Supplementary Information

Enhancing the Nucleophilicity of Aluminyl Anions: Targeting Selective C–H Activation

Authors: Fabian Kallmeier,[a] Gareth R. Nelmes[a] Claire L. McMullin,[b] Alison J. Edwards[c] and Jamie Hicks*[a]

Affiliations:

[a] Research School of Chemistry, Australian National University, Sullivans Creek Road, Acton, 2601, Australia.

[b] Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, United Kingdom.

[c] Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, NSW, 2234, Australia.

* Email address for correspondence:

jamie.hicks@anu.edu.au

This PDF file includes:

Figures S1-S28

Tables S1-S3

(63 pages total)

Contents

Materials and Methods

General Considerations

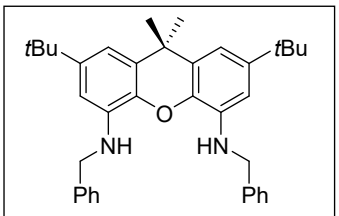
All manipulations, unless otherwise indicated, were performed under inert conditions using standard Schlenk and glovebox techniques, employing nitrogen or argon as an inert gas. Solvents (*n*-hexane, toluene, tetrahydrofuran THF, diethyl ether) were pre-dried using an MBraun solvent purification system, degassed by passing agon through, and stored over sodium. Benzene and benzene-d_6 were distilled over potassium and stored over sodium. *n*-Pentane was degassed and pre-dried for seven days by storage over 4 Å molecular sieves and then filtered onto sodium metal for storage. Benzylamine and diphenylether were fractionally distilled before use,[S1] 18-crown-6 was doubly sublimed, fluorobenzene was degassed and stored over 4 Å molecular sieves, methyl iodide was degassed and stored over 4 Å molecular sieves and a sheet of copper mesh. *n*-BuLi was purchased from Sigma Aldrich filtered and titrated against (-)-menthol using 1,10-phenanthroline as an indicator before use.[S2] Potassium graphite was prepared in a ball mill (IKA ULTRA-TURRAX Tube Drive) in a glovebox. Typically, a 20 mL polypropylene vial was charged with potassium metal (1 g), graphite (2.46 g), and 30 stainless steel balls (0.52 g each, ⌀ 5 mm). Ball milling was performed for 2 × 29 min at 4000 rpm, which was accompanied by a colour change from black to bronze. The resultant fine powder was used without further purification after the balls had been manually removed. H_2(**^{tBu}NON**), AlI(**^{TIPS}NON**) (**1**), K_2[Al(**^{Dipp}NON**)]$_2$ (**I**) and 4,5-dibromo-2,7-di-*tert*-butyl-9,9-dimethylxanthene were synthesised according to the literature.[S3,S4] All other reagents and solvents were used as received.

NMR samples were prepared in an Ar or N_2 atmosphere glovebox using Norell NMR tubes (⌀ 5 mm) with a J Young valve. NMR spectra were recorded at 298 K using a Bruker Avance 800 MHz or a Bruker Avance 400 MHz. ^{1}H and ^{13}C{^{1}H} spectra were referenced to residual protio solvent (for benzene ^{1}H: 7.16 ppm, ^{13}C: 128.06 ppm). ^{29}Si NMR spectra were referenced by adding a sealed glass capillary containing a solution of tetramethyl silane (δ = 0 ppm) in benzene. Where direct observation of the silicon nucleus was unsuccessful, two-dimensional ^{1}H-^{29}Si HMBC experiments were used to determine the silicon shift. ^{19}F{^{1}H} spectra were externally referenced to $CFCl_3$ (δ = 0 ppm). ^{27}Al NMR spectroscopy was unsuccessful due to signal broadening (I = 5/2) and artefacts from the aluminium in the probe. High-Resolution Mass Spectrometry was performed at the ANU Joint Mass Spectrometry Facility (JMSF) using a Thermo Orbitrap Elite system (Thermo Fisher Scientific, Delaware, USA) equipped with a HESI-II electron spray ionisation source (spray voltage: 2.5 kV, source heater: 300 °C) coupled to an UltiMate 3000 UHPLC (Thermo). The sample was delivered to the MS using an isocratic elution mode, the scan range was set to m/z 150-2000 at a resolution of 120000, and the data were analysed using Thermo Freestyle

software. Elemental analysis was performed by the Elemental Analysis Service of the Science Centre at London Metropolitan University, UK. Aluminium and silicon are known to form their respective carbides, leading to slightly lower carbon determinations.

Synthesis and Characterisation of New Compounds

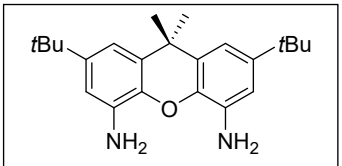
Synthesis of N^4,N^5-dibenzyl-2,7-di-*tert*-butyl-9,9-dimethyl-xanthene-4,5-diamine, H_2(**^{Bn}NON**)



Chemical Formula: $C_{37}H_{44}N_2O$
Molecular Weight: 532.77

Following a modified procedure described in the literature.[S4] To a suspension of 4,5-dibromo-2,7-di-*tert*-butyl-9,9-dimethylxanthene (19.20 g, 40 mmol), $Pd(OAc)_2$ (0.45 g, 2 mmol, 5 mol%), 2-(di-*tert*-butylphosphino)biphenyl (0.89 g, 3 mmol, 7.5 mol%), and sodium *tert*-butoxide (10.80 g, 112 mmol, 2.8 equiv.) in toluene (150 mL) was added benzylamine (17.5 mL, 160 mmol, 4 equiv.) under Ar. The flask was tightly sealed, and the mixture stirred at 120 °C overnight. After cooling to room temperature, the reaction mixture was poured into 500 mL saturated NaCl solution and extracted into toluene (3 x 350 mL). The organic phase was dried over $MgSO_4$ and the volatiles removed *in vacuo* to give an amber solid, which was subsequently refluxed in 100 mL MeOH for 10 minutes. Upon cooling to 5 °C, the colourless solid was filtered off and dried to yield H_2(**^{Bn}NON**) as a colourless solid. **Yield**: 74% (15.76 g, 29.6 mmol). **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.26–7.19 (m, 4H, *o*-Ph), 7.14 – 7.03 (m, 6H, *m*-Ph, *p*-Ph), 6.99 (d, J = 2.1 Hz, 2H, xanthene), 6.71 (d, J = 2.2 Hz, 2H, xanthene), 4.47 (s, 2H, N*H*), 4.11 (s, 4H, CH_2), 1.73 (s, 6H, C(CH_3)$_2$), 1.33 (s, 18H, C(CH_3)$_3$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 145.9, 140.2, 137.1, 136.7, 129.5, 128.9, 127.6, 127.3, 110.9, 107.4 (*C*-Ar), 48.7 (*C*H_2), 35.2 (*C*(CH$_3$)$_3$), 34.9 (*C*(CH$_3$)$_2$), 32.2 (*C*(CH$_3$)$_2$), 31.8 (*C*(CH$_3$)$_3$) ppm. **HRMS** (ESI+): *m*/*z* calcd. for $[C_{37}H_{44}N_2O+H]^+$ 533.3526; found 533.3526.

Synthesis of 2,7-di-*tert*-butyl-9,9-dimethyl-9H-xanthene-4,5-diamine, H_2(**^{H}NON**)



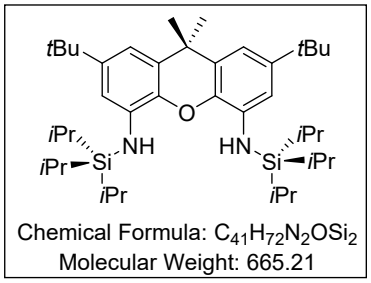
Chemical Formula: $C_{23}H_{32}N_2O$
Molecular Weight: 352.52

Route A) A suspension of H_2(**^{Bn}NON**) (10 g, 18.8 mmol) and Pd/C (400 mg, 10 %-wt.) in THF (50 mL) and MeOH (30 mL) was degassed *via* two freeze-pump-thaw cycles. The flask was then charged with H_2 (20 psi), and the mixture stirred until thin layer chromatography or NMR analysis indicated complete consumption of the starting material (approx. 24 hours). The mixture was filtered, and the residue washed with THF (3x 10 mL). The solvent was evaporated and the crude product recrystallised from toluene/hexane, yielding H_2(**^{H}NON**) as a colourless solid. **Yield**: 81% (5.36 g, 15.2 mmol). **^{1}H NMR** (400 MHz, C_6D_6): δ = 6.93 (d, J = 2.2 Hz, 2H, xanthene), 6.51 (d, J = 2.2 Hz, 2H, xanthene), 3.29 (s, 4H, NH_2), 1.64 (s, 6H, C(CH_3)$_2$), 1.33 (s,18H, C(CH_3)$_3$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 145.6, 137.2, 134.9, 130.1, 112.0, 111.1 (*C*-Ar), 35.0, 34.6, 32.3, 31.8 ppm. **HRMS** (ESI+): *m*/*z* calcd. for$[C_{23}H_{32}N_2O + H]^+$ 353.2587; found 353.2586.

Route B) Under ambient conditions, a suspension of H_2(**^{tBu}NON**) (9.50 g, 20.4 mmol) in *ortho*-phosphoric acid (0.25 L, 85 %-w/w) was heated to 145 °C for 18 hours. The mixture was cooled to room temperature and slowly

poured into excess KOH (0.60 kg, technical grade) in water (1.50 L) under strong stirring and cooling with an ice bath. Once cooled down, the mixture was filtered, the residue washed (3 x 100 mL H_2O, 2 x 20 mL EtOH 70%), and then dried *in vacuo* for 5 minutes. The solid was dissolved in $CHCl_3$ (350 mL) and dried over $MgSO_4$. After filtration through a pad of Celite® the volatiles were removed *in vacuo*, leaving H_2(**^{H}NON**) as a fine powder. The compound was further purified by trituration in hot hexane (*ca.* 50 mL per 8 g of pure compound) for 15 minutes. The mixture was then placed in a freezer for 30 minutes and the titular compound was isolated as a brown solid *via* filtration. The solid was washed with hexane (3x15 mL) and then dried *in vacuo*. **Yield**: 97% (7.01 g, 19.9 mmol) as colourless solid. NMR spectroscopic analysis matched the product obtained from Route **A**.

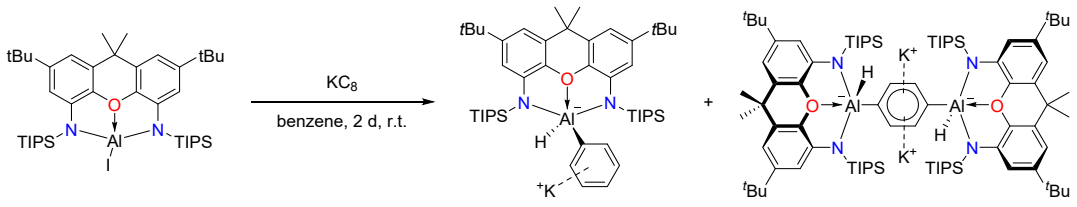
Synthesis of H_2(**^{TIPS}NON**)



Chemical Formula: $C_{41}H_{72}N_2OSi_2$
Molecular Weight: 665.21

Following a modified literature procedure by Tilley and coworkers.[S5] To a solution of H_2(**^{H}NON**) (7.68 g, 21.89 mmol) in THF (100 mL) was added *n*-BuLi (22 mL, 44 mmol, 2.0 M in cyclohexane) dropwise at 0 °C. The solution was allowed to warm to room temperature and stirred for a further 1.5 h. After cooling to 0 °C, neat chlorotriisopropylsilane (9.4 mL, 8.48 g, 44 mmol; TIPSCl) was added in one portion *via* a syringe. After stirring the solution for 2 days at room temperature, methanol (20 mL, "wet") was added under a stream of argon. After stirring for 10 minutes, the argon stream was turned off, and workup commenced under ambient conditions. The solvents were evaporated, and the residue was taken up in toluene (200 mL) and water (50 mL). The organic layer was separated, the aqueous layer extracted using toluene (2 x 50 mL), the combined organic layer was dried using $MgSO_4$ and the solids filtered off. The crude product was taken up in minimal toluene (*ca.* 50 mL) and the solution was poured into methanol at 0 °C, stirred at 0 °C for 2 hours and the colourless, crystalline precipitate was collected and dried under reduced pressure. **Yield**: 91% (13.19 g, 19.83 mmol) as colourless solid. **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.03 (d, J = 2.2 Hz, 2H, xanthene), 6.94 (d, J = 2.2 Hz, 2H, xanthene), 4.08 (s, 2H, N*H*), 1.64 (s, 6H, C(CH_3)$_2$), 1.45–1.35 (m, 24H, Si-C*H*(CH$_3$)$_2$ & C(CH_3)$_3$), 1.21 (d, J = 7.5 Hz, 36H, Si-CH(CH_3)$_2$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 145.3, 137.8, 135.9, 129.8, 111.9, 111.5 (*C*-Ar), 35.2, 34.8, 32.6, 31.9, 18.8 (Si-CH(*C*H$_3$)$_2$), 13.5 (Si-*C*H(CH$_3$)$_2$) ppm. **^{29}Si{^{1}H} NMR** (79 MHz, C_6D_6, TMS Standard): δ = 6.7 ppm. The analysis matched the reported values.

Reaction of K_n[Al(**^{TIPS}NON**)]$_n$ with benzene - Synthesis of K[AlH(Ph)(**^{TIPS}NON**)] (**2**) and K_2[{AlH(**^{TIPS}NON**)}$_2$-1,4-C_6H_4] (**3**)



1

2
29 %

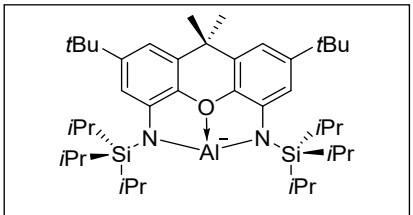
3
13 %

Solution-phase synthesis: To a mixture of **1** (1.00 g, 1.22 mmol) and KC_8 (2.50 g, 18.3 mmol, 15 eq) was added benzene (50 mL) at 5 ºC. The suspension was left to warm to room temperature and stirred for two days at room temperature. The solids were filtered off, and the volatiles of the orange solution were removed under reduced pressure, yielding a foamy residue. To this was added *n*-hexane (20 mL) and the resulting suspension was triturated overnight. Note: the supernatant at this point contains mostly K_2(**^{TIPS}NON**), **3**, and unidentified species with broad ^{1}H NMR spectrum signals, while the solid contains **2** and **3** in a ratio of ~ 5:1. The solids were filtered off and the colourless precipitate was washed with *n*-hexane (4 x 10 mL). Residual solvent was removed from the powder *in vacuo* to give **2** as colourless solid. **Yield**: 29% (285 mg, 0.35 mmol). **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.69–7.63 (m, 2H, Al-$C_6H^o_5$), 7.29 (d, J = 1.9 Hz, 2H, xanthene), 6.60 (t, J = 7.4 Hz, 2H, Al-$C_6H^m_5$), 6.44 (tt, J = 7.9, 1.5 Hz, 1H, Al-$C_6H^p_5$), 6.26 (d, J = 1.9 Hz, 2H, xanthene), 5.06 (s, 1H, Al-*H*), 2.13 (hept, J = 7.5 Hz, 6H, Si-C*H*$(CH_3)_2$), 1.61 (d, J = 7.5 Hz, 18H, Si-CH(C$H_3)_2$), 1.43 (d, J = 7.5 Hz, 18H, Si-CH(C$H_3)_2$), 1.35 (s, 3H, C(C$H_3)_2$), 1.31 (s, 21H, C(C$H_3)_3$ & C(C$H_3)_2$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 162.0 (Al-$C^{ipso}{}_6H_5$)*, 148.8, 146.1, 143.7, 141.7 (Al-$C^o{}_6H_5$), 130.3, 126.2 (Al-$C^m{}_6H_5$), 125.7 (Al-$C^p{}_6H_5$), 119.5, 104.0 (*C*-Ar), 36.0 (*C*$(CH_3)_3$), 34.9 (*C*$(CH_3)_2$), 32.0 (C(*C*$H_3)_3$), 31.5, 24.2, 20.3 (Si(CH(*C*$H_3)_2$), 20.0 (Si(CH(*C*$H_3)_2$), 14.7 (Si(*C*H$(CH_3)_2$) ppm. *resonance observed through ^{1}H-^{13}C HMBC experiment. **^{29}Si NMR** (79 MHz, C_6D_6): δ = 4.7 ppm observed *via* ^{1}H-^{29}Si HMBC. **Elemental Analysis** calcd. for $C_{47}H_{76}AlKN_2OSi_2$: C 69.92, H 9.49, N 3.47; found: C 70.35, H 9.69, N 3.52.

The combined hexane washings were concentrated under reduced pressure, and colourless crystals of **3** were obtained upon storage at 5 ºC for two weeks. **Yield**: 13% (120 mg, 0.08 mmol). **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.15 (d, J = 1.8 Hz, 4H, xanthene), 7.02 (s, 4H, Al-C_6H_4-Al), 6.34 (d, J = 1.7 Hz, 4H, xanthene), 4.57 (s, 2H, Al-*H*), 1.97 (hept, J = 7.3 Hz, 12H, Si-C*H*$(CH_3)_2$), 1.49 (d, J = 7.5 Hz, 36H, Si-CH(C$H_3)_2$), 1.36 (s, 36H, C(C$H_3)_3$), 1.29 (d, J = 7.4 Hz, 42H, Si-CH(C$H_3)_2$ & C(C$H_3)_2$), 1.24 (s, 6H, C(C$H_3)_2$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 159.6 (Al-*C*)*, 147.7, 146.9, 141.5, 139.3 (Al-CC_4H_4C-Al), 128.4*, 117.5, 104.7 (*C*-Ar), 35.5 (*C*$(CH_3)_3$), 35.1 (*C*$(CH_3)_2$), 32.2 (C(*C*$H_3)_3$), 25.3 (C(*C*$H_3)_2$), 20.1 (Si(CH(*C*$H_3)_2$), 20.0 (Si(CH(*C*$H_3)_2$), 18.8 (C(*C*$H_3)_2$), 14.7 (Si(*C*H$(CH_3)_2$) ppm. *resonances observed through ^{1}H-^{13}C HMBC experiment. **^{29}Si NMR** (79 MHz, C_6D_6): δ = 4.3 ppm observed *via* ^{1}H-^{29}Si HMBC. **Elemental Analysis** calcd. for $C_{88}H_{146}Al_2K_2N_4O_2Si_4 \cdot C_6H_{14}$: C 69.57, H 9.94, N 3.45; found: C 69.38, H 10.00, N 3.53.

Ball-mill synthesis: Crystals of **1** (200 mg, 0.24 mmol) and KC_8 (800 mg, 5.93 mmol) were combined in a 20 mL polypropylene vessel with stainless steel balls (30 pieces, diameter: 5 mm, weight per ball: 0.52 g). Milling was commenced on the highest setting (4000 rpm, 66.7 Hz) for 58 minutes using an IKA ULTRA-TURRAX® Tube Drive. From the mixture, an aliquot (130 mg) was transferred to a filter, C_6D_6 (0.5 mL) was added evenly, and filtered into a J. Young NMR tube for analysis. ^{1}H NMR spectroscopic analysis confirmed the complete conversion of the starting material, along with **2**-d_6 and **3**-d_6 in a ratio of 1.36 to 1.

Synthesis of [K(18-crown-6)][Al(**^{TIPS}NON**)] (**4**)

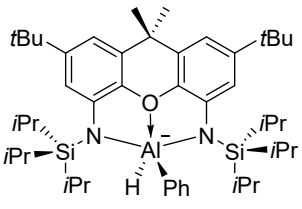


Chemical Formula: $C_{53}H_{94}AlKN_2O_7Si_2$
Molecular Weight: 993.59

To a mixture of **1** (409 mg, 0.5 mmol), KC_8 (608 mg, 4.5 mmol), and 18-crown-6 (145 mg, 0.55 mmol) was added *n*-pentane (80 mL) at 0 ºC. The suspension was stirred for two hours. The solids were filtered off and the supernatant was concentrated to *ca.* 4 mL. Keeping the flask

under static vacuum, the bottom of the flask was gently warmed to 32 ºC until orange crystals appeared (usually after *ca.* 10 minutes) and the flask was backfilled with inert gas. After crystallisation finished, the supernatant was decanted, and the crystals were washed with *n*-pentane (2 x 2.5 mL) and dried *in vacuo,* yielding **4** as red-orange crystals. **Yield:** 56% (308 mg, 0.28 mmol). **^{1}H NMR** (400 MHz, C_6D_{12}): δ = 6.70 (d, J = 1.7 Hz, 2H, xanthene), 6.25 (d, J = 1.7 Hz, 2H, xanthene), 3.46 (s, 24H, 18-crown-6), 1.66 (hept, J = 7.5 Hz, 6H, Si-C*H*$(CH_3)_2$), 1.56 (s, 6H, C(C*H*$_3)_2$), 1.22 (s, 18H, C(C*H*$_3)_3$), 1.18 (d, J = 6.8 Hz, 36H, Si-CH(C*H*$_3)_2$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_{12}): δ = 148.5, 146.9, 145.0, 135.0, 115.4, 104.0 (*C*-Ar), 70.9 (-*C*$_2$H$_4$O-), 38.4 (*C*$(CH_3)_2$), 35.5 (*C*$(CH_3)_3$), 32.5 (C(*C*$H_3)_3$), 20.6 (Si-CH(*C*$H_3)_2$), 16.1 (Si-*C*H$(CH_3)_2$) ppm. **^{29}Si NMR** (79 MHz, C_6D_{12}, TMS): δ = 2.7 ppm (*Si*-CH$(CH_3)_2$) observed *via* ^{1}H-^{29}Si HMBC. **Elemental Analysis** calcd. for $C_{53}H_{94}AlKN_2O_7Si_2 \cdot 0.5\ C_5H_{12}$: C 64.74, H 9.79, N 2.72; found: C 64.49, H 9.73, N 2.64. **Note:** Upon standing at room temperature, solutions of compound **4** decompose (*vide infra*).

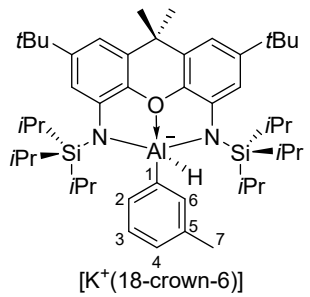
Synthesis of [K(18-crown-6)][AlH(Ph)(**^{TIPS}NON**)] (**5**)



[K^{+}(18-crown-6)]
Chemical Formula: $C_{59}H_{100}AlKN_2O_7Si_2$
Molecular Weight: 1071.71

A freshly prepared solution of **4** (0.25 mmol in 40 mL *n*-pentane) was concentrated to *ca.* 2 mL. Benzene (0.22 mL, 2.5 mmol, 10 equiv.) was added in one portion at room temperature. After 10 minutes of stirring the mixture, volatiles were removed *in vacuo*, the crude product was washed with *n*-pentane (3 mL), giving **5** as a colourless solid. **Yield**: 56% (0.151 g, 0.141 mmol) **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.82 (dd, J = 7.7, 1.3 Hz, 2H, $C_6H^{o}_5$), 7.37 (d, J = 1.9 Hz, 2H, xanthene), 6.90 (t, J = 7.5 Hz, 2H, $C_6H^{m}_5$), 6.71 (tt, J = 7.4, 1.5 Hz, 1H, $C_6H^{p}_5$), 6.64 (d, J = 1.8 Hz, 2H, xanthene), 5.16 (s, 1H, Al-*H*), 2.91 (s, 24H, 18-crown-6), 2.32 (hept, J = 7.5 Hz, 6H, Si-C*H*$(CH_3)_2$), 1.71 (d, J = 7.6 Hz, 18H, Si-CH(C*H*$_3)_2$), 1.63 (s, 3H, C(C*H*$_3)_2$), 1.61 (s, 3H, C(C*H*$_3)_2$), 1.58 (d, J = 7.5 Hz, 18H, Si-CH(C*H*$_3)_2$), 1.54 (s, 18H, C(C*H*$_3)_3$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 160.6* (*C*$^{ipso}{}_6$H$_5$), 147.1, 144.8, 141.3, 140.4 (*C*$^{o}{}_6$H$_5$), 128.3, 125.0 (*C*$^{m}{}_6$H$_5$), 123.4 (*C*$^{p}{}_6$H$_5$), 116.5, 105.8 (*C*-xanthene), 69.9 (-*C*$_2$H$_4$O-), 35.8 (*C*$(CH_3)_3$), 35.1 (*C*$(CH_3)_2$), 32.8 (C(*C*$H_3)_2$), 32.5 (C(*C*$H_3)_3$), 28.0 (C(*C*$H_3)_2$), 20.8 (Si-CH(*C*$H_3)_2$), 20.7 (Si-CH(*C*$H_3)_2$), 15.4 (Si-*C*H$(CH_3)_2$) ppm. (*observable through ^{1}H-^{13}C HMBC correlation) **^{29}Si NMR** (79 MHz, C_6D_6): δ = 2.8 (*Si*-CH$(CH_3)_2$) ppm. **Elemental Analysis** calcd. for $C_{59}H_{100}AlKN_2O_7Si_2$: C 66.12, H 9.41, N 2.61; found: C 64.62, H 9.43, N 2.44. **n.b.** Single crystals suitable for X-ray diffraction were obtained by storing a concentrated solution in cyclohexane at 5 ºC overnight.

Synthesis of [K(18-crown-6)][AlH(3-Me-C_6H_4)(**^{TIPS}NON**)] (**6**)

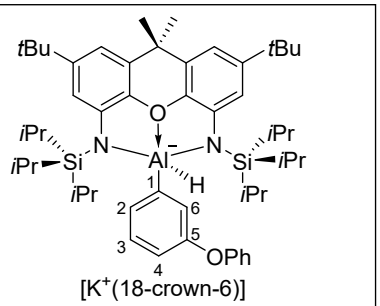


[K^{+}(18-crown-6)]
Chemical Formula: $C_{60}H_{102}AlKN_2O_7Si_2$
Molecular Weight: 1085.73

A freshly prepared solution of **4** (0.25 mmol in 40 mL *n*-pentane) was concentrated to *ca.* 2 mL. Toluene (0.26 mL, 2.5 mmol, 10 equiv.) was added in one portion at room temperature. After 10 minutes of stirring the mixture, volatiles were removed *in vacuo*, the crude product was washed with *n*-pentane (3 mL), giving **6** as a colourless solid. **Yield**: 88% (238 mg, 0.22 mmol). **^{1}H NMR** (800 MHz, C_6D_6): δ = 7.56 (d, J = 7.1 Hz, 1H, *H*-2), 7.51 (s, 1H, H-*6*), 7.44 (d, J = 1.9 Hz, 2H, xanthene), 6.68 (d, J = 1.9 Hz, 2H, xanthene), 6.65 (t, J = 7.1

Hz, 1H, *H*-3), 6.26 (d, *J* = 7.1 Hz, 1H, *H*-4), 5.01 (s, 1H, Al-*H*), 2.90 (s, 24H, 18-crown-6), 2.27 (hept, *J* = 7.5 Hz, 6H, Si-C*H*(CH_3)$_2$), *H*-7), 1.76 (d, *J* = 7.5 Hz, 18H, Si-CH(CH_3)$_2$), 1.62 – 1.59 (m, 36H, Si-CH(CH_3)$_2$ & C(CH_3)$_3$), 1.57 (s, 3H, C(CH_3)$_2$), 1.53 (s, 3H, C(CH_3)$_2$) ppm. **^{13}C{^{1}H} NMR** (201 MHz, C_6D_6): δ = 159.8* (*C*-1), 147.0, 144.3, 142.1 (*C*-6), 137.9 (*C*-2), 132.2, 128.3 (*C*-5), 124.5 (*C*-3), 123.5 (C-4), 117.3, 106.8 (*C*-xanthene), 69.9 (-C_2H_4O-), 35.9, 35.1 (*C*(CH_3)$_3$), 33.8, 32.5 (C(*C*H_3)$_3$), 25.7 (*C*(CH_3)$_2$), 22.3 (C(*C*H_3)$_2$), 21.4 (*C*-7) 20.8 (Si-CH(*C*H_3)$_2$), 20.7 (Si-CH(*C*H_3)$_2$), 18.8 (C(*C*H_3)$_2$), 15.5 (*Si*-CH(CH_3)$_2$) ppm. (*observable through ^{1}H-^{13}C HMBC correlation) **^{1}H-^{29}Si HMBC** (79 MHz, C_6D_6): δ = 2.4 (*Si*-CH(CH_3)$_2$) ppm. Direct observation of the ^{29}Si nucleus by 1D ^{29}Si NMR spectroscopy was not possible due to the low solubility of the compound in C_6D_6. **Elemental Analysis** calcd. for $C_{60}H_{102}AlKN_2O_7Si_2$: C 66.38, H 9.47, N 2.58; found: C 64.75, H 9.34, N 2.36. **n.b.** Single crystals suitable for X-ray diffraction were obtained by storing a concentrated solution in toluene at -35 ºC overnight.

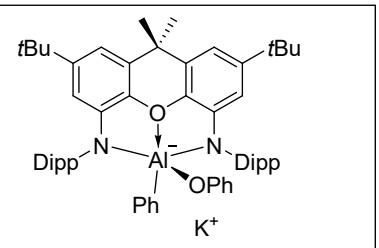
Synthesis of [K(18-crown-6)][AlH(3-OPh-C_6H_4)(**^{TIPS}NON**)] (**7**)



Chemical Formula: $C_{65}H_{104}AlKN_2O_8Si_2$
Molecular Weight: 1163.80

To a freshly prepared solution of **4** (0.25 mmol in 40 mL *n*-pentane) was added phenyl ether (0.06 mL, 0.33 mmol, 1.30 equiv.), and the mixture was stirred for one hour. After the solids had settled, the solution was removed *via* cannula filtration. The solid was dried *in vacuo*, and recrystallised from boiling benzene (1 mL). The supernatant was decanted, and the colourless crystals were dried under reduced pressure. **Yield**: 52% (0.154 g, 0.13 mmol). **^{1}H NMR** (800 MHz, C_6D_6): δ = 7.68 (dd, *J* = 7.1, 0.9 Hz, 1H, *H*-2), 7.44 (d, *J* = 2.7 Hz, 1H, *H*-6), 7.37 (d, *J* = 1.9 Hz, 2H, xanthene), 7.18 (m, 2H, OC_6H_5), 6.86 (tt, *J* = 7.4, 1.1 Hz, 1H, OC_6H_5), 6.78 (t, *J* = 7.4 Hz, 1H, *H*-3), 6.73 – 6.70 (m, 2H, , OC_6H_5), 6.68 (d, *J* = 1.9 Hz, 2H, xanthene), 6.25 (ddd, *J* = 7.7, 2.7, 1.2 Hz, 1H, *H*-4), 2.88 (s, 24H, 18-crown-6), 2.28 (hept, *J* = 7.5 Hz, 6H, Si-C*H*(CH_3)$_2$), 1.73 (d, *J* = 7.6 Hz, 18H, Si-CH(CH_3)$_2$), 1.72 (s, 3H, C(CH_3)$_2$), 1.62 (s, 3H, C(CH_3)$_2$), 1.59 (d, *J* = 7.5 Hz, 18H, Si-C*H*(CH_3)$_2$), 1.46 (s, 18H, C(CH_3)$_3$). **^{13}C NMR** (201 MHz, C_6D_6): δ = 165.2 (*C*-1), 161.0 (*C*-5), 153.0 (OC_6H_5), 146.9, 144.7, 141.2, 137.3 (*C*-2), 132.9 (*C*-6), 129.5 (OC_6H_5), 127.7, 125.6 (*C*-3), 121.3 (OC_6H_5), 117.1 (OC_6H_5), 116.9 (*C*-xanthene), 115.7 (*C*-4), 106.6 (*C*-xanthene), 69.8 (-C_2H_4O-), 35.8 (*C*(CH_3)$_2$), 35.0 (*C*(CH_3)$_2$), 34.0 (C(*C*H_3)$_2$), 32.3 (C(*C*H_3)$_3$), 27.2 (C(*C*H_3)$_2$), 20.7 (Si-CH(*C*H_3)$_2$), 20.6 (Si-CH(*C*H_3)$_2$), 15.4 (Si-*C*H(CH_3)$_2$) ppm. **^{1}H-^{29}Si HMBC** (400 MHz, 79 MHz, C_6D_6): δ = 3.0 (*Si*-CH(CH_3)$_2$) ppm. Direct observation of the ^{29}Si nucleus by 1D ^{29}Si NMR spectroscopy was not possible due to the low solubility of the compound in C_6D_6. **Elemental Analysis** calcd. for $C_{65}H_{104}AlKN_2O_8Si_2$: C 67.08, H 9.01, N 2.41; found: C 66.82, H 9.15, N 2.28.

