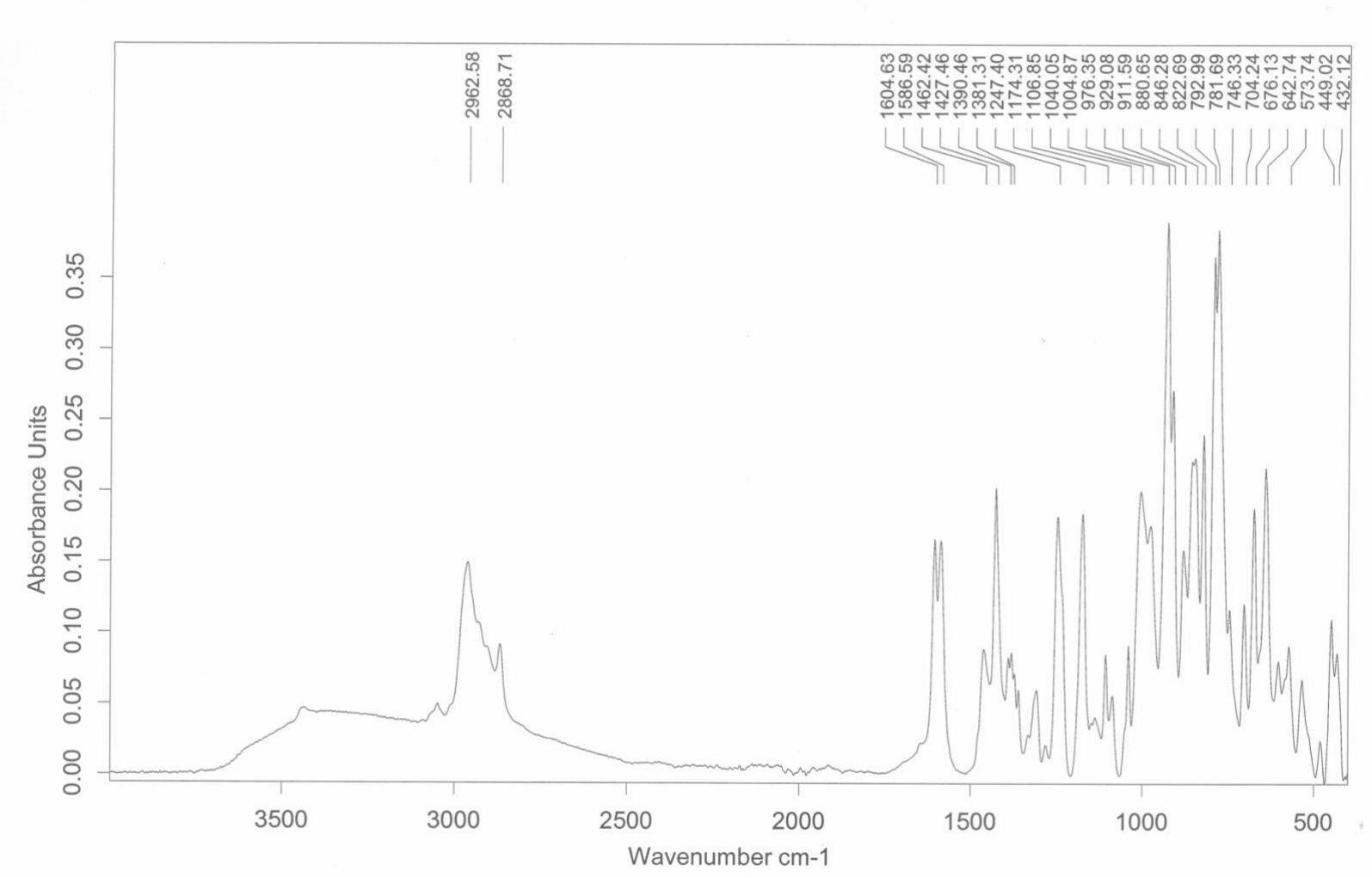
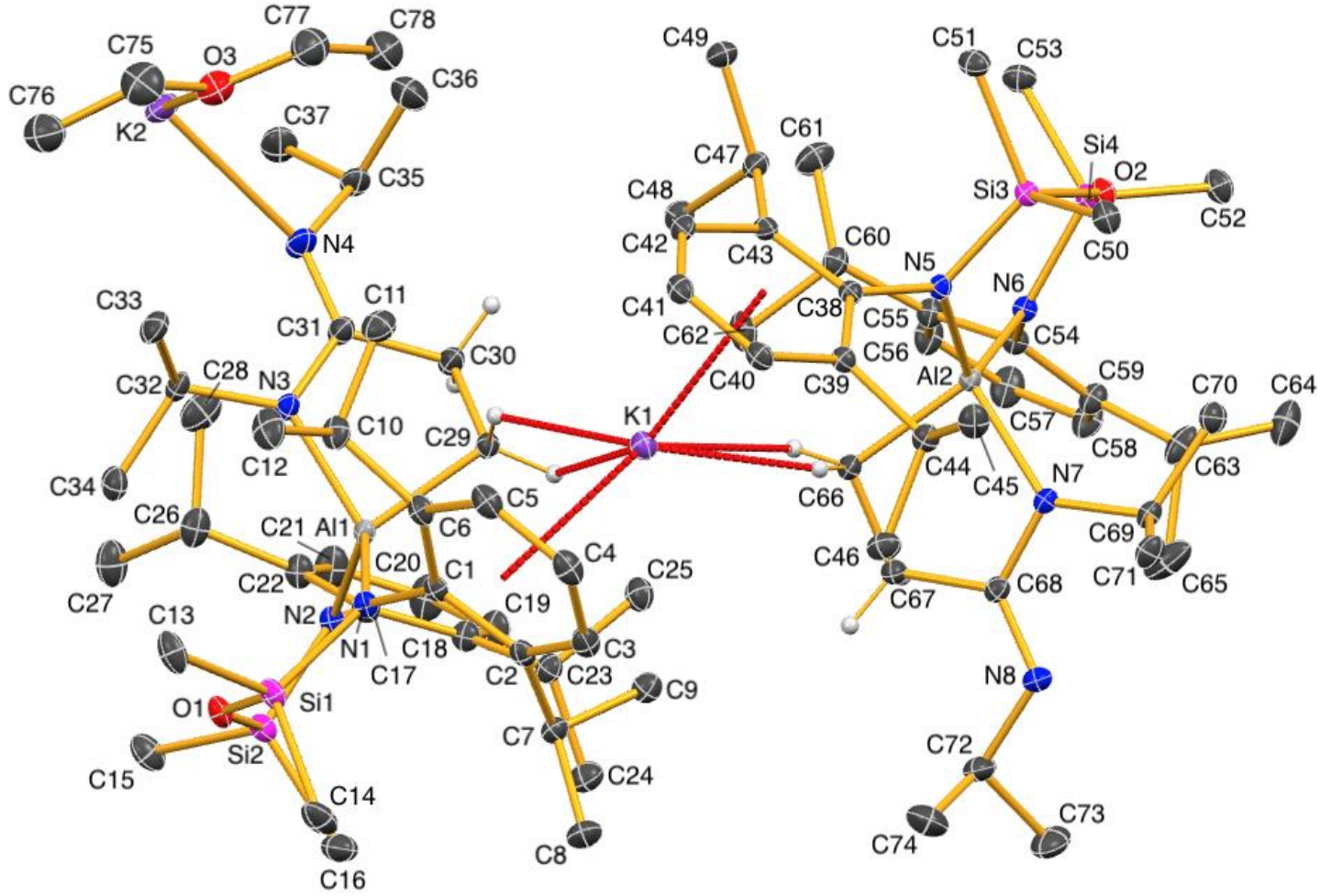


Figure S10 ORTEP (ellipsoids 30%, H-atoms {except C*H*$_2$ of metallacycle}, disordered atoms and toluene solvate omitted), of the asymmetric unit of [K(Et$_2$O)][Al(NON)(CH$_2$CH$_2$C{=N*i*Pr}N*i*Pr)]K[Al(NON)(CH$_2$CH$_2$C{=N*i*Pr}N*i*Pr)] [(**2**·**Et$_2$O**)(**2**)].



Synthesis of K[Al(NNO){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (3)

A solution of **2** (14.1 mg, 0.02 mmol) in C_6D_6 (0.6 mL) was transferred to an NMR tube fitted with a J. Young's Teflon tap and heated to 80 °C. Reaction progress was monitored by ^{1}H NMR spectroscopy, showing complete conversion after for 2 days. The reaction mixture was transferred to a scintillation vial and the solvent was reduced *in vacuo*. Crystals suitable for X-ray diffraction were obtained by slow evaporation from benzene. Yield = 4.1 mg, 29 %.

Elemental analysis: Anal. Calcd. for $C_{37}H_{64}AlKN_4OSi_2$ (*703.20*): C 63.20, H 9.17, N 7.97 %; Found: C 63.76, H 7.76, N 7.34 %.

^{1}H NMR (500 MHz, C_6D_6): δ 7.31 – 7.11 (m, 6H, C_6H_3), 4.30 (sept, *J* = 6.7, 1H, C*H*Me$_2$), 4.18 (sept, *J* = 6.7, 1H, C*H*Me$_2$), 4.02 (sept, J = 6.7, 1H, C*H*Me$_2$), 3.92 (sept, *J* = 6.7, 1H, C*H*Me$_2$), 3.63 (sept, *J* = 6.7, 1H, C*H*Me$_2$), 3.54 (sept, *J* = 6.2, 1H, C*H*Me$_2$), 2.52 (m, 1H, CH_2), 2.00 (m, 1H, CH_2), 1.55 (t, *J* = 6.7 Hz, 6H, CH*Me*$_2$), 1.52 (d, *J* = 6.7 Hz, 3H, CH*Me*$_2$), 1.47 (m, 6H, CH*Me*$_2$), 1.42 (m, 15H, CH*Me*$_2$), 1.12 (d, *J* = 6.2, 3H, CH*Me*$_2$), 0.90 (d, 3H, CH*Me*$_2$) *partial overlap with solvent peak, 0.73 (s, 3H, Si*Me*$_2$), 0.36 (s, 3H, Si*Me*$_2$), 0.13 (m, 1H, CH_2), 0.07 (s, 3H, Si*Me*$_2$), 0.01 (s, 3H, Si*Me*$_2$), –0.47 (m, 1H, CH_2).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 170.3 (*C*=N), 149.0, 148.4, 147.2, 146.9, 145.6, 141.4, 125.3, 124.9, 124.6, 124.2, 124.1, 123.0 (C_6H_3) 47.3, 45.1 (*C*HMe$_2$), 28.3 (CH*Me*$_2$), 28.0, 27.9, 27.5 (*C*HMe$_2$), 27.4 (CH*Me*$_2$), 27.3 (*C*HMe$_2$), 27.1, 26.7, 25.9 (CH*Me*$_2$), 25.9 (*C*H$_2$), 25.8, 25.1, 24.6, 23.6, 23.2 (CH*Me*$_2$), 5.8, 5.5, 4.0, 2.9 (Si*Me*$_2$).

IR (solid, cm^{-1}): 3053 (m), 2962 (m), 2868 (m), 1608 (br m, υ_{CN}), , 1459 (w), 1429 (m), 1381 (br w), 1312 (w), 1245 (m), 1172 (m), 1100 (m), 1040 (s), 961 (br vs), 926 (vs), 792 (s), 772 (s), 491 (w), 447 (w).

Figure S11 ^{1}H NMR spectrum (500 MHz, C_6D_6) of K[Al(NNO){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (**3**).

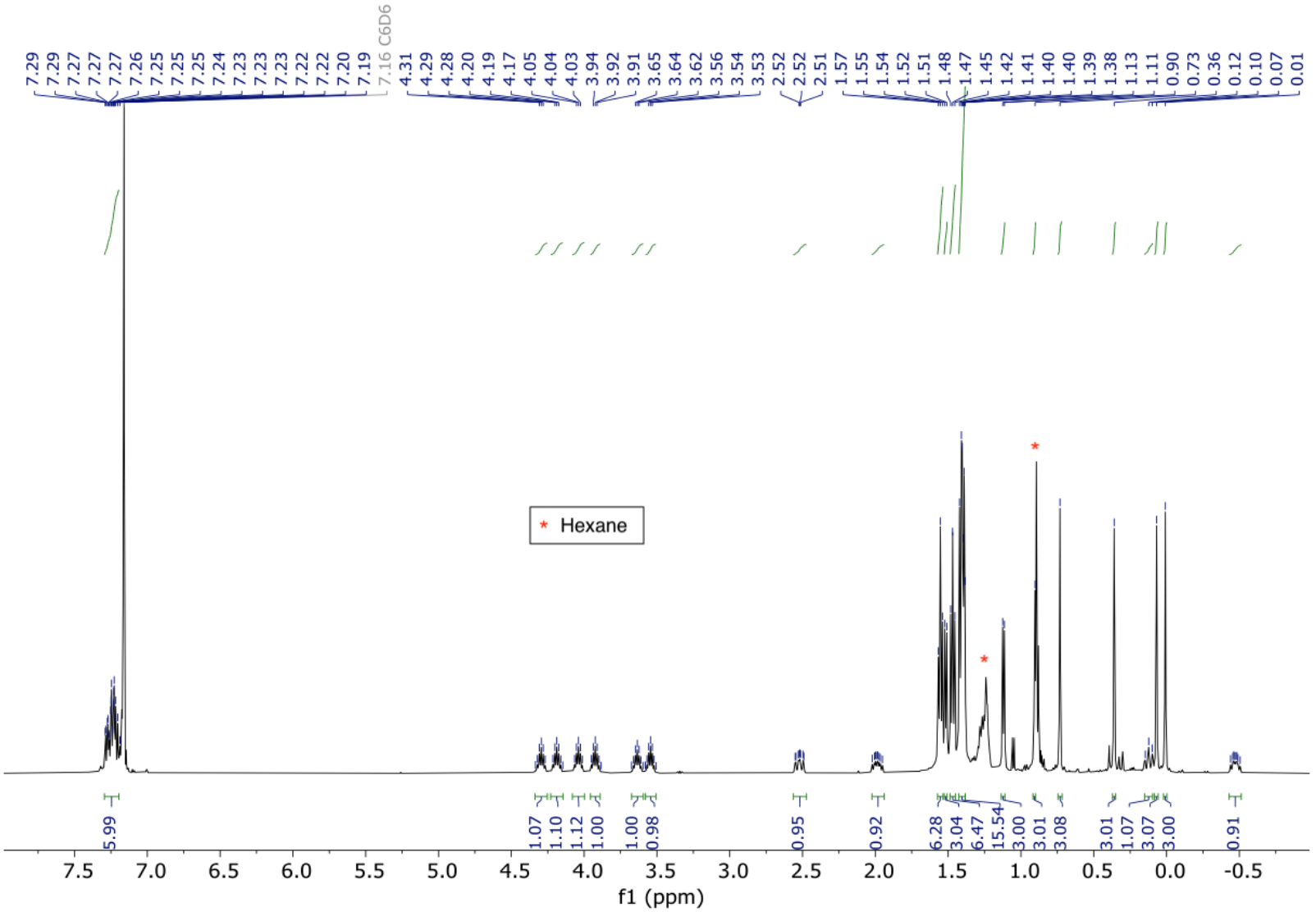


Figure S12 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of K[Al(NNO){$CH_2CH_2C(=N$*i*Pr)N*i*Pr}] (**3**).