Synthesis of K_2[AlOPh(Ph)(**^{Dipp}NON**)]$_2$ (**8**)

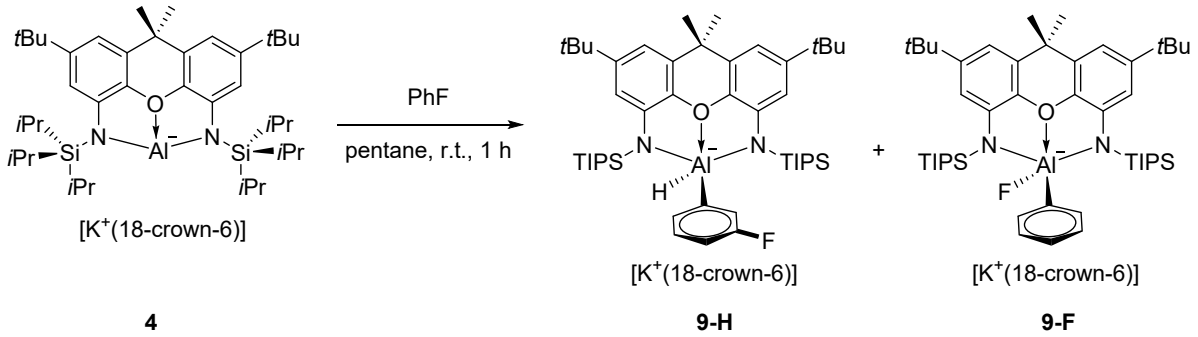


Chemical Formula: $C_{59}H_{72}AlKN_2O_2$
Molecular Weight: 907.32

A mixture of K_2[Al(**^{Dipp}NON**)]$_2$ (**I**, 34 µmol, 50 mg) and diphenyl ether (3 mL) was stirred at 50 °C overnight. Upon heating, the bright yellow colour of **I** gradually faded and the solution turned colourless. The temperature was increased to 65 °C and the solution reduced to ca 1 mL *in vacuo*. Crystalline **8** was obtained over 3 days by addition

of 15 mL hexane, followed by filtration and removal of volatiles *in vacuo*. **Yield**: 66 % (41 mg, 35 µmol) as colourless solid. **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.96 (d, J = 5.2 Hz, 2H, O-*o*-Ph), 7.41 (t, J = 7.0 Hz, 2H, O-*m*-Ph), 7.07 – 6.83 (m, 11H, Ar*H*), 6.78 (s, 2H, xanthene), 6.51 (t, J = 7.0 Hz, 1H, O-*p*-Ph), 6.08 (s, 2H, xanthene), 3.94 (hept, J = 6.4 Hz, 2H, C*H*(CH_3)$_2$), 3.45 (hept, J = 6.4 Hz, 2H, C*H*(CH_3)$_2$), 1.81 (s, 3H, C(CH_3)$_2$), 1.70 (s, 3H, C(CH_3)$_2$), 1.34 (s, 18H, C(CH_3)$_3$), 1.23 (d, J = 6.6 Hz, 6H, CH(CH_3)$_2$), 1.11 (d, J = 6.6 Hz, 6H, CH(CH_3)$_2$), 0.99 (d, J = 6.7 Hz, 6H, CH(CH_3)$_2$), 0.54 (d, J = 6.6 Hz, 6H, CH(CH_3)$_2$) ppm. **^{13}C NMR** (101 MHz, C_6D_6): δ = 160.7, 149.1 (Dipp), 149.0 (Dipp), 148.0, 146.6 ((*t*Bu)$C_{xanthene}$), 145.3, 140.1, 138.6 (O-*o*-Ph), 131.6, 129.4, 127.5 (O-*m*-Ph), 126.2, 124.7, 124.5, 123.6, 119.6, 117.2 (O-*p*-Ph), 110.4 ($C_{xanthene}$H), 105.5 ($C_{xanthene}$H), 36.8, 35.2, 33.9 (C(CH$_3$)$_2$), 32.1 (C(CH$_3$)$_3$), 29.6 (*C*H(CH_3)$_2$), 27.4 (*C*H(CH_3)$_2$), 26.0 (CH(*C*H$_3$)$_2$), 25.7 (CH(*C*H$_3$)$_2$), 24.3 (CH(*C*H$_3$)$_2$), 23.6 (CH(*C*H$_3$)$_2$), 23.1 (C(*C*H$_3$)$_2$) ppm.

Reaction of **4** with fluorobenzene. Synthesis of [K(18-crown-6)][AlH(3-F-C_6H_4)(**^{TIPS}NON**)] (**9-H**) and [K(18-crown-6)][AlF(Ph)(**^{TIPS}NON**)] (**9-F**)

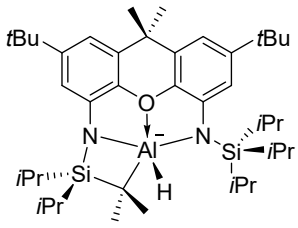


4 **9-H** **9-F**

To a freshly prepared solution of **4** (0.38 mmol in 50 mL *n*-hexane) was added fluorobenzene (0.05 mL, 0.53 mmol, 1.4 equiv.) at 0 °C. The reaction was stirred at room temperature for one hour. After the solids had settled, the supernatant solution was removed *via* cannula filtration. The solid was dried *in vacuo*, and recrystallised from boiling benzene/hexane (1 mL each). The supernatant was carefully decanted, and the colourless crystals (suitable for X-ray diffractometry) were dried under reduced pressure. **Yield**: 38% (0.156 g, 0.14 mmol) as an inseparable mixture of **9-H** and **9-F** (*ca.* 2.7 : 1 by NMR). **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.71–7.67 (m, 2H, **9-F**, Al-$C_6H^o_5$), 7.59 (dd, J = 10.6, 3.0 Hz, 1H, **9-H**, Al-C_6H_4F), 7.56–7.52 (m, 1H, **9-H,** Al-C_6H_4F), 7.46 (d, J = 1.9 Hz, 2H, **9-F**, xanthene), 7.42 (d, J = 1.9 Hz, 2H, **9-H**, xanthene), 6.86 (t, J = 7.3 Hz, 2H, **9-F**, Al-$C_6H^m_5$), 6.78 (td, J = 7.4, 5.8 Hz, 1H, **9-H**, Al-C_6H_4F), 6.71 (t, J = 1.7 Hz, 1H, **9-F**, Al-$C_6H^p_5$), 6.69 (d, J = 1.9 Hz, 2H, **9-F**, xanthene), 6.68 (d, J = 1.9 Hz, 2H, **9-H**, xanthene), 6.29 (dddd, J = 9.4, 7.9, 3.0, 1.1 Hz, 1H, **9-H**, Al-C_6H_4F), 5.12 (s, 1H, **9-H**, Al-*H*), 2.87 (s, 48H, **9-H + 9-F,** 18-crown-6), 2.30 (hept, J = 7.6 Hz, 6H, **9-H**, Si-C*H*(CH_3)$_2$), 2.26 (hept, J = 7.6 Hz, 6H, **9-F**, Si-C*H*(CH_3)$_2$), 1.73 (d, J = 7.6 Hz, 18H, **9-H**, Si-CH(CH_3)$_2$), 1.72 (d, J = 7.3 Hz, 18H, **9-F**, Si-CH(CH_3)$_2$), 1.65 (s, 6H, **9-F**, C(CH_3)$_2$), 1.60 (s, 6H, **9-H**, C(CH_3)$_2$), 1.58 (d, J = 7.1 Hz, 21H, **9-H**, Si-CH(CH_3)$_2$ & C(CH_3)$_2$), 1.56 (s, 18H, **9-H**, C(CH_3)$_3$), 1.56 (s, 18H, **9-F**, C(CH_3)$_3$) ppm. **^{13}C NMR** (101 MHz, C_6D_6): δ = 165.9* (**9-H,** Al-$C^{ipso}_6H_4$F) 163.4 (**9-H**, Al-C_6H_4F), 160.9 (**9-H**, Al-C_6H_4F), 158.1* (**9-F**, Al-C_6H_5), 147.0 (**9-H**, xanthene), 146.8 (**9-F**, xanthene), 145.1, 144.9, 141.9 (**9-F**, xanthene), 141.7 (**9-H**, xanthene), 140.5 (**9-F**, Al-$C^o_6H_5$), 135.9 (**9-H,** Al-C_6H_4F), 129.0, 128.7, 125.6, 125.6 (**9-H**, Al-C_6H_4F), 125.5 (**9-H**, Al-C_6H_4F), 125.0 (**9-F**, Al-$C^m_6H_5$), 123.7 (**9-F**, Al-$C^p_6H_5$), 117.5 (**9-F**, xanthene), 116.9 (**9-H**, xanthene), 109.6 (**9-H**, Al-C_6H_4F), 106.7 (**9-F**, xanthene), 106.2

(**9-H**, xanthene), 69.8 (-C_2H_4O-), 36.0, 35.8, 35.2, 35.2, 33.3, 32.8, 32.4 (**9-H** + **9-F**, C(CH_3)$_3$), 27.1 (**A**, C(CH_3)$_2$), 26.9 (**9-F**, C(CH_3)$_2$), 20.9, 20.7 (**9-H**, Si-CH(CH_3)$_2$), 20.7 (**9-F**, Si-CH(CH_3)$_2$), 15.5 (**9-H**, *Si*-CH(CH_3)$_2$), 15.3 (**9-F**, *Si*-CH(CH_3)$_2$) ppm. **^{19}F{^{1}H} NMR** (376 MHz, C_6D_6): δ = –119.7 (s, **9-H**, C-*F*), –135.7 (br, **9-F**, Al-*F*) ppm. **^{29}Si{^{1}H} NMR** (79 MHz, C_6D_6): δ = 3.4 (**9-F**, *Si*-CH(CH_3)$_2$), 2.9 (**9-H**, *Si*-CH(CH_3)$_2$) ppm. **Elemental Analysis** calcd. for $C_{59}H_{99}AlFKN_2O_7Si_2$: C 65.03, H 9.16, N 2.57; found: C 63.46, H 8.77, N 2.39.

Synthesis of [K(18-crown-6)][(**^{TIPS}NON**)Al(H)(Si(*i*Pr)$_2$C-κ^1*Al*-Me$_2$)] (**10**)



[K$^+$(18-crown-6)]

Chemical Formula: $C_{53}H_{94}AlKN_2O_7Si_2$

Molecular Weight: 993.59

A solid sample of **1** (200 mg, 0.201 mmol) was heated at 100 °C under Ar for 2 hours, giving **10** in quantitative yield. **^{1}H NMR** (400 MHz, C_6D_6): δ = 7.26 (d, J = 2.0 Hz, 1H, xanthene), 6.92 (d, J = 2.0 Hz, 1H, xanthene), 6.79 (d, J = 1.9 Hz, 1H, xanthene), 6.62 (d, J = 2.0 Hz, 1H, xanthene), 4.45 (s, 1H, Al-*H*), 3.09 (s, 24H, 18-crown-6), 2.01 (hept, J = 7.5 Hz, 5H, Si-C*H*(CH_3)$_2$), 1.94 (s, 3H, C(CH_3)$_2$), 1.88 (s, 3H, C(CH_3)$_2$), 1.83 (s, 3H, C(CH_3)$_2$), 1.66 – 1.54 (m, 30H, Si-CH(CH_3)$_2$), 1.49 (s, 9H, C(CH_3)$_3$), 1.47 (s, 9H, C(CH_3)$_3$), 1.09 (d, J = 7.3 Hz, 3H, C(CH_3)$_2$) ppm. **^{13}C{^{1}H} NMR** (101 MHz, C_6D_6): δ = 147.2, 146.7, 146.4, 146.4, 145.4, 144.8, 134.9, 133.3, 117.2, 113.1, 106.4, 104.1 (*C*-Ar), 70.0 (-C_2H_4O-), 37.7, 35.2, 35.0, 32.5, 32.4, 31.8, 31.0, 27.6, 25.1, 23.4, 21.4, 21.3, 20.9, 20.1, 19.7, 19.4, 18.8, 16.9, 15.3, 14.5, 13.5 (Si-*C*H(CH_3)$_2$) ppm. **^{29}Si{^{1}H} NMR** (79 MHz, C_6D_6): δ = 5.4, 1.9 ppm. **Elemental Analysis** calcd. for $C_{53}H_{94}AlKN_2O_7Si_2$: C 64.07, H 9.54, N 2.82; found: C 64.11, H 9.70, N 2.74. **n.b.** Crystals suitable for SCXRD analysis were grown by layering a concentrated solution of **10** in benzene with *n*-pentane.

NMR Spectra of New Compounds

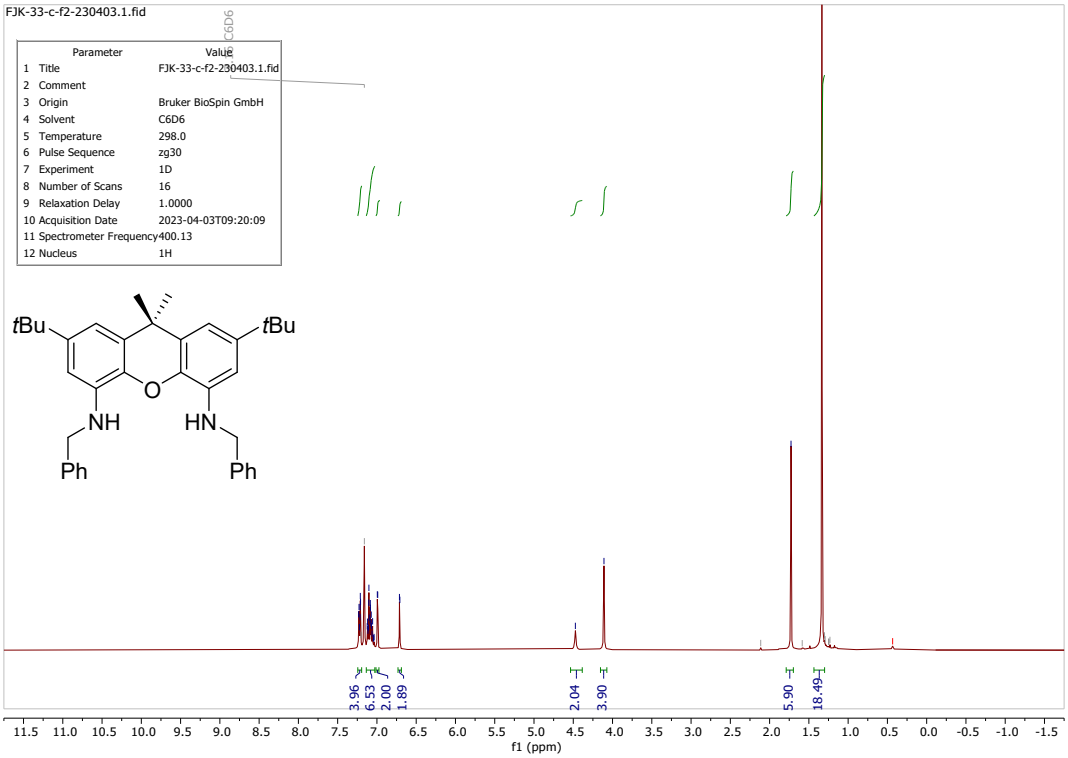


Figure S1: ^{1}H NMR spectrum of H_2(**^{Bn}NON**) (400 MHz, C_6D_6, 298 K)

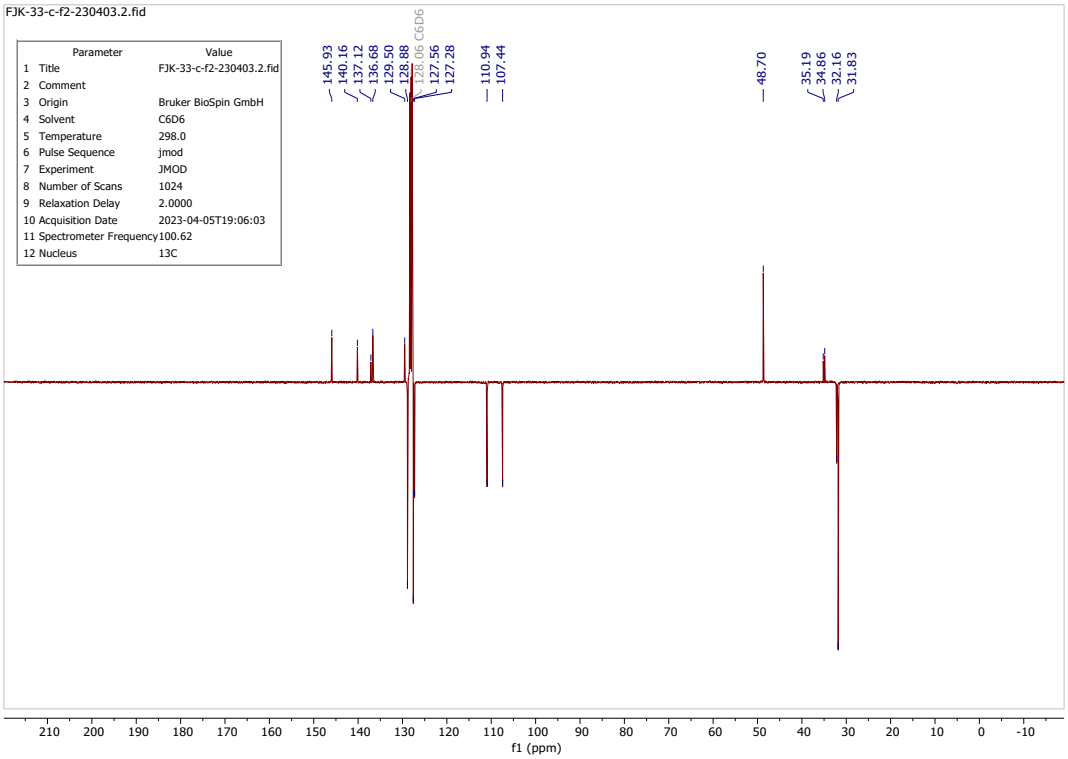


Figure S2: ^{13}C-APT NMR spectrum of H_2(**^{Bn}NON**) (101 MHz, C_6D_6, 298 K)

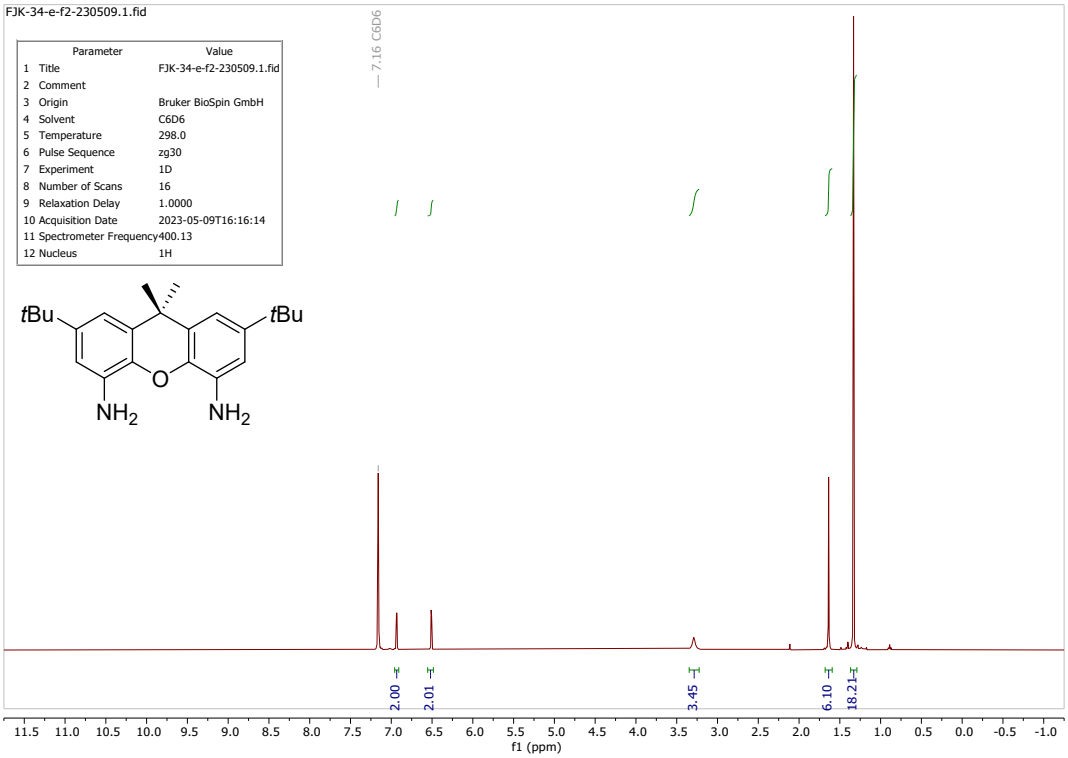


Figure S3: ^{1}H NMR spectrum of H_2(**^{H}NON**) (400 MHz, C_6D_6, 298 K)

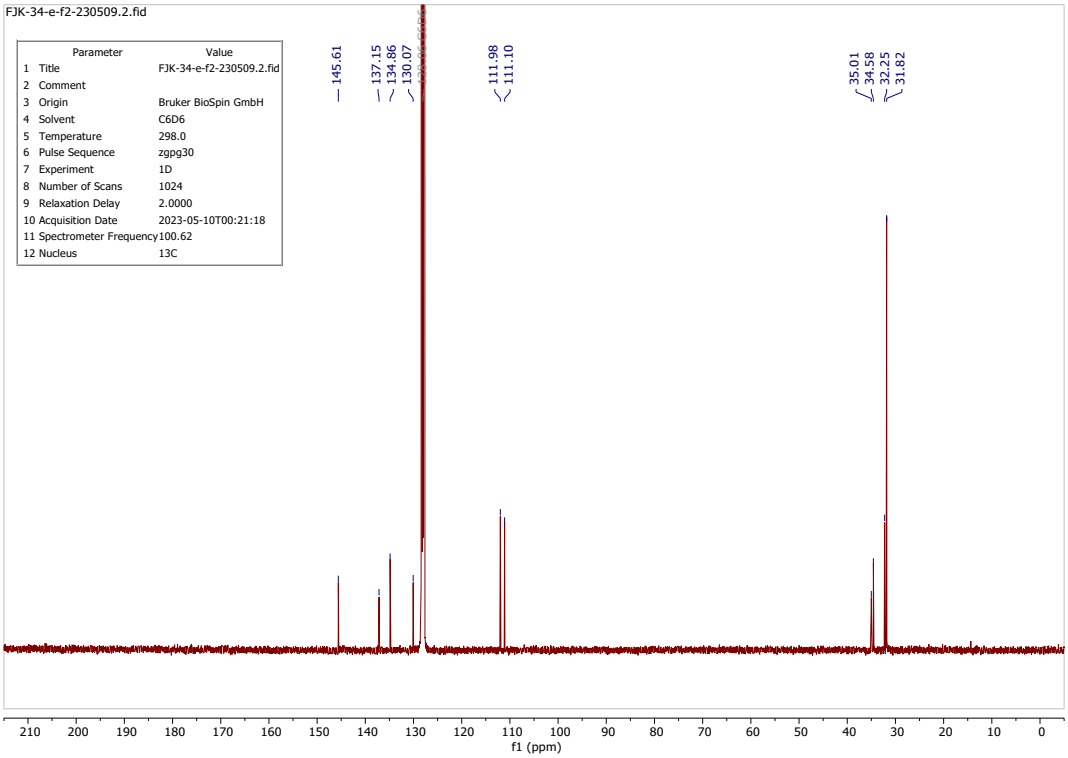


Figure S4: ^{13}C{^{1}H} spectrum of H_2(**^{H}NON**) (101 MHz, C_6D_6, 298 K)

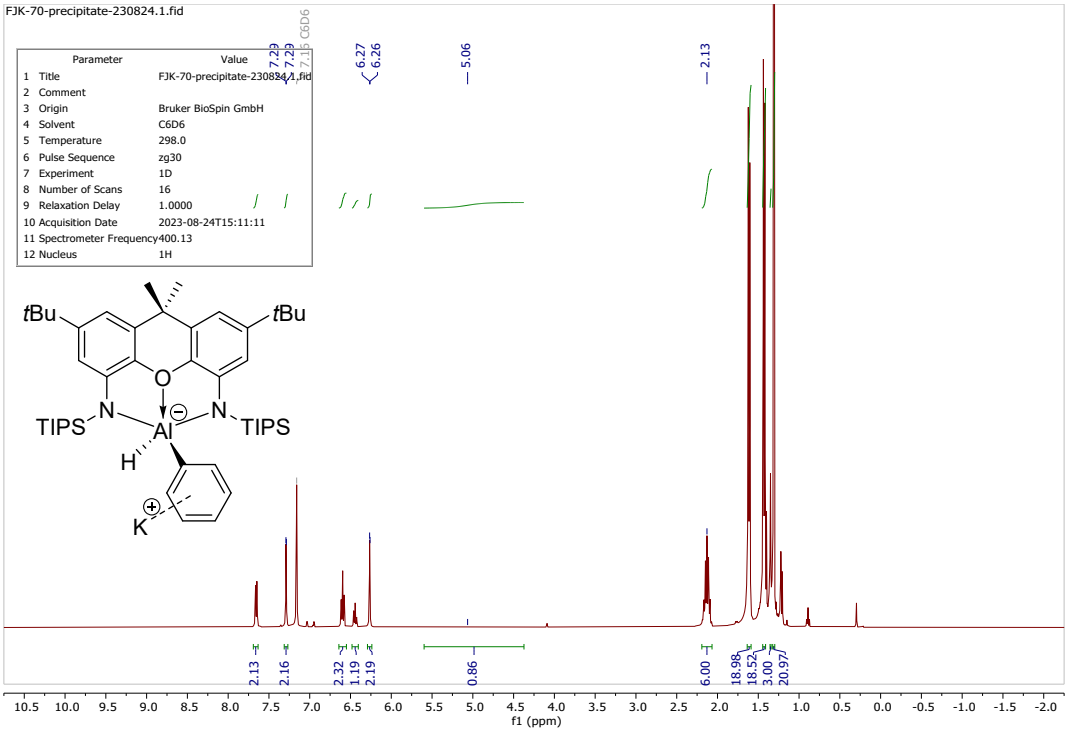


Figure S5: ^{1}H NMR spectrum of **2** (400 MHz, C_6D_6, 298 K)

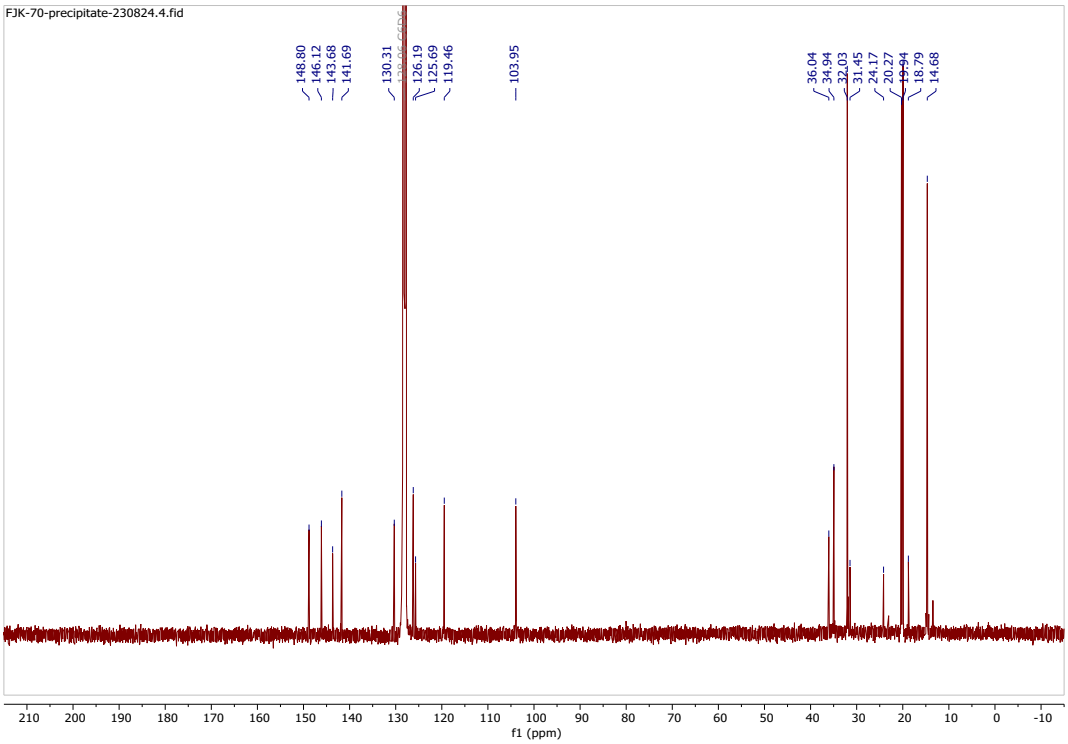


Figure S6: ^{13}C{^{1}H} spectrum of **2** (101 MHz, C_6D_6, 298 K)

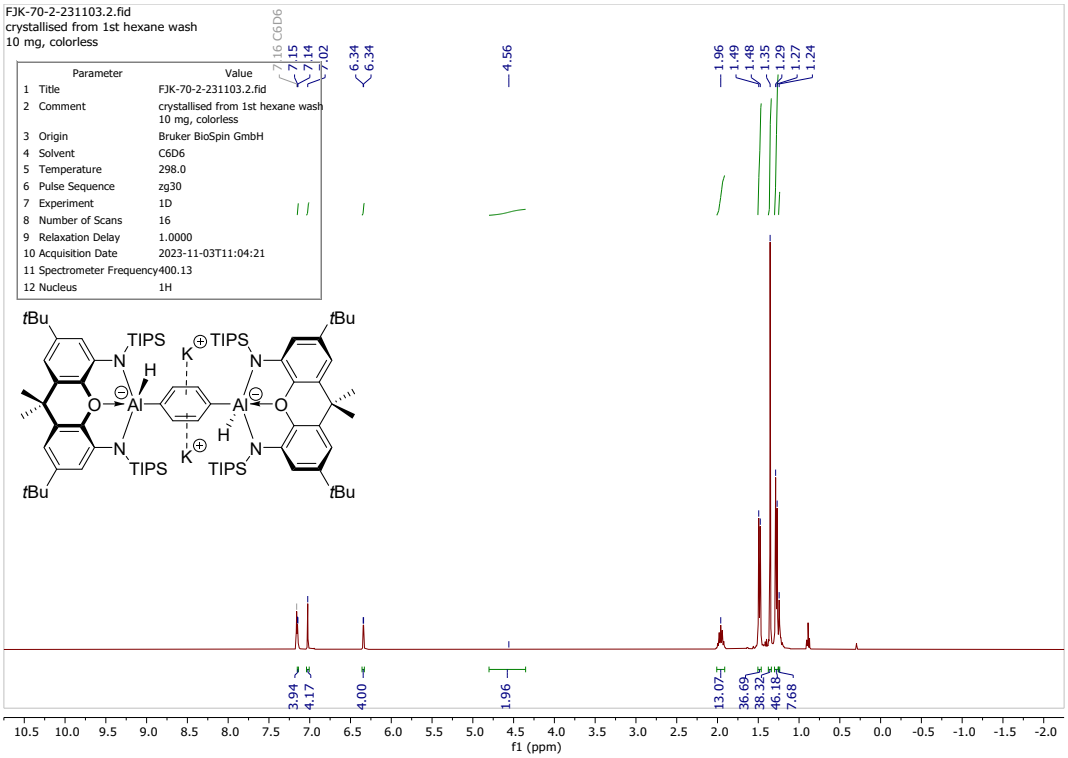


Figure S7: ^{1}H NMR spectrum of **3** (400 MHz, C_6D_6, 298 K)

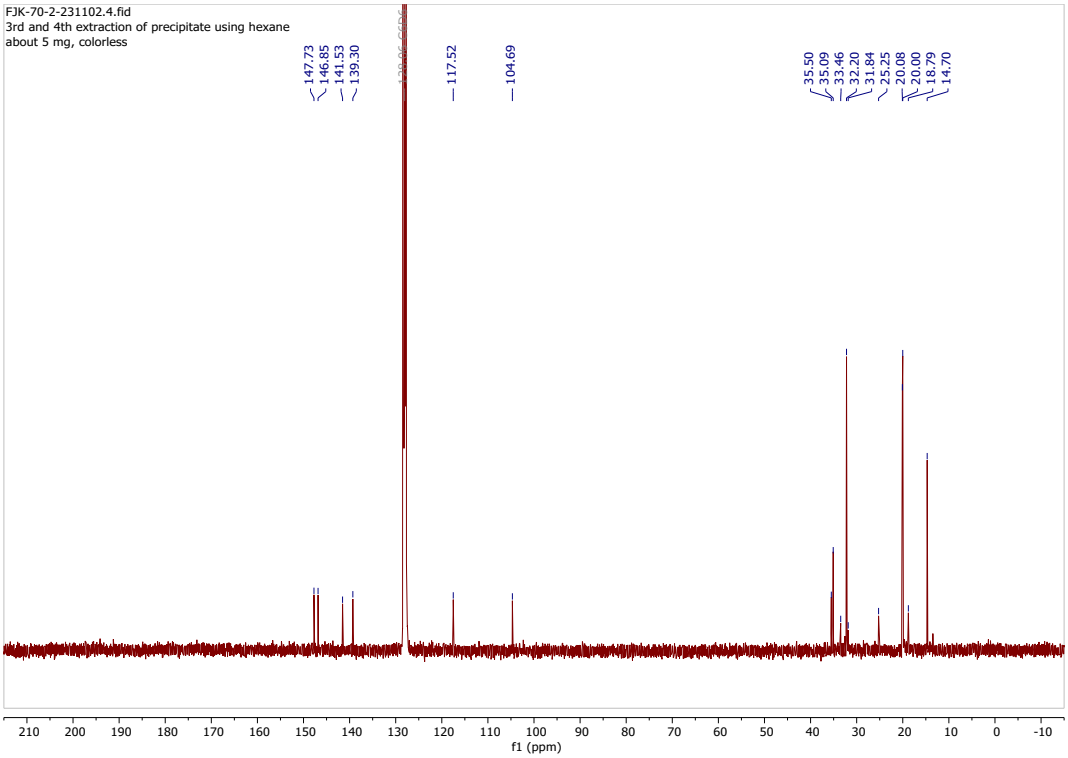


Figure S8: $^{13}C\{^{1}H\}$ spectrum of **3** (101 MHz, C_6D_6, 298 K)

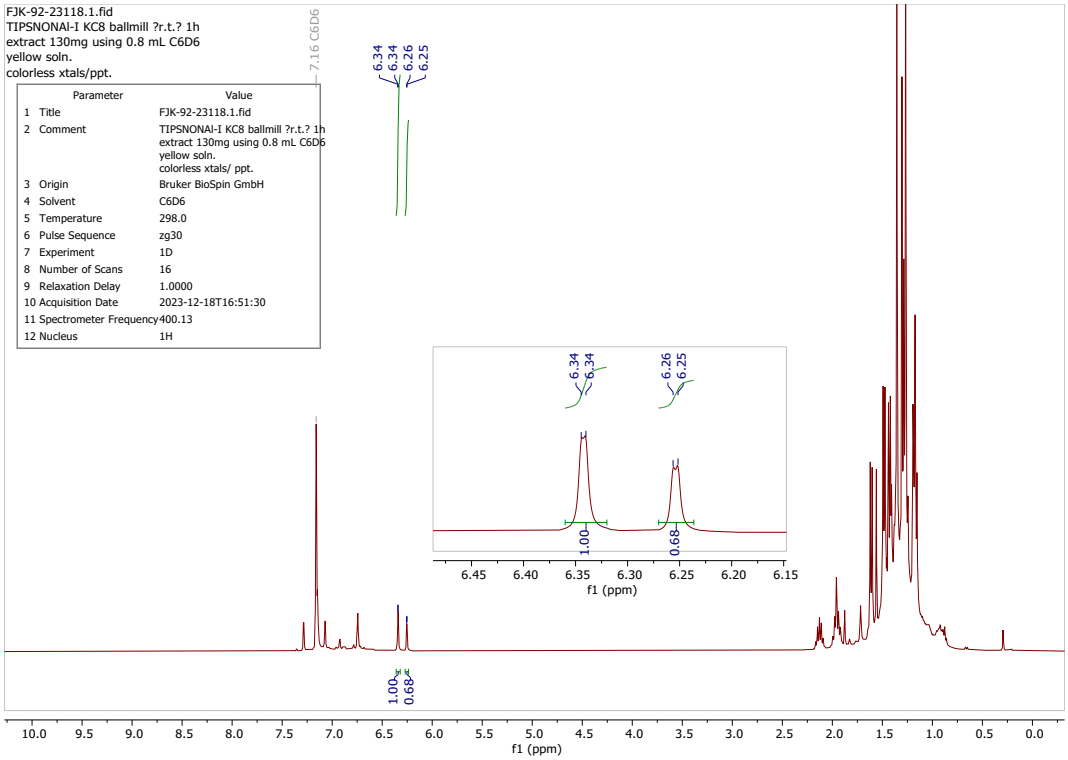


Figure S9: ^{1}H NMR analysis of the C_6D_6 extraction of the reduction of **1** with KC_8 using a ball mill (400 MHz, C_6D_6, 298 K)

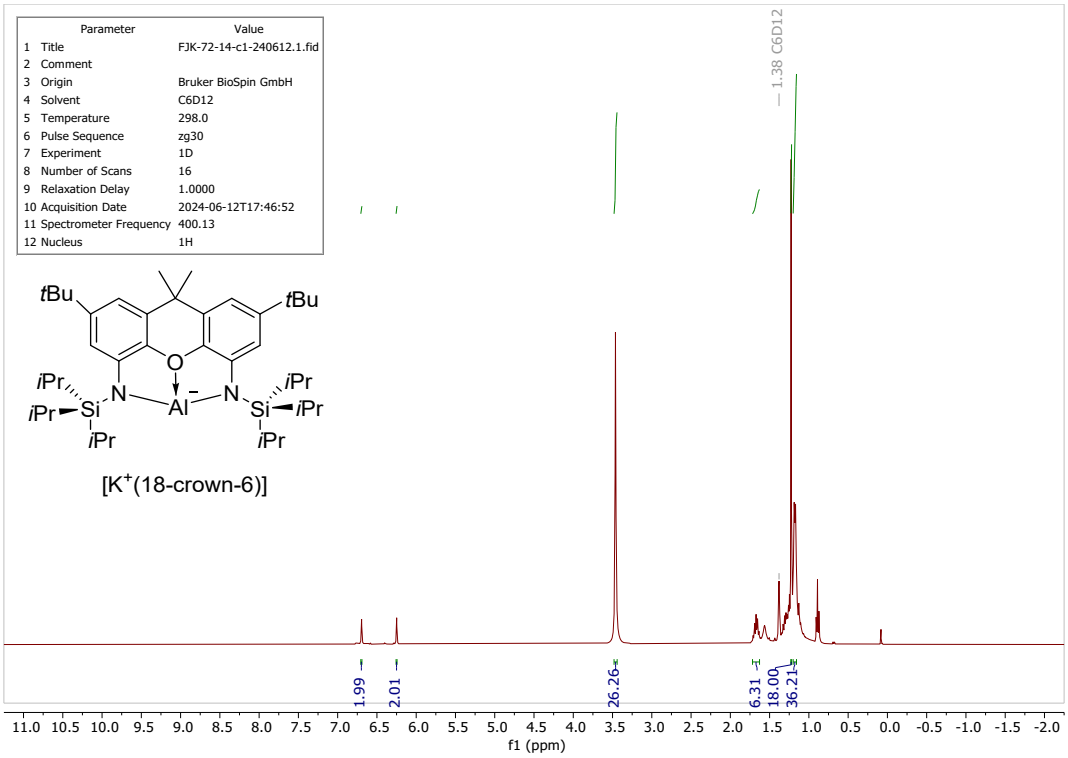


Figure S10: ^{1}H NMR spectrum of **4** (400 MHz, C_6D_{12}, 298 K)

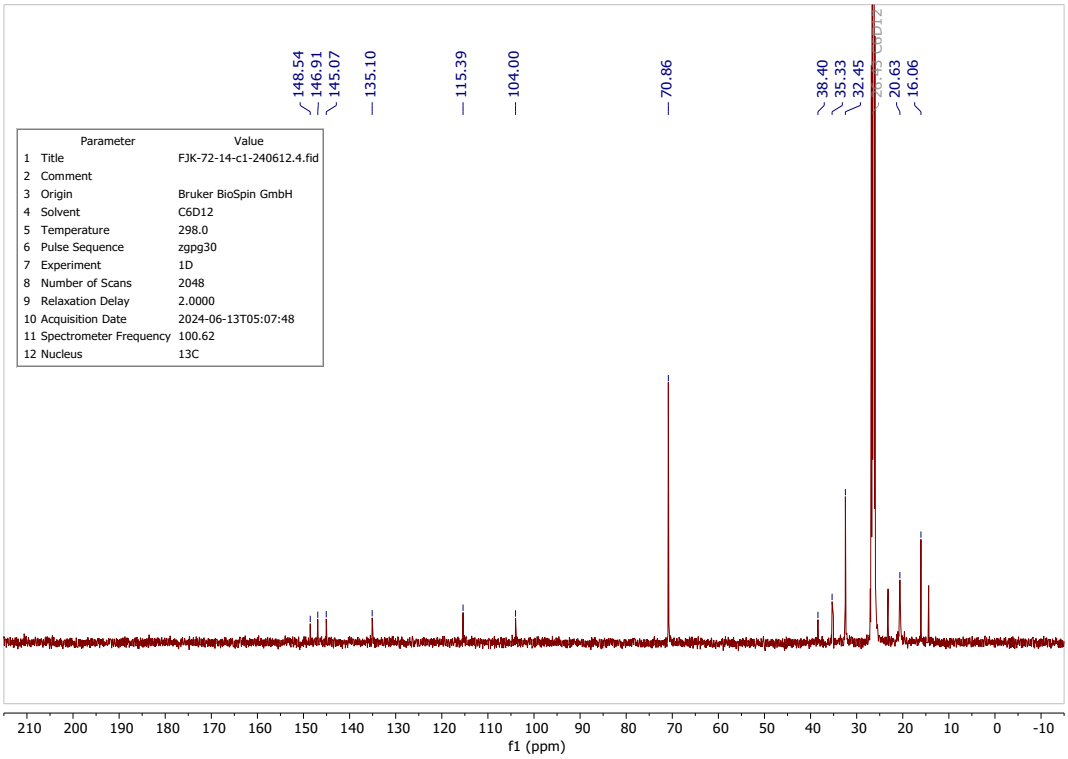


Figure S11: $^{13}C\{^{1}H\}$ spectrum of **4** (101 MHz, C_6D_{12}, 298 K)

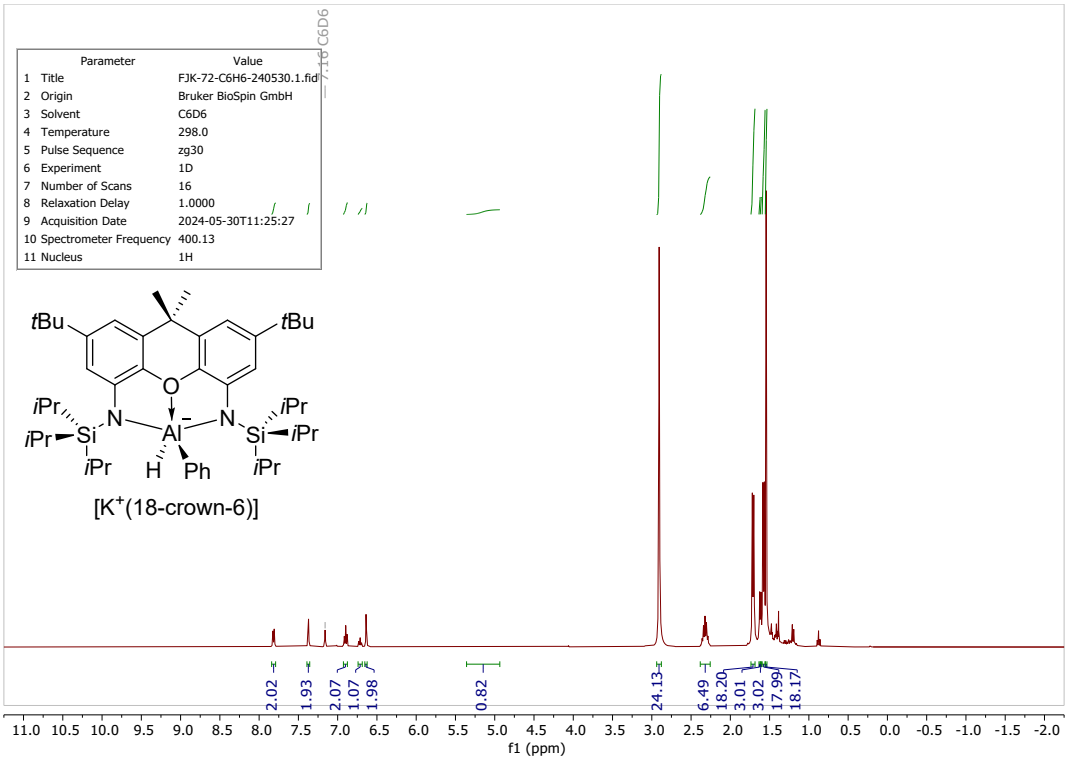


Figure S12: ^{1}H NMR spectrum of **5** (400 MHz, C_6D_6, 298 K)

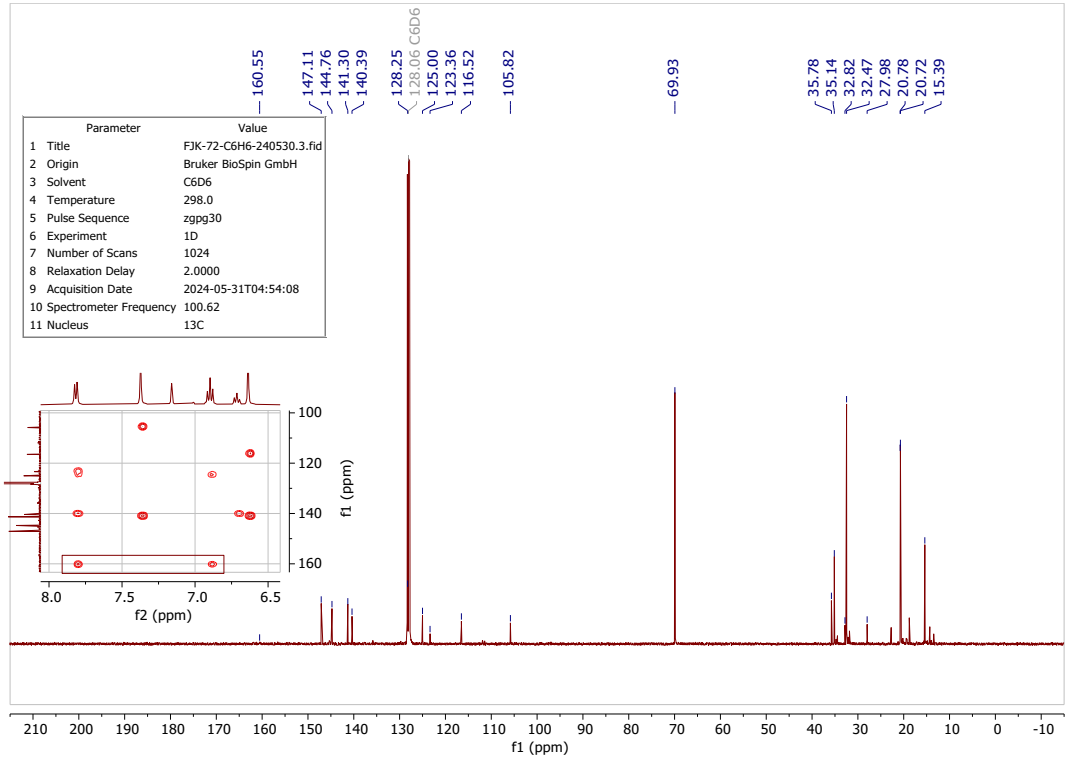


Figure S13: $^{13}C\{^{1}H\}$ spectrum of **5** (101 MHz, C_6D_6, 298 K), Insert: Excerpt of the ^{1}H-^{13}C HMBC experiment of the aromatic signals to elucidate the Al-C^{ipso} signal.

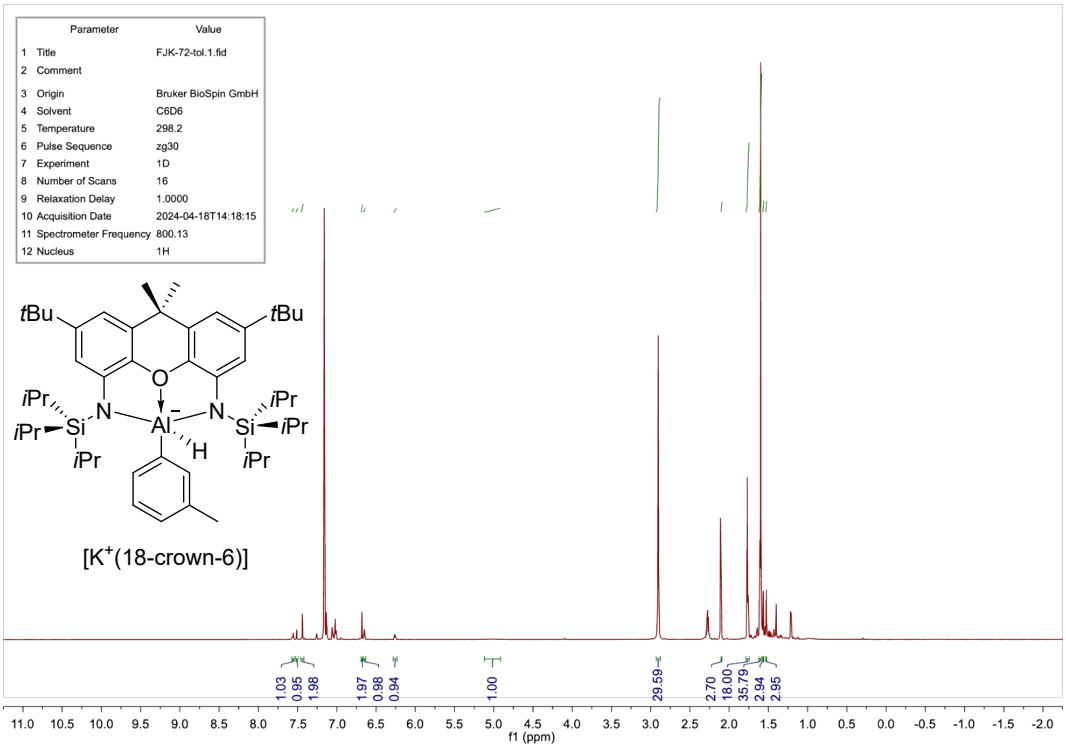


Figure S14: ^{1}H NMR spectrum of **6** (800 MHz, C_6D_6, 298 K)

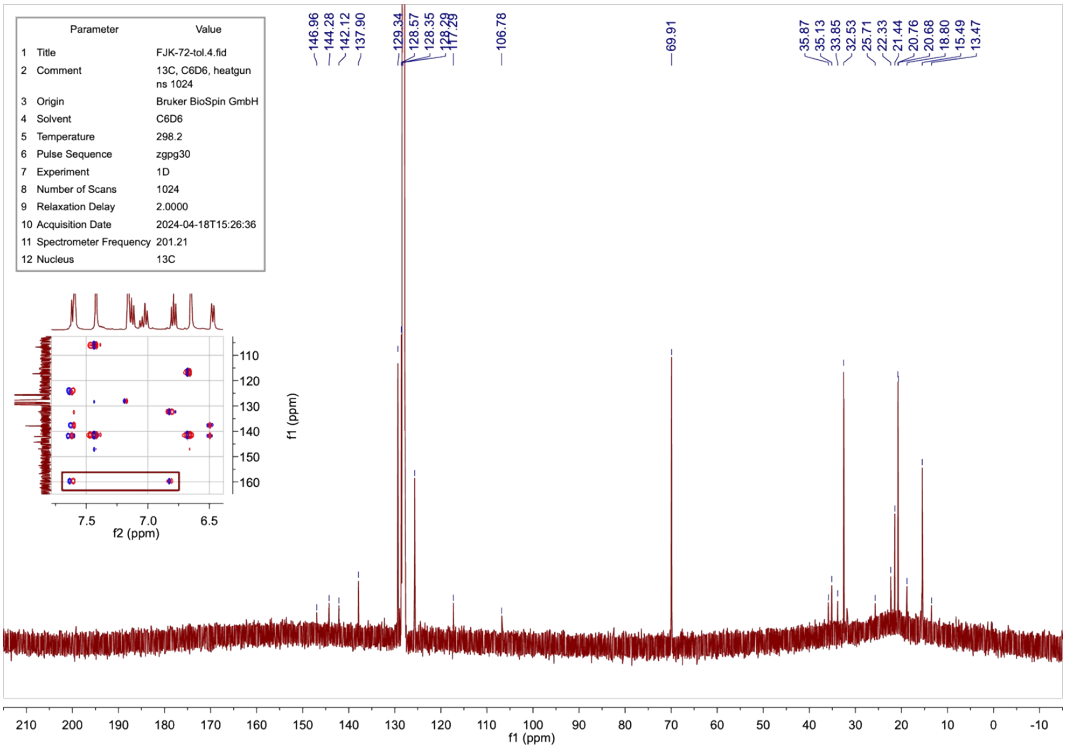


Figure S15: ^{13}C{^{1}H} spectrum of **6** (201 MHz, C_6D_6, 298 K), Insert: Excerpt of the ^{1}H-^{13}C HMBC experiment of the aromatic signals to elucidate the Al-C^{ipso} signal

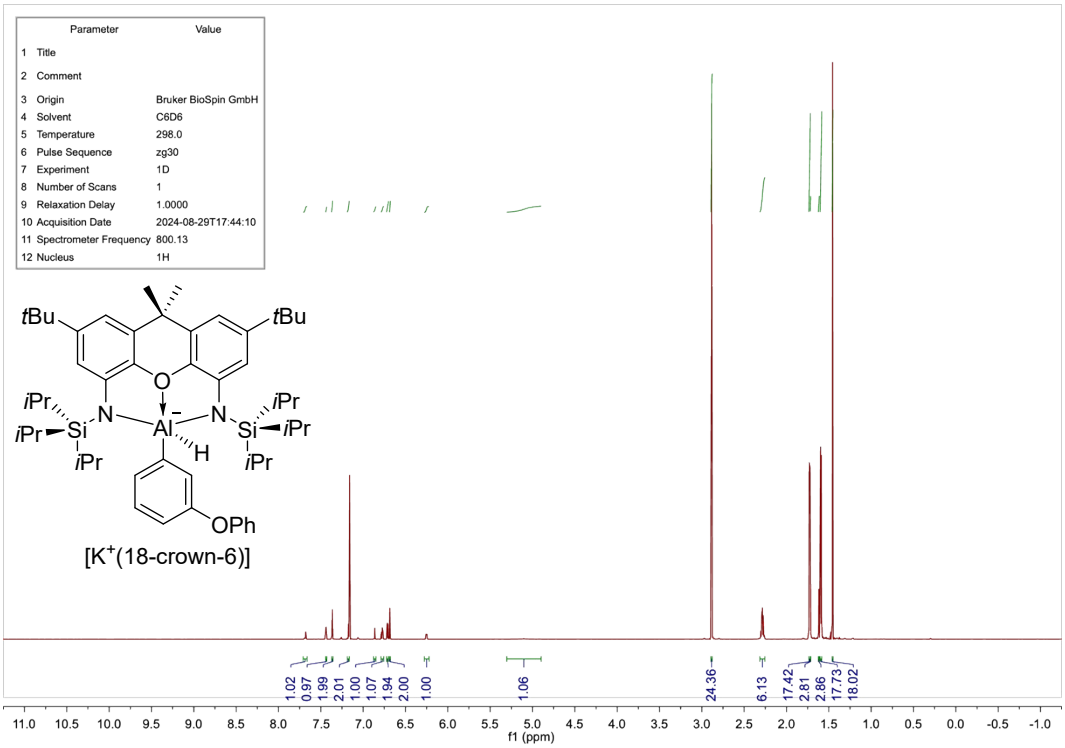


Figure S16: ^{1}H NMR spectrum of **7** (800 MHz, C_6D_6, 298 K)

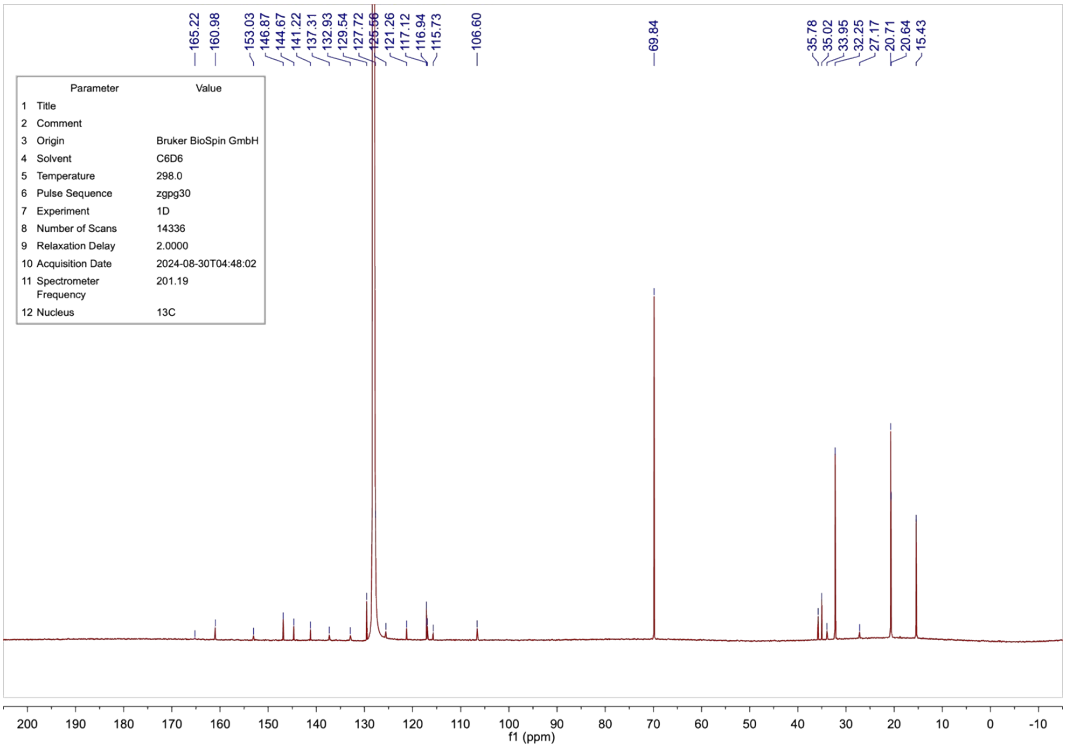


Figure S17: ^{1}H{^{13}C} NMR spectrum of **7** (201 MHz, C_6D_6, 298 K)

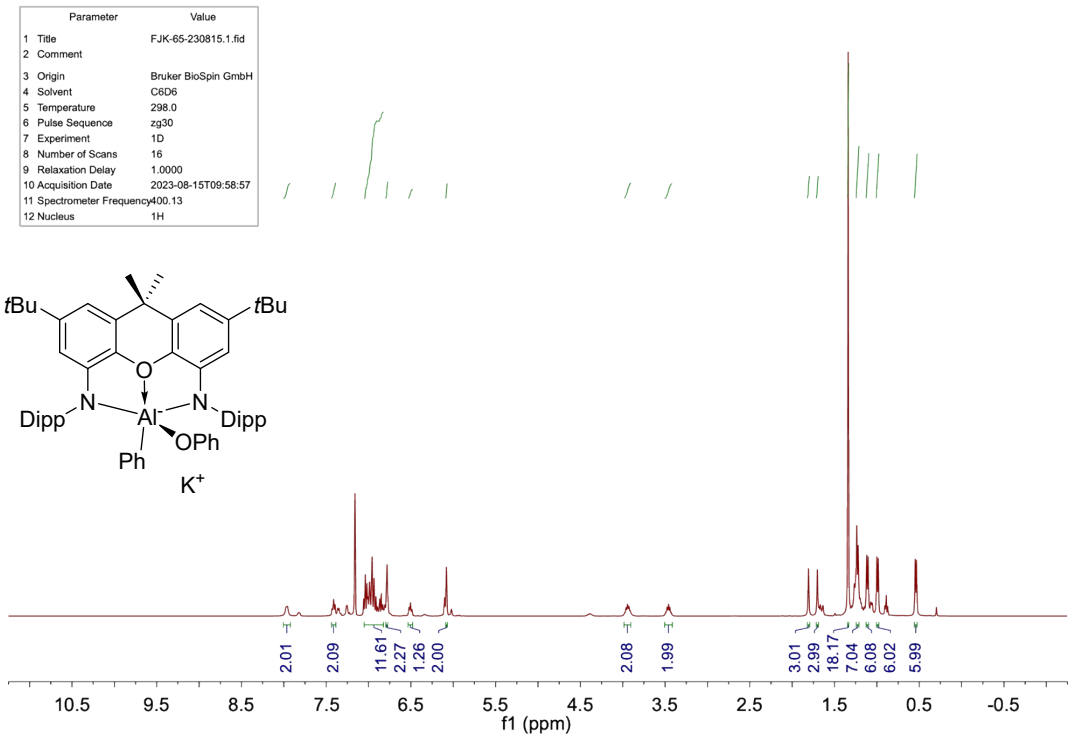


Figure S18: ^{1}H NMR spectrum of **8** (400 MHz, C_6D_6, 298 K)

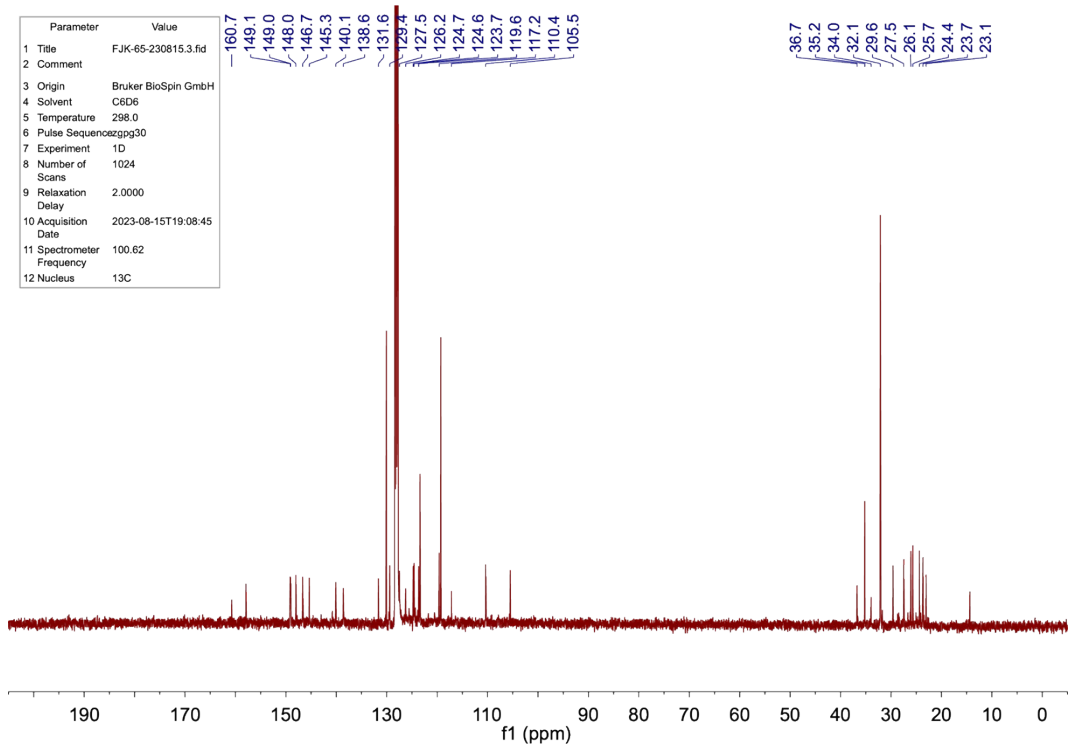


Figure S19: ^{1}H{^{13}C} NMR spectrum of **8** (101 MHz, C_6D_6, 298 K).