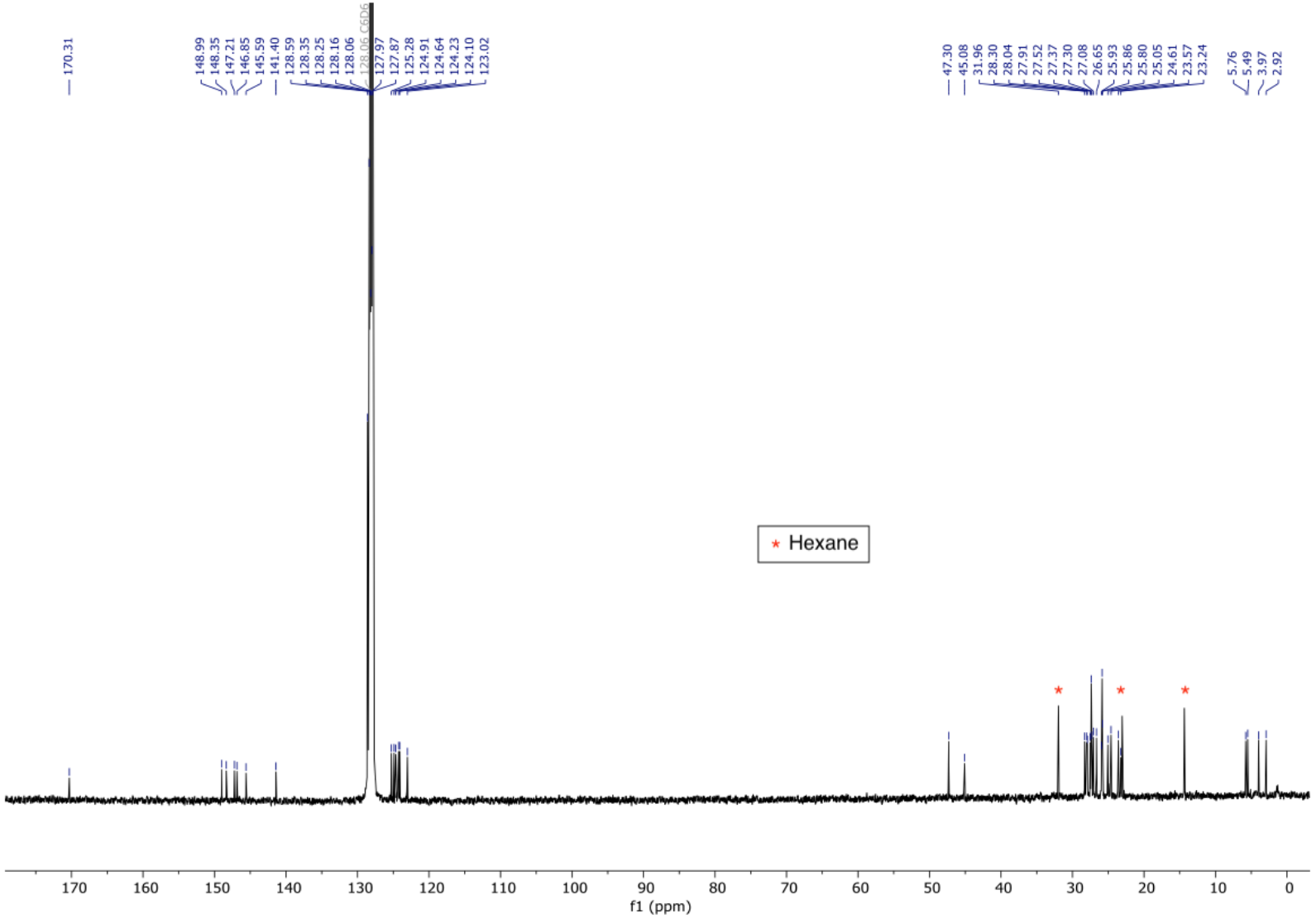


Figure S13 ^{1}H NMR spectra (500 MHz, C_6D_6, 353 K) charting the conversion of K[Al(NON){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (**2**) K[Al(NNO){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (**3**).

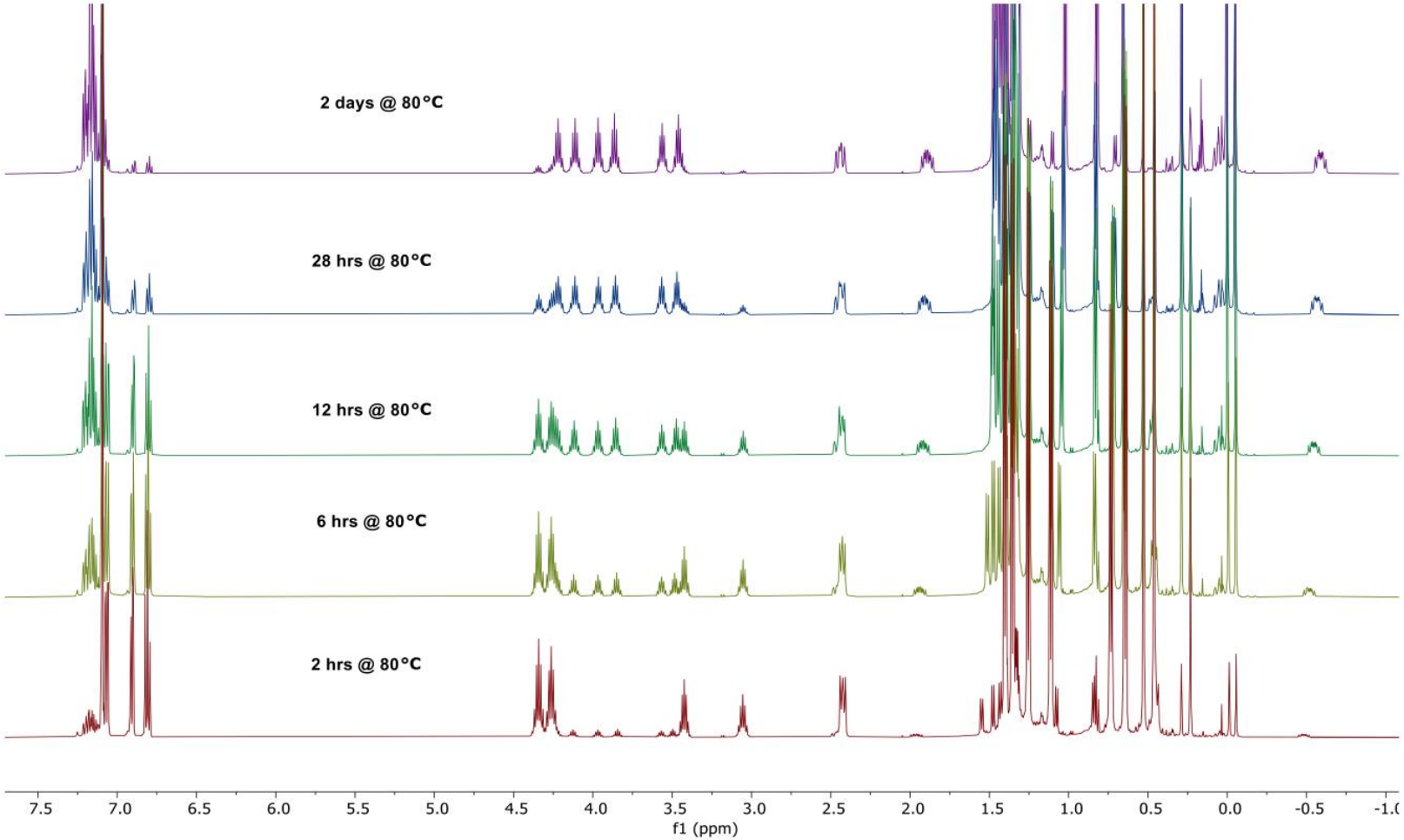


Figure S14 IR spectrum (solid, cm^{-1}) of K[Al(NNO){CH_2CH_2C(=N*i*Pr)N*i*Pr}] (**3**).

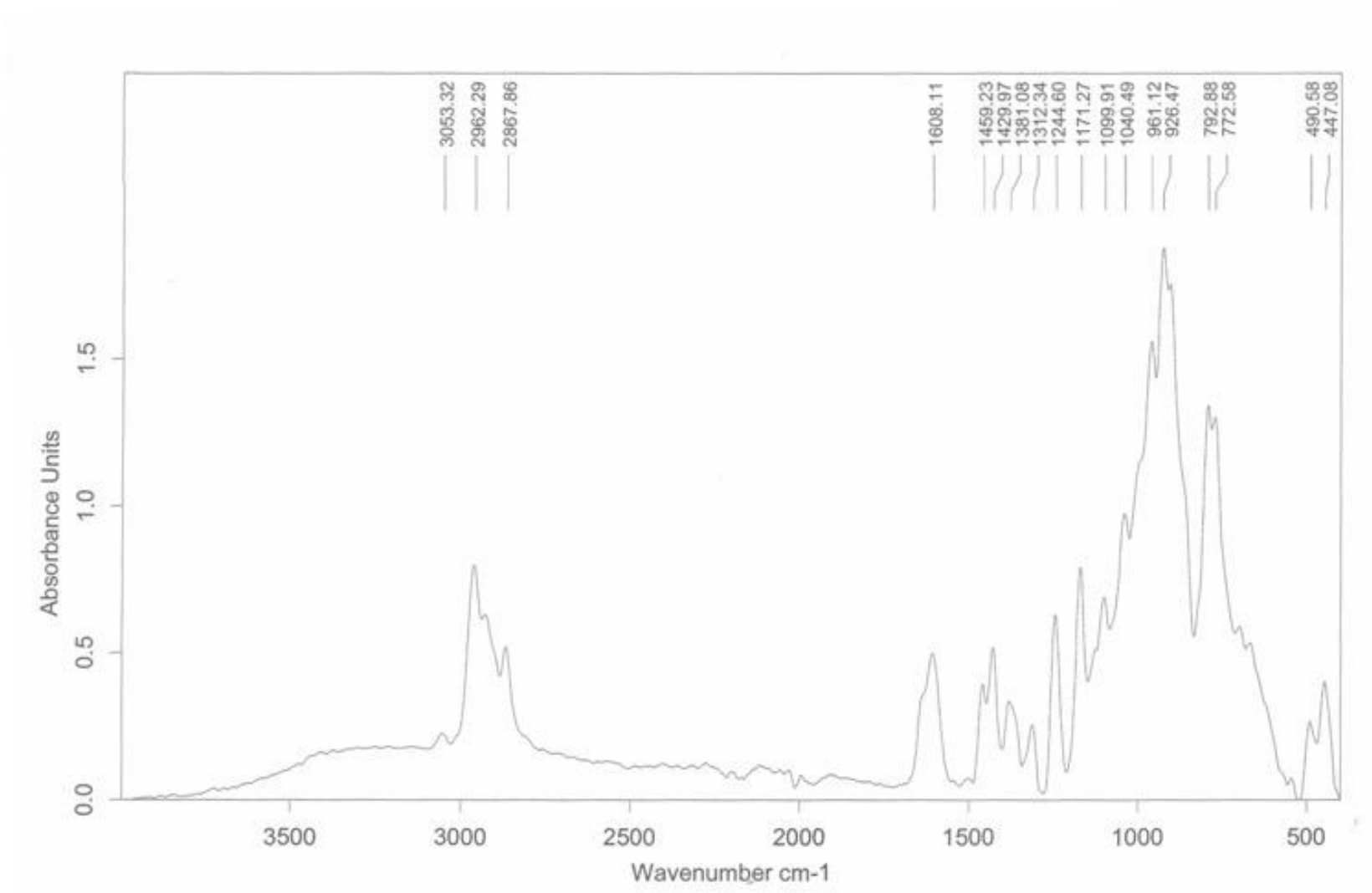


Figure S14 ORTEP (ellipsoids 30%, H-atoms {except C*H*$_2$ of metallacycle} omitted), of the asymmetric unit of [K(C$_6$H$_6$)][Al(NNO)(CH$_2$CH$_2$C{=N*i*Pr}N*i*Pr] **3·(C$_6$H$_6$)**