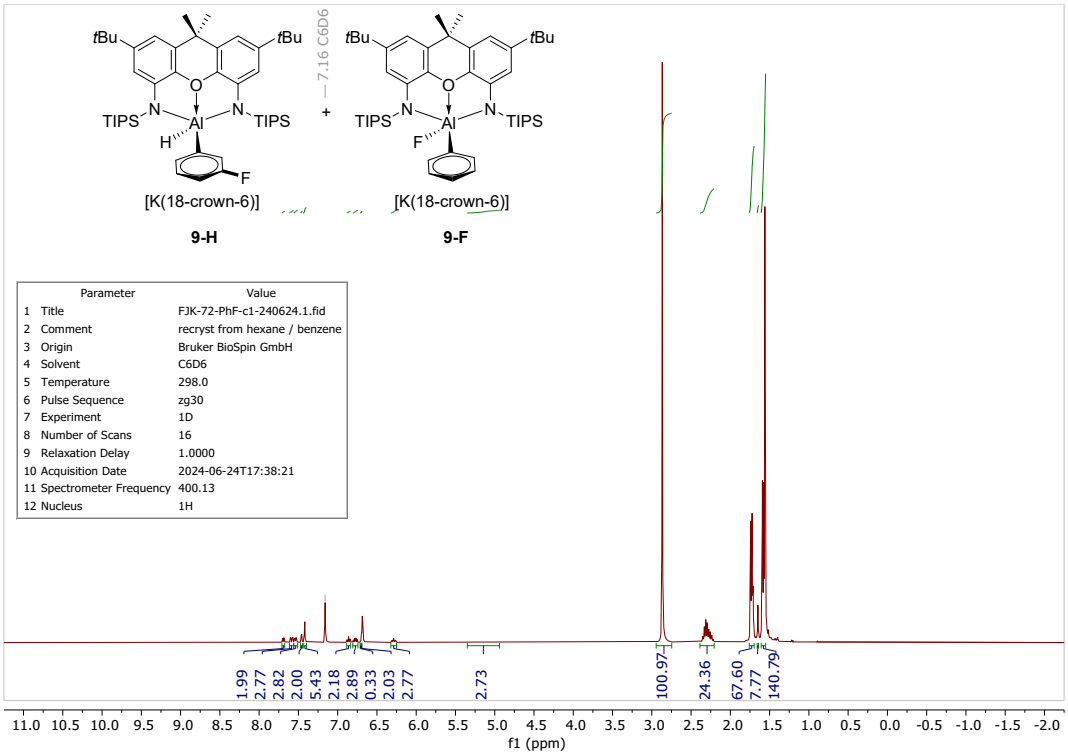


Figure S20: ^{1}H NMR spectrum of a mixture of **9-H** and **9-F** (400 MHz, C_6D_6, 298 K)

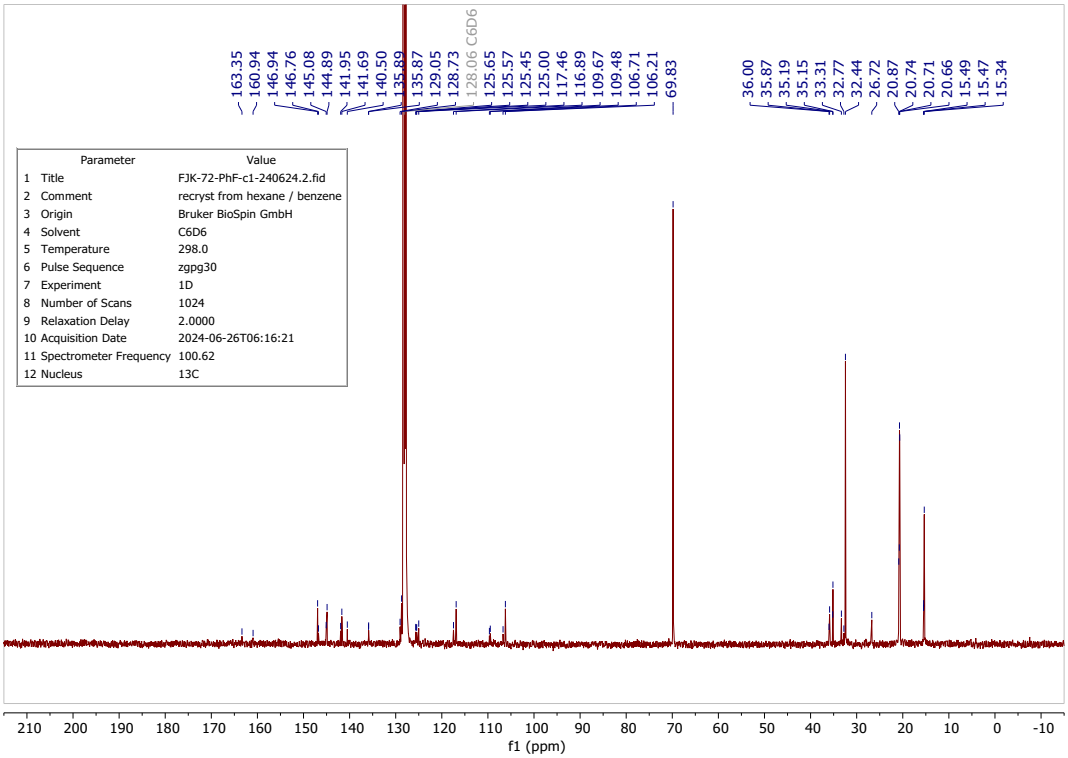


Figure S21: $^{13}C\{^{1}H\}$ spectrum of a mixture of **9-H** and **9-F** (101 MHz, C_6D_6, 298 K)

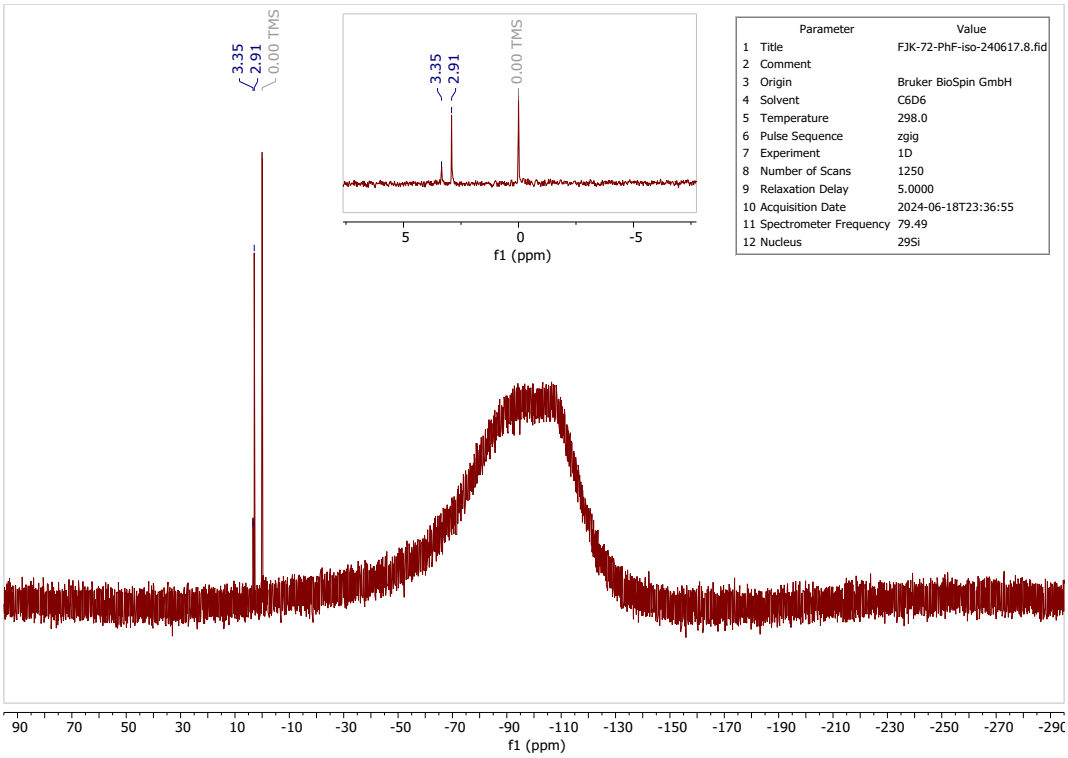


Figure S22: $^{29}Si\{^{1}H\}$ NMR of a mixture of **9-H** and **9-F** (79 MHz, C_6D_6, 298 K), Insert: Region of interest.

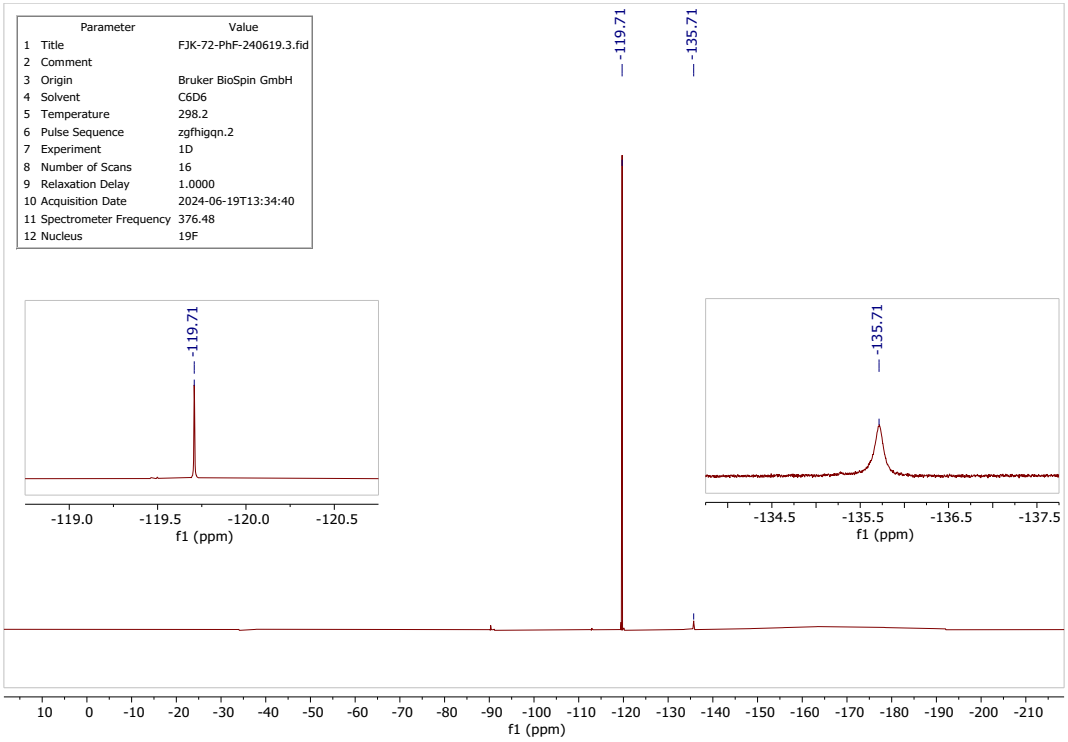


Figure S23: $^{19}F\{^{1}H\}$ NMR spectrum of a mixture of **9-H** and **9-F** (376 MHz, C_6D_6, 298 K), Inserts: Regions of interest.

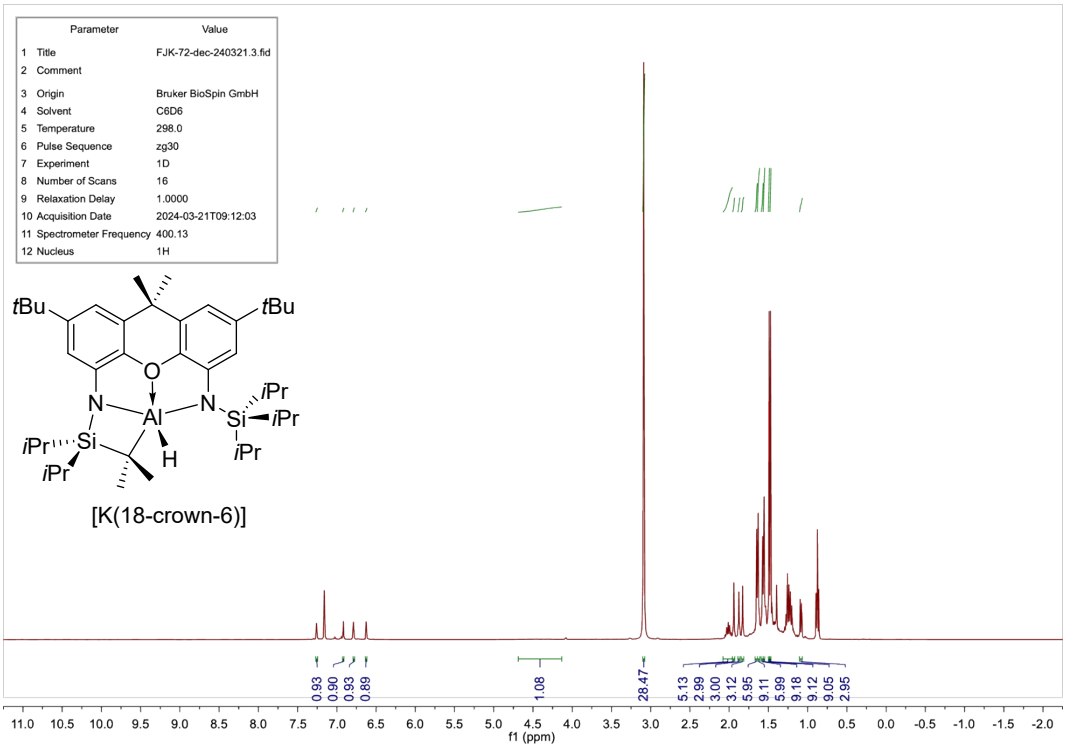


Figure S24: ^{1}H NMR spectrum of **10** (400 MHz, C_6D_6, 298 K)

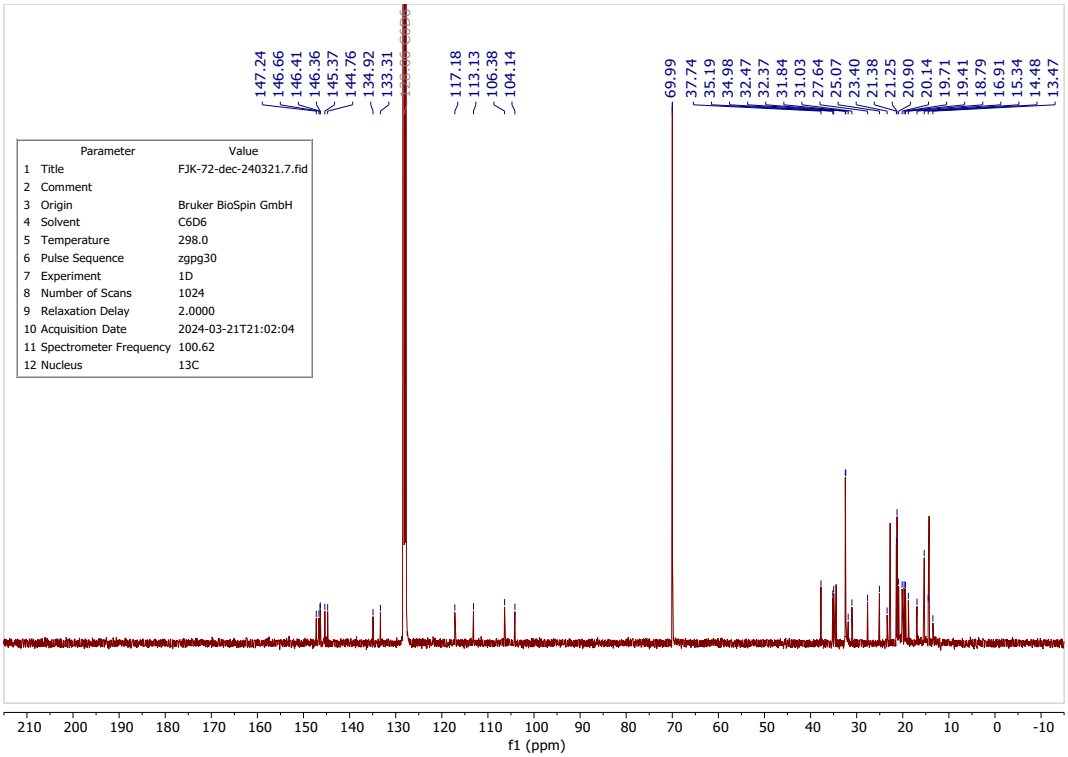


Figure S25: $^{13}C\{^{1}H\}$ spectrum of **10** (101 MHz, C_6D_6, 298 K)

X-ray Crystallographic Studies

X-ray diffraction experiments were performed using a Rigaku Supernova dual-source diffractometer using Cu Kα radiation equipped with a Rigaku Hybrid Pixel 2-dimensional detector (HyPix-6000HE). Crystals were suspended in immersion oil, mounted on Micromount loops, and quench-cooled to 150 K using an Oxford Cryostream N_2 cooler. Data were processed using the CrysAlisPro package (v171.41.93a) by Rigaku, solved and refined using the SHELX software package[S6,S7] using the graphical interface Olex2[S8] and visualised using Mercury.[S9]

Finalised CIFs for all diffraction structures (2432683-2432692) have been deposited at the Cambridge Crystallographic Data Centre. These can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Table S1: Crystallographic and refinement parameters for **2**, **3** and **4**.

	2	**3·benzene**	**4·1.5pentane**
Formula	$C_{47}H_{76}AlKN_2OSi_2$	$C_{94}H_{152}Al_2K_2N_4O_2Si_4$	$C_{60.5}H_{112}AlKN_2O_7Si_2$
M	807.35	1614.71	1101.77
Cell setting	Triclinic	Monoclinic	Monoclinic
Space group	P-1	C2/c	$P2_1/n$
a [Å]	14.41060(10)	22.4566(3)	15.8565(3)
b [Å]	15.42140(10)	18.6939(2)	22.3423(5)
c [Å]	24.1204(2)	23.7291(2)	19.5531(5)
α [°]	101.4380(10)	90	90
β [°]	105.3220(10)	107.2990(10)	102.317(2)
γ [°]	103.9550(10)	90	90
V [A^3]	4816.58(7)	9510.91(19)	6767.6(3)
Z	4	4	4
Reflections (unique)	20375	9803	11922
Reflections (I > 2σI)	18603	8025	8299
R_{int}	0.0445	0.0741	0.0395
Parameters	1071	519	1103
R1 (all data)	0.0385	0.0694	0.1095
R1 (I > 2σI)	0.0356	0.0554	0.0851
wR2 (all data)	0.0965	0.1444	0.2762
wR2 (I > 2σI)	0.0946	0.1372	0.2492
GooF	1.068	1.023	1.04
Residual max	0.487	0.525	0.502
Residual min	-0.711	-0.646	-0.436
T [K]	150.00(10)	150.00(10)	150.00(10)
CCDC Deposition No.	2432683	2432684	2432685

Table S2: Crystallographic and refinement parameters for **5**, **6** and **7**.

	5·2cyclohexane	**6**	**7·3.75benzene**
Formula	$C_{74}H_{130}AlKN_2O_7Si_2$	$C_{60}H_{102}AlKN_2O_7Si_2$	$C_{175}H_{253}Al_2K_2N_4O_{16}Si_4$
M	1282.05	1085.69	2913.32
Cell setting	Monoclinic	Orthorhombic	Triclinic
Space group	$P2_1/n$	Pnma	P-1
a [Å]	14.8101(4)	13.52700(10)	11.57270(10)
b [Å]	24.0778(3)	23.84830(10)	26.0715(4)
c [Å]	22.5799(4)	20.00370(10)	28.9632(4)
α [°]	90	90	88.4050(10)
β [°]	98.984(2)	90	79.7730(10)
γ [°]	90	90	89.7800(10)
V [A^3]	7953.1(3)	6453.11(6)	8596.53(19)
Z	4	4	2
Reflections (unique)	13965	7075	35979
Reflections (I > 2σI)	9520	6677	29802
R_{int}	0.0634	0.0375	0.0604
Parameters	1041	543	1899
R1 (all data)	0.1463	0.0795	0.0852
R1 (I > 2σI)	0.1124	0.0772	0.0745
wR2 (all data)	0.3242	0.2269	0.217
wR2 (I > 2σI)	0.2972	0.224	0.2061
GooF	1.049	1.082	1.021
Residual max	0.69	0.664	1.286
Residual min	-0.507	-0.608	-0.602
T [K]	150.00(10)	150.00(10)	150.00(10)
CCDC Deposition No.	2432686	2432687	2432689

Table S3: Crystallographic and refinement parameters for **8**, **9** and **10**.

	8·11benzene	**9**	**10·pentane**
Formula	$C_{302}H_{354}Al_4K_4N_8O_8$	$C_{59}H_{99}AlFKN_2O_7Si_2$	$C_{58}H_{106}AlKN_2O_7Si_2$
M	4488.23	1089.66	1065.7
Cell setting	Monoclinic	Orthorhombic	Monoclinic
Space group	P2/n	Pnma	$P2_1/n$
a [Å]	20.4545(3)	13.3496(2)	16.7297(3)
b [Å]	14.2108(2)	23.9758(6)	22.5628(2)
c [Å]	45.7301(8)	20.1328(3)	17.7034(3)
α [°]	90	90	90
β [°]	96.745(2)	90	104.568(2)
γ [°]	90	90	90
V [A^3]	13200.6(4)	6443.9(2)	6467.64(18)
Z	4	4	4
Reflections (unique)	26583	5824	13622
Reflections (I > 2σI)	19540	4593	11095
R_{int}	0.0759	0.0612	0.0461
Parameters	1455	558	740
R1 (all data)	0.1149	0.1109	0.0719
R1 (I > 2σI)	0.0863	0.0945	0.0581
wR2 (all data)	0.2317	0.2831	0.1598
wR2 (I > 2σI)	0.2152	0.2662	0.1506
GooF	1.093	1.055	1.036
Residual max	0.623	0.883	0.37
Residual min	-0.421	-0.679	-0.347
T [K]	150.00(10)	150.00(10)	150.00(10)
CCDC Deposition No.	2432690	2432691	2432692

Neutron Laue diffraction experiment details

The structure of compound **6** was investigated using single-crystal neutron Laue diffraction. The unit-cell dimensions employed were those determined from the X-ray diffraction studies, as these cannot be reliably determined from Laue neutron diffraction. Care was taken to ensure that the temperature of the experiment was matched to the X-ray experiment (150 K) using an Oxford Cryosystems COBRA™ wide-bore cryostream, which also served to protect the crystal from moisture and oxygen. The sample was handled immersed in argon to ensure compound stability while the crystal was transferred to the coldstream. Neutron Laue data were collected on the KOALA instrument at ANSTO (Sydney). Data for **6** were collected from a colourless single-crystal (3.0 × 1.7 × 1.0 mm) mounted to the phi axis of the newly commissioned KOALA2 diffractometer, which stands at an end guide position of TG3 - a supermirror thermal neutron guide at the OPAL nuclear reactor at ANSTO. A total 12 Laue diffraction images were collected in a single run (6000s exposures) with 17° rotations of the crystal around the phi axis occurring between exposures. An example of one of these images is shown in Figure S26. A total of 25654 reflections from neutrons of wavelengths between 0.85 and 1.70 Å covering the full sphere of reciprocal space to a maximum resolution of 0.90 Å were reduced [L4R(int) = 8.2(6.6) for 4σ observations] to yield 3013 independent reflections with I > 4σ(I). Data reduction was by means of the LAUEG suite.[S10,S11]

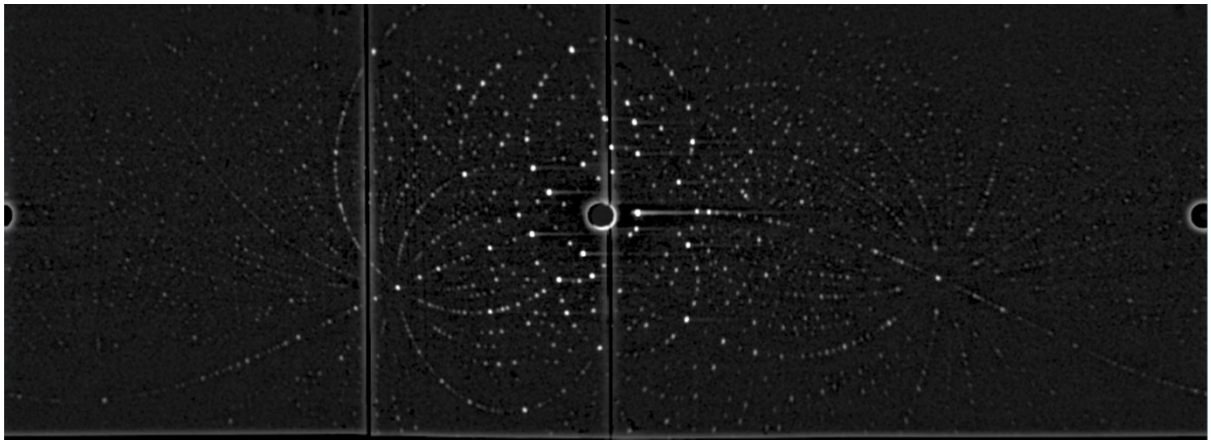


Figure S26: An example diffraction image acquired from the KOALA2 beamline at ANSTO during the neutron diffraction experiment of **6**

Establishing the optimum model for this structure has involved iterating between the X-ray and neutron studies and ultimately, the models presented here represent choices made by the analysts. The initial X-ray derived model employed for refinement against the neutron data arose from the automatically chosen conventional choice of the highest symmetry space group consistent with the X-ray diffraction data. The Pnma choice could, for the available X-ray data, be refined to an adequate fit to the data albeit with very significant disorder within both the anion and cation. When tested against the neutron data in the CRYSTALS[S12] program system, initial success in exploring the difference density followed initial refinement of the scale factor. Subsequent deletion of all H atoms associated with the ordered parts of the anion returned every hydrogen atomic site in sensible locations. There was some disquiet regarding the difficulties in refinement and some aspects of the structure were reminiscent of problems encountered previously in our model building to fit neutron diffraction data.[S13] In this instance, we first explored

a shift of space group to the non-centrosymmetric $Pn2_1a$ (indistinguishable on the basis of the diffraction pattern from Pnma because the 0k0 k odd absence is a subset of the 0kl k+l odd absence – noting that the "standard setting" is the permuted $Pna2_1$). Similar observations regarding difference density were noted, and the ROTAX[S14] program built into the CRYSTALS[S12] system revealed the potential presence of a mirror twin – i.e. that the crystal may in fact be a merohedral twin. Review of the X-ray study incorporating $Pna2_1$ as the space group yielded a satisfactory model which when explored via ROTAX[S14] in CRYSTALS[S13] yielded the same possible mirror twin operator in the X-ray data and we provide here a fully refined model for a structure in $Pna2_1$ incorporating the mirror twin law for which the fraction refines to 0.53(2) as an acceptable model for the crystals studied.

The fact that the choice of space group is part of the modelling process in crystallography (and that this may be a choice made by software without adequate consideration of the options which the analyst should survey) has become reinforced for us in the context of application of neutrons as a radiation source. Indeed, one study known to us deliberately exploited the possibility that using neutrons might enhance subtle but perceptible differences arising from the absence of crystallographic inversion symmetry to reveal a true structure differing from that which had been reported in the literature.[S14] Recollecting this, we have now carefully examined all of the possible glide absence observations available in the neutron data and it appears that there are absence violations for both the n and a cases sufficient to suggest that the true space group of the structure is in fact $P2_12_12_1$ (possibly twinned by merohedry to varying degrees in all three principal directions) and that the combined effect of disorder and twinning means that for each crystal examined, and for each radiation type employed a description as Pnma or $Pna2_1$ may be a valid and acceptable (if imperfect) choice for building a suitable model for understanding the structural chemistry which is the motivation for the study. Carried to its logical conclusion, and restricting the discussion to space groups (i.e. not exploring whether the crystal class may also be only approximately orthorhombic) we are choosing to model this structure in either $Pna2_1$ or Pnma for the X-ray data and we are choosing to report the structure in Pnma for the neutron data. The challenges posed in building a model in $P2_12_12_1$ and properly directing the path of a refinement in the context of disorder and twinning could occupy a student for many months without appreciable "improvement" in the final structure – nonetheless, we suggest that $P2_12_12_1$ is likely the true space group of the structure.

The Pnma model for the neutron diffraction study of **6** was refined against F^2 using the SHELXL 2018 package and the graphical interface Olex2 (Figure S34).[S7,S8] The starting model was from the X-ray diffraction experiment with all hydrogen atoms removed. The structure was then refined against the neutron data and the hydrogen atoms of the more ordered parts of the anion were included from the difference map. It should be noted that the hydride attached to the Al atom was clearly evident in the difference map having a magnitude similar to the most geometrically constrained hydrogens of the ligand while those hydrogen atoms which are less geometrically constrained such as those of the ^{t}Bu groups were of lesser magnitude – the stable anisotropic refinement of the "ordered" hydrogen atoms of the anion without need for restraints arises directly from the data. Hydrogen atoms of the cation and the disordered isopropyl groups of the anion were added in the calculated positions using the appropriate HFIX commands. The structure was refined against the available data using a mixed isotropic/anisotropic model with care taken not over-parameterise the model and to make the most out of the

available data. The ordered hydrogen atoms, including the aluminium hydride, were refined anisotropically without restraints.

The compound crystallises in the space group $P2_12_12_1$ but a combination of merohedral twinning (first identified within the neutron diffraction data via the CRYSTALS[S12] software using the embedded ROTAX[S14] analysis) but is modelled in the approximate Pnma spacegroup, with the molecules lying aross a mirror plane in a disordered manner (Figure S27). As such, only half the molecule appears in the asymmetric unit. There is significant disorder in the structure, with the Si^iPr_3 and 18-crown-6 both being disordered. The Si^iPr_3 was modelled as a two-part disordered with fixed 50% occupancy for each part. The 18-crown-6 was found to be significantly disordered, modelled as four-part disordered with fixed 25% occupancy for each part. Due to the high level of disorder, the 18-crown-6 could only reasonably be modelled isotropically.

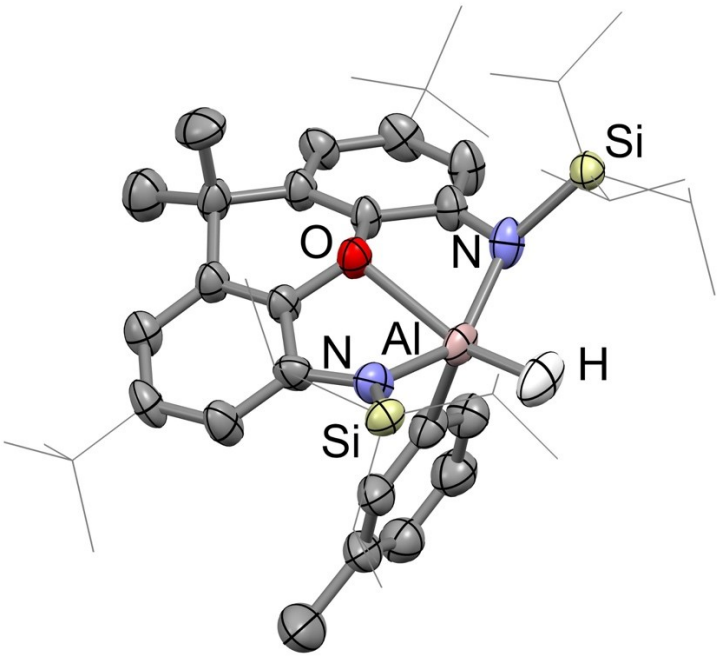


Figure S27: Molecular structure of the anionic part of **6** as determined by single crystal Laue neutron diffraction. Solvent molecules, [K(18-crown-6)] cation and hydrogen atoms (apart from the Al-H) have been omitted, and selected groups are shown in wireframe for clarity. Displacement ellipsoids set at 50% probability level.

The CIF for the refined structure model has been deposited at the Cambridge Crystallographic Data Centre (2432688). This can be obtained free-of-charge via www.ccdc.cam.ac.uk/data_request/cif, by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Computational Studies

Methodology

Density functional theory (DFT) calculations for geometry optimisations were performed using the Gaussian 16 program[S15] using the PBE0 hybrid density functional approximation[S16] with Grimme's D3 dispersion correction with Becke-Johnson dampening, [S17] Stuttgart ECPs and associated basis sets[S18] for Si (ζ_d = 0.284), K (ζ_d = 1.000), and Al (ζ_d = 0.190), with listed additional polarisation functions and Pople's 6-31G** basis set[S19] for all other atoms (BS1), and the ultrafine integration grid. The method used for geometry optimisation was taken from recent benchmarking for low-valent main group species within the group to accurately reproduce important bond lengths.[S20]

The structures were confirmed as minima on the potential energy surface *via* analytical frequency calculations, yielding no negative eigenvalues, except for transition states, which were verified as saddle points on the potential energy surface with a single negative eigenvalue. The corresponding imaginary modes were verified as connecting the appropriate intermediates *via* the intrinsic reaction coordinate method. Thermochemical properties were calculated at a pressure of 1.0 atmospheres, unscaled frequencies, and a temperature of 298.15 K. Single point calculations were performed on the optimised geometries again using PBE0-D3BJ, with the Def2-TZVPP basis[S21] and conductor-like polarisable continuum model[S22] solvation correction (CPCM) with benzene as the solvent. Gibb's free energies were obtained by adding the thermal contribution to Gibb's free energy calculated at the PBE0-D3BJ/BS1 level of theory to the electronic energy calculated at PBE0-D3BJ-(CPCM=benzene)/Def2-TZVPP level.

Reaction Pathways

For di-activations involving species which exist in either monomeric and dimeric (or oligo- or poly- meric) forms, or equilibria between them, multiple possible pathways exist: in the presented case, the difference is in whether the first activation occurs from a monomer, or from a dimer. The second activation is necessarily dimeric in nature due to the phenyl moiety already being tethered to an aluminium centre.

Figure S28 shows the possible pathways between the aluminyl (in either monomeric or dimeric forms) and the observed 1,4-diactivation product (**3**), as well as the observed monomeric activation product necessarily *inter viam* (**2**).