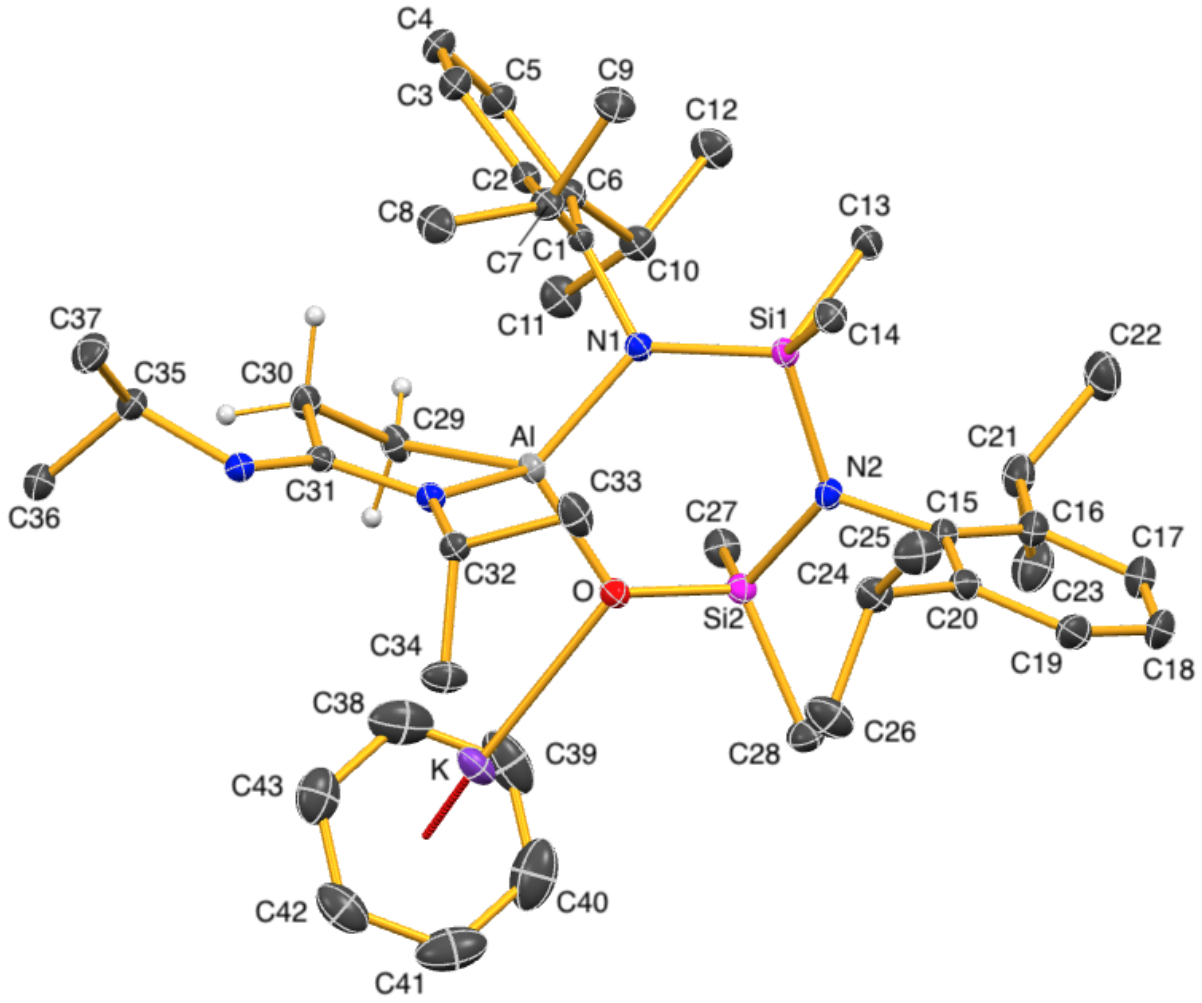


Figure S15 ORTEP (ellipsoids 30%, H-atoms {except C*H*$_2$ of metallacycle} omitted), of dimer unit of [{K(C_6H_6)}(Al{NNO}{CH_2CH_2C(=N*i*Pr)N*i*Pr})]$_2$ [**3**·(**C_6H_6**)]$_2$.

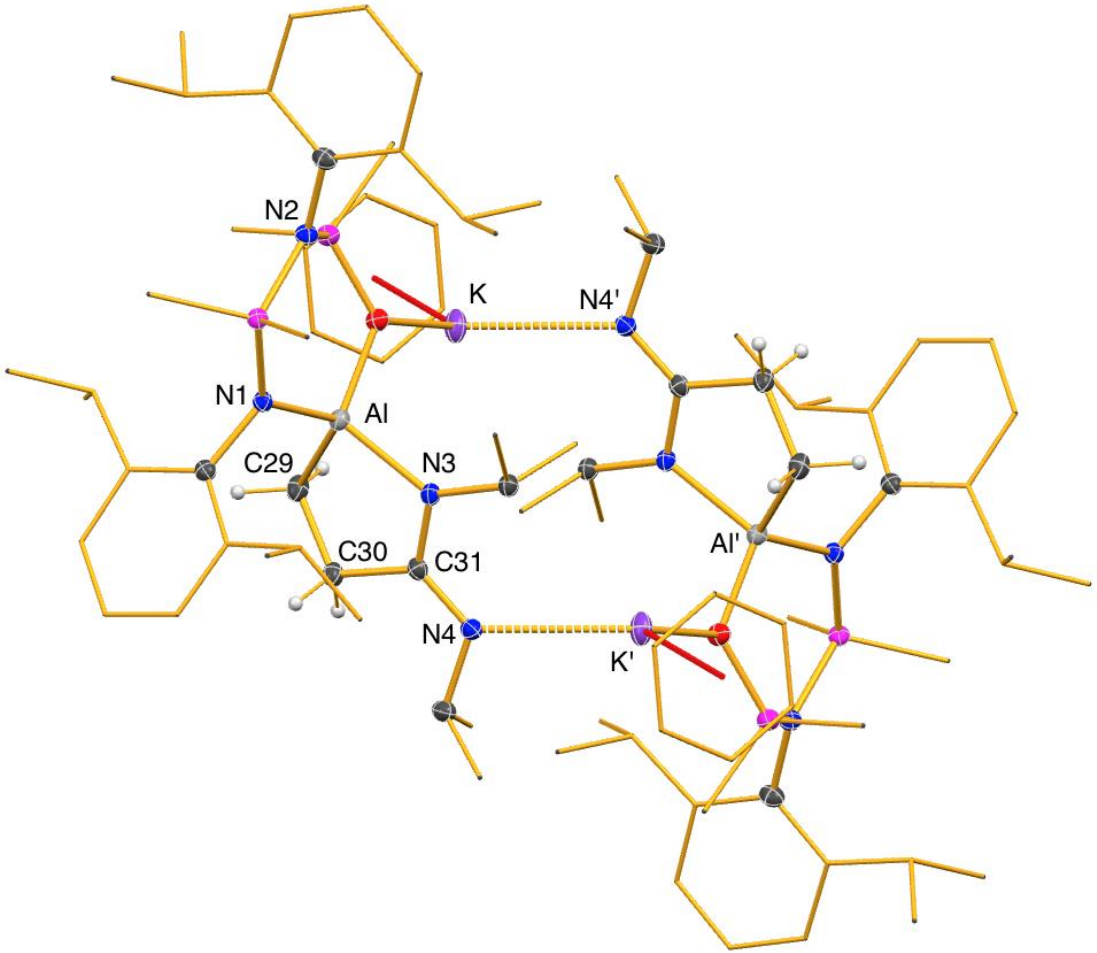
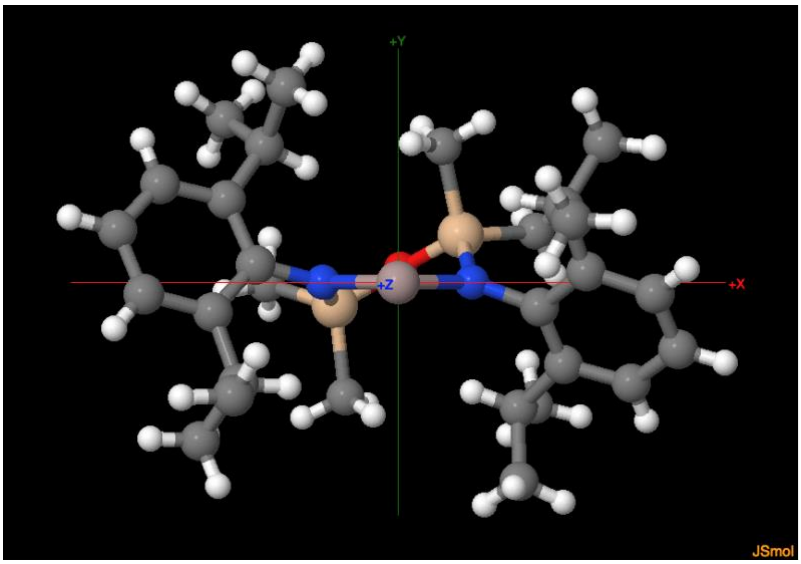
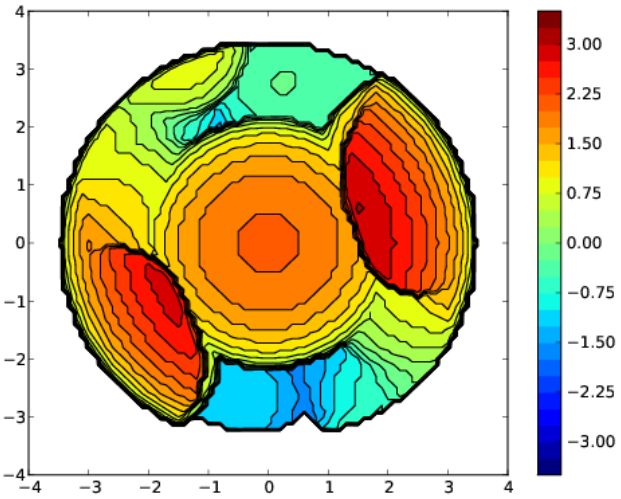


Figure S16 Summary of % volume buried calculations[S2] for the 'Al(NON)' fragment

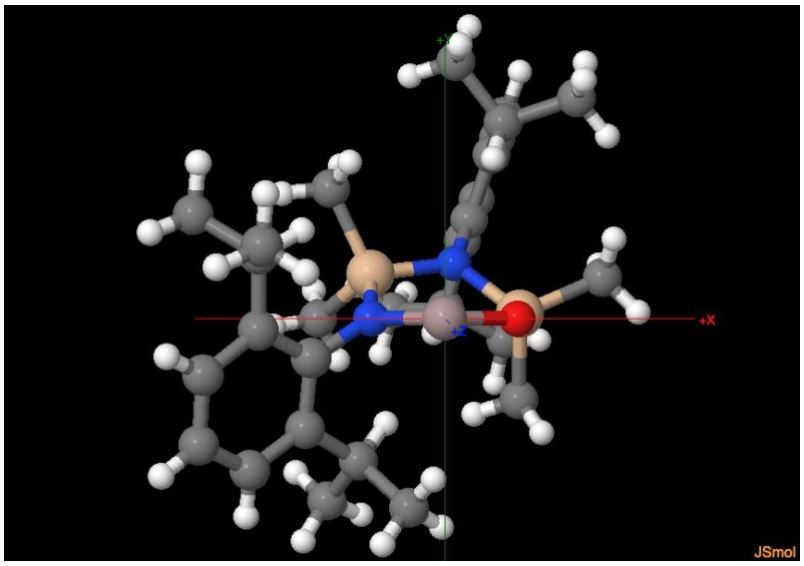


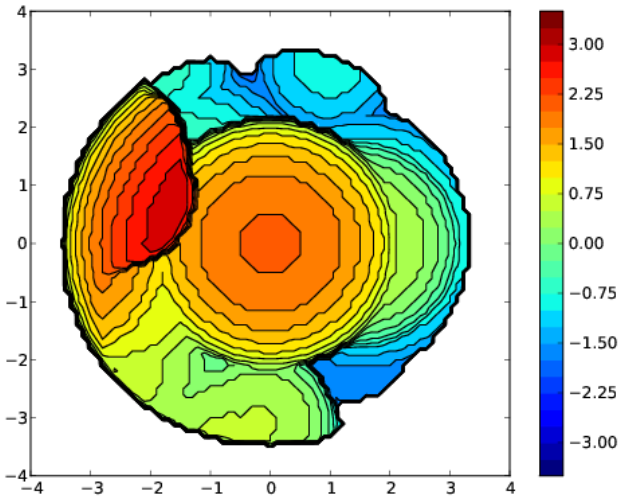


%V Free	%V Buried	% V Tot/V Ex
27.3	**72.7**	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	10.1	34.7	44.9	**22.6**	77.4
NW	13.7	31.1	44.9	**30.6**	69.4
NE	8.9	36.0	44.9	**19.8**	80.2
SE	16.3	28.6	44.9	**36.3**	63.7

Figure S17 Summary of % volume buried calculations[S2] for the 'Al(NNO)' fragment





%V Free	%V Buried	% V Tot/V Ex
36.7	**63.3**	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	11.7	33.2	44.9	**26.0**	74.0
NW	11.7	33.1	44.9	**26.1**	73.9
NE	21.8	23.1	44.9	**48.6**	51.4
SE	20.7	24.2	44.9	**46.1**	53.9

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 150 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.[S3] Space groups were determined from systematic absences and checked for higher symmetry. All structures were solved using direct methods with SHELXS,[S4] refined on F^2 using all data by full matrix least-squares procedures with SHELXL-97,[S5] within the OLEX2 ([**1·(Et$_2$O)$_2$**]$_2$)[S6] or WinGX ([(**2·Et$_2$O**)(**2**)] and **3·C$_6$H$_6$**)[S7] programs. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in calculated positions or manually assigned from residual electron density where appropriate, unless otherwise stated. The functions minimized were Σ*w*(*F2o-F2c),* with *w* = [σ2(*F2o*) + *a*P2 + *bP*]–1, where *P* = [max(*Fo*)2 + 2*F2c*]/3. The isotropic displacement parameters are 1.2 or 1.5 times the isotropic equivalent of their carrier atoms.

Additional Information:

[1·(Et$_2$O)$_2$]$_2$: The crystal was twinned with a two-fold rotation twin law with the ratio of components refining to 0.5100(7) / 0.4900(7).

[(2·Et$_2$O)(2)]: One of the *i*Pr groups is disordered and was modelled over two positions with the lower occupancy orientation having isotopic C and N atoms and C–C bond lengths restrained to be equal using the SADI command.

Table S1 Crystal structure and refinement data for [**1**·**(Et$_2$O)$_2$**]$_2$, [(**2**·**Et$_2$O**)(**2**)] and **3**·**C$_6$H$_6$**

	[**1**·**(Et$_2$O)$_2$**]$_2$	[**(2**·**Et$_2$O)(2)**]	**3**·**C$_6$H$_6$**
Empirical formula	$C_{78}H_{140}Al_2K_2N_4O_{10}Si_4$	$C_{85}H_{146}Al_2K_2N_8O_3Si_4$	$C_{116}H_{170}Al_2K_2N_8O_2Si_4$
CCDC Number	2310396	2310397	2310398
M_r	1538.45	1572.61	1953.11
T [K]	120.0(1)	120.0(1)	120.0(1)
Crystal size [mm]	0.35 × 0.25 × 0.22	0.27 × 0.26 × 0.19	0.33 × 0.31 × 0.23
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1$ (No. 4)	$P2_1/c$ (No. 14)	$P2_1/c$ (No. 14)
a [Å]	15.7613(2)	21.7767(2)	13.45606(16)
b [Å]	13.63024(18)	16.40993(13)	23.22737(19)
c [Å]	21.2238(18)	25.5079(2)	19.4534(2)
α [°]	90	90	90
β [°]	89.397(3)	98.7193(9)	108.1459(13)
γ [°]	90	90	90
V [Å^3]	4559.3(4)	9010.03(14)	5777.77(11)
Z	2	4	2
$D_{calc.}$ [mg m^{-3}]	1.121	1.159	1.123
Absorption coefficient [mm^{-1}]	2.016	2.004	1.650
θ range for data collection [°]	3.475 to 68.245	3.668 to 74.744	3.538 to 73.591
Reflections collected	48991	122864	49574
Independent reflections	24344 [R_{int} 0.053]	18081 [R_{int} 0.035]	11593 [R_{int} 0.030]
Reflections with $I > 2\sigma(I)$	23544	16660	10469
Data/restraints/parameters	24344 / 2 / 954	18081 / 2 / 1019	11593 / 0 / 636
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.027, wR_2 = 0.074	R_1 = 0.043, wR_2 = 0.114	R_1 = 0.037, wR_2 = 0.095
Final R indices (all data)	R_1 = 0.028, wR_2 = 0.075	R_1 = 0.047, wR_2 = 0.117	R_1 = 0.042, wR_2 = 0.100
GOOF on F^2	1.052	1.06	1.016
Largest diff. peak/hole [e.Å^{-3}]	0.15 and –0.24	1.25 and –0.63	0.32 and –0.42

Computational Details

DFT calculations were run with Gaussian 16 (C.01).[S8] The Al, Si and K centres were described with the Stuttgart RECPs and associated basis sets,[S9] and the 6-31G** basis set was used for all other atoms (BS1).[S10] A polarization function was also added to Al (ζ_d = 0.190), Si (ζ_d = 0.284) and K (ζ_d = 1.000).[S11] Initial BP86 optimizations were performed using the 'grid = ultrafine' option,[S12] with all stationary points being fully characterized via analytical frequency calculations as minima (all positive eigenvalues) or transition states (one imaginary eigenvalue), and with intrinsic reaction coordinate calculations confirming the connectivity of the reaction pathway. All energies were recomputed with a larger basis set featuring 6-311++G** basis sets on all atoms (BS2). Corrections for the effect of benzene (ε = 2.2706) solvent were run using the polarizable continuum model and BS1[S13] using the keyword "scrf=benzene" within Gaussian. Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[S14]

Breakdown of Energy Contributions

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

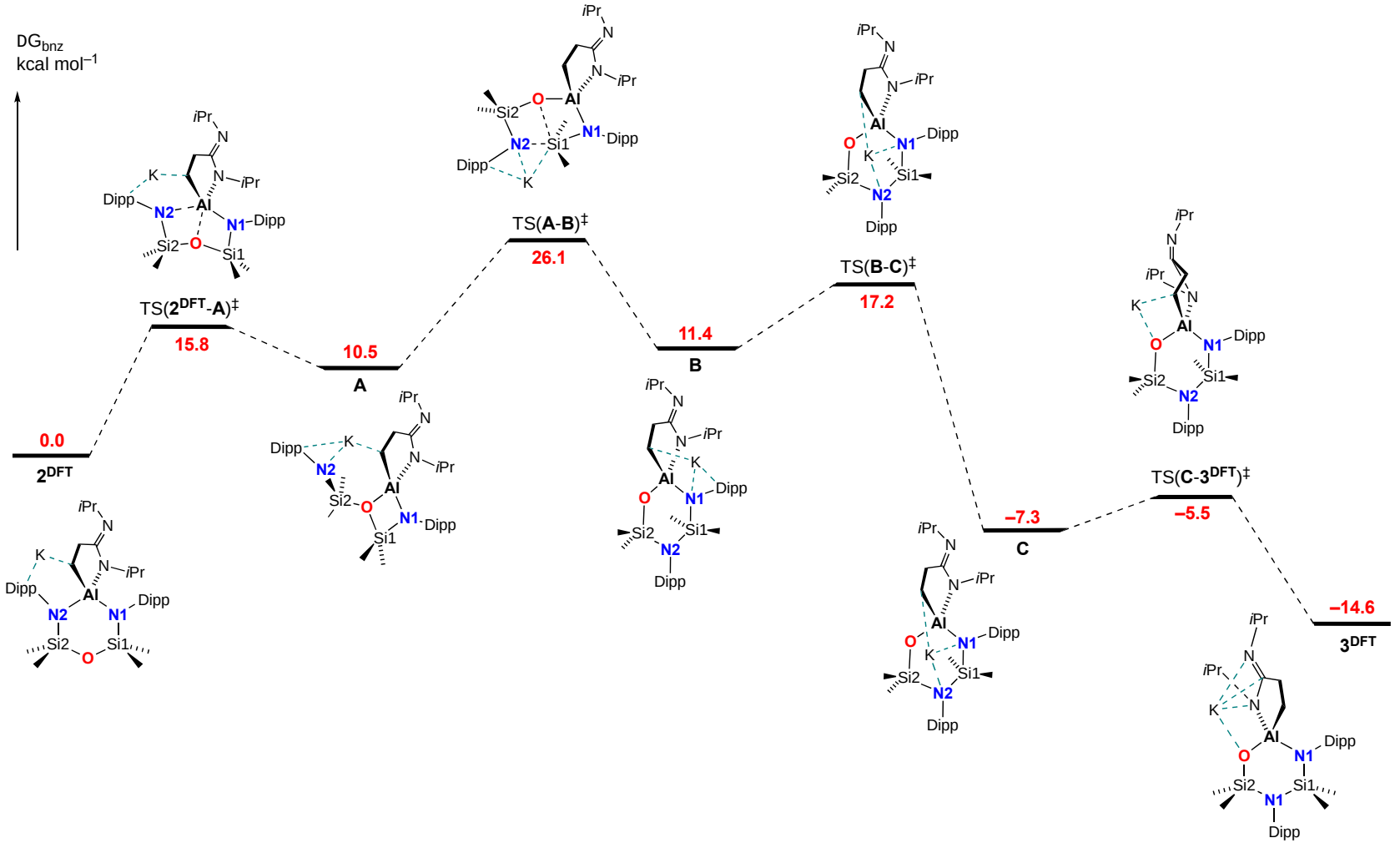
$\mathbf{\Delta E_{BSI}}$	SCF energy computed with the BP86 functional with BS1
$\mathbf{\Delta H_{BSI}}$	Enthalpy at 0 K with BS1
$\mathbf{\Delta G_{BSI}}$	Free energy at 298.15 K and 1 atm with BS1
$\mathbf{\Delta G_{BSI/}}\boldsymbol{bnz}$	Free energy corrected for benzene solvent with BS1
$\mathbf{\Delta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

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

Table S2 Relative energies for computed structures. Data in bold are those used in the main text. Free energies are quoted relative to compound **2**$^{\mathbf{DFT}}$ at 0.0 kcal mol^{-1}.

	ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/bnz}$	$\Delta G_{BSI/bnz+D3BJ}$	ΔE_{BS2}	ΔG_{bnz}
2$^{\mathbf{DFT}}$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
2 (Dimer crystal with Et_2O)	-32.8	-31.9	-12.0	-24.2	-28.1	-25.7	**-21.0**
TS(2$^{\mathbf{DFT}}$-A)	9.0	7.5	4.8	11.6	16.1	8.7	**15.8**
A	3.6	1.8	-3.8	7.3	11.1	3.0	**10.5**
TS(A-B)	16.9	16.2	14.6	20.8	24.2	18.8	**26.1**
B	7.6	7.8	7.6	11.7	9.4	9.7	**11.4**
TS(B-C)	9.8	10.03	11.0	14.4	15.8	11.2	**17.2**
C	-8.2	-8.0	-8.0	-5.0	-8.9	-6.6	**-7.3**
TS(C-3$^{\mathbf{DFT}}$)	-7.4	-7.3	-5.8	-6.4	-6.6	-6.3	**-5.5**
3$^{\mathbf{DFT}}$	-19.6	-19.2	-19.2	-15.9	-16.1	-18.1	**-14.6**
3 (Monomer crystal with benzene)	-26.6	-25.9	-16.9	-20.5	-17.5	-23.0	**-13.8**

Figure S18 Computed free energy profile (BP86-D3BJ(PCM=C_6H_6)/BS2//BP86/BS1 in kcal mol^{-1}) for 1,3-silyl retro-Brook rearrangement converting K[Al(NON){$CH_2CH_2C(=NiPr)NiPr$}] (**2**^{DFT}) to K[Al(NNO){$CH_2CH_2C(=NiPr)NiPr$}] (**3**^{DFT}).



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Cartesian Coordinates and Electronic Energies (in Hartrees)

2^{DFT}

SCF (BP86) Energy = -1781.18571943
Enthalpy 0K = -1780.263562
Enthalpy 298K = -1780.203970
Free Energy 298K = -1780.353799
Lowest Frequency = 10.4822 cm^{-1}
Second Frequency = 20.5881 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.48546681
SCF (C6H6) Energy = -1781.20285752
SCF (BS2) Energy = -3164.95223072

K	2.82093	0.90357	-3.02882
Si	1.80325	-0.85651	2.42773
Si	-0.79441	-2.42300	1.75701
Al	-0.14758	0.17063	0.13202
O	0.24654	-1.45045	2.70610
N	1.68381	-0.15897	0.79742
N	-1.23247	-1.40218	0.38659
N	-1.03387	1.84812	0.57780
N	-2.21862	3.60171	-0.45382
C	2.87187	0.21410	0.11893
C	3.34302	1.58084	0.09242
C	4.54901	1.90726	-0.56728
H	4.89335	2.94830	-0.54416
C	5.34038	0.93747	-1.20172
H	6.29864	1.20583	-1.66084
C	4.88963	-0.39195	-1.19957
H	5.49595	-1.16497	-1.68725
C	3.67771	-0.76815	-0.57827
C	2.59912	2.71196	0.79835
H	1.68055	2.27633	1.22410
C	3.44603	3.30662	1.94786
H	2.85725	4.05380	2.50780
H	4.34833	3.81574	1.56276
H	3.77456	2.53019	2.65639
C	2.17606	3.83595	-0.17377
H	1.62877	4.62249	0.37051
H	1.49471	3.46462	-0.95852
H	3.05116	4.31088	-0.65628
C	3.21918	-2.21647	-0.75331
H	2.36918	-2.36587	-0.06820
C	2.69339	-2.42720	-2.19173
H	2.33171	-3.45940	-2.33834
H	3.49737	-2.25608	-2.93570
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C	4.31079	-3.26426	-0.44817
H	3.87794	-4.27934	-0.47177
H	4.76414	-3.11072	0.54264
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C	2.20113	0.38375	3.81137
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H	1.89834	-0.04817	4.78118
H	1.69702	1.35501	3.69853
C	3.09679	-2.23100	2.65355
H	4.10683	-1.87995	2.38034
H	2.87393	-3.14530	2.08391
H	3.12072	-2.49729	3.72496
C	-2.19534	-2.94321	2.91721
H	-2.98466	-3.48956	2.37494
H	-2.65225	-2.08166	3.42696
H	-1.78433	-3.61957	3.68687
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H	-0.59986	-4.79410	0.95396
H	0.58613	-4.45532	2.23259
H	0.89761	-3.91683	0.55438
C	-2.37613	-1.73070	-0.43697
C	-2.22677	-2.49650	-1.64528
C	-3.35532	-2.83300	-2.41953
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C	-4.79953	-1.67354	-0.89929
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H	-4.81544	-2.18533	2.33471
H	-6.07810	-1.18066	1.58431
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H	-5.47182	0.86475	0.18417
H	-3.79638	1.48335	0.16521
C	0.01395	0.87932	-1.74517
H	0.87605	1.57967	-1.70302
H	0.12615	0.18864	-2.60391
C	-1.25042	1.74910	-1.87501
H	-1.19668	2.48089	-2.70287
H	-2.12333	1.10288	-2.09519
C	-1.53073	2.49349	-0.55353
C	-1.44994	2.47261	1.85955
H	-2.50435	2.78535	1.72765
C	-1.36292	1.49919	3.03822
H	-1.70814	1.99822	3.96086
H	-0.33143	1.15721	3.21453
H	-1.98274	0.60279	2.88685
C	-0.66711	3.76457	2.17853
H	0.39057	3.54811	2.41246
H	-1.10650	4.26538	3.06050
H	-0.72836	4.45667	1.32560
C	-2.79731	4.23983	-1.63339
H	-2.97210	3.53021	-2.47430
C	-4.16790	4.82575	-1.24158
H	-4.84196	4.02772	-0.88903
H	-4.64708	5.33736	-2.09579
H	-4.04663	5.55029	-0.41765
C	-1.85997	5.35551	-2.14537
H	-2.30602	5.90596	-2.99373
H	-0.89137	4.93844	-2.47505
H	-1.65476	6.07281	-1.33141

2

SCF (BP86) Energy = -3796.07874358
Enthalpy 0K = -3794.099896
Enthalpy 298K = -3793.970297
Free Energy 298K = -3794.278954
Lowest Frequency = 1.9957 cm^{-1}
Second Frequency = 3.1688 cm^{-1}
SCF (BP86-D3BJ) Energy = -3796.73176868
SCF (C6H6) Energy = -3796.10037484
SCF (BS2) Energy = -6563.66457982