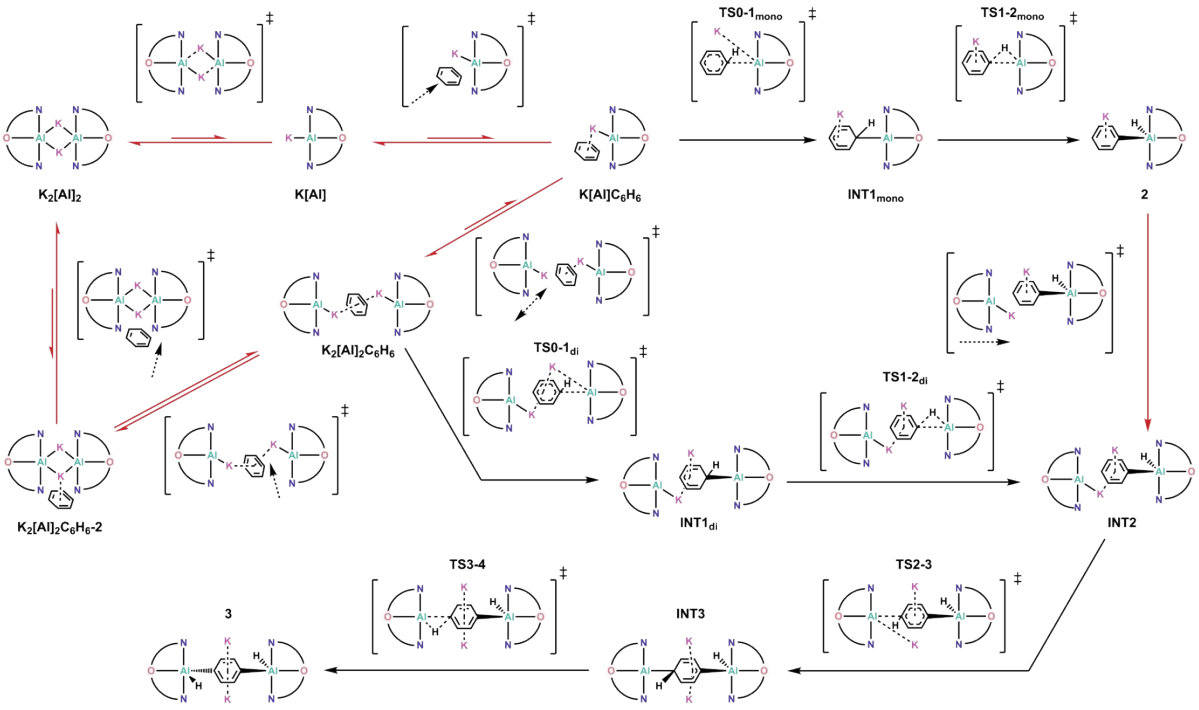


Figure S28: Theorised reaction pathways from the proposed aluminyl dimer, $\mathbf{K_2[Al]_2}$ to the experimentally observed 1,4-activated benzene dialuminate **3**. Structures above arrows within brackets and with double-daggers are transition states, and structures between reaction arrows are local minima. The "a" pathway indicates that the first C-H activation occurred in the monomeric form, and the "b" pathway indicates the alternative, dimeric pathway. Both pathways necessarily link in **INT2**, as the second activation must occur on the already activated ring.

The reaction pathways for both the monomeric and dimeric mechanisms were elucidated along the entirety of each pathway with the exception of associative/dissociative steps, for which we were (expectedly) unable to discern a local maximum on the potential energy surfaces (PESs) to identify the transition states between the minima, due to their flat shapes and absence of critical points between the connected intermediates.

Reaction Profile

Figure 3 in the manuscript shows the elucidated reaction profile for both the monomeric and dimeric pathways with approximate relative energies to the arbitrary 0 of the potassium bridged aluminyl dimer **$K_2[Al]_2$**. Each process proceeds in a similar fashion, starting with nucleophilic attack of a benzene carbon by the aluminyl, with the potassium associated with the aluminium serving to polarise and presumably activate the benzene in the transition state, leading to a Meisenheimer complex, followed by hydride transfer from the C_6H_6 to the aluminium, forming an aluminate. Once the aluminate is formed, the process is repeated on the 4 position of the phenyl moiety with a second equivalent of aluminyl.

The Al-C nucleophilic attack is evidently the rate determining step in each part of the process for both the monomeric and dimeric pathways. This barrier is similar in both the monomeric (29.9 kcal mol^{-1}) and dimeric (31.7 kcal mol^{-1}) pathways, with the monomeric pathway slightly higher by 1.8 kcal mol^{-1}. However, if the monomeric aluminyl is formed and then reacts with benzene before being able to dimerise as if it were reduced from the corresponding aluminium iodide complex (which is monomeric, at least in the solid state) in dilute conditions and thus considering the monomer as the free energyzero, then the monomeric pathway is more energetically favoured, having a barrier height of only 24.4 kcal mol^{-1}. In each case, the hydride transfer has an activation barrier of less than 1.6 kcal mol^{-1}, and is essentially barrierless.

These results are similar to those reported by Harder and co-workers,[S23] showing that a Meisenheimer-intermediate mechanism is more facile that an oxidative addition-type mechanism for aluminyls, with a calculated barrier of 30.3 kcal mol^{-1} (using the ωB97XD-PCM(benzene)/6-311+G**//ωB97XD-PCM(benzene)/6-31+G**[S19,S24] method) for Roesky's (deprotonated) β-diketiminate potassium aluminyl,[S25] which experimentally performs C-H activation of benzene over a period of 7 days at 35 °C. This activation barrier size does not agree well with the experiment, with the Eyring equation predicting a $t_{1/2}$ of *ca.* 10 years for such an energy, suggested to be due to overestimation of entropic factors in the original report.

The activation barrier herein reported (24-32 kcal mol^{-1}) agrees with the previously reported results. Harder and co-workers also shed light on the para-selectivity, showing a thermodynamic preference for the 1,4-substitution using the parent AlH_2^{2-} aluminyl, suggesting a templating effect by the potassiums. They also calculate barriers of $\Delta G^{\ddagger}$ = 31.8 kcal mol^{-1} for the first, and $\Delta G^{\ddagger}$ = 34.3 kcal mol^{-1} for the second aluminations of benzene for the Roesky potassium aluminyl (diisopropylphenyl moieties computationally pruned to phenyl, almost certainly lowering the activation barrier by decreasing steric interactions). In contrast, the second nucleophilic attack transition state for **INT2-3** is calculated to have an activation barrier of only 10.4 kcal mol^{-1}, significantly lower (by at least 14 kcal mol^{-1}) than the initial Meisenheimer intermediate formation barrier of 24-32 kcal mol^{-1}.

McMullin, Coles, and Mulvey[S26] also report similar results for the differences between the monomeric and dimeric forms of the first C-H activation of benzene for rubidium and caesium aluminyls, calculating the dimeric forms to have a barrier *ca.* 18 kcal mol^{-1} lower than the monomeric forms.

Energetic Data and Optimised xyz Coordinates

C_6H_6

SCF (PBE0-D3BJ-(CPCM=benzene)/def2-TZVPP) Energy =
-232.058175 Eh
Thermal Gibb's Corr. = 0.073935 Eh
Gibb's Free Energy= -231.905572 Eh
Lowest Frequency = 412.6381 cm^{-1}
Second Frequency = 412.6645 cm^{-1}

C	0.98451	0.98519	0.00000
C	-0.36097	1.34520	0.00000
C	-1.34546	0.36001	-0.00000
C	-0.98450	-0.98520	0.00000
C	0.36096	-1.34520	0.00000
C	1.34547	-0.36000	-0.00000
H	1.75232	1.75359	-0.00000
H	-0.64248	2.39435	0.00000
H	-2.39482	0.64074	-0.00000
H	-1.75234	-1.75357	-0.00000
H	0.64251	-2.39434	0.00000
H	2.39482	-0.64077	-0.00000

$K_2[Al]_2$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy =
-6650.159606 Eh
Thermal Gibb's Corr. = 1.921640 Eh
Gibb's Free Energy= -6416.054708Eh
Lowest Frequency = 7.2513 cm^{-1}
Second Frequency = 11.4960 cm^{-1}

K	0.10289	-1.80892	-1.75741
Al	-2.75220	-0.16704	-0.59801
O	-4.22332	1.12129	-1.32184
N	-4.37291	-1.31762	-0.32622
N	-2.53545	1.42768	0.68235
C	-5.51301	0.59872	-1.19241
C	-5.57214	-0.68393	-0.63495
C	-6.88374	-1.14392	-0.42995
H	-7.02481	-2.11000	0.03504
C	-8.01362	-0.38464	-0.75926
C	-7.85717	0.89522	-1.30115
H	-8.72395	1.49965	-1.53436
C	-6.57769	1.41484	-1.51454
C	-6.23883	2.81640	-2.03850
C	-5.11157	3.33007	-1.13943
C	-5.03133	4.58883	-0.54584
H	-5.76377	5.34719	-0.79882
C	-4.03682	4.86929	0.40395
C	-3.16027	3.85635	0.80114
H	-2.45293	4.04322	1.59881
C	-3.23055	2.55143	0.26299
C	-4.14269	2.40799	-0.78680
C	-5.73086	2.70079	-3.48957
H	-4.86030	2.04342	-3.55347
H	-5.44878	3.68824	-3.86966
H	-6.51769	2.29134	-4.13081
C	-7.45004	3.74142	-2.00616
H	-8.24559	3.34914	-2.64591
H	-7.18609	4.73124	-2.38995
H	-7.84335	3.85437	-0.99179
C	-9.39341	-0.98353	-0.47348
C	-9.52238	-1.26051	1.03240
H	-8.76367	-1.96751	1.38085
H	-10.50687	-1.68495	1.25989
H	-9.40498	-0.33635	1.60721
C	-9.55177	-2.29943	-1.24964
H	-10.53700	-2.73974	-1.05863
H	-8.79495	-3.03439	-0.95984
H	-9.45521	-2.12976	-2.32694
C	-10.52987	-0.04641	-0.88621
H	-11.49346	-0.51919	-0.67073
H	-10.50085	0.17651	-1.95790
H	-10.49449	0.89949	-0.33589
C	-3.97530	6.26646	1.02576
C	-3.75646	7.30523	-0.08396
H	-4.55901	7.27788	-0.82647
H	-2.81155	7.12204	-0.60652
H	-3.72235	8.31565	0.33863
C	-2.83987	6.40628	2.04220
H	-2.82730	7.42574	2.44051
H	-1.86141	6.21539	1.58811
H	-2.96532	5.72319	2.88898
C	-5.29971	6.55781	1.74796
H	-5.27440	7.55346	2.20486
H	-5.47884	5.82166	2.53807
H	-6.15111	6.52524	1.06226
K	-0.30958	2.16088	-0.98788
Al	2.70769	0.39327	-1.06086
O	3.21884	0.07095	0.93118
N	4.47134	1.33810	-0.99605
N	2.78018	-1.68701	-1.00913
C	4.50059	0.52259	1.24883
C	5.16488	1.15560	0.19835
C	6.49805	1.49721	0.49802
H	7.09476	1.95452	-0.27609
C	7.07719	1.23202	1.74051
C	6.32904	0.58528	2.73719
H	6.78689	0.35878	3.69368
C	5.01127	0.20470	2.49404
C	4.07694	-0.53691	3.45944
C	3.34645	-1.59635	2.62797
C	3.06209	-2.90567	3.01075
H	3.28255	-3.22754	4.02227
C	2.49989	-3.81252	2.09906
C	2.35138	-3.43281	0.75950
H	1.99067	-4.15127	0.03315
C	2.70540	-2.14245	0.30715
C	3.02154	-1.24679	1.33128
C	3.05748	0.47050	4.02429
H	2.49940	0.95853	3.22168
H	2.34556	-0.04055	4.68099
H	3.57167	1.24557	4.60136
C	4.84538	-1.17092	4.61389
H	5.37041	-0.40321	5.18921
H	4.15931	-1.67382	5.30142
H	5.57736	-1.90041	4.25570
C	8.53089	1.61061	2.03423
C	9.19817	2.32506	0.85681
H	8.67890	3.25528	0.60217
H	10.22939	2.58148	1.12016
H	9.23176	1.69355	-0.03713
C	8.57547	2.55107	3.24767
H	9.60976	2.83276	3.47547
H	8.00700	3.46545	3.04887
H	8.15189	2.08179	4.14032
C	9.33221	0.33620	2.33905
H	10.37881	0.58249	2.55136

H	8.92975	-0.19627	3.20574
H	9.30613	-0.34868	1.48535
C	2.12756	-5.21277	2.59515
C	1.18988	-5.09259	3.80649
H	1.65798	-4.55352	4.63452
H	0.27270	-4.55820	3.53796
H	0.91085	-6.08767	4.17033
C	1.41182	-6.04904	1.53228
H	1.13452	-7.01882	1.95779
H	0.49230	-5.56492	1.18848
H	2.04589	-6.24478	0.66282
C	3.40853	-5.95323	3.00887
H	3.16949	-6.95756	3.37639
H	4.08956	-6.05260	2.15731
H	3.94203	-5.42157	3.80224
Si	-4.26480	-3.08578	-0.45759
Si	3.71959	-2.63269	-2.18701
Si	4.74033	2.85067	-1.89383
Si	-2.28158	1.21823	2.43045
C	-1.66101	-0.58085	2.58606
H	-2.34748	-1.12473	1.91508
C	-1.80186	-1.20370	3.97542
H	-2.83572	-1.18906	4.33256
H	-1.47082	-2.25032	3.96351
H	-1.18755	-0.68569	4.71808
C	-0.24138	-0.76537	2.05336
H	0.04037	-1.82571	2.01355
H	-0.12406	-0.35501	1.04250
H	0.49870	-0.27341	2.69075
C	-1.02820	2.47902	3.18805
H	-1.63043	3.36901	3.42881
C	0.08162	2.91831	2.23194
H	0.64755	2.06554	1.83637
H	-0.32148	3.49429	1.39075
H	0.80593	3.57149	2.73559
C	-0.42211	1.98444	4.50448
H	0.19345	2.76672	4.96722
H	-1.18494	1.69272	5.23165
H	0.22813	1.11995	4.34421
C	-3.98095	1.49129	3.26708
H	-4.32163	2.44047	2.82527
C	-3.95597	1.67865	4.78344
H	-4.96629	1.87091	5.16732
H	-3.58259	0.78834	5.30179
H	-3.32867	2.52425	5.08454
C	-4.97916	0.41150	2.84797
H	-4.71509	-0.56596	3.26817
H	-5.99071	0.65169	3.19928
H	-5.02372	0.29285	1.76233
C	-5.51333	-4.06534	0.62348
H	-6.48006	-3.92209	0.12120
C	-5.23358	-5.56977	0.56939
H	-6.02476	-6.13426	1.07886
H	-5.18080	-5.93983	-0.46080
H	-4.29068	-5.82970	1.06000
C	-5.66139	-3.55473	2.05576
H	-5.85046	-2.47663	2.08183
H	-6.49099	-4.05688	2.57034
H	-4.75920	-3.74150	2.64620
C	-2.44060	-3.51081	0.01066
H	-1.95973	-2.52428	-0.12154
C	-1.75557	-4.50175	-0.93068
H	-0.69347	-4.63012	-0.66977
H	-2.20755	-5.49778	-0.86425
H	-1.81935	-4.20210	-1.98364
C	-2.19938	-3.91469	1.46390
H	-2.68593	-3.23734	2.16860
H	-2.56129	-4.92590	1.67397
H	-1.12538	-3.90445	1.69094
C	-4.57887	-3.62395	-2.28062
H	-4.07920	-4.59821	-2.39239
C	-3.93452	-2.63978	-3.25733
H	-4.43682	-1.66713	-3.21360
H	-2.87974	-2.44451	-3.03001
H	-3.99751	-3.00281	-4.29174
C	-6.05394	-3.81945	-2.63960
H	-6.16001	-4.14248	-3.68363
H	-6.53863	-4.57759	-2.01595
H	-6.61733	-2.88749	-2.52749
C	3.81462	-1.41721	-3.66408
H	4.19366	-0.50295	-3.17590
C	4.80689	-1.76629	-4.77309
H	4.56240	-2.70883	-5.27167
H	4.80556	-0.98465	-5.54410
H	5.82864	-1.84641	-4.39521
C	2.43589	-1.07949	-4.24257
H	1.84156	-0.49547	-3.52624
H	2.53133	-0.45367	-5.13861
H	1.86953	-1.97102	-4.53785
C	2.83293	-4.29657	-2.68306
H	1.76929	-4.14456	-2.43019
C	2.90004	-4.64651	-4.17297
H	2.49390	-3.86554	-4.82027
H	3.93458	-4.82290	-4.48721
H	2.34347	-5.57001	-4.37947
C	3.31782	-5.51357	-1.88543
H	3.40601	-5.32388	-0.81360
H	2.64082	-6.36638	-2.02306
H	4.30596	-5.83195	-2.23098
C	5.42747	-3.08920	-1.45605
H	5.17399	-3.78259	-0.63953
C	6.36215	-3.82765	-2.41875
H	7.18955	-4.29567	-1.87105
H	5.86441	-4.61429	-2.99447
H	6.81204	-3.13722	-3.13840
C	6.13519	-1.88872	-0.83288
H	6.29481	-1.08580	-1.56131
H	5.56365	-1.46304	-0.00662
H	7.11849	-2.17392	-0.43692
C	3.52005	2.85345	-3.37983
H	2.66182	2.27317	-3.00172
C	4.03522	2.13091	-4.62505
H	4.40772	1.12879	-4.40065
H	3.23588	2.02759	-5.37087
H	4.84960	2.68199	-5.10630
C	3.01058	4.24545	-3.75933
H	2.29882	4.18127	-4.59352
H	2.50145	4.74756	-2.93034
H	3.82372	4.90398	-4.08528
C	4.30084	4.35537	-0.77375
H	4.20375	5.20648	-1.46427
C	2.94659	4.14247	-0.09625
H	2.64250	5.02307	0.48585
H	2.15728	3.93834	-0.83067
H	2.98094	3.28532	0.58613
C	5.35924	4.72772	0.26637
H	5.50372	3.92612	0.99700
H	6.33233	4.93411	-0.19168
H	5.06184	5.62947	0.81823
C	6.55188	3.09615	-2.48495
H	7.11737	3.34566	-1.57664
C	6.68824	4.30656	-3.41205
H	7.74158	4.49927	-3.65265
H	6.16598	4.15631	-4.36227

H 6.28553 5.21827 -2.95651
C 7.17963 1.83938 -3.08747
H 7.08776 0.98145 -2.41319
H 6.70078 1.56166 -4.03157
H 8.24642 1.99125 -3.29753

K[Al]

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -3208.966817 Eh

Thermal Gibb's Corr. = 0.948242 Eh

Gibb's Free Energy= -3208.018575 Eh

Lowest Frequency = 15.5757 cm^{-1}

Second Frequency = 20.6035 cm^{-1}

Si 1.78399 -2.05951 1.09109
Si -3.48837 -1.16083 -0.60372
Al -0.31635 -1.27312 -1.46362
K 2.21880 -2.62351 -2.80263
O 0.21524 0.76194 -1.54042
N 1.54105 -1.26640 -0.47284
N -1.83715 -0.49778 -0.46508
C 2.24548 -0.08980 -0.69972
C -1.15870 3.62484 0.23048
H -0.95260 4.67521 0.40443
C -2.24131 3.00833 0.87779
C 1.54722 1.00673 -1.21408
C -2.48924 1.64954 0.67388
H -3.29931 1.17200 1.20450
C -1.70042 0.85838 -0.18310
C 3.31528 2.52796 -0.80151
H 3.70285 3.53953 -0.75360
C 4.14756 1.44660 -0.47366
C 3.60719 0.15888 -0.42272
H 4.21448 -0.66378 -0.06688
C 1.98363 2.31904 -1.15789
C -3.11779 3.84265 1.81500
C 0.91405 3.39683 -1.35361
C 3.51250 -2.90118 1.25566
H 4.20281 -2.08058 1.49793
C 0.58060 3.52880 -2.85289
H -0.21696 4.26450 -2.99614
H 0.24643 2.57553 -3.26935
H 1.46507 3.85843 -3.40797
C 0.35774 -3.33480 1.17559
H -0.48093 -2.77150 0.73267
C 1.59328 -0.86743 2.57798
H 1.41715 -1.54229 3.43017
C -3.30410 -2.95578 -1.26336
H -2.39920 -2.90842 -1.89150
C -4.47430 -1.11089 1.04566
H -4.75971 -0.05772 1.17757
C 5.60951 1.71693 -0.10978
C 1.37492 4.74896 -0.82186
H 2.25334 5.09896 -1.37199
H 1.62641 4.69841 0.24152
H 0.58966 5.49787 -0.95842
C -2.25342 4.39350 2.95885
H -2.86187 4.99421 3.64455
H -1.44412 5.02738 2.58471
H -1.80027 3.57519 3.52766
C -4.47983 -0.16012 -1.91100
H -5.29280 -0.83763 -2.21172
C 0.35285 0.00808 2.39607
H 0.51439 0.75097 1.60846
H 0.11356 0.55759 3.31538
H -0.53244 -0.56694 2.10650
C 4.03308 -3.56003 -0.02060
H 3.34858 -4.33406 -0.38982
H 5.00359 -4.04582 0.14472
H 4.18652 -2.81446 -0.81149
C -4.25894 3.02740 2.42758
H -3.88527 2.19435 3.03217
H -4.92468 2.62286 1.65772
H -4.85806 3.66919 3.08164
C 6.31200 2.38517 -1.30058
H 5.82969 3.32767 -1.57497
H 6.29214 1.73243 -2.17969
H 7.35872 2.59990 -1.05727
C 0.57948 -4.57585 0.31134
H 0.75248 -4.31008 -0.73843
H -0.30401 -5.22621 0.32477
H 1.42774 -5.17347 0.66268
C -3.73545 5.00786 1.02778
H -4.36568 5.62050 1.68251
H -4.35580 4.63360 0.20692
H -2.96799 5.65757 0.59713
C -0.07630 -3.72754 2.58797
H 0.71996 -4.24357 3.13563
H -0.93540 -4.41014 2.54972
H -0.37811 -2.85861 3.17958
C -3.04467 -4.00568 -0.18222
H -2.22727 -3.72413 0.48579
H -2.78242 -4.97051 -0.63639
H -3.92968 -4.17586 0.43975
C 2.80935 -0.00640 2.92308
H 3.71226 -0.60328 3.09446
H 2.62385 0.57110 3.83809
H 3.02788 0.70865 2.12404
C 3.54900 -3.87286 2.43704
H 3.21292 -3.39554 3.36367
H 4.56477 -4.25039 2.61193
H 2.90597 -4.74278 2.26655
C 5.66658 2.65059 1.10918
H 6.70744 2.85424 1.38503
H 5.16649 2.19479 1.96964
H 5.17969 3.60913 0.90911
C -4.45929 -3.40318 -2.16149
H -5.41935 -3.39593 -1.63201
H -4.29456 -4.43018 -2.51311
H -4.56487 -2.76964 -3.04684
C -5.78598 -1.89290 0.94037
H -6.39141 -1.56233 0.08878
H -6.39430 -1.76337 1.84486
H -5.61337 -2.96724 0.82151
C 6.37110 0.43678 0.24024
H 6.37299 -0.27499 -0.59244
H 5.94573 -0.06053 1.11841
H 7.41300 0.68033 0.47135
C -3.65798 -1.52105 2.27014
H -3.35053 -2.57046 2.22001
H -4.23903 -1.39705 3.19359
H -2.74783 -0.91978 2.36317
C -5.13148 1.13559 -1.42447
H -4.38132 1.87572 -1.12948
H -5.79124 0.97081 -0.56532
H -5.74079 1.58460 -2.22020
C -3.60448 0.10249 -3.13799
H -2.79804 0.80317 -2.89334
H -4.18696 0.54291 -3.95782
H -3.12903 -0.80991 -3.51627
C -0.32910 2.88795 -0.61174
C -0.64859 1.55322 -0.78007

$K_2[Al]_2C_6H_6$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.053213 Eh
Thermal Gibb's Corr. = 2.016765 Eh
Gibb's Free Energy= -3881.325046 Eh
Lowest Frequency = 8.7366 cm-1
Second Frequency = 10.8291 cm-1

K	0.21780	1.55739	2.00236
Al	-2.70688	0.26419	0.55277
O	-4.33945	-0.95447	1.04601
N	-4.21189	1.58199	0.33529
N	-2.56484	-1.18940	-0.90172
C	-5.56893	-0.30530	0.89647
C	-5.47866	1.03089	0.48934
C	-6.72814	1.62722	0.24841
H	-6.75149	2.64660	-0.11151
C	-7.93884	0.94128	0.40405
C	-7.93154	-0.39905	0.80373
H	-8.86066	-0.94497	0.90215
C	-6.72018	-1.05196	1.04520
C	-6.54288	-2.52609	1.43028
C	-5.38853	-3.04321	0.56720
C	-5.35432	-4.24850	-0.13576
H	-6.15704	-4.96604	-0.00766
C	-4.31275	-4.51945	-1.03814
C	-3.34688	-3.54123	-1.28516
H	-2.59448	-3.71041	-2.04496
C	-3.36170	-2.29098	-0.62899
C	-4.33019	-2.17529	0.37200
C	-6.16194	-2.60487	2.92162
H	-5.28668	-1.98747	3.13734
H	-5.94088	-3.63904	3.20619
H	-6.98942	-2.24158	3.53896
C	-7.81622	-3.33229	1.19988
H	-8.63308	-2.93637	1.80964
H	-7.66850	-4.37471	1.49713
H	-8.12253	-3.30900	0.15019
C	-9.23706	1.68809	0.08669
C	-9.21515	2.13596	-1.38305
H	-8.37654	2.80746	-1.58961
H	-10.14048	2.66659	-1.63467
H	-9.12152	1.27237	-2.04923
C	-9.35473	2.92133	0.99454
H	-10.28150	3.46590	0.78126
H	-8.51934	3.61265	0.84928
H	-9.36434	2.62834	2.04941
C	-10.47572	0.81668	0.30240
H	-11.37665	1.39380	0.07070
H	-10.55565	0.47768	1.34057
H	-10.46965	-0.06363	-0.34867
C	-4.29628	-5.86158	-1.77317
C	-4.26440	-7.00259	-0.74571
H	-5.13088	-6.97286	-0.07912
H	-3.36416	-6.94184	-0.12455
H	-4.26254	-7.97423	-1.25204
C	-3.07972	-6.01175	-2.68921
H	-3.10001	-6.99544	-3.16883
H	-2.14000	-5.93214	-2.13166
H	-3.07237	-5.25824	-3.48373
C	-5.56284	-5.98191	-2.63423
H	-5.57106	-6.93659	-3.17203
H	-5.60718	-5.17266	-3.37005
H	-6.47089	-5.93061	-2.02667
K	-0.25137	-2.15077	0.57678
Al	2.82336	-0.44239	0.87423
O	3.26308	0.20638	-1.05862
N	4.59816	-1.33406	0.60187
N	2.87419	1.63614	1.14811
C	4.53832	-0.17092	-1.48468
C	5.24828	-0.94738	-0.56941
C	6.57548	-1.20964	-0.96303
H	7.20664	-1.77029	-0.29204
C	7.10602	-0.74762	-2.16850
C	6.31248	0.02651	-3.02927
H	6.72993	0.40311	-3.95645
C	5.00026	0.34002	-2.68424
C	4.02266	1.20391	-3.49010
C	3.32956	2.11915	-2.47633
C	3.06061	3.47646	-2.63630
H	3.25987	3.95181	-3.58984
C	2.55704	4.23830	-1.57108
C	2.43432	3.64834	-0.30684
H	2.11613	4.24878	0.53673
C	2.77096	2.29477	-0.07692
C	3.04691	1.57031	-1.23951
C	2.98733	0.27753	-4.15628
H	2.48349	-0.34676	-3.41460
H	2.23197	0.86973	-4.68370
H	3.48126	-0.38259	-4.87627
C	4.73593	2.01022	-4.56993
H	5.24028	1.34170	-5.27331
H	4.01698	2.59965	-5.14621
H	5.47830	2.68869	-4.13993
C	8.55164	-1.05279	-2.56782
C	9.27697	-1.91088	-1.52893
H	8.78571	-2.88024	-1.39189
H	10.30189	-2.10273	-1.86252
H	9.33256	-1.41237	-0.55553
C	8.55725	-1.81459	-3.90152
H	9.58433	-2.04366	-4.20768
H	8.00817	-2.75738	-3.80960
H	8.09056	-1.23300	-4.70183
C	9.32317	0.26615	-2.72314
H	10.36281	0.07094	-3.00977
H	8.87818	0.90699	-3.48987
H	9.32479	0.82471	-1.78157
C	2.24634	5.71848	-1.81713
C	1.31297	5.85950	-3.02942
H	1.76105	5.45656	-3.94164
H	0.36901	5.33213	-2.86011
H	1.08582	6.91608	-3.20947
C	1.56698	6.39341	-0.62348
H	1.33453	7.43252	-0.87817
H	0.62755	5.89979	-0.35844
H	2.20897	6.41299	0.26139
C	3.56470	6.45619	-2.09925
H	3.37698	7.51970	-2.28575
H	4.24488	6.37244	-1.24525
H	4.07593	6.04393	-2.97417
Si	-3.97552	3.30679	0.68891
Si	3.82086	2.40455	2.44256
Si	4.93614	-2.96646	1.22549
Si	-2.29705	-0.79891	-2.61866
C	-1.60114	0.97779	-2.57384
H	-2.27800	1.47748	-1.85992
C	-1.68547	1.74985	-3.89105
H	-2.71000	1.81303	-4.26913
H	-1.31715	2.77582	-3.75972
H	-1.07116	1.29157	-4.67196
C	-0.18503	1.03513	-2.00477
H	0.16100	2.06916	-1.88399
H	-0.11699	0.55056	-1.02246
H	0.53588	0.54171	-2.66190

C	-1.10544	-2.02712	-3.52037
H	-1.75920	-2.84710	-3.85734
C	-0.01772	-2.64174	-2.63945
H	0.61398	-1.87512	-2.17262
H	-0.44577	-3.27687	-1.85526
H	0.65216	-3.28370	-3.22613
C	-0.47110	-1.41791	-4.77417
H	0.08872	-2.17797	-5.33452
H	-1.21233	-0.98831	-5.45336
H	0.23758	-0.62575	-4.51597
C	-3.99860	-0.90740	-3.49050
H	-4.38616	-1.88123	-3.15368
C	-3.96467	-0.93704	-5.01813
H	-4.97863	-1.04345	-5.42525
H	-3.54860	-0.01459	-5.43863
H	-3.37185	-1.77325	-5.40312
C	-4.95550	0.16596	-2.97221
H	-4.64216	1.16921	-3.28343
H	-5.97091	0.00960	-3.35810
H	-5.01399	0.17132	-1.88152
C	-5.05008	4.51222	-0.35053
H	-6.06445	4.39855	0.05613
C	-4.65673	5.96889	-0.09023
H	-5.35169	6.65780	-0.58687
H	-4.66635	6.21037	0.97871
H	-3.65602	6.19775	-0.46881
C	-5.11421	4.18570	-1.84174
H	-5.38740	3.13925	-2.01277
H	-5.85251	4.81677	-2.35344
H	-4.15183	4.35519	-2.33423
C	-2.09398	3.62376	0.40661
H	-1.70809	2.58893	0.44437
C	-1.41253	4.42957	1.51270
H	-0.32701	4.50058	1.34275
H	-1.78218	5.46071	1.54462
H	-1.58024	4.00863	2.51139
C	-1.70153	4.17463	-0.96266
H	-2.17229	3.62413	-1.77952
H	-1.97202	5.22931	-1.07518
H	-0.61587	4.10267	-1.10380
C	-4.39223	3.64892	2.53858
H	-3.82468	4.55240	2.80851
C	-3.91128	2.49853	3.42404
H	-4.49295	1.59129	3.22655
H	-2.86336	2.23109	3.24235
H	-4.02105	2.74052	4.48953
C	-5.87016	3.93473	2.81577
H	-6.03253	4.14308	3.88156
H	-6.23994	4.80072	2.25711
H	-6.49720	3.07712	2.55152
C	3.97046	0.98159	3.71656
H	4.38321	0.17365	3.08819
C	4.95254	1.19084	4.86882
H	4.64863	2.00768	5.53003
H	5.01220	0.28384	5.48478
H	5.96184	1.40945	4.51444
C	2.61319	0.49759	4.24006
H	2.03880	0.00064	3.44550
H	2.74536	-0.25038	5.03206
H	2.01187	1.30812	4.67002
C	2.92142	3.96117	3.20076
H	1.86629	3.85920	2.89385
C	2.94436	4.05006	4.72969
H	2.52867	3.16771	5.22246
H	3.96803	4.17552	5.09912
H	2.37314	4.92157	5.07547
C	3.42596	5.29626	2.64005
H	3.53744	5.29610	1.55367
H	2.74660	6.11512	2.90915
H	4.40659	5.54423	3.05746
C	5.50913	2.98910	1.75710
H	5.23470	3.81354	1.08186
C	6.47308	3.54995	2.80710
H	7.26563	4.13974	2.33020
H	5.98792	4.19215	3.54926
H	6.96926	2.74256	3.35431
C	6.19559	1.91820	0.91278
H	6.36530	0.99752	1.48203
H	5.60342	1.64895	0.03661
H	7.17189	2.26734	0.55228
C	3.79768	-3.29954	2.73877
H	2.84778	-2.80817	2.47261
C	4.28624	-2.67565	4.04608
H	4.52221	-1.61501	3.93953
H	3.52443	-2.76810	4.83240
H	5.18691	-3.17533	4.41758
C	3.52375	-4.79080	2.95275
H	2.87077	-4.94735	3.82213
H	3.04131	-5.25589	2.08839
H	4.44363	-5.35056	3.14995
C	4.47058	-4.27838	-0.10354
H	4.52850	-5.24477	0.41968
C	3.02568	-4.07606	-0.56539
H	2.71525	-4.85936	-1.27054
H	2.32147	-4.08609	0.27611
H	2.91370	-3.10953	-1.07118
C	5.40547	-4.35688	-1.31163
H	5.37478	-3.43740	-1.90338
H	6.44775	-4.52078	-1.01774
H	5.11790	-5.18613	-1.97186
C	6.78223	-3.23005	1.70210
H	7.31217	-3.33499	0.74532
C	7.02588	-4.53782	2.45853
H	8.10055	-4.71002	2.60038
H	6.57200	-4.52500	3.45458
H	6.62467	-5.40515	1.92260
C	7.38689	-2.03500	2.44041
H	7.24296	-1.10199	1.88645
H	6.92921	-1.89857	3.42559
H	8.46456	-2.17165	2.59944
C	-2.33353	-3.40800	3.06404
C	-1.14189	-3.15940	3.74712
C	-0.02585	-3.96667	3.52238
C	-0.10457	-5.02471	2.61426
C	-1.29717	-5.27084	1.93101
C	-2.41366	-4.46314	2.15361
H	-3.19653	-2.77160	3.22837
H	-1.08244	-2.33169	4.44838
H	0.90394	-3.76981	4.04770
H	0.76200	-5.65676	2.44627
H	-1.35846	-6.09606	1.22636
H	-3.33845	-4.64541	1.61362