K	-0.91431	-0.51186	-1.90410
K	6.91793	3.67738	0.14182
Si	4.64263	-3.78450	-1.85060
Si	5.33322	-3.69851	1.15337
Si	-6.17159	2.74998	-2.07260
Si	-6.63448	3.08996	0.97043
Al	3.67679	-1.29984	-0.04192
Al	-5.16365	0.48934	-0.03030
O	5.68734	-3.70700	-0.51711
O	-7.09374	2.88494	-0.66223
O	9.27285	4.95407	-0.39306
N	3.42326	-2.54149	-1.50531
N	4.55264	-2.13499	1.45430
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C	1.12000	-3.38205	-2.03107
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C	-0.02960	-2.64723	-4.07842
H	-0.88048	-2.71909	-4.76423
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C	2.16443	-1.70291	-3.49985
C	1.03003	-4.22309	-0.75707
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H	0.71653	-6.27604	-0.07754
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H	4.07491	-0.83669	-3.14673
C	2.74422	0.74565	-3.77707
H	3.51697	1.46496	-4.10027
H	2.46945	0.99974	-2.73947
H	1.86119	0.90137	-4.42312
C	3.82791	-0.96944	-5.29504
H	4.67592	-0.29249	-5.50249
H	3.06878	-0.79035	-6.07721
H	4.18460	-2.00544	-5.40601
C	5.71103	-3.52210	-3.40394
H	5.14045	-3.81196	-4.30326
H	6.58611	-4.19268	-3.34099
H	6.08107	-2.49674	-3.55086
C	3.96585	-5.54349	-2.06876
H	3.22309	-5.58362	-2.88357
H	3.50503	-5.94793	-1.15598
H	4.80379	-6.20503	-2.35046
C	7.00151	-3.96023	2.01011
H	6.92542	-3.82321	3.10130
H	7.77653	-3.28370	1.61838
H	7.32984	-4.99728	1.82246
C	4.30359	-5.23886	1.58493
H	4.31747	-5.40733	2.67514
H	4.75884	-6.12581	1.11084
H	3.25110	-5.17516	1.26712
C	4.48789	-1.66658	2.82217
C	3.35398	-1.94899	3.66109
C	3.35729	-1.54930	5.01298
H	2.48637	-1.78827	5.63380
C	4.43214	-0.86589	5.58335
H	4.41622	-0.57483	6.63900
C	5.52297	-0.55322	4.77000
H	6.36814	-0.00159	5.19903
C	5.57444	-0.92773	3.41249
C	2.09133	-2.65762	3.16809
H	2.23004	-2.87167	2.09385
C	1.84303	-3.99344	3.90699
H	0.96029	-4.51081	3.49052
H	1.64470	-3.82126	4.97972
C	0.84903	-1.75067	3.33860
H	-0.04618	-2.22209	2.89778
H	0.99196	-0.76501	2.86699
H	0.63005	-1.57321	4.40599
C	6.80580	-0.46436	2.63027
H	6.72943	-0.89106	1.61680
C	8.14378	-0.90976	3.26500
H	8.99188	-0.63676	2.61020
H	8.18348	-1.99517	3.43436
H	8.31011	-0.41468	4.23839
C	6.81004	1.07984	2.51306
H	7.70238	1.40823	1.93807
H	6.87828	1.54432	3.51377
H	5.89664	1.45731	2.02259
C	1.99672	-0.23585	0.14815
H	1.62658	-0.16909	-0.89727
H	1.17474	-0.61078	0.77785
C	2.45303	1.15528	0.61293
H	1.75862	1.96141	0.30732
H	2.46499	1.18582	1.72079
C	3.87216	1.51670	0.13078
C	5.91550	0.72021	-0.92823
H	6.49756	1.20117	-0.11195
C	5.92656	1.65054	-2.16639
H	6.96389	1.94122	-2.43062
H	5.31323	2.55045	-1.99857
H	5.51531	1.11806	-3.03857
C	6.64590	-0.58042	-1.27410
H	7.69238	-0.37254	-1.56009
H	6.15947	-1.07696	-2.12752
H	6.64993	-1.29412	-0.43698
C	-3.82213	1.41417	-2.54694
C	-3.81530	0.39943	-3.57221
C	-2.74885	0.32716	-4.49431
H	-2.78810	-0.43316	-5.28360
C	-1.66696	1.21762	-4.45265
H	-0.87182	1.17169	-5.20511
C	-1.63536	2.17832	-3.43085

H	-0.79267	2.87857	-3.37858
C	-2.67241	2.28728	-2.47908
C	-4.94135	-0.62235	-3.71503
H	-5.68980	-0.38474	-2.94122
C	-5.62076	-0.55075	-5.10144
H	-6.48919	-1.23168	-5.13516
H	-4.93153	-0.85692	-5.90962
H	-5.97613	0.46651	-5.33021
C	-4.43388	-2.05830	-3.45003
H	-5.25336	-2.78609	-3.56741
H	-4.05685	-2.16780	-2.41934
H	-3.63130	-2.33779	-4.15879
C	-2.49710	3.31137	-1.35824
H	-3.46237	3.36894	-0.82781
C	-1.43870	2.80886	-0.35108
H	-1.31681	3.51895	0.48516
H	-0.45057	2.70342	-0.84100
H	-1.72977	1.83864	0.08522
C	-2.10562	4.72082	-1.85289
H	-2.11450	5.43419	-1.01010
H	-2.79622	5.09557	-2.62349
H	-1.08516	4.73602	-2.27765
C	-7.35818	2.25184	-3.47310
H	-6.88172	2.42911	-4.45327
H	-8.25722	2.89079	-3.42210
H	-7.68459	1.20199	-3.43493
C	-5.52408	4.45666	-2.60807
H	-4.83565	4.36993	-3.46642
H	-5.01141	4.99731	-1.79854
H	-6.38430	5.06775	-2.93346
C	-8.24877	3.42584	1.90193
H	-8.08561	3.46148	2.99172
H	-9.01140	2.66207	1.68625
H	-8.64559	4.40624	1.58537
C	-5.63342	4.70794	1.11024
H	-5.56387	5.02323	2.16547
H	-6.15778	5.51017	0.56190
H	-4.60877	4.62667	0.71315
C	-5.57691	1.34018	2.82316
C	-4.38290	1.76048	3.50636
C	-4.24619	1.55215	4.89369
H	-3.33190	1.89626	5.39209
C	-5.23647	0.92041	5.64749
H	-5.11254	0.77032	6.72564
C	-6.38260	0.47162	4.98863
H	-7.16039	-0.04771	5.56032
C	-6.57780	0.66267	3.60619
C	-3.19459	2.41261	2.79835
H	-3.44808	2.47031	1.72528
C	-2.91041	3.84117	3.31682
H	-2.08195	4.30775	2.75171
H	-2.61302	3.82482	4.38074
H	-3.79171	4.49423	3.22770
C	-1.92056	1.55077	2.96867
H	-1.07033	1.98198	2.41033
H	-2.08146	0.51765	2.62016
H	-1.61999	1.49528	4.02979
C	-7.86192	0.08101	3.01536
H	-7.91216	0.41101	1.96642
C	-9.13802	0.56135	3.74610
H	-10.03734	0.21068	3.20876
H	-9.19211	1.65827	3.82339
H	-9.19444	0.15070	4.77030
C	-7.82524	-1.46478	3.03377
H	-8.75397	-1.87864	2.60202
H	-7.74543	-1.83908	4.07102
H	-6.97983	-1.86985	2.45688
C	-3.48838	-0.59084	0.20142
H	-3.20693	-0.82598	-0.84781
H	-2.60896	-0.17390	0.72423
C	-3.99522	-1.88419	0.86478
H	-3.32079	-2.75018	0.71737
H	-4.05182	-1.73636	1.96196
C	-5.40814	-2.26132	0.36978
C	-7.51987	-1.53088	-0.55376
H	-7.93761	-2.12732	0.28133
C	-8.36652	-0.27020	-0.74968
H	-9.41531	-0.54757	-0.95593
H	-8.00805	0.32289	-1.60619
H	-8.35575	0.38881	0.13138
C	-7.62762	-2.42533	-1.80816
H	-7.31870	-1.87753	-2.71604
H	-8.67578	-2.74577	-1.95277
H	-7.00656	-3.32394	-1.68173
C	-5.21208	-4.53744	1.13559
H	-4.42007	-4.18303	1.83464
C	-6.20892	-5.37168	1.96408
H	-6.68216	-4.74767	2.74016
H	-5.71019	-6.22615	2.45677
H	-7.01048	-5.75813	1.31066
C	-4.53249	-5.41959	0.06474
H	-4.02480	-6.29219	0.51540
H	-3.78446	-4.84047	-0.50597
H	-5.28855	-5.78558	-0.65211
C	10.39570	4.99793	0.50938
H	10.74390	6.04702	0.60996
H	11.23505	4.40846	0.08442
C	9.98188	4.44238	1.86596
H	9.16136	5.03398	2.30772
H	10.83271	4.48536	2.56502
H	9.67273	3.38470	1.79563
C	9.61009	5.50613	-1.68081
H	10.44091	4.92107	-2.12810
H	9.97024	6.54782	-1.54996
C	8.38469	5.47662	-2.58542
H	8.03457	4.44450	-2.76248
H	8.63310	5.90842	-3.56843
H	7.55933	6.07458	-2.16145
C	3.54008	3.78170	0.86899
H	2.75899	3.35867	1.53089
C	2.83566	4.59506	-0.23738
H	2.21439	5.40536	0.18340
H	2.18727	3.94858	-0.85129
H	3.58380	5.05084	-0.91336
C	4.37092	4.72518	1.76574
H	3.71575	5.42464	2.31174
H	5.06012	5.36267	1.17219
H	4.95016	4.15715	2.51542
H	2.70402	-4.67493	3.83309

TS(2^{DFT}-A)

SCF (BP86) Energy = -1781.17139089
Enthalpy 0K = -1780.251685
Enthalpy 298K = -1780.191412
Free Energy 298K = -1780.346158
Lowest Frequency = -55.9372 cm-1
Second Frequency = 14.3051 cm^{-1}

SCF (BP86-D3BJ) Energy = -1781.45727263
SCF (C6H6) Energy = -1781.18434153
SCF (BS2) Energy = -3164.93844155

K	2.47820	0.00047	-2.81726
Si	1.78194	-0.24849	2.41638
Si	-0.84616	-2.14608	1.84278
Al	-0.61552	0.17846	0.37408
O	0.07354	-0.63999	2.04712
N	2.26745	0.20354	0.87011
N	-1.48327	-1.54247	0.34392
N	-1.54894	1.80615	0.71927
N	-2.57574	3.57216	-0.44391
C	3.30172	0.50477	0.04280
C	3.44384	1.85240	-0.50275
C	4.40436	2.12266	-1.49374
H	4.49083	3.14507	-1.88133
C	5.28229	1.13268	-1.98070
H	6.04564	1.37771	-2.72702
C	5.20547	-0.15639	-1.42239
H	5.91778	-0.92398	-1.75309
C	4.24755	-0.49360	-0.44549
C	2.59479	2.98056	0.07737
H	1.67535	2.50973	0.46996
C	3.33095	3.62269	1.27856
H	2.69710	4.38469	1.76558
H	4.26449	4.11283	0.94772
H	3.59539	2.86405	2.03273
C	2.18824	4.06531	-0.93861
H	1.48792	4.77774	-0.47142
H	1.68080	3.63570	-1.82141
H	3.05454	4.65042	-1.29831
C	4.22341	-1.91088	0.11883
H	3.28698	-1.98710	0.69874
C	4.19193	-3.00875	-0.96697
H	4.13917	-4.01137	-0.50743
H	5.09367	-2.99203	-1.60553
H	3.30788	-2.91111	-1.62624
C	5.40866	-2.14355	1.08378
H	5.34811	-3.13886	1.55952
H	5.42534	-1.38247	1.88100
H	6.37226	-2.08273	0.54634
C	1.69529	1.12684	3.71877
H	2.71681	1.40058	4.03752
H	1.14184	0.79930	4.61604
H	1.21207	2.03304	3.32336
C	2.52756	-1.74193	3.33995
H	3.52053	-1.44573	3.72252
H	2.66240	-2.64511	2.72771
H	1.91023	-2.00124	4.21854
C	-1.98499	-2.36034	3.33756
H	-2.66697	-3.21265	3.17177
H	-2.59346	-1.46374	3.52579
H	-1.39417	-2.57909	4.24411
C	0.24949	-3.68807	1.75164
H	-0.38470	-4.53840	1.44319
H	0.68146	-3.94057	2.73346
H	1.06305	-3.58885	1.01655
C	-2.37932	-2.09985	-0.61182
C	-1.89033	-2.86700	-1.72115
C	-2.79601	-3.37234	-2.67397
H	-2.41246	-3.96588	-3.51309
C	-4.17173	-3.13988	-2.57368
H	-4.86036	-3.53926	-3.32587
C	-4.65200	-2.39012	-1.49474
H	-5.72871	-2.20220	-1.40731
C	-3.78977	-1.86814	-0.51188
C	-0.40419	-3.17963	-1.89970
H	0.13180	-2.63552	-1.10161
C	-0.11419	-4.69036	-1.74637
H	0.96959	-4.89823	-1.80949
H	-0.61456	-5.27046	-2.54203
H	-0.47892	-5.07402	-0.78069
C	0.13548	-2.69281	-3.26602
H	1.23020	-2.85912	-3.33425
H	-0.09302	-1.62445	-3.43335
H	-0.31852	-3.24897	-4.10490
C	-4.39667	-1.07219	0.64240
H	-3.56068	-0.77404	1.29640
C	-5.37364	-1.93367	1.47463
H	-5.74622	-1.36691	2.34631
H	-4.88989	-2.85355	1.84520
H	-6.25203	-2.23895	0.87829
C	-5.08755	0.22123	0.15594
H	-5.51368	0.77584	1.01053
H	-5.91383	-0.00087	-0.54316
H	-4.37673	0.89150	-0.35415
C	-0.16985	0.82853	-1.46016
H	0.77008	1.41128	-1.42015
H	-0.11539	0.04944	-2.24367
C	-1.35029	1.78403	-1.74313
H	-1.10004	2.55782	-2.49230
H	-2.19415	1.20904	-2.17280
C	-1.86345	2.48046	-0.46483
C	-2.09196	2.44259	1.94265
H	-3.09110	2.83603	1.67100
C	-2.25285	1.44657	3.09593
H	-2.68273	1.95836	3.97459
H	-1.29038	1.00243	3.39895
H	-2.93870	0.62872	2.81633
C	-1.24542	3.66106	2.36177
H	-0.21378	3.36052	2.61583
H	-1.68521	4.15691	3.24603
H	-1.21572	4.38809	1.53624
C	-2.96766	4.24647	-1.67880
H	-2.91034	3.58871	-2.57591
C	-4.43504	4.69672	-1.53750
H	-5.09349	3.82724	-1.37426
H	-4.78003	5.23209	-2.44030
H	-4.54165	5.36643	-0.66663
C	-2.04693	5.46050	-1.92494
H	-2.36021	6.03263	-2.81696
H	-1.00017	5.14004	-2.06840
H	-2.07414	6.13340	-1.05007

A

SCF (BP86) Energy = -1781.18000056
Enthalpy 0K = -1780.260696
Enthalpy 298K = -1780.199131
Free Energy 298K = -1780.359815
Lowest Frequency = 8.9634 cm^{-1}
Second Frequency = 10.1451 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.46195808
SCF (C6H6) Energy = -1781.19128436
SCF (BS2) Energy = -3164.94739985

K	2.01650	-0.09131	-2.00772
Si	1.86121	0.36904	1.86224
Si	-0.37797	-1.94904	1.34349
Al	-1.13629	0.38719	0.16144
O	0.22559	-0.27556	1.38645
N	2.78348	0.19700	0.46857
N	-1.57573	-1.46833	0.16395
N	-2.21831	1.81975	0.72342
N	-3.54908	3.50708	-0.22429
C	4.07629	0.41785	0.01574
C	4.45349	1.66639	-0.61655
C	5.72212	1.81025	-1.20962
H	5.98677	2.77134	-1.66939
C	6.66022	0.76999	-1.21408
H	7.64384	0.90447	-1.67605
C	6.31445	-0.44303	-0.60182
H	7.04429	-1.26299	-0.58929
C	5.06144	-0.64209	0.00294
C	3.50039	2.86207	-0.60606
H	2.54258	2.49092	-0.19527
C	4.01173	3.97833	0.33341
H	3.28586	4.80844	0.40065
H	4.96895	4.39263	-0.03094
H	4.18601	3.59010	1.35027
C	3.23298	3.44452	-2.01313
H	2.50088	4.26987	-1.96697
H	2.83238	2.68990	-2.71891
H	4.15462	3.84362	-2.47210
C	4.75317	-1.98871	0.65283
H	3.70799	-1.92091	1.00317
C	4.84464	-3.16025	-0.35031
H	4.56716	-4.11665	0.12817
H	5.86730	-3.27453	-0.75208
H	4.17083	-3.01050	-1.21463
C	5.65656	-2.25436	1.87767
H	5.38783	-3.20594	2.37156
H	5.56622	-1.44488	2.62101
H	6.72011	-2.31904	1.58533
C	1.41703	2.11332	2.46544
H	2.33782	2.66464	2.72381
H	0.77901	2.07902	3.36505
H	0.88660	2.69189	1.69116
C	2.32668	-0.65473	3.40025
H	3.27462	-0.25943	3.80711
H	2.49431	-1.72075	3.17581
H	1.56568	-0.57270	4.19533
C	-0.96073	-2.45571	3.06764
H	-1.52649	-3.40197	3.00683
H	-1.61604	-1.69383	3.51620
H	-0.10121	-2.62062	3.73898
C	0.93764	-3.18693	0.78368
H	0.45069	-4.15787	0.58215
H	1.68997	-3.34982	1.57260
H	1.46489	-2.86977	-0.12812
C	-2.49016	-2.27061	-0.58690
C	-2.12716	-2.78156	-1.87586
C	-3.05303	-3.54766	-2.61004
H	-2.76438	-3.93457	-3.59477
C	-4.33057	-3.82452	-2.11396
H	-5.03852	-4.41919	-2.70065
C	-4.68831	-3.32747	-0.85667
H	-5.68926	-3.53548	-0.46158
C	-3.79680	-2.56245	-0.08086
C	-0.75693	-2.52151	-2.50311
H	-0.20217	-1.91130	-1.76462
C	0.02869	-3.82999	-2.74787
H	1.03631	-3.62463	-3.15730
H	-0.49208	-4.47351	-3.47779
H	0.14971	-4.41102	-1.82010
C	-0.87876	-1.71951	-3.82001
H	0.11732	-1.49221	-4.25167
H	-1.42278	-0.77217	-3.67323
H	-1.42452	-2.29704	-4.58590
C	-4.26977	-2.04058	1.27330
H	-3.38697	-1.60422	1.76862
C	-4.81466	-3.16161	2.18488
H	-5.06084	-2.75982	3.18341
H	-4.07923	-3.97423	2.31399
H	-5.73722	-3.61128	1.77713
C	-5.31331	-0.91306	1.10060
H	-5.63741	-0.52514	2.08261
H	-6.21022	-1.28105	0.57112
H	-4.90029	-0.07036	0.52176
C	-0.67214	1.35778	-1.52001
H	0.18399	2.04205	-1.35012
H	-0.48558	0.79750	-2.45556
C	-1.95875	2.20976	-1.70330
H	-1.76055	3.13531	-2.27281
H	-2.69396	1.64006	-2.30538
C	-2.63877	2.59035	-0.36811
C	-2.82151	2.17519	2.02870
H	-3.90793	2.31253	1.85959
C	-2.60329	1.05933	3.05618
H	-3.06799	1.33201	4.01912
H	-1.52671	0.89262	3.24095
H	-3.05267	0.10957	2.72260
C	-2.27303	3.51416	2.56276
H	-1.19002	3.44373	2.76262
H	-2.78001	3.78420	3.50652
H	-2.45835	4.31302	1.83039
C	-4.02104	4.28684	-1.36742
H	-3.78620	3.81269	-2.34714
C	-5.55472	4.40185	-1.27027
H	-6.02235	3.40330	-1.29548
H	-5.96497	5.00066	-2.10286
H	-5.83728	4.88103	-0.31707
C	-3.36463	5.68320	-1.35004
H	-3.74662	6.31804	-2.16948
H	-2.26819	5.60696	-1.45375
H	-3.57679	6.18570	-0.39029

TS(A-B)

SCF (BP86) Energy = -1781.15876993
Enthalpy 0K = -1780.237816
Enthalpy 298K = -1780.178234
Free Energy 298K = -1780.330603
Lowest Frequency = -96.6549 cm^{-1}
Second Frequency = 10.9651 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.44926941
SCF (C6H6) Energy = -1781.16975097
SCF (BS2) Energy = -3164.92234120

K	1.93811	-0.12386	2.19753
Si	1.29403	-1.84766	-1.20172
Si	0.69131	1.01588	-0.79075
Al	-1.61031	-0.45299	-0.03491
O	-0.02398	-0.71079	-1.05220

N	2.40290	-0.77141	-0.43264
N	-0.85046	1.29017	0.09695
N	-3.18508	-1.05078	-0.87671
N	-5.20018	-2.14888	-0.39370
C	3.77237	-0.77291	-0.11824
C	4.31416	-1.60010	0.94505
C	5.63897	-1.41677	1.38908
H	6.02467	-2.05709	2.19150
C	6.48338	-0.46056	0.81580
H	7.50604	-0.32449	1.18213
C	6.00531	0.28181	-0.27086
H	6.67827	0.98784	-0.77030
C	4.69538	0.13569	-0.76125
C	3.52385	-2.77940	1.52163
H	2.46047	-2.63507	1.25394
C	3.97098	-4.09617	0.84039
H	3.36174	-4.95249	1.18069
H	5.02820	-4.30901	1.07709
H	3.88723	-4.02397	-0.25615
C	3.62308	-2.94469	3.05692
H	2.94419	-3.74204	3.40583
H	3.37629	-2.02409	3.62244
H	4.64224	-3.22618	3.37144
C	4.31104	0.86015	-2.04943
H	3.21252	0.87673	-2.08566
C	4.81643	2.31444	-2.14363
H	4.40323	2.80178	-3.04390
H	5.91650	2.36656	-2.22890
H	4.51931	2.91307	-1.26630
C	4.80286	0.04679	-3.27202
H	4.48055	0.52073	-4.21679
H	4.41154	-0.98362	-3.25350
H	5.90593	-0.01358	-3.28231
C	0.67759	-3.46548	-0.41158
H	1.41600	-4.27621	-0.52761
H	-0.24369	-3.77880	-0.93399
H	0.43260	-3.36970	0.65843
C	1.60746	-2.24548	-3.02893
H	2.46006	-2.94151	-3.12179
H	1.84109	-1.34700	-3.62022
H	0.72618	-2.73708	-3.47563
C	0.79931	1.49203	-2.63502
H	1.12830	2.53554	-2.76461
H	-0.18957	1.37589	-3.10552
H	1.49904	0.84634	-3.18774
C	1.90830	2.19062	0.16414
H	1.91166	3.14764	-0.38730
H	2.95123	1.83726	0.20767
H	1.53537	2.44338	1.17358
C	-1.23745	2.50961	0.73134
C	-1.21175	2.65989	2.16082
C	-1.56049	3.88892	2.75427
H	-1.53579	3.97880	3.84711
C	-1.94412	4.99259	1.98876
H	-2.20533	5.94240	2.46672
C	-2.00848	4.84718	0.60026
H	-2.33683	5.69500	-0.01229
C	-1.67917	3.63801	-0.04063
C	-0.85136	1.51332	3.10380
H	-0.58506	0.65445	2.45972
C	0.33249	1.86896	4.03843
H	0.63959	1.00176	4.65775
H	0.04943	2.66354	4.74894
H	1.20848	2.26253	3.48783
C	-2.06594	1.07300	3.95212
H	-1.81331	0.21627	4.60325
H	-2.90866	0.77509	3.30852
H	-2.41284	1.89752	4.59900
C	-1.86634	3.57334	-1.55523
H	-1.55411	2.56834	-1.87810
C	-1.00075	4.61354	-2.30064
H	-1.09238	4.48613	-3.39366
H	0.06604	4.52403	-2.03406
H	-1.31404	5.64528	-2.06076
C	-3.35635	3.74277	-1.93466
H	-3.49635	3.63552	-3.02500
H	-3.73286	4.74026	-1.64592
H	-3.98693	2.99061	-1.43182
C	-1.98193	-1.60892	1.54583
H	-1.54336	-2.60963	1.36442
H	-1.67194	-1.30957	2.56227
C	-3.52802	-1.72927	1.46816
H	-3.89631	-2.65140	1.95264
H	-3.99808	-0.89286	2.02443
C	-4.05623	-1.68353	0.01691
C	-3.62518	-1.01863	-2.28664
H	-4.71306	-0.81143	-2.28417
C	-2.89518	0.08053	-3.06434
H	-3.25041	0.11385	-4.10891
H	-1.80732	-0.11257	-3.08944
H	-3.06627	1.07143	-2.61406
C	-3.42505	-2.39223	-2.95879
H	-2.35180	-2.65565	-2.99242
H	-3.80725	-2.38088	-3.99560
H	-3.97157	-3.16441	-2.39683
C	-6.14556	-2.76362	0.53463
H	-5.93052	-2.52653	1.60112
C	-7.55295	-2.21881	0.22021
H	-7.58272	-1.12341	0.34610
H	-8.31451	-2.66745	0.88306
H	-7.81915	-2.44335	-0.82720
C	-6.10451	-4.29786	0.37561
H	-6.85705	-4.79148	1.01668
H	-5.10932	-4.69502	0.64102
H	-6.30590	-4.57076	-0.67509

B

SCF (BP86) Energy = -1781.19877995
Enthalpy 0K = -1780.276258
Enthalpy 298K = -1780.216639
Free Energy 298K = -1780.366591
Lowest Frequency = 15.5986 cm^{-1}
Second Frequency = 21.3976 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.47702315
SCF (C6H6) Energy = -1781.18425767
SCF (BS2) Energy = -3164.93679883

K	0.37738	1.00517	2.83549
Si	1.50453	-1.85134	1.11059
Si	1.21818	0.15636	-1.26349
Al	-1.36475	-0.38121	0.65599
O	-0.01147	-1.25731	1.50084
N	2.25800	-0.59261	0.05862
N	-0.34865	0.69320	-0.59123
N	-2.91786	-1.42319	0.33619
N	-5.22107	-1.44843	0.78671
C	3.70420	-0.44319	0.06764

C	4.31530	0.60954	0.82986
C	5.71766	0.69848	0.91938
H	6.16378	1.49950	1.51975
C	6.55424	-0.20430	0.25927
H	7.64293	-0.12011	0.33983
C	5.97025	-1.20824	-0.51404
H	6.61482	-1.91355	-1.05040
C	4.57170	-1.35112	-0.62611
C	3.50963	1.67701	1.57077
H	2.46418	1.55662	1.23076
C	3.58609	1.49377	3.10682
H	2.99770	2.26916	3.63871
H	4.62700	1.60361	3.45614
H	3.25684	0.49138	3.42838
C	3.96336	3.10981	1.21450
H	3.31134	3.85709	1.70017
H	3.93933	3.28649	0.12780
H	4.99298	3.30383	1.56077
C	4.07228	-2.48783	-1.51829
H	2.97473	-2.51390	-1.44153
C	4.44717	-2.23640	-2.99864
H	4.01961	-3.02004	-3.64879
H	5.54285	-2.24915	-3.13682
H	4.08341	-1.25811	-3.35472
C	4.61809	-3.86483	-1.07320
H	4.14157	-4.67492	-1.65223
H	4.43523	-4.05420	-0.00249
H	5.70744	-3.94036	-1.23776
C	2.52068	-2.07596	2.71020
H	3.60617	-2.05465	2.51853
H	2.27119	-3.06078	3.14189
H	2.30239	-1.32555	3.49039
C	1.35521	-3.59621	0.37558
H	2.31097	-4.13990	0.44809
H	1.03443	-3.61488	-0.67690
H	0.60580	-4.15118	0.96633
C	0.95634	-1.12677	-2.64734
H	1.91358	-1.47780	-3.06223
H	0.38973	-0.66527	-3.47208
H	0.38317	-2.00541	-2.31017
C	2.21646	1.57200	-2.03713
H	3.08634	1.16703	-2.58089
H	2.58878	2.29406	-1.29568
H	1.58620	2.11614	-2.76094
C	-1.10501	1.79734	-1.15018
C	-0.92986	3.13931	-0.66156
C	-1.80825	4.16371	-1.06605
H	-1.66871	5.17332	-0.66134
C	-2.84596	3.93164	-1.97110
H	-3.52561	4.73847	-2.26458
C	-2.97600	2.65181	-2.51320
H	-3.75799	2.46194	-3.25689
C	-2.12950	1.58860	-2.13887
C	0.21706	3.55766	0.26075
H	0.84028	2.65870	0.42533
C	1.09519	4.64047	-0.41154
H	1.94686	4.92234	0.23072
H	0.50848	5.55549	-0.60196
H	1.49083	4.29514	-1.37917
C	-0.26956	4.09138	1.63070
H	0.58382	4.30593	2.30381
H	-0.96949	3.39773	2.13020
H	-0.82258	5.03880	1.51022
C	-2.31804	0.26741	-2.88489
H	-1.66772	-0.47782	-2.39968
C	-1.86680	0.42545	-4.35853
H	-1.89557	-0.54579	-4.88423
H	-0.84424	0.83267	-4.43908
H	-2.53529	1.11826	-4.90039
C	-3.76629	-0.26687	-2.84140
H	-3.82878	-1.23527	-3.36919
H	-4.46882	0.41961	-3.34671
H	-4.11440	-0.42285	-1.80909
C	-2.41274	0.77302	1.93994
H	-2.41057	0.33829	2.96555
H	-2.21111	1.85689	2.04292
C	-3.84399	0.60291	1.36358
H	-4.62387	0.85048	2.10457
H	-3.98094	1.31155	0.52285
C	-4.07855	-0.82193	0.82946
C	-3.08393	-2.81350	-0.13754
H	-4.09318	-2.88101	-0.58673
C	-2.03812	-3.17620	-1.19573
H	-2.14906	-4.23098	-1.50279
H	-1.01616	-3.05914	-0.79602
H	-2.13562	-2.54838	-2.09589
C	-3.04836	-3.79752	1.04957
H	-2.07026	-3.75456	1.56170
H	-3.22061	-4.83564	0.71094
H	-3.84016	-3.53431	1.76823
C	-6.45420	-0.81975	1.25170
H	-6.38999	0.29110	1.29740
C	-7.57876	-1.17068	0.25762
H	-7.33531	-0.79601	-0.75070
H	-8.54327	-0.73179	0.57040
H	-7.69424	-2.26639	0.18956
C	-6.79736	-1.33098	2.66689
H	-7.76603	-0.93215	3.01885
H	-6.01780	-1.03714	3.39134
H	-6.85254	-2.43371	2.66224