K[Al]C_6H_6

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -3441.042004 Eh

Thermal Gibb's Corr. = 1.040980 Eh

Gibb's Free Energy= -3440.001024 Eh

Lowest Frequency = 9.3409 cm^{-1}

Second Frequency = 17.8127 cm^{-1}

Si	-1.46736	-2.14176	-1.62868
Si	3.66740	-1.50436	0.73850

```
Al  0.41215 -1.22357  1.07833
K  -2.47732 -2.03789  2.17014
O   0.04830  0.85147  0.99517
N  -1.27745 -1.07314 -0.23295
N   2.18154 -0.57960  0.39819
C   1.15084  1.57259  0.53220
C  -1.81952  0.19914 -0.28200
C   1.01732  2.93951  0.37344
C   2.11741  3.62388 -0.13733
H   2.06531  4.69707 -0.28359
C   3.28441  2.92476 -0.48174
C  -1.12599  1.23387  0.35481
C   3.33519  1.53946 -0.32320
H   4.22501  1.00957 -0.62408
C   2.25889  0.79129  0.19837
C  -2.56110  2.94030 -0.45502
H  -2.80949  3.98797 -0.58208
C  -3.38968  1.95113 -1.00970
C  -3.01344  0.61047 -0.91712
H  -3.61860 -0.14321 -1.40044
C  -1.39571  2.58542  0.22461
C   4.47888  3.70304 -1.03938
C  -0.33445  3.54635  0.76282
C  -3.30329 -2.62539 -1.98586
H  -3.73057 -1.76561 -2.52110
C  -0.43362  3.59963  2.30108
H   0.34416  4.25441  2.70618
H  -0.30292  2.60583  2.73726
H  -1.41165  3.99103  2.60278
C  -5.06812  0.27622  2.09125
C  -0.41436 -3.68865 -1.21366
H   0.46664 -3.25612 -0.71314
C  -0.73719 -1.35180 -3.21351
H  -0.62540 -2.18780 -3.92077
C   3.10766 -3.32771  0.94624
H   2.08572 -3.23734  1.35314
C   5.03453 -1.34852 -0.60817
H   5.47612 -0.35465 -0.45240
C  -5.53389 -0.64737  3.02898
H  -6.38703 -1.27848  2.79424
C  -3.98463  1.10242  2.39653
H  -3.62081  1.81308  1.66032
C  -4.65768  2.37577 -1.75472
C  -0.50830  4.95333  0.20300
H  -1.47438  5.37004  0.50306
H  -0.44841  4.96112 -0.88912
H   0.26564  5.61747  0.59778
C   4.06022  4.42498 -2.32862
H   4.90250  4.99256 -2.74058
H   3.23849  5.12512 -2.15177
H   3.72881  3.70524 -3.08384
C   4.44122 -0.91366  2.39504
H   5.10258 -1.73647  2.70615
C   0.65346 -0.78965 -2.90909
H   0.59161  0.05743 -2.21762
H   1.14637 -0.43506 -3.82333
H   1.31489 -1.52530 -2.43978
C  -4.14959 -2.83919 -0.73101
H  -3.75425 -3.65598 -0.11307
H  -5.18297 -3.11000 -0.98514
H  -4.19885 -1.92627 -0.12448
C   5.66791  2.79601 -1.36465
H   5.41355  2.04803 -2.12300
H   6.03254  2.27300 -0.47412
H   6.49307  3.39940 -1.75685
C  -5.46464  1.18014 -2.26574
H  -5.77380  0.51667 -1.45019
H  -4.89683  0.58812 -2.99105
H  -6.37111  1.53497 -2.76633
C  -1.03996 -4.65558 -0.20978
H  -1.23735 -4.16344  0.74942
H  -0.35309 -5.48381  0.00829
H  -1.97318 -5.09621 -0.57690
C   4.93816  4.73463  0.00186
H   5.79335  5.30649 -0.37627
H   5.24067  4.23793  0.92943
H   4.14174  5.44345  0.24689
C   0.08907 -4.44398 -2.44457
H  -0.73342 -4.85911 -3.03681
H   0.72947 -5.28320 -2.14583
H   0.68046 -3.80427 -3.10616
C   3.00957 -4.09198 -0.37469
H   2.49040 -3.52375 -1.15150
H   2.46862 -5.03833 -0.23993
H   3.99978 -4.34429 -0.76827
C  -3.82826  0.07733  4.58302
H  -3.34855  0.00556  5.55517
C  -1.60735 -0.29188 -3.89148
H  -2.60396 -0.66982 -4.14672
H  -1.14132  0.05035 -4.82467
H  -1.73802  0.58524 -3.25029
C  -3.40587 -3.82005 -2.93590
H  -2.83193 -3.65720 -3.85432
H  -4.44747 -4.00582 -3.22852
H  -3.03151 -4.74013 -2.47529
C  -3.36486  1.00006  3.64267
H  -2.51703  1.63753  3.87558
C  -5.55534  3.19699 -0.81766
H  -6.46271  3.51817 -1.34123
H  -5.04562  4.09251 -0.45136
H  -5.85759  2.60769  0.05480
C   3.92693 -4.12452  1.96220
H   4.98170 -4.19644  1.67192
H   3.54579 -5.15094  2.04516
H   3.88858 -3.68048  2.96123
C   6.17001 -2.34704 -0.36722
H   6.57398 -2.26918  0.64849
H   6.99989 -2.17152 -1.06401
H   5.84413 -3.38182 -0.51181
C  -4.26160  3.23414 -2.96599
H  -3.61746  2.66736 -3.64581
H  -3.71723  4.13272 -2.66201
H  -5.15273  3.55061 -3.51986
C   4.52237 -1.40147 -2.04669
H   4.12528 -2.39009 -2.29677
H   5.32871 -1.18773 -2.76097
H   3.72020 -0.67609 -2.21668
C  -4.91393 -0.74635  4.27756
H  -5.28653 -1.45139  5.01585
C   5.29501  0.35255  2.30316
H   4.69914  1.21410  1.98426
H   6.12528  0.24388  1.59667
H   5.73086  0.59939  3.28055
C   3.35415 -0.74998  3.45792
H   2.68882  0.08291  3.20290
H   3.78846 -0.53825  4.44409
H   2.71908 -1.63808  3.55103
H  -5.54322  0.35505  1.11765
```

$K_2[Al]_2C_6H_6$-2

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy =
-6650.053212 Eh
Thermal Gibb's Corr. = 2.013754 Eh

Gibb's Free Energy= -6650.0262375 Eh
Lowest Frequency = 8.2766 cm^{-1}
Second Frequency = 12.4888 cm^{-1}

K	1.31666	-3.51112	-1.67510
Si	4.53490	-0.03842	-3.65898
Si	5.41885	-2.86982	1.43298
Al	3.52235	-1.21520	-0.72520
O	3.05221	0.49503	0.39380
N	3.70614	0.22073	-2.12601
N	4.93637	-1.33165	0.68295
C	5.03111	-0.18656	1.47455
C	2.83698	1.61742	-0.41491
C	3.14443	1.42603	-1.76490
C	3.92389	1.95938	2.05856
C	4.01114	0.76470	1.37272
C	2.89301	2.55456	-2.57663
H	3.02929	2.45716	-3.64407
C	2.48845	3.94901	-0.64186
H	2.33135	4.93098	-0.21022
C	2.57610	3.80096	-2.03581
C	2.63119	2.84203	0.19387
C	6.04432	0.16424	2.38146
H	6.89445	-0.49686	2.48612
C	4.94589	2.23968	2.96940
H	4.92040	3.16726	3.52651
C	6.01068	1.34746	3.13107
C	2.73141	2.86159	1.72041
C	5.67998	-1.53154	-3.31166
H	5.04248	-2.19089	-2.69267
C	5.51237	1.49603	-4.27799
H	4.76197	2.16810	-4.71640
C	3.31882	-0.55145	-5.06268
H	3.94899	-0.84278	-5.91635
C	7.27252	-2.96812	1.93221
H	7.35598	-2.34807	2.83584
C	7.17086	1.63183	4.08918
C	2.38905	5.03079	-2.92823
C	4.39162	-3.18546	3.03137
H	4.49310	-4.26498	3.21960
C	6.11030	-2.33616	-4.53731
H	5.25929	-2.68682	-5.13048
H	6.68856	-3.21981	-4.23671
H	6.74919	-1.74656	-5.20313
C	4.95841	-4.25944	0.18883
H	4.05968	-3.83258	-0.28655
C	2.49433	-1.76489	-4.63828
H	3.12453	-2.61257	-4.34386
H	1.82665	-2.10436	-5.44370
H	1.87452	-1.49564	-3.77385
C	0.99442	5.63021	-2.69656
H	0.21442	4.91184	-2.96817
H	0.85865	6.53069	-3.30658
H	0.84048	5.90590	-1.64936
C	2.91379	4.27566	2.25874
H	2.99083	4.26019	3.34997
H	2.04660	4.89257	2.00482
H	3.81136	4.75104	1.85242
C	2.38549	0.56978	-5.51746
H	1.73728	0.89849	-4.69647
H	1.73355	0.23740	-6.33740
H	2.93190	1.44823	-5.87642
C	7.26580	0.50526	5.12876
H	6.33810	0.42823	5.70502
H	8.08911	0.69682	5.82653
H	7.44483	-0.46550	4.65725
C	1.45739	2.25370	2.33613
H	1.26802	1.25396	1.94454
H	0.58623	2.87112	2.10404
H	1.55910	2.18570	3.42357
C	8.48258	1.70066	3.29243
H	8.68850	0.76154	2.77041
H	9.32625	1.90522	3.96167
H	8.43795	2.49622	2.54196
C	8.23344	-2.40053	0.88926
H	8.24372	-3.01096	-0.01928
H	9.26225	-2.37182	1.27189
H	7.95356	-1.38537	0.59047
C	7.66347	-4.38764	2.35011
H	7.00483	-4.78171	3.13237
H	8.68878	-4.41446	2.74118
H	7.62540	-5.08437	1.50600
C	3.46132	6.07320	-2.57644
H	3.38604	6.39469	-1.53375
H	3.35501	6.96098	-3.21050
H	4.46395	5.66000	-2.72717
C	2.91560	-2.88293	2.77687
C	4.56379	-5.58973	0.82858
H	5.38821	-6.03770	1.39438
H	4.27760	-6.32062	0.05793
H	3.71737	-5.48594	1.51531
C	6.88918	-1.13371	-2.46405
H	7.55386	-0.45859	-3.01280
H	7.48880	-2.01167	-2.19193
H	6.58929	-0.64114	-1.53380
C	6.22379	2.27196	-3.16829
H	5.52967	2.58680	-2.38471
H	6.70424	3.17248	-3.57371
H	7.00649	1.67280	-2.69406
C	6.99588	2.95537	4.83608
H	6.95666	3.80596	4.14783
H	7.84398	3.11256	5.51047
H	6.08356	2.95988	5.44162
C	5.97861	-4.47533	-0.92649
H	6.24891	-3.53788	-1.41719
H	5.57968	-5.14860	-1.69920
H	6.90189	-4.93174	-0.55405
C	6.47921	1.12673	-5.40632
H	7.29772	0.49500	-5.04519
H	6.93691	2.02643	-5.83739
H	5.98334	0.58893	-6.22245
C	2.52038	4.69907	-4.41636
H	3.51963	4.32312	-4.66144
H	2.35288	5.60346	-5.01040
H	1.78384	3.95185	-4.73020
C	4.87173	-2.45737	4.28747
H	5.91444	-2.68978	4.52813
H	4.26612	-2.74332	5.15821
H	4.79486	-1.37192	4.17453
H	-1.65744	-4.99216	-4.88300
H	2.76839	-1.81149	2.60284
H	2.29045	-3.16960	3.63368
H	2.53064	-3.39988	1.88942
C	-1.61482	-4.19708	-4.14381
C	-1.51044	-2.14990	-2.24624
C	-1.13174	-2.93554	-4.50328
C	-1.98048	-3.41666	-1.87992
C	-1.08331	-1.91145	-3.55577
C	-2.03743	-4.43719	-2.83323
K	-4.50142	-1.60883	-3.32866
Si	-3.68494	3.78544	-0.48395
Si	-6.98121	-1.16535	-0.19259
Al	-4.20434	0.64874	-1.13419
O	-2.86761	-0.25364	0.26973

```
N  -3.95480  2.13221  0.14450
N  -5.23950 -1.11564 -0.52917
C  -4.43344 -2.00978  0.15305
C  -2.65508  0.55878  1.38594
C  -3.28771  1.79879  1.32130
C  -2.42564 -2.19080  1.58572
C  -3.19930 -1.55069  0.63816
C  -3.15636  2.56817  2.49300
H  -3.65667  3.52494  2.53144
C  -1.80192  0.86725  3.56336
H  -1.24371  0.51852  4.42505
C  -2.42236  2.12685  3.59688
C  -1.92196  0.04896  2.44142
C  -4.70525 -3.35574  0.46184
H  -5.61723 -3.79390  0.07335
C  -2.76667 -3.51256  1.90028
H  -2.17582 -4.05293  2.62831
C  -3.88454 -4.11310  1.30947
C  -1.33398 -1.35613  2.26012
C  -4.42807  3.82049 -2.25037
H  -4.14752  2.83724 -2.66124
C  -4.42502  5.15206  0.64615
H  -3.72083  5.22728  1.48705
C  -1.79667  4.09816 -0.63970
H  -1.70277  4.86362 -1.42364
C  -7.30112 -1.61391  1.64252
H  -7.04534 -2.68055  1.71691
C  -4.26784 -5.56766  1.59153
C  -2.30690  2.97856  4.86443
C  -8.01921 -2.41425 -1.24935
H  -9.03114 -2.00143 -1.12833
C  -3.82420  4.88291 -3.17014
H  -2.74655  4.74728 -3.30349
H  -4.28382  4.83028 -4.16606
H  -3.98423  5.90035 -2.79744
C  -7.62945  0.57182 -0.68969
H  -6.98096  0.86574 -1.53459
C  -1.08967  2.83231 -1.13403
H  -1.57934  2.40718 -2.01943
H  -0.04087  3.02841 -1.38396
H  -1.09576  2.05837 -0.35819
C  -2.95477  2.22331  6.03478
H  -2.46340  1.26256  6.21493
H  -2.88837  2.81374  6.95573
H  -4.01141  2.02461  5.82896
C  -0.89871 -1.96440  3.58895
H  -0.45612 -2.95289  3.43468
H  -0.12824 -1.34272  4.05293
H  -1.73859 -2.05961  4.28314
C  -1.11522  4.65745  0.60982
H  -1.21819  3.97755  1.46109
H  -0.04205  4.79711  0.42877
H  -1.53106  5.62619  0.90814
C  -4.26394 -6.35327  0.27093
H  -3.26519 -6.34181 -0.18109
H  -4.54611 -7.39808  0.44220
H  -4.96808 -5.92854 -0.45137
C  -0.11122 -1.27764  1.32724
H  -0.34712 -0.77867  0.38413
H   0.70356 -0.72321  1.79756
H   0.26294 -2.28457  1.11336
C  -5.67258 -5.62057  2.21101
H  -6.43028 -5.21304  1.53566
H  -5.95092 -6.65542  2.43937
H  -5.70657 -5.04275  3.13980
C  -6.39856 -0.87480  2.63260
H  -6.58869  0.20187  2.63793
H  -6.56877 -1.24087  3.65333
H  -5.33833 -1.01652  2.40524
C  -8.78006 -1.47281  2.01297
H  -9.43458 -2.04965  1.34954
H  -8.96300 -1.82313  3.03684
H  -9.11024 -0.42931  1.96935
C  -3.00464  4.33314  4.72197
H  -4.07850  4.22244  4.53931
H  -2.88364  4.90645  5.64675
H  -2.57560  4.92406  3.90561
C  -7.68837 -2.35180 -2.74018
C  -9.07712  0.61695 -1.18049
H  -9.77612  0.27184 -0.40931
H  -9.36166  1.64633 -1.43225
H  -9.24448  0.00695 -2.07372
C  -5.95460  3.88318 -2.26812
H  -6.32789  4.84445 -1.89750
H  -6.33933  3.75914 -3.28945
H  -6.40085  3.09690 -1.65204
C  -5.80109  4.82385  1.22128
H  -5.80668  3.85956  1.73879
H  -6.12523  5.59358  1.93422
H  -6.56104  4.76991  0.43514
C  -3.29500 -6.24995  2.55488
H  -3.28124 -5.75649  3.53174
H  -3.60019 -7.28920  2.71289
H  -2.27312 -6.25914  2.16081
C  -7.42481  1.60090  0.42445
H  -6.37788  1.67802  0.73363
H  -7.73555  2.59797  0.08885
H  -8.02989  1.36011  1.30444
C  -4.42108  6.51654 -0.04674
H  -5.12951  6.54474 -0.88163
H  -4.71366  7.31268  0.65007
H  -3.43333  6.77537 -0.44472
C  -0.82734  3.24043  5.18054
H  -0.34634  3.78885  4.36473
H  -0.73403  3.83553  6.09600
H  -0.27178  2.30989  5.32877
C  -8.08756 -3.86983 -0.79199
H  -8.30419 -3.96145  0.27666
H  -8.87095 -4.41703 -1.33255
H  -7.14853 -4.40241 -0.98640
H  -1.48831 -1.34560 -1.51732
H  -6.78440 -2.94394 -2.94499
H  -8.48043 -2.79445 -3.35743
H  -7.53091 -1.32541 -3.09661
H  -2.41636 -5.41635 -2.55225
H  -2.31840 -3.59562 -0.86246
H  -0.78931 -2.75191 -5.51744
H  -0.71594 -0.92661 -3.82936
```

TS0-1$_{mono}$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -3441.008226 Eh

Thermal Gibb's Corr. = 1.046070 Eh

Gibb's Free Energy= -3439.962156 Eh

Lowest Frequency = -118.1402 cm^{-1}

Second Frequency = 10.8571 cm^{-1}

```
Si -2.92918 -1.99189 -0.72858
Si  2.73992 -1.99500 -0.73176
Al -0.07482 -1.06741  0.68563
K   2.34788  0.12685  2.64883
O  -0.05996  0.97473  0.69338
N  -1.85656 -0.71763 -0.10473
N   1.81030 -0.61240 -0.09137
```

C	1.05911	1.61529	0.18276
C	-2.23440	0.61285	-0.07924
C	1.07164	2.99696	0.12801
C	2.22915	3.58654	-0.37479
H	2.29210	4.66631	-0.44509
C	3.31078	2.79692	-0.78983
C	-1.27576	1.54688	0.32171
C	3.21995	1.40264	-0.72983
H	4.05258	0.80990	-1.07068
C	2.06288	0.74092	-0.25982
C	-2.63240	3.43129	-0.09193
H	-2.78139	4.50391	-0.13835
C	-3.68881	2.56550	-0.41175
C	-3.47926	1.18517	-0.41047
H	-4.28784	0.52783	-0.69321
C	-1.39074	2.92123	0.28431
C	4.56982	3.49732	-1.31039
C	-0.15555	3.73927	0.66038
C	-4.63943	-1.97679	0.14261
H	-5.20716	-1.16435	-0.33250
C	-0.05423	3.79118	2.19912
H	0.84408	4.34041	2.50210
H	-0.01219	2.78411	2.62396
H	-0.93117	4.29550	2.61721
C	-0.60017	-1.21995	3.05545
C	-1.98369	-3.63802	-0.43977
H	-0.93322	-3.37255	-0.64744
C	-3.19845	-1.84977	-2.62330
H	-3.62923	-2.82376	-2.90156
C	1.84003	-2.61001	-2.29942
H	0.84470	-2.87258	-1.90344
C	4.61559	-1.61036	-1.06147
H	4.89815	-0.83223	-0.33671
C	0.22765	-2.04317	3.92136
H	0.24513	-3.11768	3.75572
C	-0.76276	0.14859	3.52250
H	-1.53346	0.76851	3.07152
C	-5.04891	3.16411	-0.78042
C	-0.23369	5.16177	0.11465
H	-1.10669	5.67856	0.52192
H	-0.30238	5.16933	-0.97675
H	0.64538	5.73908	0.41456
C	4.20836	4.32312	-2.55455
H	5.09570	4.83403	-2.94475
H	3.45421	5.08311	-2.33103
H	3.80889	3.67833	-3.34356
C	2.76673	-3.43802	0.53753
H	3.53977	-4.09415	0.11348
C	-1.84959	-1.70528	-3.32574
H	-1.36164	-0.76883	-3.03503
H	-1.96241	-1.69768	-4.41777
H	-1.16134	-2.51832	-3.07136
C	-4.54664	-1.65320	1.63362
H	-3.99645	-2.42484	2.18196
H	-5.54499	-1.58564	2.08499
H	-4.03590	-0.70048	1.80546
C	5.67617	2.51462	-1.69734
H	5.36810	1.85563	-2.51415
H	5.98305	1.89094	-0.85053
H	6.55691	3.06989	-2.03522
C	-6.11060	2.09247	-1.03751
H	-6.25919	1.45282	-0.16094
H	-5.84955	1.45618	-1.88894
H	-7.06767	2.57250	-1.26581
C	-2.03451	-4.14518	1.00156
H	-1.67598	-3.39621	1.71340
H	-1.40256	-5.03431	1.12180
H	-3.04959	-4.42889	1.29694
C	5.12151	4.42898	-0.22051
H	6.01723	4.94769	-0.57979
H	5.39496	3.85990	0.67471
H	4.39162	5.18772	0.07533
C	-2.36711	-4.75988	-1.40720
H	-3.41929	-5.04657	-1.30177
H	-1.76812	-5.65758	-1.20645
H	-2.20379	-4.48565	-2.45329
C	1.62952	-1.52016	-3.35046
H	1.23078	-0.60294	-2.90506
H	0.92229	-1.84891	-4.12105
H	2.56352	-1.26679	-3.85974
C	0.99559	-0.10659	5.20040
H	1.53488	0.29036	6.05421
C	-4.16913	-0.77317	-3.10687
H	-5.14659	-0.84232	-2.61651
H	-4.34077	-0.86459	-4.18730
H	-3.77297	0.23097	-2.92508
C	-5.43001	-3.26068	-0.11967
H	-5.52995	-3.46982	-1.19080
H	-6.44321	-3.18857	0.29587
H	-4.95631	-4.13290	0.34238
C	0.03351	0.67387	4.52189
H	-0.12457	1.70739	4.82802
C	-5.54263	4.05352	0.37045
H	-6.51664	4.49043	0.12292
H	-4.85043	4.87504	0.57599
H	-5.65230	3.47063	1.29047
C	2.44595	-3.87553	-2.90678
H	3.44130	-3.68409	-3.32344
H	1.82460	-4.25616	-3.72727
H	2.54843	-4.68167	-2.17243
C	5.54094	-2.80565	-0.80631
H	5.52209	-3.14454	0.23293
H	6.57847	-2.53782	-1.04429
H	5.27989	-3.66144	-1.43941
C	-4.89895	4.00849	-2.05469
H	-4.55025	3.39081	-2.88858
H	-4.17983	4.82155	-1.91771
H	-5.86071	4.45278	-2.33530
C	4.89673	-1.08007	-2.47211
H	4.75453	-1.87275	-3.21361
H	5.93640	-0.74020	-2.56125
H	4.24770	-0.25072	-2.76492
C	1.01150	-1.49678	4.91029
H	1.63070	-2.15806	5.51472
C	3.24593	-2.99603	1.92249
H	2.41400	-2.55996	2.48958
H	4.07711	-2.27786	1.87821
H	3.59613	-3.85006	2.51605
C	1.49928	-4.27601	0.67473
H	0.68963	-3.67225	1.10542
H	1.66834	-5.13767	1.33486
H	1.14600	-4.66069	-0.28736
H	-1.52085	-1.67745	2.69816

TS0-1$_{di}$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.00607Eh

Thermal Gibb's Corr. = 2.017566 Eh

Gibb's Free Energy= -6647.988504 Eh

Lowest Frequency = -78.68 cm^{-1}

Second Frequency = 8.48 cm^{-1}

K	1.04710	-2.64883	-2.04384

Si	4.35417	1.02243	-3.33384
Si	5.75670	-3.61265	0.00458
Al	3.76393	-1.11936	-0.85523
O	3.87821	0.07479	0.86637
N	3.87519	0.73097	-1.66481
N	5.42704	-1.86580	-0.01367
C	5.89056	-1.12494	1.07247
C	3.68123	1.42957	0.59101
C	3.61698	1.74286	-0.77079
C	5.32517	0.71800	2.64303
C	5.05648	-0.12577	1.58472
C	3.32819	3.10153	-1.02917
H	3.16734	3.40476	-2.05439
C	3.62763	3.68664	1.30142
H	3.72267	4.44063	2.07424
C	3.32538	4.06353	-0.01712
C	3.81774	2.34186	1.61925
C	7.11918	-1.23219	1.74479
H	7.84279	-1.95202	1.38594
C	6.55143	0.54341	3.29086
H	6.80891	1.18426	4.12417
C	7.45232	-0.42818	2.84299
C	4.26336	1.77584	2.96845
C	5.28064	-0.58285	-3.81468
H	4.69129	-1.36783	-3.30390
C	5.43966	2.59367	-3.53047
H	4.74098	3.43887	-3.46483
C	2.85917	1.20712	-4.53556
H	3.27264	1.02816	-5.53914
C	7.62322	-4.07256	-0.03605
H	7.99309	-3.84949	0.97455
C	8.81780	-0.63608	3.50429
C	3.08163	5.54126	-0.33193
C	5.01520	-4.40881	1.59319
H	4.96436	-5.48542	1.37005
C	5.28868	-0.92228	-5.30386
H	4.27776	-1.01290	-5.71523
H	5.80254	-1.87630	-5.48135
H	5.81351	-0.16057	-5.89147
C	4.82442	-4.37073	-1.49460
H	3.94279	-3.71087	-1.55304
C	1.81447	0.12754	-4.25486
H	2.24719	-0.87834	-4.33264
H	0.97014	0.18742	-4.95664
H	1.42165	0.24083	-3.23647
C	2.07369	6.13153	0.66429
H	1.12803	5.58254	0.63316
H	1.87042	7.18101	0.42323
H	2.44252	6.09342	1.69277
C	4.80943	2.86541	3.88382
H	5.13013	2.43726	4.83800
H	4.03187	3.60259	4.10454
H	5.66016	3.38223	3.43034
C	2.21275	2.59065	-4.54191
H	1.80961	2.84972	-3.55772
H	1.37380	2.63562	-5.24947
H	2.92112	3.37560	-4.82590
C	8.91716	-2.07659	4.02805
H	8.12757	-2.27998	4.75866
H	9.88615	-2.24227	4.51300
H	8.81663	-2.80719	3.22004
C	3.06381	1.09358	3.65695
H	2.63645	0.31249	3.02383
H	2.28099	1.83068	3.86567
H	3.37956	0.63943	4.60177
C	9.92795	-0.39246	2.47075
H	9.84844	-1.07808	1.62205
H	10.91390	-0.53640	2.92763
H	9.87552	0.62872	2.08013
C	8.44860	-3.25207	-1.02560
H	8.17775	-3.48480	-2.06026
H	9.52128	-3.46052	-0.91702
H	8.29530	-2.17697	-0.88898
C	7.82296	-5.57575	-0.24305
H	7.27156	-6.16874	0.49538
H	8.88290	-5.84817	-0.15669
H	7.49069	-5.89559	-1.23639
C	4.41559	6.29403	-0.21510
H	4.83543	6.19928	0.79098
H	4.27958	7.36057	-0.42965
H	5.14824	5.89001	-0.92137
C	3.58997	-3.90440	1.82349
C	4.32619	-5.79988	-1.28503
H	5.15014	-6.50955	-1.15017
H	3.75542	-6.14321	-2.16048
H	3.67365	-5.88906	-0.41069
C	6.69348	-0.62041	-3.23103
H	7.33053	0.14800	-3.68118
H	7.17815	-1.58541	-3.42683
H	6.68729	-0.47329	-2.14656
C	6.47788	2.78609	-2.42426
H	6.01538	2.78995	-1.43348
H	7.00539	3.74097	-2.55194
H	7.23341	1.99531	-2.43224
C	9.04453	0.31535	4.68059
H	9.01383	1.36319	4.36453
H	10.02999	0.12941	5.12008
H	8.29655	0.17068	5.46715
C	5.55453	-4.24260	-2.82973
H	5.88428	-3.21832	-3.01709
H	4.90095	-4.53586	-3.66418
H	6.43794	-4.88843	-2.87716
C	6.07771	2.65399	-4.92078
H	6.81337	1.85471	-5.06207
H	6.60574	3.60472	-5.07014
H	5.33583	2.56201	-5.72262
C	2.52465	5.75144	-1.74251
H	3.23664	5.44551	-2.51589
H	2.30951	6.81349	-1.89936
H	1.59459	5.19225	-1.89498
C	5.84865	-4.24654	2.86519
H	6.86297	-4.64308	2.74970
H	5.38456	-4.78097	3.70531
H	5.93860	-3.19492	3.15331
H	-2.05696	-4.89574	-3.52540
H	3.58963	-2.83337	2.05499
H	3.11051	-4.42629	2.66289
H	2.95558	-4.03216	0.93837
C	-1.99838	-3.90985	-3.07567
C	-1.83296	-1.31311	-1.90360
C	-1.75117	-2.76457	-3.87252
C	-1.92225	-2.48883	-1.09930
C	-1.64094	-1.50601	-3.30475
C	-2.04482	-3.74638	-1.67974
K	-4.67439	-2.41434	-2.71390
Si	-2.25602	3.07750	-0.41453
Si	-7.38974	0.08992	-1.34365
Al	-4.03189	0.33692	-1.02193
O	-3.77455	-0.75690	0.79910
N	-3.33178	1.76021	0.15562
N	-5.85814	-0.62366	-0.79175
C	-5.87020	-1.62441	0.17394
C	-3.48537	0.10305	1.86890
C	-3.29173	1.43973	1.50839