TS(B-C)

SCF (BP86) Energy = -1781.17009116
Enthalpy 0K = -1780.247204
Enthalpy 298K = -1780.188518
Free Energy 298K = -1780.336329
Lowest Frequency = -20.4839 cm^{-1}
Second Frequency = 10.2955 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.46946752
SCF (C6H6) Energy = -1781.17985494
SCF (BS2) Energy = -3164.93445088

K	0.48613	-0.27744	2.35563
Si	1.38907	-2.28014	-0.48298
Si	1.21491	0.69634	-0.79392
Al	-1.47176	-0.76154	-0.16908
O	-0.11123	-1.69840	-0.89777
N	2.23305	-0.72778	-0.08626
N	-0.44198	0.89818	-0.02511
N	-3.15895	-1.01436	-0.97916
N	-5.39600	-1.52484	-0.49293
C	3.67494	-0.62136	0.13518
C	4.23166	-0.76301	1.45437
C	5.59365	-0.49658	1.69500
H	5.97773	-0.58561	2.71750
C	6.46409	-0.13009	0.66882
H	7.51605	0.09265	0.87417

C	5.96318	-0.10034	-0.63226
H	6.64400	0.12310	-1.46102
C	4.61006	-0.36398	-0.92936
C	3.42777	-1.22764	2.66773
H	2.46608	-1.59137	2.27677
C	4.06441	-2.44673	3.37506
H	3.40342	-2.82004	4.17777
H	5.03284	-2.19251	3.83749
H	4.24138	-3.27040	2.66463
C	3.21960	-0.07927	3.68731
H	2.55593	-0.37621	4.52343
H	2.83384	0.84456	3.21741
H	4.18470	0.20227	4.14070
C	4.26562	-0.41341	-2.41890
H	3.19745	-0.64537	-2.50718
C	4.53567	0.92536	-3.14394
H	4.21323	0.86489	-4.19825
H	5.61272	1.16927	-3.14474
H	4.00684	1.76929	-2.67235
C	5.04664	-1.54698	-3.12857
H	4.71840	-1.63864	-4.17906
H	4.89262	-2.52047	-2.63672
H	6.13201	-1.34469	-3.13669
C	1.29224	-3.49605	0.98922
H	2.28944	-3.81436	1.33792
H	0.76581	-4.39886	0.63212
H	0.71924	-3.13345	1.86098
C	2.14200	-3.29104	-1.89497
H	3.15206	-3.65469	-1.64206
H	2.20160	-2.73032	-2.84026
H	1.50128	-4.17348	-2.06675
C	1.11955	0.48812	-2.69598
H	1.88315	1.09370	-3.20820
H	0.13987	0.79104	-3.08622
H	1.25224	-0.56495	-2.98365
C	2.25617	2.20634	-0.26838
H	3.31965	2.05159	-0.50872
H	2.18107	2.36894	0.82198
H	1.91485	3.13534	-0.74762
C	-0.82422	2.25499	0.32424
C	-1.19682	2.64310	1.66472
C	-1.19268	4.00409	2.03573
H	-1.43443	4.26655	3.07251
C	-0.93141	5.02467	1.11922
H	-0.89932	6.07268	1.43391
C	-0.81831	4.66818	-0.22632
H	-0.75729	5.45417	-0.98796
C	-0.81684	3.32335	-0.64531
C	-1.79194	1.68439	2.70203
H	-1.76775	0.66178	2.29018
C	-1.09531	1.72597	4.08827
H	-1.44181	0.90026	4.73738
H	-1.33740	2.66346	4.61636
H	0.01063	1.70482	4.03844
C	-3.29878	1.99500	2.89523
H	-3.76113	1.28069	3.59982
H	-3.83791	1.93486	1.93651
H	-3.44156	3.01268	3.29749
C	-0.98762	3.07742	-2.14586
H	-0.94082	1.99188	-2.30117
C	0.07051	3.75412	-3.04253
H	-0.10360	3.49785	-4.10224
H	1.09633	3.44432	-2.78620
H	0.02346	4.85464	-2.96213
C	-2.40665	3.53044	-2.57355
H	-2.58463	3.29275	-3.63762
H	-2.53385	4.61977	-2.44453
H	-3.18466	3.02847	-1.97485
C	-2.17962	-1.63372	1.52041
H	-1.96314	-2.71017	1.35705
H	-1.89149	-1.44112	2.57582
C	-3.70961	-1.41750	1.38976
H	-4.28176	-2.21840	1.89227
H	-4.00291	-0.47958	1.89951
C	-4.17664	-1.33100	-0.07779
C	-3.53831	-1.07506	-2.40787
H	-4.54495	-0.62374	-2.49888
C	-2.54619	-0.29499	-3.27345
H	-2.84460	-0.33850	-4.33538
H	-1.53202	-0.72698	-3.19710
H	-2.50613	0.76555	-2.97657
C	-3.64226	-2.53872	-2.88375
H	-2.66031	-3.03924	-2.80983
H	-3.97681	-2.58471	-3.93614
H	-4.37418	-3.08080	-2.26618
C	-6.47448	-1.82169	0.44560
H	-6.23029	-1.54614	1.49701
C	-7.71107	-0.99819	0.03417
H	-7.48744	0.08148	0.06692
H	-8.56823	-1.19824	0.70206
H	-8.00292	-1.24823	-1.00054
C	-6.79045	-3.33216	0.41682
H	-7.64786	-3.57973	1.06860
H	-5.91999	-3.92378	0.74998
H	-7.03253	-3.64347	-0.61438

C

SCF (BP86) Energy = -1781.19878031
Enthalpy 0K = -1780.276261
Enthalpy 298K = -1780.216641
Free Energy 298K = -1780.366591
Lowest Frequency = 15.5763 cm^{-1}
Second Frequency = 21.4724 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.50496745
SCF (C6H6) Energy = -1781.21088821
SCF (BS2) Energy = -3164.96271581

K	-0.37596	1.00072	-2.84220
Si	-1.50489	-1.85108	-1.10936
Si	-1.21835	0.15648	1.26481
Al	1.36396	-0.38081	-0.65551
O	0.01096	-1.25720	-1.50073
N	-2.25804	-0.59234	-0.05746
N	0.34866	0.69266	0.59278
N	2.91705	-1.42304	-0.33597
N	5.22021	-1.44851	-0.78686
C	-3.70411	-0.44211	-0.06764
C	-4.31415	0.61036	-0.83106
C	-5.71641	0.70001	-0.92138
H	-6.16178	1.50087	-1.52254
C	-6.55385	-0.20184	-0.26108
H	-7.64245	-0.11708	-0.34227
C	-5.97086	-1.20563	0.51321
H	-6.61613	-1.91025	1.04965
C	-4.57246	-1.34917	0.62614
C	-3.50750	1.67698	-1.57213
H	-2.46191	1.55497	-1.23302

C	-3.58540	1.49485	-3.10824
H	-2.99614	2.26967	-3.64000
H	-4.62635	1.60659	-3.45683
H	-3.25799	0.49216	-3.43073
C	-3.95926	3.11016	-1.21483
H	-3.30687	3.85696	-1.70076
H	-3.93408	3.28635	-0.12809
H	-4.98903	3.30535	-1.56005
C	-4.07393	-2.48564	1.51912
H	-2.97636	-2.51218	1.44284
C	-4.44935	-2.23334	2.99919
H	-4.02254	-3.01694	3.64987
H	-5.54510	-2.24537	3.13689
H	-4.08514	-1.25511	3.35498
C	-4.62005	-3.86264	1.07441
H	-4.14433	-4.67262	1.65424
H	-4.43645	-4.05269	0.00395
H	-5.70956	-3.93759	1.23819
C	-2.52140	-2.07684	-2.70852
H	-3.60674	-2.06212	-2.51541
H	-2.26686	-3.05921	-3.14285
H	-2.30882	-1.32317	-3.48712
C	-1.35573	-3.59577	-0.37383
H	-2.31160	-4.13926	-0.44648
H	-1.03540	-3.61414	0.67879
H	-0.60623	-4.15114	-0.96408
C	-0.95711	-1.12672	2.64876
H	-0.39041	-0.66541	3.47354
H	-0.38421	-2.00557	2.31167
H	-1.91452	-1.47741	3.06355
C	-2.21636	1.57240	2.03826
H	-3.08650	1.16773	2.58183
H	-2.58823	2.29461	1.29675
H	-1.58606	2.11628	2.76224
C	1.10566	1.79661	1.15117
C	0.93111	3.13843	0.66199
C	1.81033	4.16244	1.06566
H	1.67128	5.17195	0.66052
C	2.84817	3.93013	1.97050
H	3.52846	4.73666	2.26336
C	2.97753	2.65051	2.51328
H	3.75960	2.46052	3.25685
C	2.13027	1.58765	2.13966
C	-0.21630	3.55702	-0.25959
H	-0.83988	2.65825	-0.42371
C	-1.09329	4.64033	0.41341
H	-1.94580	4.92209	-0.22777
H	-0.50613	5.55532	0.60260
H	-1.48766	4.29552	1.38176
C	0.26918	4.09030	-1.63007
H	-0.58488	4.30564	-2.30205
H	0.96760	3.39577	-2.13044
H	0.82341	5.03712	-1.51038
C	2.31810	0.26659	2.88608
H	1.66735	-0.47839	2.40104
C	1.86691	0.42529	4.35965
H	1.89537	-0.54576	4.88570
H	0.84447	0.83284	4.44003
H	2.53560	1.11810	4.90127
C	3.76606	-0.26848	2.84269
H	3.82804	-1.23682	3.37065
H	4.46896	0.41770	3.34790
H	4.11409	-0.42479	1.81040
C	2.41217	0.77372	-1.93913
H	2.41044	0.33939	-2.96495
H	2.21051	1.85762	-2.04169
C	3.84334	0.60325	-1.36265
H	4.62331	0.85117	-2.10342
H	3.98016	1.31149	-0.52156
C	4.07776	-0.82182	-0.82917
C	3.08295	-2.81353	0.13725
H	4.09234	-2.88144	0.58607
C	2.03742	-3.17630	1.19570
H	2.14808	-4.23125	1.50229
H	1.01536	-3.05866	0.79646
H	2.13551	-2.54887	2.09607
C	3.04675	-3.79718	-1.05016
H	2.06848	-3.75384	-1.56194
H	3.21889	-4.83545	-0.71192
H	3.83837	-3.53392	-1.76900
C	6.45331	-0.81975	-1.25186
H	6.38947	0.29117	-1.29618
C	7.57831	-1.17228	-0.25886
H	7.33555	-0.79876	0.75005
H	8.54280	-0.73333	-0.57163
H	7.69346	-2.26810	-0.19220
C	6.79548	-1.32941	-2.66786
H	7.76412	-0.93057	-3.01989
H	6.01564	-1.03437	-3.39153
H	6.85019	-2.43217	-2.66458

TS(C-3^{DFT})

SCF (BP86) Energy = -1781.19747465
Enthalpy 0K = -1780.275127
Enthalpy 298K = -1780.216434
Free Energy 298K = -1780.363023
Lowest Frequency = -12.3144 cm^{-1}
Second Frequency = 17.9933 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.50010629
SCF (C6H6) Energy = -1781.21302035
SCF (BS2) Energy = -3164.96222652

K	-0.31681	-0.51091	-3.54114
Si	-1.70826	-1.99999	-0.65027
Si	-1.23990	0.34553	1.33518
Al	1.17927	-0.54897	-0.63697
O	-0.16986	-1.63586	-1.21971
N	-2.32084	-0.50895	0.12257
N	0.36300	0.65175	0.61869
N	2.80009	-1.49306	-0.30329
N	5.11584	-1.28371	-0.62958
C	-3.70936	-0.14673	-0.07389
C	-4.08028	0.77729	-1.10619
C	-5.43927	1.07857	-1.32279
H	-5.70900	1.78599	-2.11584
C	-6.45124	0.50558	-0.54819
H	-7.50185	0.75526	-0.72969
C	-6.09545	-0.38850	0.46434
H	-6.88072	-0.84160	1.08028
C	-4.75207	-0.73195	0.71609
C	-3.05698	1.48998	-1.99289
H	-2.05620	1.18536	-1.63119
C	-3.20715	1.11014	-3.48750
H	-2.43920	1.61656	-4.10662
H	-4.18474	1.43761	-3.88106
H	-3.16426	0.01934	-3.65809
C	-3.17354	3.02552	-1.87132

H	-2.37378	3.52884	-2.44230
H	-3.10268	3.35397	-0.82383
H	-4.14076	3.38211	-2.26670
C	-4.48230	-1.73381	1.83917
H	-3.39940	-1.93353	1.84677
C	-4.87071	-1.15542	3.21969
H	-4.62521	-1.86986	4.02533
H	-5.95418	-0.94852	3.27551
H	-4.34231	-0.21027	3.42864
C	-5.21058	-3.07733	1.60434
H	-4.92779	-3.81134	2.37920
H	-4.96641	-3.50914	0.61864
H	-6.30762	-2.95824	1.64758
C	-2.82439	-2.49950	-2.11782
H	-3.84714	-2.70725	-1.76120
H	-2.43287	-3.43274	-2.56123
H	-2.93151	-1.74884	-2.91919
C	-1.66863	-3.54916	0.44680
H	-2.68963	-3.92592	0.62404
H	-1.19514	-3.37953	1.42517
H	-1.10201	-4.34321	-0.06988
C	-1.10359	-0.76202	2.88259
H	-0.56918	-0.21957	3.67868
H	-0.54238	-1.69127	2.69123
H	-2.09609	-1.03226	3.27737
C	-2.14236	1.91620	1.89276
H	-3.02886	1.64943	2.49226
H	-2.47890	2.53949	1.05153
H	-1.47261	2.52158	2.52645
C	1.22909	1.71438	1.10608
C	1.19617	3.02813	0.51878
C	2.15263	3.99350	0.89348
H	2.12035	4.98041	0.41722
C	3.13294	3.73445	1.85268
H	3.87220	4.49683	2.12053
C	3.13232	2.48611	2.47599
H	3.87419	2.27443	3.25414
C	2.20495	1.48006	2.13770
C	0.13846	3.49066	-0.48634
H	-0.53938	2.63746	-0.66499
C	-0.67660	4.67561	0.08882
H	-1.45809	5.00170	-0.61931
H	-0.02232	5.54494	0.27519
H	-1.16010	4.41836	1.04407
C	0.75019	3.92280	-1.83942
H	-0.04399	4.18512	-2.56350
H	1.37899	3.13249	-2.27871
H	1.38681	4.81728	-1.72121
C	2.28044	0.19173	2.95611
H	1.55627	-0.51449	2.51942
C	1.88008	0.46350	4.42765
H	1.81401	-0.48042	4.99779
H	0.91167	0.98586	4.50865
H	2.63279	1.10081	4.92531
C	3.67881	-0.46490	2.92099
H	3.65788	-1.43653	3.44629
H	4.42804	0.16256	3.43646
H	4.03006	-0.63652	1.89213
C	2.12456	0.34585	-2.19261
H	2.25507	-0.34722	-3.05745
H	1.81099	1.32441	-2.60406
C	3.53464	0.47953	-1.55277
H	4.31329	0.70873	-2.30155
H	3.53816	1.32360	-0.83515
C	3.91007	-0.81787	-0.80658
C	3.07211	-2.81506	0.29619
H	4.01369	-2.73431	0.87310
C	1.93694	-3.24960	1.22779
H	2.15203	-4.24224	1.66073
H	0.98798	-3.32726	0.67155
H	1.79971	-2.54072	2.06106
C	3.30663	-3.87090	-0.80493
H	2.39460	-4.00028	-1.41636
H	3.56850	-4.85006	-0.36389
H	4.13750	-3.55197	-1.45286
C	6.28579	-0.56390	-1.12586
H	6.08817	0.51635	-1.31096
C	7.39280	-0.64787	-0.05682
H	7.05459	-0.18818	0.88669
H	8.31186	-0.13176	-0.38806
H	7.63600	-1.70407	0.15263
C	6.76191	-1.19082	-2.45362
H	7.68945	-0.71391	-2.81914
H	5.98952	-1.08973	-3.23637
H	6.95496	-2.26848	-2.30988

3^{DFT}

SCF (BP86) Energy = -1781.21695297
Enthalpy 0K = -1780.294216
Enthalpy 298K = -1780.234575
Free Energy 298K = -1780.384335
Lowest Frequency = 21.7656 cm^{-1}
Second Frequency = 24.6761 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.51776029
SCF (C6H6) Energy = -1781.22812099
SCF (BS2) Energy = -3164.98109217

K	2.48635	-2.47855	-2.05765
Si	-1.60818	0.94506	0.79526
Si	-1.21651	-1.06006	-1.62224
Al	1.36015	0.24793	-0.41508
O	0.44183	-1.04921	-1.31736
N	0.04445	1.39827	0.31035
N	-2.08970	-0.53869	-0.14450
N	2.71310	-0.87814	0.47647
N	4.73491	-1.81889	-0.26171
C	0.46990	2.77632	0.47858
C	1.17302	3.18986	1.65694
C	1.66676	4.50696	1.75393
H	2.21222	4.80155	2.65824
C	1.47984	5.44025	0.73225
H	1.87647	6.45716	0.82378
C	0.76721	5.05266	-0.40648
H	0.60522	5.77962	-1.21069
C	0.25044	3.75096	-0.55398
C	1.42580	2.25659	2.84126
H	0.91677	1.30489	2.61839
C	2.93274	1.96180	3.02066
H	3.34245	1.43641	2.14180
H	3.50811	2.89355	3.16431
H	3.10698	1.32572	3.90782
C	0.83370	2.82065	4.15347
H	1.35668	3.73976	4.47253
H	-0.23480	3.07138	4.04448
H	0.93142	2.08445	4.97100
C	-0.52404	3.44237	-1.83633
H	-1.00351	2.46168	-1.68444

C	0.40771	3.32804	-3.06500
H	0.96013	4.27116	-3.22601
H	1.14699	2.52218	-2.93974
H	-0.17633	3.12163	-3.98045
C	-1.63171	4.48149	-2.12649
H	-2.28753	4.64020	-1.25564
H	-1.20612	5.46127	-2.40692
H	-2.25730	4.14718	-2.97355
C	-2.81001	2.39631	0.53265
H	-2.37226	3.31365	0.96263
H	-3.05277	2.59469	-0.52119
H	-3.74954	2.19113	1.07283
C	-1.79031	0.58537	2.65360
H	-1.03692	-0.11329	3.04642
H	-1.68854	1.53596	3.20460
H	-2.79348	0.18136	2.87119
C	-3.31546	-1.21579	0.25559
C	-4.57763	-0.85086	-0.31943
C	-5.75378	-1.49410	0.11637
H	-6.71160	-1.20411	-0.33020
C	-5.72820	-2.49176	1.09318
H	-6.65462	-2.97441	1.42258
C	-4.49656	-2.87460	1.63002
H	-4.46370	-3.67423	2.37867
C	-3.28840	-2.26870	1.23085
C	-4.72054	0.16692	-1.45372
H	-3.73707	0.64371	-1.59617
C	-5.75286	1.27574	-1.14851
H	-6.77653	0.86805	-1.07533
H	-5.53060	1.79624	-0.20422
H	-5.75822	2.02656	-1.95832
C	-5.10914	-0.54590	-2.77231
H	-4.39731	-1.34660	-3.03395
H	-6.10767	-1.01044	-2.68716
H	-5.14514	0.17209	-3.61136
C	-1.99936	-2.82666	1.83971
H	-1.16999	-2.18763	1.49128
C	-2.01157	-2.83032	3.38647
H	-2.24835	-1.84176	3.80657
H	-2.75444	-3.54786	3.77790
H	-1.02531	-3.14047	3.77447
C	-1.73620	-4.27213	1.35106
H	-2.52582	-4.95605	1.71033
H	-1.71776	-4.34183	0.25276
H	-0.77138	-4.64358	1.73993
C	-1.52056	-0.00351	-3.17637
H	-1.32327	1.06584	-3.01211
H	-0.83296	-0.34761	-3.97066
H	-2.54806	-0.11032	-3.55874
C	-1.72120	-2.83548	-2.09449
H	-1.54111	-2.99401	-3.17314
H	-1.13764	-3.58398	-1.53356
H	-2.78827	-3.03358	-1.90288
C	2.83772	1.10111	-1.47130
H	2.81408	2.20209	-1.50574
H	2.81662	0.76984	-2.53261
C	4.15093	0.60818	-0.80541
H	4.42799	1.30248	0.01086
H	5.00783	0.59224	-1.50267
C	3.93443	-0.77434	-0.17540
C	2.59404	-1.96742	1.47475
H	3.61200	-2.14060	1.87575
C	1.67279	-1.52580	2.61879
H	0.65637	-1.30927	2.24660
H	1.58942	-2.31970	3.38138
H	2.05925	-0.61833	3.10565
C	2.12136	-3.32569	0.90412
H	2.90111	-3.75432	0.24987
H	1.96277	-4.05339	1.71923
H	1.16062	-3.21724	0.36787
C	6.09026	-1.68055	-0.80580
H	6.44337	-0.62718	-0.79831
C	6.13337	-2.17500	-2.26836
H	5.50402	-1.54118	-2.92172
H	7.15769	-2.15543	-2.67968
H	5.77180	-3.22041	-2.32540
C	7.05610	-2.50009	0.07079
H	6.75960	-3.56386	0.07674
H	8.09461	-2.42602	-0.29775
H	7.02890	-2.13923	1.11183

3

SCF (BP86) Energy = -2013.47020801
Enthalpy 0K = -2012.449137
Enthalpy 298K = -2012.382594
Free Energy 298K = -2012.552592
Lowest Frequency = 8.5305 cm^{-1}
Second Frequency = 13.0081 cm^{-1}
SCF (BP86-D3BJ) Energy = -2013.79756845
SCF (C6H6) Energy = -2013.47866298
SCF (BS2) Energy = -3397.28884192

K	-3.11376	1.50367	0.32712
Si	2.47025	-0.84328	-0.32017
Si	0.89481	1.65992	0.80689
Al	-0.77209	-0.90984	0.19084
O	-0.54822	0.88831	0.40750
N	0.97267	-1.65029	0.20419
N	2.23239	0.95450	-0.16052
N	-2.14530	-0.91203	-1.21910
N	-4.48953	-0.76694	-1.25031
C	1.04405	-3.02021	0.67831
C	0.80752	-4.11957	-0.21050
C	0.77319	-5.43572	0.29398
H	0.57802	-6.26227	-0.39946
C	0.98041	-5.71115	1.64718
H	0.94346	-6.74012	2.02098
C	1.24736	-4.64677	2.51359
H	1.42416	-4.85161	3.57587
C	1.29457	-3.31355	2.06241
C	0.58557	-3.93731	-1.71221
H	0.71263	-2.86465	-1.93042
C	-0.84630	-4.34212	-2.13079
H	-1.59815	-3.69847	-1.64461
H	-1.06103	-5.39114	-1.85978
H	-0.97763	-4.24944	-3.22448
C	1.62623	-4.72176	-2.54438
H	1.50049	-5.81290	-2.42708
H	2.65852	-4.47555	-2.24391
H	1.51744	-4.49051	-3.61892
C	1.61210	-2.23180	3.09626
H	1.78857	-1.30167	2.53188
C	0.43005	-1.98320	4.06158
H	0.17097	-2.90729	4.60893
H	-0.46933	-1.64746	3.52292
H	0.69232	-1.21324	4.81014
C	2.88494	-2.54958	3.91478

H	3.74233	-2.79232	3.26705
H	2.72720	-3.40570	4.59448
H	3.16143	-1.68442	4.54386
C	3.96229	-1.47322	0.67921
H	3.94464	-2.57655	0.70184
H	3.99532	-1.11070	1.71663
H	4.89338	-1.16564	0.17400
C	2.97668	-1.24215	-2.10981
H	2.16426	-1.11633	-2.84060
H	3.31128	-2.29270	-2.15368
H	3.82751	-0.61044	-2.41660
C	3.25112	1.82042	-0.73588
C	4.37946	2.24297	0.04189
C	5.37039	3.05226	-0.54985
H	6.22789	3.36654	0.05595
C	5.28313	3.46775	-1.88030
H	6.06717	4.09159	-2.32290
C	4.16864	3.08605	-2.63143
H	4.07911	3.42710	-3.66909
C	3.14650	2.27965	-2.09202
C	4.54027	1.91996	1.52937
H	3.74744	1.20335	1.79921
C	5.90482	1.27802	1.86682
H	6.73840	1.98093	1.69169
H	6.09453	0.37577	1.26514
H	5.93940	0.99040	2.93253
C	4.34898	3.19792	2.38243
H	3.38336	3.68947	2.17691
H	5.14389	3.93457	2.16872
H	4.39388	2.96118	3.46082
C	1.94488	1.98651	-2.99379
H	1.29744	1.27583	-2.45293
C	2.34463	1.36379	-4.35206
H	2.97581	0.47061	-4.23459
H	2.89952	2.08746	-4.97536
H	1.44192	1.07333	-4.91791
C	1.12679	3.27199	-3.26824
H	1.72474	4.00089	-3.84421
H	0.81029	3.76843	-2.33849
H	0.22495	3.03715	-3.86129
C	1.10059	1.54363	2.69680
H	1.24990	0.51199	3.04722
H	0.17459	1.92104	3.16823
H	1.93568	2.15919	3.06714
C	0.71803	3.51662	0.41654
H	0.28008	4.03454	1.28845
H	0.05464	3.67951	-0.44855
H	1.68547	3.99496	0.19386
C	-2.11361	-1.74233	1.43066
H	-1.74361	-2.60414	2.00885
H	-2.47435	-1.01133	2.18746
C	-3.29427	-2.16918	0.51988
H	-3.11369	-3.19507	0.14546
H	-4.26184	-2.20920	1.05261
C	-3.39081	-1.25534	-0.70978
C	-2.13162	-0.37546	-2.59957
H	-2.99544	-0.82823	-3.12439
C	-0.83795	-0.78953	-3.31065
H	0.04741	-0.39479	-2.78274
H	-0.81662	-0.39697	-4.34235
H	-0.74806	-1.88510	-3.35674
C	-2.32927	1.15584	-2.68811
H	-3.34980	1.42300	-2.36135
H	-2.23289	1.50000	-3.73308
H	-1.56532	1.68730	-2.09130
C	-5.81142	-1.25838	-0.85775
H	-5.85752	-1.55824	0.21556
C	-6.83688	-0.12813	-1.06445
H	-6.58866	0.75009	-0.44023
H	-7.85701	-0.45655	-0.79903
H	-6.83577	0.19920	-2.11882
C	-6.19289	-2.49536	-1.69819
H	-6.15489	-2.24606	-2.77297
H	-7.21073	-2.84993	-1.45578
H	-5.48715	-3.32329	-1.51755
C	-3.74038	3.47614	3.01873
H	-3.08406	3.30301	3.87782
C	-3.38404	4.42419	2.04087
H	-2.45065	4.98769	2.13932
C	-4.23517	4.65843	0.94419
H	-3.96477	5.40678	0.19175
C	-5.44327	3.94551	0.82596
H	-6.11280	4.13733	-0.01893
C	-5.80014	2.99819	1.80444
H	-6.74633	2.45413	1.71924
C	-4.94836	2.76297	2.90038
H	-5.23231	2.03592	3.66845