C	-4.79788	-2.30195	2.29088
C	-4.80276	-1.64097	1.09011
C	-3.07885	2.30445	2.59695
H	-2.94945	3.35765	2.39515
C	-3.23981	0.48562	4.18544
H	-3.21872	0.13403	5.21080
C	-3.03071	1.84525	3.91479
C	-3.48518	-0.41841	3.15281
C	-6.83477	-2.62447	0.37909
H	-7.65724	-2.71008	-0.32187
C	-5.83178	-3.22490	2.49971
H	-5.85405	-3.77896	3.42850
C	-6.82345	-3.42752	1.53195
C	-3.72811	-1.92582	3.31738
C	-2.35986	3.00440	-2.32759
H	-2.44735	1.92364	-2.53680
C	-2.70971	4.82087	0.25950
H	-2.29205	4.83991	1.27584
C	-0.43223	2.75969	0.10245
H	0.14994	3.44273	-0.53573
C	-8.79958	-0.08629	-0.05655
H	-9.10648	-1.14063	-0.08905
C	-7.94612	-4.45008	1.72043
C	-2.73791	2.79509	5.07874
C	-7.95407	-0.73206	-2.99488
H	-8.89206	-0.23365	-3.27458
C	-1.10849	3.51551	-3.04022
H	-0.21161	2.96823	-2.73756
H	-1.20586	3.40476	-4.12835
H	-0.92555	4.57768	-2.84251
C	-6.98296	1.90461	-1.76323
H	-6.01780	1.82207	-2.29521
C	0.00494	1.33701	-0.23823
H	-0.08528	1.12923	-1.31119
H	1.05381	1.17091	0.03068
H	-0.59795	0.60350	0.31258
C	-3.88055	2.72765	6.10227
H	-4.01331	1.71714	6.49945
H	-3.67460	3.39443	6.94706
H	-4.82730	3.03473	5.64657
C	-4.16307	-2.27508	4.73818
H	-4.30766	-3.35370	4.84567
H	-3.38833	-1.98713	5.45375
H	-5.09318	-1.76760	5.00852
C	-0.05028	3.07878	1.55011
H	-0.50543	2.36877	2.24691
H	1.03730	3.02198	1.66830
H	-0.35568	4.08582	1.85449
C	-7.98646	-5.39824	0.51255
H	-7.03885	-5.93799	0.41094
H	-8.78765	-6.13572	0.63284
H	-8.17073	-4.85789	-0.42125
C	-2.41914	-2.67712	3.00684
H	-2.06272	-2.44701	2.00082
H	-1.63767	-2.38165	3.71350
H	-2.57212	-3.75877	3.08057
C	-9.28843	-3.71088	1.83316
H	-9.51209	-3.13922	0.92715
H	-10.10646	-4.42261	1.99108
H	-9.27491	-3.00938	2.67304
C	-8.37811	0.22239	1.38203
H	-8.09704	1.27285	1.50060
H	-9.20818	0.02807	2.07328
H	-7.52968	-0.38597	1.70505
C	-10.02242	0.74539	-0.45474
H	-10.35708	0.54329	-1.47832
H	-10.86707	0.53578	0.21338
H	-9.81633	1.81819	-0.38064
C	-2.59422	4.24859	4.62223
H	-3.50381	4.61186	4.13225
H	-2.40546	4.88829	5.49034
H	-1.75535	4.37415	3.93023
C	-6.92711	-0.45863	-4.10862
C	-7.96708	2.60427	-2.70200
H	-8.94280	2.74626	-2.22648
H	-7.59362	3.60014	-2.97116
H	-8.13520	2.05719	-3.63364
C	-3.62040	3.65777	-2.89421
H	-3.60037	4.74631	-2.77638
H	-3.72181	3.45049	-3.96807
H	-4.52671	3.29362	-2.40243
C	-4.20295	5.11187	0.37665
H	-4.72703	4.32984	0.93467
H	-4.37870	6.06808	0.88667
H	-4.67372	5.18169	-0.60920
C	-7.75546	-5.29465	2.98180
H	-7.79278	-4.68274	3.88866
H	-8.55707	-6.03657	3.05299
H	-6.80158	-5.83199	2.96759
C	-6.75596	2.75634	-0.51399
H	-6.02034	2.31826	0.16783
H	-6.38866	3.75222	-0.78681
H	-7.69110	2.90061	0.03742
C	-1.98511	5.92164	-0.51997
H	-2.36717	6.01096	-1.54233
H	-2.12284	6.89849	-0.03909
H	-0.90724	5.74244	-0.58826
C	-1.42114	2.36848	5.74654
H	-0.59459	2.40083	5.02904
H	-1.17933	3.03871	6.57930
H	-1.48053	1.34950	6.14034
C	-8.27647	-2.22092	-2.86331
H	-9.08757	-2.40144	-2.15017
H	-8.58515	-2.65278	-3.82438
H	-7.42339	-2.81254	-2.50360
H	-1.48518	-0.39699	-1.45292
H	-5.90706	-0.29383	-3.72826
H	-6.89951	-1.27228	-4.84816
H	-7.16274	0.45352	-4.66225
H	-2.15388	-4.61891	-1.03899
H	-1.95242	-2.38383	-0.02107
H	-1.62477	-2.87845	-4.94700
H	-1.45103	-0.63951	-3.93236

INT1$_{mono}$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -3441.016075 Eh

Thermal Gibb's Corr. = 1.041226 Eh

Gibb's Free Energy= -3439.974849 Eh

Lowest Frequency = 12.9407 cm^{-1}

Second Frequency = 20.3413 cm^{-1}

Si	3.16811	2.11813	-0.07829
Si	-2.71081	2.49745	-0.42240
Al	0.12106	0.83678	0.44044
K	-1.44573	-2.82161	2.10263
O	0.02941	-0.53834	-1.00850
N	1.94470	0.84072	-0.20754
N	-1.70703	1.05008	-0.22177
C	-1.18440	-1.16112	-0.87537
C	2.25580	-0.48112	-0.52045
C	-1.32975	-2.51353	-1.09017
C	-2.62841	-3.00840	-0.88811

H	-2.83426	-4.05829	-1.06960
C	-3.67855	-2.15623	-0.49791
C	1.18750	-1.28376	-0.94358
C	-3.43689	-0.79404	-0.27338
H	-4.23346	-0.15157	0.07658
C	-2.15761	-0.23879	-0.44837
C	2.41825	-3.27349	-1.00864
H	2.50088	-4.34180	-1.17629
C	3.55836	-2.54721	-0.63045
C	3.47011	-1.17103	-0.38745
H	4.33967	-0.62919	-0.04283
C	1.18041	-2.64144	-1.16649
C	-5.07600	-2.75407	-0.29931
C	-0.12622	-3.32166	-1.59886
C	4.43915	1.78981	1.31271
H	5.12303	1.02815	0.90870
C	-0.17746	-4.76280	-1.08675
H	-1.10914	-5.25296	-1.38133
H	-0.08370	-4.80893	0.00374
H	0.63919	-5.35181	-1.51127
C	0.07864	0.29092	2.33919
C	2.11547	3.69168	0.19523
H	1.30379	3.54947	-0.53354
C	4.08458	2.34144	-1.74607
H	4.59542	3.31163	-1.64585
C	-1.43484	3.84532	-0.87017
H	-0.67675	3.71606	-0.07914
C	-4.03005	2.18574	-1.77790
H	-4.78311	1.53518	-1.30988
C	-1.32482	0.01490	2.84804
H	-2.18262	0.49375	2.38529
C	0.86196	-1.00568	2.51454
H	1.68870	-1.26402	1.85690
C	4.88488	-3.29384	-0.46281
C	-0.18522	-3.33323	-3.13920
H	0.66958	-3.88255	-3.54626
H	-0.15534	-2.31383	-3.53336
H	-1.10998	-3.80737	-3.48427
C	-5.54181	-3.40575	-1.61009
H	-6.54513	-3.82886	-1.49009
H	-4.87376	-4.21255	-1.92518
H	-5.57560	-2.66627	-2.41600
C	-3.59949	3.06959	1.17156
H	-4.12437	3.99019	0.87032
C	3.07774	2.44820	-2.89277
H	2.50456	1.51974	-2.99214
H	3.58224	2.63329	-3.84973
H	2.35640	3.25757	-2.73862
C	3.81170	1.22174	2.58547
H	3.14185	1.94471	3.06204
H	4.58540	0.96751	3.32124
H	3.21887	0.32237	2.39503
C	-6.11027	-1.70000	0.10236
H	-6.20690	-0.92019	-0.65998
H	-5.85891	-1.22023	1.05406
H	-7.09000	-2.17371	0.21890
C	6.02327	-2.37003	-0.02360
H	5.81742	-1.90535	0.94636
H	6.20743	-1.57616	-0.75502
H	6.94643	-2.94968	0.07623
C	1.48946	3.79583	1.58665
H	0.97499	2.88119	1.91044
H	0.75932	4.61462	1.63145
H	2.24998	4.00011	2.34773
C	-5.02405	-3.81675	0.80990
H	-6.00933	-4.27307	0.95382
H	-4.72827	-3.36472	1.76474
H	-4.31924	-4.61968	0.57014
C	2.81068	5.00260	-0.17506
H	3.66993	5.20449	0.47304
H	2.11939	5.84837	-0.06686
H	3.16913	5.00374	-1.20878
C	-0.75100	3.60308	-2.21535
H	-0.37614	2.57843	-2.31103
H	0.09688	4.28634	-2.35630
H	-1.44396	3.78276	-3.04453
C	-0.40754	-1.46636	4.55602
H	-0.50546	-1.98537	5.50435
C	5.15526	1.29695	-2.06564
H	5.89015	1.19352	-1.25966
H	5.70520	1.57190	-2.97495
H	4.71088	0.31199	-2.24045
C	5.28289	3.03273	1.60577
H	5.74907	3.44431	0.70316
H	6.08698	2.80348	2.31625
H	4.67655	3.82644	2.05626
C	0.70005	-1.69230	3.70297
H	1.40079	-2.49649	3.94487
C	4.72049	-4.38755	0.60333
H	5.66284	-4.92903	0.74296
H	3.95493	-5.11693	0.32244
H	4.43013	-3.94935	1.56357
C	-1.93574	5.28596	-0.76539
H	-2.68418	5.50692	-1.53328
H	-1.10956	5.99399	-0.90894
H	-2.38914	5.50229	0.20632
C	-4.73829	3.48607	-2.16798
H	-5.13011	4.02837	-1.30088
H	-5.58247	3.28558	-2.83971
H	-4.05996	4.16134	-2.70100
C	5.27820	-3.93395	-1.80254
H	5.40201	-3.16881	-2.57559
H	4.52045	-4.64186	-2.15132
H	6.22472	-4.47704	-1.70316
C	-3.50735	1.46138	-3.01948
H	-2.75439	2.05629	-3.54523
H	-4.32443	1.27403	-3.72837
H	-3.05411	0.49708	-2.77503
C	-1.46421	-0.67698	4.03175
H	-2.44335	-0.70782	4.51939
C	-4.65447	2.08483	1.67770
H	-4.19540	1.14447	2.00286
H	-5.40441	1.84905	0.91376
H	-5.18987	2.49363	2.54385
C	-2.61441	3.43392	2.28626
H	-2.05501	2.55721	2.62972
H	-3.14407	3.83808	3.15822
H	-1.88801	4.18946	1.96958
H	0.55649	1.08247	2.96783

INT1$_{di}$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.019806Eh

Thermal Gibb's Corr. = 2.014272 Eh

Gibb's Free Energy= -6648.005534 Eh

Lowest Frequency = 4.2331 cm^{-1}

Second Frequency = 7.8963 cm^{-1}

K	-0.35058	-1.99984	-1.38517
Si	-3.92403	-1.13639	3.24098
Si	-5.28382	-3.08529	-2.07779
Al	-3.38312	-1.30658	-0.04099
O	-3.85887	0.65156	-0.70088

N	-3.59172	-0.31217	1.71764
N	-5.10390	-1.64283	-1.06067
C	-5.77930	-0.48679	-1.44124
C	-3.71959	1.59575	0.31687
C	-3.51085	1.05185	1.59061
C	-5.60038	1.98892	-1.60983
C	-5.11386	0.73627	-1.29784
C	-3.30150	2.02443	2.59646
H	-3.05499	1.68323	3.59236
C	-3.91141	3.82420	1.09223
H	-4.15806	4.86772	0.93160
C	-3.50247	3.38669	2.36259
C	-4.04960	2.90977	0.04715
C	-7.07957	-0.35839	-1.95908
H	-7.68208	-1.25014	-2.06569
C	-6.88949	2.04920	-2.14761
H	-7.31584	3.01000	-2.40544
C	-7.63226	0.87699	-2.32153
C	-4.67491	3.17978	-1.32507
C	-4.78487	-2.75671	2.70362
H	-4.18246	-3.06882	1.83010
C	-5.00916	-0.10049	4.44487
H	-4.33141	0.64311	4.88731
C	-2.31060	-1.60712	4.16806
H	-2.61717	-2.17384	5.06036
C	-7.09422	-3.71213	-2.27553
H	-7.57260	-2.98425	-2.94598
C	-9.05499	0.89320	-2.88753
C	-3.37059	4.41609	3.48853
C	-4.65269	-2.72169	-3.86431
H	-4.59048	-3.70580	-4.35368
C	-4.73932	-3.90022	3.71680
H	-3.72332	-4.12185	4.05737
H	-5.14851	-4.82064	3.27962
H	-5.33894	-3.67338	4.60467
C	-4.15894	-4.45028	-1.33159
H	-3.31317	-3.86795	-0.92921
C	-1.42938	-2.50299	3.30029
H	-1.93464	-3.42394	2.99173
H	-0.51023	-2.78855	3.83073
H	-1.14160	-1.97961	2.38021
C	-2.32964	5.47357	3.09522
H	-1.34913	5.00989	2.95003
H	-2.23465	6.23402	3.87907
H	-2.60134	5.97944	2.16411
C	-5.43426	4.50186	-1.34293
H	-5.87869	4.67427	-2.32756
H	-4.75468	5.33585	-1.14380
H	-6.23071	4.51607	-0.59354
C	-1.51115	-0.38690	4.61925
H	-1.20668	0.21031	3.75297
H	-0.59419	-0.68245	5.14909
H	-2.07887	0.26724	5.29056
C	-9.10415	0.04370	-4.16645
H	-8.40986	0.43302	-4.91818
H	-10.11389	0.05021	-4.59323
H	-8.82986	-0.99683	-3.96922
C	-3.57708	3.21848	-2.40580
H	-2.98460	2.29985	-2.39935
H	-2.90648	4.06646	-2.23008
H	-4.02717	3.33129	-3.39749
C	-10.02468	0.30779	-1.84984
H	-9.76686	-0.72363	-1.59230
H	-11.04964	0.31124	-2.23875
H	-10.00463	0.89630	-0.92713
C	-7.89799	-3.74514	-0.97634
H	-7.51926	-4.51199	-0.29341
H	-8.95392	-3.97739	-1.16973
H	-7.85220	-2.79095	-0.44248
C	-7.14895	-5.06060	-2.99734
H	-6.61652	-5.03822	-3.95467
H	-8.18651	-5.35288	-3.20596
H	-6.70716	-5.86004	-2.39315
C	-4.73144	5.09416	3.71060
H	-5.07633	5.61524	2.81304
H	-4.66603	5.82800	4.52244
H	-5.49026	4.35164	3.97754
C	-3.24714	-2.12178	-3.83763
C	-3.60142	-5.44283	-2.35272
H	-4.39395	-6.02732	-2.83330
H	-2.92786	-6.16071	-1.86443
H	-3.03449	-4.95102	-3.14988
C	-6.21483	-2.51719	2.21949
H	-6.86472	-2.21601	3.04827
H	-6.64742	-3.43230	1.79561
H	-6.25952	-1.74644	1.44453
C	-6.15163	0.66296	3.77263
H	-5.79251	1.31757	2.97458
H	-6.68353	1.28626	4.50451
H	-6.88644	-0.01839	3.33395
C	-9.52584	2.30638	-3.23631
H	-9.54238	2.95570	-2.35484
H	-10.54310	2.26711	-3.63963
H	-8.88488	2.77010	-3.99348
C	-4.78391	-5.19562	-0.15255
H	-5.19614	-4.51178	0.59298
H	-4.03722	-5.82308	0.35292
H	-5.59387	-5.85913	-0.47563
C	-5.53189	-0.96123	5.59805
H	-6.26474	-1.69564	5.24689
H	-6.03607	-0.34188	6.35146
H	-4.73226	-1.51117	6.10679
C	-2.93881	3.78667	4.81491
H	-3.67822	3.06458	5.17706
H	-2.83851	4.56735	5.57636
H	-1.97453	3.27641	4.73015
C	-5.58003	-1.84377	-4.70647
H	-6.58427	-2.27009	-4.79763
H	-5.18429	-1.72200	-5.72426
H	-5.68911	-0.84483	-4.27318
H	1.42488	-2.38823	-4.36569
H	-3.24492	-1.16021	-3.31056
H	-2.86209	-1.95158	-4.85283
H	-2.53902	-2.77934	-3.31919
C	1.77018	-1.92930	-3.44528
C	2.54541	-0.71066	-0.88620
C	2.50260	-2.66990	-2.47264
C	2.23719	0.10242	-2.13671
C	2.99803	-2.09615	-1.32265
C	1.75290	-0.51364	-3.26828
K	4.64824	-0.95585	-3.45899
Si	2.00425	3.05076	1.08888
Si	4.49532	-2.17184	2.74580
Al	3.67768	0.19836	0.46459
O	5.51019	0.86043	-0.00820
N	3.31371	2.08006	0.35456
N	4.76831	-1.16275	1.30321
C	5.74496	-1.40342	0.34751
C	5.27237	1.82573	-0.97529
C	4.07037	2.51255	-0.72951
C	7.04289	-0.27350	-1.46710
C	6.16283	-0.29154	-0.40718
C	3.78283	3.49871	-1.68253
H	2.86822	4.06892	-1.57910

C	5.75878	2.94661	-2.98632
H	6.38727	3.11655	-3.85114
C	4.60897	3.72366	-2.79370
C	6.11827	1.96365	-2.05294
C	6.33612	-2.61046	-0.04945
H	6.03989	-3.52174	0.45687
C	7.59707	-1.51621	-1.81842
H	8.31544	-1.56997	-2.62707
C	7.25237	-2.67704	-1.10913
C	7.37782	1.08837	-2.09015
C	1.77339	2.22384	2.79339
H	1.74910	1.14033	2.56463
C	2.57085	4.87915	1.17920
H	2.44276	5.26957	0.15934
C	0.32072	2.96149	0.19444
H	-0.36606	3.48791	0.87560
C	6.10391	-3.07268	3.26873
H	6.22847	-3.88081	2.53397
C	7.83126	-4.04792	-1.47005
C	4.19680	4.81502	-3.78491
C	3.13913	-3.49365	2.49595
H	2.91994	-3.84773	3.51484
C	0.45287	2.56597	3.48259
H	-0.42414	2.34185	2.86873
H	0.35034	2.00564	4.41988
H	0.41072	3.62959	3.73993
C	3.87138	-0.91230	4.04005
H	3.24753	-0.21582	3.45489
C	-0.17792	1.52184	0.05794
H	-0.18136	0.97592	1.00769
H	-1.20780	1.50364	-0.31334
H	0.44702	0.97652	-0.65774
C	5.19399	4.96440	-4.93533
H	5.27120	4.04692	-5.52891
H	4.86146	5.76189	-5.60673
H	6.19343	5.22982	-4.57509
C	8.45417	1.75586	-1.20898
H	9.36188	1.14444	-1.18876
H	8.70088	2.74744	-1.60098
H	8.09686	1.87330	-0.18255
C	0.24997	3.66641	-1.15918
H	0.84631	3.13605	-1.91045
H	-0.78232	3.68269	-1.52564
H	0.59718	4.70553	-1.11568
C	6.68656	-4.99495	-1.86379
H	6.14088	-4.60898	-2.73231
H	7.08181	-5.98262	-2.12424
H	5.96631	-5.12689	-1.05149
C	7.92629	0.94741	-3.50849
H	7.20062	0.50165	-4.19908
H	8.20368	1.92473	-3.91086
H	8.82737	0.32903	-3.51673
C	8.57148	-4.61912	-0.25067
H	7.90512	-4.73998	0.60830
H	8.99398	-5.60135	-0.48813
H	9.38891	-3.95763	0.05271
C	7.38463	-2.23761	3.24572
H	7.36038	-1.43871	3.99145
H	8.25504	-2.86651	3.47290
H	7.55789	-1.77519	2.27017
C	5.90711	-3.74742	4.63057
H	5.02460	-4.39600	4.65068
H	6.77540	-4.36668	4.88751
H	5.79152	-3.00979	5.43190
C	4.11053	6.15988	-3.04702
H	5.07748	6.42687	-2.60906
H	3.81582	6.95511	-3.74026
H	3.37436	6.13224	-2.23837
C	1.86101	-2.87885	1.92389
C	2.98467	-1.49347	5.14156
H	3.52390	-2.22874	5.74899
H	2.64451	-0.70187	5.82115
H	2.09228	-1.98490	4.74263
C	2.94569	2.48650	3.73561
H	2.96607	3.53825	4.04052
H	2.85216	1.89092	4.65157
H	3.91310	2.25614	3.27782
C	4.04016	5.07081	1.55588
H	4.71002	4.53761	0.87544
H	4.31015	6.13415	1.52337
H	4.24763	4.71516	2.56952
C	8.81658	-3.97698	-2.63794
H	9.67245	-3.33354	-2.40964
H	9.20331	-4.97766	-2.85293
H	8.33957	-3.60691	-3.55245
C	5.02619	-0.10278	4.63169
H	5.65568	0.33970	3.85249
H	4.65739	0.71128	5.26555
H	5.66483	-0.73214	5.26020
C	1.65169	5.70506	2.08286
H	1.74053	5.40258	3.13201
H	1.91165	6.76985	2.03417
H	0.59789	5.61252	1.80051
C	2.82345	4.46878	-4.38075
H	2.04870	4.40632	-3.61172
H	2.51765	5.23515	-5.10122
H	2.85628	3.50533	-4.90075
C	3.57205	-4.70282	1.66695
H	4.44257	-5.21213	2.09407
H	2.76290	-5.44127	1.60107
H	3.81908	-4.41384	0.63875
H	1.61209	-0.79033	-0.25352
H	2.01691	-2.60140	0.87667
H	1.02718	-3.59067	1.95785
H	1.53486	-1.98625	2.46985
H	1.42522	0.11494	-4.09929
H	2.30453	1.18624	-2.10936
H	2.76631	-3.70816	-2.68965
H	3.66485	-2.66922	-0.68649

TS1-2$_{mono}$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -3441.01108 Eh

Thermal Gibb's Corr. = 1.038791 Eh

Gibb's Free Energy= -3439.972289 Eh

Lowest Frequency = -351.5155 cm^{-1}

Second Frequency = 12.5542 cm^{-1}

Si	2.99573	2.30407	-0.25360
Si	-2.89502	2.37493	-0.17167
Al	0.03111	0.78713	0.33576
K	-0.40075	-3.11275	1.90662
O	0.04418	-0.44023	-1.33390
N	1.85862	0.94879	-0.17901
N	-1.77319	1.00785	-0.27196
C	-1.14396	-1.11921	-1.12706
C	2.20370	-0.36374	-0.49812
C	-1.22368	-2.47844	-1.36469
C	-2.45483	-3.07860	-1.07783
H	-2.58822	-4.14092	-1.25465
C	-3.52646	-2.31775	-0.57717
C	1.20661	-1.15431	-1.08703
C	-3.36005	-0.95098	-0.33206

H	-4.16548	-0.37917	0.10895
C	-2.14125	-0.29622	-0.57912
C	2.45866	-3.14783	-1.00181
H	2.56719	-4.21370	-1.17281
C	3.53391	-2.41944	-0.46420
C	3.39591	-1.05089	-0.21523
H	4.20128	-0.50261	0.25383
C	1.25578	-2.51467	-1.32496
C	-4.84552	-3.02553	-0.25402
C	0.01634	-3.16231	-1.95378
C	4.45658	2.12217	0.96774
H	5.08705	1.32710	0.54158
C	-0.00716	-4.67240	-1.73395
H	-0.88987	-5.11771	-2.20029
H	-0.01323	-4.93781	-0.67030
H	0.86915	-5.14066	-2.18958
C	-0.04611	-0.06905	2.05589
C	1.90959	3.83962	0.07551
H	0.99191	3.59410	-0.47919
C	3.68493	2.43102	-2.03570
H	4.16515	3.41962	-2.09388
C	-1.75690	3.87390	-0.49078
H	-0.91641	3.67126	0.19487
C	-4.28580	2.15123	-1.47016
H	-4.96090	1.39206	-1.04904
C	-1.33520	-0.54308	2.64727
H	-2.26394	-0.38712	2.10418
C	1.10806	-0.80861	2.65288
H	2.05196	-0.86150	2.11506
C	4.82815	-3.15995	-0.11768
C	0.04189	-2.88206	-3.47085
H	0.93412	-3.32701	-3.92253
H	0.05910	-1.80674	-3.66646
H	-0.84776	-3.30369	-3.94940
C	-5.38023	-3.72039	-1.51482
H	-6.32479	-4.23082	-1.29686
H	-4.67870	-4.46658	-1.89923
H	-5.56085	-2.99074	-2.31025
C	-3.69005	2.63728	1.54755
H	-4.23281	3.59002	1.43788
C	2.53580	2.39634	-3.04537
H	2.00276	1.44038	-2.99433
H	2.90361	2.51895	-4.07215
H	1.79829	3.18555	-2.86269
C	4.03894	1.68748	2.37240
H	3.48719	2.48004	2.88706
H	4.91723	1.45463	2.98826
H	3.38713	0.80923	2.36201
C	-5.91933	-2.05812	0.24860
H	-6.14140	-1.28288	-0.49212
H	-5.62416	-1.56733	1.18158
H	-6.84565	-2.60785	0.44285
C	5.90335	-2.22398	0.43902
H	5.58567	-1.74698	1.37197
H	6.16528	-1.43874	-0.27791
H	6.81182	-2.79596	0.65256
C	1.53066	4.04529	1.54290
H	1.12698	3.13716	2.00798
H	0.77026	4.83153	1.64246
H	2.39682	4.35887	2.13556
C	-4.59364	-4.07176	0.84354
H	-5.52208	-4.59389	1.09957
H	-4.21479	-3.59005	1.75229
H	-3.86632	-4.82491	0.52265
C	2.45299	5.13687	-0.52561
H	3.40016	5.43340	-0.06198
H	1.74493	5.96033	-0.36570
H	2.62444	5.05653	-1.60327
C	-1.20085	3.90454	-1.91431
H	-0.79692	2.93309	-2.21899
H	-0.40025	4.64980	-2.01191
H	-1.98059	4.17933	-2.63337
C	-0.19643	-1.37993	4.64399
H	-0.24056	-1.76860	5.65567
C	4.74355	1.38246	-2.38336
H	5.59704	1.41262	-1.69732
H	5.13331	1.54332	-3.39698
H	4.32926	0.36932	-2.35168
C	5.30961	3.39262	1.00452
H	5.63875	3.70270	0.00625
H	6.20825	3.24699	1.61713
H	4.75528	4.22926	1.44438
C	1.02550	-1.31020	3.93570
H	1.92279	-1.74113	4.38587
C	4.52617	-4.22830	0.94451
H	5.43969	-4.76890	1.21580
H	3.79920	-4.96250	0.58305
H	4.12060	-3.76540	1.85058
C	-2.32821	5.23501	-0.09516
H	-3.18556	5.50968	-0.71876
H	-1.57373	6.02229	-0.22072
H	-2.65779	5.26028	0.94759
C	-5.09901	3.43812	-1.63318
H	-5.46987	3.82360	-0.67722
H	-5.96912	3.27356	-2.28129
H	-4.49954	4.22907	-2.09755
C	5.38675	-3.83113	-1.38112
H	5.60550	-3.08439	-2.15094
H	4.68148	-4.55176	-1.80554
H	6.31413	-4.36680	-1.14998
C	-3.80437	1.63252	-2.82564
H	-3.12897	2.34298	-3.31181
H	-4.65382	1.47648	-3.50338
H	-3.27256	0.68149	-2.73542
C	-1.36971	-1.04620	3.93358
H	-2.34133	-1.26490	4.38278
C	-4.70944	1.57434	1.95749
H	-4.21943	0.61168	2.13941
H	-5.48969	1.42388	1.20250
H	-5.21087	1.85402	2.89262
C	-2.63292	2.81307	2.64099
H	-2.08773	1.87820	2.81318
H	-3.09934	3.09219	3.59441
H	-1.90141	3.59073	2.39751
H	0.07611	1.10842	2.35090

INT1-2$_{di}$

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.017739 Eh

Thermal Gibb's Corr. = 2.014402 Eh

Gibb's Free Energy= -6648.003337 Eh

Lowest Frequency = -271.9576 cm-1

Second Frequency = 8.1406 cm-1

K	-0.14462	-1.93634	-1.02922
Si	-3.84849	-1.25394	3.18197
Si	-5.15545	-3.01575	-2.22203
Al	-3.32707	-1.28128	-0.10249
O	-3.86713	0.69200	-0.67804
N	-3.54620	-0.35774	1.69521
N	-5.03649	-1.62770	-1.12180
C	-5.75547	-0.48087	-1.44629
C	-3.75005	1.59915	0.37549

```
C  -3.51367  1.01198  1.62494
C  -5.66462  2.00413 -1.51354
C  -5.13096  0.75762 -1.25892
C  -3.32849  1.94842  2.66885
H  -3.06532  1.57466  3.64897
C  -4.00623  3.78682  1.24249
H  -4.28594  4.82784  1.12573
C  -3.57211  3.31238  2.49106
C  -4.12577  2.91109  0.16223
C  -7.06544 -0.37801 -1.94448
H  -7.63748 -1.28591 -2.08054
C  -6.96129  2.04054 -2.03508
H  -7.42404  2.99546 -2.24838
C  -7.66496  0.85097 -2.24991
C  -4.77710  3.21422 -1.19104
C  -4.62260 -2.89375  2.57314
H  -4.01654 -3.12903  1.67805
C  -4.99128 -0.31312  4.40897
H  -4.35504  0.45115  4.87671
C  -2.22800 -1.69269  4.11503
H  -2.52164 -2.37026  4.93097
C  -6.93692 -3.71134 -2.44367
H  -7.45369 -2.96712 -3.06600
C  -9.09355  0.84012 -2.80101
C  -3.45494  4.30092  3.65460
C  -4.55000 -2.51546 -3.98255
H  -4.40403 -3.46652 -4.51720
C  -4.49533 -4.07936  3.52903
H  -3.45854 -4.27468  3.82007
H  -4.88435 -4.99472  3.06377
H  -5.06848 -3.91841  4.44859
C  -3.96173 -4.36496 -1.55992
H  -3.14528 -3.76295 -1.12750
C  -1.26221 -2.43431  3.19387
H  -1.70627 -3.32771  2.74216
H  -0.35703 -2.74631  3.73310
H  -0.95730 -1.78226  2.36597
C  -2.43677  5.39266  3.29576
H  -1.44744  4.95524  3.12946
H  -2.35355  6.12582  4.10651
H  -2.72385  5.92639  2.38498
C  -5.58099  4.50902 -1.14659
H  -6.04440  4.70490 -2.11799
H  -4.92755  5.35743 -0.92248
H  -6.36715  4.46606 -0.38751
C  -1.52815 -0.48009  4.72386
H  -1.22969  0.22359  3.93960
H  -0.61431 -0.77299  5.26005
H  -2.16309  0.06249  5.43291
C  -9.12585  0.04514 -4.11510
H  -8.45508  0.49228 -4.85593
H  -10.13994  0.03222 -4.53133
H  -8.81063 -0.99182 -3.96616
C  -3.69617  3.33300 -2.28274
H  -3.08057  2.43068 -2.32658
H  -3.04579  4.19008 -2.07701
H  -4.16336  3.47812 -3.26225
C  -10.03037  0.17587 -1.78075
H  -9.73309 -0.85565 -1.57048
H  -11.05886  0.15881 -2.15982
H  -10.02170  0.72461 -0.83366
C  -7.72527 -3.85778 -1.14304
H  -7.30444 -4.64405 -0.50858
H  -8.77125 -4.12767 -1.34163
H  -7.71801 -2.93486 -0.55494
C  -6.93515 -5.01542 -3.24470
H  -6.41446 -4.90995 -4.20306
H  -7.95955 -5.34509 -3.46264
H  -6.44866 -5.82710 -2.69329
C  -4.82717  4.94354  3.90938
H  -5.18711  5.49294  3.03493
H  -4.77104  5.64619  4.74899
H  -5.57031  4.17681  4.15074
C  -3.19868 -1.80407 -3.90930
C  -3.35664 -5.26156 -2.64046
H  -4.11883 -5.84877 -3.16504
H  -2.65202 -5.97879 -2.19655
H  -2.80974 -4.68969 -3.39722
C  -6.07024 -2.71453  2.11591
H  -6.72638 -2.48929  2.96369
H  -6.45469 -3.63250  1.65343
H  -6.16801 -1.91319  1.37758
C  -6.16431  0.41328  3.74877
H  -5.82927  1.10957  2.97570
H  -6.73262  0.98687  4.49370
H  -6.86070 -0.28833  3.28054
C  -9.61840  2.24900 -3.08359
H  -9.64757  2.85883 -2.17467
H  -10.63827  2.19040 -3.47784
H  -9.00332  2.76754 -3.82654
C  -4.53898 -5.20761 -0.42319
H  -4.97445 -4.58854  0.36498
H  -3.75835 -5.82772  0.03870
H  -5.32045 -5.88905 -0.77772
C  -5.47405 -1.23345  5.53318
H  -6.15853 -2.00109  5.15622
H  -6.02068 -0.66541  6.29734
H  -4.64724 -1.74793  6.03585
C  -3.00324  3.63074  4.95410
H  -3.72408  2.87787  5.29016
H  -2.91809  4.38352  5.74490
H  -2.02758  3.14714  4.84692
C  -5.54218 -1.67860 -4.79201
H  -6.50437 -2.18534 -4.92014
H  -5.14829 -1.46962 -5.79629
H  -5.74198 -0.71668 -4.30986
H   1.17989 -2.28479 -4.37335
H  -3.28676 -0.85609 -3.36593
H  -2.80781 -1.58120 -4.91211
H  -2.44664 -2.40249 -3.38194
C   1.62841 -1.83880 -3.49309
C   2.80282 -0.63331 -1.07315
C   2.47926 -2.57819 -2.63684
C   2.10959  0.14962 -2.13521
C   3.09353 -2.02121 -1.53130
C   1.51355 -0.45114 -3.22522
K   4.63056 -0.41916 -3.37576
Si  1.90616  2.98846  1.15135
Si  4.43044 -2.30658  2.60416
Al  3.66206  0.19019  0.45822
O   5.53913  0.97394  0.14055
N   3.20638  2.03404  0.38216
N   4.72095 -1.18891  1.25000
C   5.75810 -1.33118  0.33500
C   5.25162  1.91447 -0.83973
C   3.98508  2.50422 -0.66819
C   7.12859 -0.07041 -1.32295
C   6.20799 -0.15838 -0.29912
C   3.65443  3.43906 -1.65811
H   2.68578  3.92088 -1.60659
C   5.73001  3.05042 -2.85623
H   6.38519  3.26247 -3.69184
C   4.50708  3.72352 -2.73459
C   6.12579  2.11517 -1.88792
```

C	6.37242	-2.50206	-0.12660
H	6.05418	-3.44924	0.29253
C	7.70885	-1.27830	-1.74175
H	8.45425	-1.26674	-2.52720
C	7.34290	-2.48932	-1.13937
C	7.44178	1.32973	-1.86194
C	1.72165	2.18191	2.86816
H	1.67764	1.10041	2.64192
C	2.44762	4.82570	1.19282
H	2.31930	5.18565	0.16174
C	0.20814	2.85496	0.29078
H	-0.48831	3.36992	0.96998
C	6.07525	-3.12463	3.15298
H	6.30420	-3.85557	2.36483
C	7.95126	-3.82682	-1.56842
C	4.04094	4.75160	-3.76848
C	3.20613	-3.72019	2.19134
H	2.96601	-4.15225	3.17472
C	0.42685	2.54649	3.59382
H	-0.46952	2.33528	3.00334
H	0.34114	1.98672	4.53334
H	0.40559	3.61015	3.85377
C	3.64389	-1.20066	3.94973
H	3.01399	-0.49103	3.38698
C	-0.24215	1.39750	0.18806
H	-0.31989	0.90664	1.16343
H	-1.23089	1.32768	-0.27722
H	0.46080	0.83259	-0.43526
C	5.07329	4.97401	-4.87511
H	5.26625	4.05711	-5.44308
H	4.69961	5.72279	-5.58002
H	6.02455	5.34044	-4.47547
C	8.40227	2.02464	-0.87524
H	9.34140	1.46690	-0.80521
H	8.61816	3.04299	-1.21300
H	7.96149	2.08121	0.12324
C	0.10081	3.53848	-1.07146
H	0.69444	3.01294	-1.82836
H	-0.93709	3.52850	-1.42087
H	0.42758	4.58480	-1.04691
C	6.83667	-4.75690	-2.07272
H	6.31936	-4.31676	-2.93256
H	7.25657	-5.71886	-2.38561
H	6.08852	-4.95582	-1.30013
C	8.10388	1.27836	-3.23588
H	7.47186	0.79605	-3.99116
H	8.33512	2.28655	-3.58864
H	9.04765	0.72916	-3.18807
C	8.64705	-4.47164	-0.35956
H	7.94602	-4.65602	0.45978
H	9.09146	-5.43172	-0.64341
H	9.44257	-3.82418	0.02225
C	7.28397	-2.19456	3.26417
H	7.16423	-1.46740	4.07147
H	8.19176	-2.77232	3.48045
H	7.46055	-1.63742	2.33992
C	5.86830	-3.92457	4.44341
H	5.04776	-4.64542	4.35937
H	6.77365	-4.48747	4.70232
H	5.64461	-3.27016	5.29264
C	3.79142	6.09528	-3.06641
H	4.70545	6.46031	-2.58764
H	3.45913	6.84641	-3.79103
H	3.02067	6.01222	-2.29464
C	1.90917	-3.18789	1.58191
C	2.73501	-1.93425	4.93630
H	3.28765	-2.68366	5.51411
H	2.29873	-1.22989	5.65560
H	1.90535	-2.44520	4.43985
C	2.92661	2.43242	3.77105
H	2.97889	3.48652	4.06446
H	2.84922	1.84859	4.69528
H	3.87438	2.17579	3.28652
C	3.91068	5.05436	1.57329
H	4.59617	4.51550	0.91311
H	4.16176	6.12117	1.51286
H	4.11712	4.73096	2.59783
C	8.98299	-3.66612	-2.68617
H	9.82038	-3.03172	-2.37805
H	9.39093	-4.64581	-2.95266
H	8.53940	-3.23800	-3.59199
C	4.70599	-0.38796	4.69238
H	5.34793	0.17368	4.00616
H	4.24530	0.32921	5.38051
H	5.34827	-1.03833	5.29512
C	1.51032	5.65817	2.07172
H	1.60972	5.38974	3.12917
H	1.74478	6.72684	1.98974
H	0.45802	5.53157	1.79652
C	2.73593	4.26438	-4.41747
H	1.93697	4.13539	-3.68204
H	2.38916	4.98715	-5.16380
H	2.88565	3.30261	-4.92074
C	3.78029	-4.83790	1.32142
H	4.68180	-5.28570	1.75284
H	3.04861	-5.64498	1.18792
H	4.03055	-4.47088	0.31912
H	2.04305	-0.69283	-0.06904
H	2.10534	-2.84707	0.55826
H	1.14120	-3.97193	1.53741
H	1.48619	-2.35207	2.14713
H	0.98248	0.18213	-3.93668
H	2.05926	1.23030	-2.03746
H	2.71457	-3.61315	-2.88989
H	3.81321	-2.61568	-0.97550

compound 2

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -3441.087753 Eh

Thermal Gibb's Corr. = 1.040838 Eh

Gibb's Free Energy= -3440.046915 Eh

Lowest Frequency = 16.7234 cm^{-1}

Second Frequency = 20.8797 cm^{-1}

Si	2.96523	2.30095	-0.22887
Si	-2.96625	2.34451	0.01939
Al	0.00590	1.21716	0.89905
K	-0.08882	-3.06200	1.14639
O	0.05062	-0.19191	-1.38458
N	1.80990	1.01287	0.17598
N	-1.77159	1.02970	0.07581
C	-1.10183	-0.90135	-1.16282
C	2.10581	-0.26734	-0.27152
C	-1.18017	-2.22379	-1.58139
C	-2.34225	-2.93430	-1.26723
H	-2.44719	-3.96612	-1.58812
C	-3.38328	-2.31055	-0.55529
C	1.17053	-0.92300	-1.08469
C	-3.23342	-0.98656	-0.13751
H	-4.00438	-0.52339	0.46426
C	-2.07250	-0.22877	-0.40189
C	2.37734	-2.97708	-1.10295
H	2.48491	-4.01137	-1.41552

C	3.37902	-2.37368	-0.32025
C	3.22768	-1.04475	0.08124
H	3.96566	-0.59041	0.72880
C	1.25187	-2.24833	-1.49609
C	-4.63660	-3.12041	-0.21252
C	0.05739	-2.76843	-2.30057
C	4.64324	2.03836	0.67097
H	5.06031	1.13584	0.19956
C	0.04635	-4.28919	-2.40906
H	-0.81867	-4.62544	-2.98711
H	0.00776	-4.78595	-1.43141
H	0.94265	-4.64250	-2.92617
C	-0.05424	-0.28910	2.26579
C	2.16330	3.98936	0.18596
H	1.09779	3.84064	-0.03626
C	3.33912	2.26220	-2.11351
H	3.89528	3.19274	-2.30449
C	-1.97993	3.94455	-0.33221
H	-1.19158	3.90015	0.43230
C	-4.28046	1.93084	-1.32166
H	-4.81034	1.04664	-0.93944
C	-1.27394	-0.77779	2.77341
H	-2.20097	-0.38484	2.36308
C	1.10973	-0.82143	2.85319
H	2.07677	-0.46320	2.50882
C	4.59169	-3.20555	0.10476
C	0.11469	-2.17322	-3.72167
H	1.02070	-2.51095	-4.23461
H	0.12466	-1.08182	-3.68723
H	-0.75904	-2.49283	-4.29825
C	-5.27886	-3.64325	-1.50600
H	-6.17997	-4.22339	-1.27812
H	-4.59763	-4.28941	-2.06734
H	-5.56224	-2.81116	-2.15773
C	-3.89957	2.61150	1.67567
H	-4.52175	3.50172	1.49508
C	2.04587	2.31122	-2.92852
H	1.42254	1.43229	-2.73459
H	2.25646	2.34109	-4.00580
H	1.43867	3.18933	-2.68761
C	4.51719	1.76158	2.16853
H	4.20518	2.65582	2.71585
H	5.47468	1.43560	2.59630
H	3.77041	0.98871	2.37806
C	-5.68167	-2.29073	0.53628
H	-6.00493	-1.42556	-0.05138
H	-5.30486	-1.92733	1.49792
H	-6.56421	-2.90624	0.73754
C	5.59181	-2.39698	0.93384
H	5.14983	-2.03153	1.86662
H	5.97281	-1.53521	0.37670
H	6.44624	-3.02854	1.19703
C	2.26907	4.37737	1.66108
H	1.89922	3.58741	2.31951
H	1.67503	5.27785	1.86493
H	3.30407	4.60538	1.94008
C	-4.24018	-4.30783	0.67954
H	-5.11881	-4.90905	0.93810
H	-3.78974	-3.95210	1.61407
H	-3.52287	-4.96646	0.17863
C	2.66771	5.13304	-0.69815
H	3.74238	5.30645	-0.57004
H	2.15901	6.06968	-0.43528
H	2.48903	4.95182	-1.76201
C	-1.29172	3.92606	-1.69668
H	-0.79058	2.97127	-1.88633
H	-0.53858	4.72222	-1.76905
H	-2.00946	4.09129	-2.50812
C	-0.16017	-2.27360	4.31458
H	-0.20014	-3.02107	5.10300
C	4.22189	1.10192	-2.57877
H	5.17446	1.06001	-2.03974
H	4.45537	1.19840	-3.64759
H	3.72419	0.13654	-2.44222
C	5.62765	3.17692	0.39631
H	5.76830	3.35015	-0.67621
H	6.61457	2.96193	0.82672
H	5.28363	4.11825	0.83871
C	1.06994	-1.79693	3.85405
H	1.99431	-2.17345	4.28722
C	4.11580	-4.39428	0.95508
H	4.96550	-5.00976	1.27041
H	3.42767	-5.03897	0.39834
H	3.60384	-4.04015	1.85791
C	-2.75241	5.24596	-0.11813
H	-3.56766	5.36398	-0.84016
H	-2.08919	6.11213	-0.24069
H	-3.18871	5.31011	0.88378
C	-5.31697	3.04723	-1.46889
H	-5.76840	3.33052	-0.51209
H	-6.13073	2.74064	-2.13903
H	-4.87057	3.94887	-1.90192
C	5.31679	-3.72608	-1.14516
H	5.65634	-2.89227	-1.76726
H	4.66797	-4.35763	-1.75919
H	6.19171	-4.32083	-0.86013
C	-3.70248	1.55081	-2.68568
H	-3.19689	2.39872	-3.15695
H	-4.50094	1.23003	-3.36802
H	-2.97900	0.73389	-2.61644
C	-1.33821	-1.75093	3.77529
H	-2.30307	-2.09030	4.14645
C	-4.83805	1.46974	2.06254
H	-4.27347	0.56215	2.30864
H	-5.54712	1.21707	1.26599
H	-5.42493	1.72419	2.95474
C	-2.94398	2.93008	2.82592
H	-2.26972	2.09001	3.02496
H	-3.49606	3.13885	3.75198
H	-2.31016	3.79567	2.61179
H	-0.03497	2.63782	1.63206

INT2

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.08668 Eh

Thermal Gibb's Corr. = 2.013937 Eh

Gibb's Free Energy= -6648.072743 Eh

Lowest Frequency = 6.9976 cm^{-1}

Second Frequency = 10.5570 cm^{-1}

K	-0.30587	-0.10053	1.47316
Si	-4.05330	-0.36201	3.35971
Si	-5.13032	-3.24536	-1.37484
Al	-3.06572	-1.26453	0.23821
O	-3.32994	0.61000	-0.69183
N	-3.16962	0.14394	1.90820
N	-4.75283	-1.59342	-0.83943
C	-5.20890	-0.50058	-1.55961
C	-3.18914	1.72907	0.12362
C	-3.08003	1.45548	1.49490
C	-4.73196	1.87325	-2.14085
C	-4.45007	0.67725	-1.51531
C	-2.85592	2.60731	2.28700

H	-2.67233	2.46316	3.34251
C	-3.22595	4.08352	0.40709
H	-3.35738	5.08401	0.01052
C	-2.93822	3.90037	1.76952
C	-3.35577	2.98206	-0.43875
C	-6.36922	-0.38264	-2.34520
H	-7.03285	-1.23386	-2.41423
C	-5.89527	1.92403	-2.91512
H	-6.16275	2.84416	-3.41807
C	-6.71597	0.79638	-3.01751
C	-3.73467	3.01610	-1.92000
C	-5.63957	-1.17335	2.67120
H	-5.21702	-1.90283	1.96070
C	-4.43342	1.01097	4.66499
H	-3.48107	1.53053	4.84329
C	-3.03866	-1.68026	4.31579
H	-3.67553	-1.95218	5.17032
C	-7.00185	-3.63604	-1.60650
H	-7.28955	-3.11664	-2.53151
C	-8.01250	0.80665	-3.83236
C	-2.77118	5.12980	2.66665
C	-4.30690	-3.57901	-3.08436
H	-4.27032	-4.67431	-3.18036
C	-6.49611	-1.94042	3.67529
H	-5.91034	-2.65087	4.26915
H	-7.28619	-2.50940	3.16711
H	-6.99591	-1.25911	4.37339
C	-4.33026	-4.42719	-0.08716
H	-3.46141	-3.85371	0.27862
C	-2.75872	-2.95763	3.52856
H	-3.68379	-3.45972	3.22873
H	-2.17570	-3.67282	4.12649
H	-2.20086	-2.75583	2.60446
C	-1.69398	6.05774	2.08730
H	-0.72545	5.54928	2.04877
H	-1.58448	6.95164	2.71161
H	-1.93883	6.38568	1.07310
C	-4.31585	4.36560	-2.32527
H	-4.57798	4.36480	-3.38712
H	-3.57979	5.16087	-2.17451
H	-5.21211	4.60619	-1.74639
C	-1.74976	-1.08235	4.87880
H	-1.08889	-0.73740	4.07480
H	-1.17935	-1.82038	5.45802
H	-1.93612	-0.22041	5.52830
C	-7.93780	-0.26720	-4.92795
H	-7.09464	-0.07785	-5.60036
H	-8.85803	-0.27183	-5.52351
H	-7.80644	-1.26748	-4.50518
C	-2.47051	2.73798	-2.76079
H	-2.02660	1.77665	-2.48876
H	-1.72475	3.52271	-2.59239
H	-2.72417	2.71426	-3.82579
C	-9.19865	0.50471	-2.90364
H	-9.10076	-0.47552	-2.42790
H	-10.13831	0.51229	-3.46807
H	-9.26821	1.25453	-2.10923
C	-7.90838	-3.11894	-0.49197
H	-7.68248	-3.59114	0.46907
H	-8.96454	-3.32254	-0.71408
H	-7.79576	-2.03899	-0.35721
C	-7.22269	-5.12684	-1.87675
H	-6.61425	-5.48598	-2.71444
H	-8.27307	-5.32848	-2.12418
H	-6.97543	-5.74147	-1.00553
C	-4.11109	5.87869	2.73243
H	-4.43788	6.20289	1.73997
H	-4.02391	6.76746	3.36802
H	-4.89234	5.23409	3.14764
C	-2.87364	-3.05118	-3.08893
C	-3.79064	-5.72607	-0.68839
H	-4.58392	-6.32873	-1.14619
H	-3.32573	-6.34519	0.09027
H	-3.03198	-5.54275	-1.45536
C	-6.47977	-0.20932	1.83362
H	-7.02318	0.50256	2.46223
H	-7.22270	-0.75513	1.24204
H	-5.86665	0.36274	1.13131
C	-5.46424	2.04830	4.21389
H	-5.25357	2.45309	3.22047
H	-5.50495	2.88989	4.91893
H	-6.46584	1.60737	4.18865
C	-8.26531	2.15715	-4.50498
H	-8.36071	2.96294	-3.76984
H	-9.19871	2.11574	-5.07587
H	-7.46095	2.41881	-5.20050
C	-5.21325	-4.73391	1.12327
H	-5.60470	-3.82913	1.59622
H	-4.64602	-5.28500	1.88506
H	-6.07241	-5.35748	0.85447
C	-4.86279	0.41791	6.01199
H	-5.76588	-0.19421	5.91768
H	-5.09251	1.21954	6.72633
H	-4.08766	-0.20775	6.46393
C	-2.35642	4.76131	4.09279
H	-3.11601	4.15276	4.59408
H	-2.22142	5.67321	4.68341
H	-1.40867	4.21161	4.10700
C	-5.07461	-3.03209	-4.28857
H	-6.08361	-3.45117	-4.36319
H	-4.55489	-3.27211	-5.22653
H	-5.17270	-1.94273	-4.23803
H	-0.49952	-1.76449	-3.44081
H	-2.87255	-1.95648	-3.03031
H	-2.34562	-3.34209	-4.00974
H	-2.29104	-3.40423	-2.23024
C	0.22262	-1.40818	-2.71337
C	2.05445	-0.46184	-0.73667
C	0.77524	-2.29029	-1.78226
C	1.45577	0.39885	-1.68056
C	1.67854	-1.81854	-0.82474
C	0.56416	-0.05556	-2.65752
K	3.46041	-1.28516	-3.23874
Si	3.13946	3.60139	0.84130
Si	4.09418	-2.19216	2.95251
Al	3.22361	0.23569	0.78021
O	5.31041	0.14600	-0.28191
N	3.62310	2.04862	0.11484
N	4.10592	-1.43633	1.34296
C	4.77569	-2.03519	0.29687
C	5.14452	0.97768	-1.36454
C	4.22711	2.01665	-1.12538
C	6.10103	-1.57364	-1.75424
C	5.43890	-1.18308	-0.60489
C	3.99080	2.84144	-2.23700
H	3.26682	3.64069	-2.13521
C	5.50098	1.56996	-3.64089
H	5.99460	1.41062	-4.59172
C	4.60889	2.63726	-3.47798
C	5.78423	0.71629	-2.56261
C	4.82585	-3.39479	-0.04775
H	4.30255	-4.10053	0.58654
C	6.11590	-2.94709	-2.04919
H	6.64115	-3.29733	-2.92938

C	5.48447	-3.86043	-1.19447
C	6.75792	-0.46393	-2.57657
C	3.19502	3.35233	2.73780
H	2.76468	2.35096	2.87525
C	4.30858	5.00105	0.23905
H	4.02300	5.19309	-0.80449
C	1.34353	4.11764	0.40993
H	1.15020	4.97520	1.07134
C	5.63885	-3.31669	3.15585
H	5.45103	-4.18297	2.50625
C	5.46834	-5.36437	-1.47904
C	4.25869	3.58782	-4.62554
C	2.55607	-3.29702	3.27707
H	2.61358	-3.52683	4.35145
C	2.34287	4.33794	3.54023
H	1.28538	4.30328	3.25941
H	2.40108	4.11043	4.61254
H	2.67971	5.37261	3.41487
C	4.04484	-0.75619	4.21587
H	3.35309	-0.03433	3.75965
C	0.36565	3.00451	0.77808
H	0.45723	2.71774	1.83224
H	-0.67333	3.30022	0.60051
H	0.57597	2.12484	0.15929
C	5.02236	3.25746	-5.90907
H	4.78735	2.25193	-6.27561
H	4.74519	3.96628	-6.69540
H	6.10542	3.32767	-5.76532
C	8.05736	-0.03416	-1.86606
H	8.75884	-0.87326	-1.82092
H	8.52696	0.79364	-2.40669
H	7.85025	0.29595	-0.84525
C	1.07788	4.58434	-1.01960
H	1.16144	3.75427	-1.73147
H	0.05601	4.97416	-1.11282
H	1.76375	5.37611	-1.34145
C	4.01524	-5.83621	-1.64520
H	3.53259	-5.32545	-2.48672
H	3.98217	-6.91329	-1.84170
H	3.41898	-5.64170	-0.74922
C	7.10384	-0.91557	-3.99219
H	6.22440	-1.23360	-4.56623
H	7.58448	-0.10518	-4.54623
H	7.80602	-1.75294	-3.96776
C	6.11288	-6.10897	-0.29962
H	5.56822	-5.93681	0.63327
H	6.12102	-7.18802	-0.48837
H	7.14511	-5.77794	-0.14894
C	6.96687	-2.70545	2.70643
H	7.25388	-1.85473	3.33034
H	7.77308	-3.44723	2.77890
H	6.93149	-2.35857	1.67018
C	5.74093	-3.84806	4.58863
H	4.81799	-4.33533	4.92149
H	6.55002	-4.58437	4.67584
H	5.96286	-3.04398	5.29871
C	4.60675	5.02716	-4.21633
H	5.67225	5.11792	-3.98341
H	4.37127	5.72257	-5.02941
H	4.04480	5.34344	-3.33270
C	1.26088	-2.52770	3.02957
C	3.48854	-1.12969	5.59097
H	4.10055	-1.88972	6.08909
H	3.46996	-0.25177	6.24948
H	2.46602	-1.51658	5.53752
C	4.62535	3.31123	3.27534
H	5.10154	4.29654	3.22325
H	4.63784	3.00555	4.32883
H	5.25261	2.60805	2.71811
C	5.79621	4.64706	0.23879
H	6.00478	3.75447	-0.35737
H	6.38788	5.47146	-0.18040
H	6.16866	4.46317	1.25059
C	6.23776	-5.72548	-2.75082
H	7.29095	-5.43422	-2.68379
H	6.20215	-6.80784	-2.90784
H	5.80445	-5.25087	-3.63845
C	5.40394	-0.06874	4.35041
H	5.82411	0.20276	3.37625
H	5.32193	0.84924	4.94424
H	6.12881	-0.71450	4.85807
C	4.05261	6.29711	1.01350
H	4.35501	6.20336	2.06203
H	4.62939	7.12762	0.58689
H	2.99716	6.59077	1.00029
C	2.75385	3.49318	-4.92301
H	2.14940	3.76550	-4.05309
H	2.48231	4.16709	-5.74287
H	2.47821	2.47399	-5.21754
C	2.52319	-4.62479	2.52233
H	3.43207	-5.21752	2.67263
H	1.67381	-5.24049	2.84425
H	2.39933	-4.46387	1.44427
H	2.21721	0.51794	2.03169
H	1.15670	-2.33630	1.95527
H	0.37784	-3.09619	3.34566
H	1.25020	-1.56705	3.55746
H	0.11647	0.64775	-3.35585
H	1.70656	1.45602	-1.65615
H	0.48087	-3.33627	-1.78796
H	2.10788	-2.52573	-0.11826

TS2-3

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.072156 Eh

Thermal Gibb's Corr. = 2.015902 Eh

Gibb's Free Energy= -6648.056254 Eh

Lowest Frequency = -126.7122 cm^{-1}

Second Frequency = 7.7643 cm^{-1}

K	-0.03383	0.72950	-1.89655
Si	3.61592	0.64291	-3.79388
Si	4.58766	-3.59394	0.35155
Al	2.85961	-1.08426	-1.00784
O	3.09105	0.42136	0.47373
N	2.98830	0.64187	-2.12936
N	4.33902	-1.84727	0.11450
C	4.90730	-0.95944	1.02207
C	2.99236	1.72117	-0.00939
C	2.88274	1.81414	-1.40141
C	4.59925	1.23507	2.14023
C	4.22145	0.23419	1.27017
C	2.69248	3.12711	-1.88695
H	2.52256	3.26196	-2.94651
C	3.11863	4.06630	0.29890
H	3.29226	4.93032	0.93001
C	2.81104	4.24546	-1.05829
C	3.22079	2.78583	0.84375
C	6.11600	-1.08009	1.72569
H	6.73078	-1.95346	1.54762
C	5.80058	1.04851	2.83133
H	6.14369	1.81467	3.51387
C	6.56989	-0.09889	2.61749

C	3.66714	2.44348	2.26541
C	4.49187	-1.04016	-3.99780
H	3.78090	-1.73898	-3.51920
C	4.78843	2.12528	-4.14416
H	4.13895	3.00410	-4.25730
C	2.19393	0.68486	-5.08859
H	2.69458	0.63828	-6.06703
C	6.41995	-4.17051	0.21016
H	6.88183	-3.85819	1.15722
C	7.92551	-0.30344	3.29991
C	2.68009	5.66638	-1.61252
C	4.03858	-4.19919	2.10594
H	3.99270	-5.29293	1.98519
C	4.70422	-1.51109	-5.43736
H	3.78554	-1.50583	-6.03094
H	5.09557	-2.53633	-5.44937
H	5.43326	-0.88458	-5.96105
C	3.46545	-4.44229	-0.95422
H	2.61026	-3.75184	-1.05075
C	1.30396	-0.55430	-4.97175
H	1.84428	-1.47242	-5.21746
H	0.43626	-0.49195	-5.64072
H	0.92942	-0.70935	-3.95248
C	1.64202	6.45426	-0.79944
H	0.65251	5.99183	-0.87193
H	1.56621	7.48036	-1.17584
H	1.90784	6.50716	0.26006
C	4.35587	3.62558	2.93904
H	4.66632	3.35766	3.95283
H	3.66633	4.46996	3.02782
H	5.23716	3.95133	2.37915
C	1.36925	1.97158	-5.07220
H	0.87915	2.14429	-4.10548
H	0.57546	1.94914	-5.83001
H	1.98313	2.85740	-5.26640
C	7.91160	-1.60824	4.10864
H	7.12923	-1.58492	4.87418
H	8.87563	-1.75707	4.60802
H	7.72804	-2.47790	3.47165
C	2.44331	2.03297	3.10759
H	1.87792	1.23529	2.61966
H	1.77631	2.88867	3.24363
H	2.76451	1.67764	4.09181
C	9.01951	-0.38490	2.22393
H	8.84704	-1.21771	1.53566
H	10.00207	-0.52905	2.68765
H	9.05003	0.53558	1.63243
C	7.21989	-3.51941	-0.91410
H	6.85858	-3.83484	-1.89758
H	8.28015	-3.79833	-0.85454
H	7.15427	-2.42787	-0.87654
C	6.52791	-5.69695	0.16615
H	6.01400	-6.17260	1.00869
H	7.57742	-6.01633	0.20095
H	6.09946	-6.10696	-0.75430
C	4.04684	6.36095	-1.51024
H	4.38884	6.42219	-0.47290
H	3.98988	7.38030	-1.90850
H	4.80285	5.80997	-2.07915
C	2.64555	-3.72427	2.51488
C	2.92716	-5.81227	-0.54090
H	3.73290	-6.54068	-0.39532
H	2.26596	-6.21739	-1.31821
H	2.35228	-5.77287	0.38986
C	5.80733	-1.10674	-3.22317
H	6.55601	-0.43889	-3.66218
H	6.22720	-2.11856	-3.25521
H	5.68745	-0.83767	-2.16873
C	5.78023	2.43201	-3.01957
H	5.28055	2.61646	-2.06547
H	6.37163	3.32449	-3.26335
H	6.48552	1.60953	-2.86969
C	8.27506	0.84244	4.25141
H	8.34306	1.79997	3.72492
H	9.24734	0.65038	4.71642
H	7.53635	0.94139	5.05375
C	4.10649	-4.51562	-2.34129
H	4.50012	-3.54704	-2.66067
H	3.37314	-4.83660	-3.09262
H	4.93306	-5.23367	-2.36864
C	5.52209	1.94399	-5.47638
H	6.24780	1.12568	-5.42396
H	6.08209	2.85099	-5.73702
H	4.84183	1.72944	-6.30798
C	2.24159	5.68159	-3.07861
H	2.98212	5.20689	-3.73130
H	2.12385	6.71611	-3.41611
H	1.28093	5.17380	-3.21799
C	5.02330	-3.91375	3.24157
H	6.02680	-4.29711	3.03324
H	4.68441	-4.38863	4.17215
H	5.11238	-2.84063	3.43363
H	1.46810	-2.71556	0.44458
H	2.59345	-2.62994	2.54408
H	2.38763	-4.09152	3.51811
H	1.86946	-4.07844	1.82843
C	0.71046	-1.99321	0.17569
C	-1.79695	-0.52023	0.04301
C	-0.38095	-2.43723	-0.64330
C	-0.78432	-0.22591	0.99354
C	-1.54640	-1.69841	-0.72771
C	0.37830	-0.97826	1.13476
K	-2.07816	-2.65360	2.02172
Si	-3.16999	3.70781	1.03172
Si	-5.13532	-0.49351	-2.98231
Al	-3.33033	0.68904	-0.41404
O	-4.89846	-0.11782	1.19567
N	-3.35663	1.94690	1.10535
N	-4.54857	-0.58860	-1.31367
C	-4.80413	-1.68381	-0.51660
C	-4.22718	0.13081	2.36864
C	-3.40757	1.27265	2.30973
C	-5.13542	-2.41275	1.83631
C	-4.97971	-1.44534	0.86063
C	-2.67388	1.51850	3.48006
H	-1.99931	2.36673	3.48943
C	-3.54930	-0.45718	4.57213
H	-3.60621	-1.11022	5.43441
C	-2.72991	0.67714	4.59978
C	-4.32316	-0.74287	3.43597
C	-4.82290	-3.04096	-0.87540
H	-4.65502	-3.29476	-1.91571
C	-5.14078	-3.75419	1.41743
H	-5.28358	-4.54039	2.14889
C	-4.99360	-4.07063	0.06096
C	-5.29338	-1.91530	3.27441
C	-4.09963	4.27779	-0.54245
H	-3.90151	3.46840	-1.25866
C	-3.83694	4.52598	2.63487
H	-3.10574	4.26744	3.41346
C	-1.33617	4.25225	0.83595
H	-1.37344	5.29059	0.47577
C	-6.68826	-1.60431	-3.20923
H	-6.31279	-2.63684	-3.18735

C	-4.98566	-5.51637	-0.44215
C	-1.85322	1.01997	5.80659
C	-3.85197	-1.06998	-4.29577
H	-4.30390	-0.78234	-5.25686
C	-3.57911	5.57697	-1.15870
H	-2.52734	5.50326	-1.45388
H	-4.15256	5.83362	-2.05903
H	-3.66784	6.42520	-0.47014
C	-5.49367	1.35485	-3.32110
H	-4.65041	1.86613	-2.83610
C	-0.66021	3.39167	-0.22836
H	-1.20140	3.42760	-1.18172
H	0.38011	3.69109	-0.39681
H	-0.66303	2.35266	0.12204
C	-2.03104	0.02754	6.95682
H	-1.74617	-0.98900	6.66385
H	-1.39260	0.31856	7.79686
H	-3.06500	0.00585	7.31636
C	-6.73159	-1.38848	3.45399
H	-7.45315	-2.19793	3.30305
H	-6.86097	-0.97974	4.46126
H	-6.94635	-0.59711	2.73188
C	-0.50410	4.23528	2.11487
H	-0.39854	3.21430	2.49913
H	0.51273	4.60148	1.92142
H	-0.93763	4.85176	2.90929
C	-3.64109	-5.81346	-1.12473
H	-2.80961	-5.68863	-0.42131
H	-3.61862	-6.84446	-1.49470
H	-3.46012	-5.14897	-1.97432
C	-5.04848	-3.01649	4.30165
H	-4.03667	-3.43656	4.24277
H	-5.18680	-2.63146	5.31535
H	-5.75950	-3.83569	4.16562
C	-6.12356	-5.70406	-1.45728
H	-6.00880	-5.03946	-2.31852
H	-6.13996	-6.73510	-1.82771
H	-7.09281	-5.48759	-0.99736
C	-7.74038	-1.49065	-2.10479
H	-8.19515	-0.49656	-2.07931
H	-8.54987	-2.21382	-2.27074
H	-7.31989	-1.68752	-1.11517
C	-7.32087	-1.39051	-4.58722
H	-6.59882	-1.50690	-5.40300
H	-8.13139	-2.10983	-4.76162
H	-7.75766	-0.38982	-4.67526
C	-2.21811	2.42109	6.31987
H	-3.26975	2.46273	6.62041
H	-1.60127	2.68340	7.18669
H	-2.06080	3.18554	5.55331
C	-2.52583	-0.32378	-4.15898
C	-5.49332	1.75530	-4.79707
H	-6.28157	1.24537	-5.36196
H	-5.67040	2.83353	-4.90300
H	-4.54171	1.53296	-5.29005
C	-5.61152	4.34595	-0.32841
H	-5.88541	5.16018	0.35162
H	-6.13234	4.53273	-1.27551
H	-6.00663	3.41420	0.08887
C	-5.19668	4.01861	3.11547
H	-5.20095	2.93383	3.25301
H	-5.45991	4.47620	4.07836
H	-5.99494	4.26645	2.41043
C	-5.18115	-6.52848	0.68809
H	-6.13775	-6.38392	1.20044
H	-5.17313	-7.54372	0.27940
H	-4.37919	-6.46764	1.43248
C	-6.77598	1.82421	-2.63408
H	-6.79328	1.55404	-1.57326
H	-6.88016	2.91372	-2.70180
H	-7.66437	1.38915	-3.10532
C	-3.82802	6.05162	2.50371
H	-4.55658	6.39445	1.76095
H	-4.09150	6.53001	3.45583
H	-2.84757	6.43800	2.20277
C	-0.37681	1.00257	5.38009
H	-0.17448	1.73334	4.59232
H	0.27224	1.23963	6.23060
H	-0.09175	0.01569	4.99864
C	-3.59740	-2.57586	-4.33723
H	-4.51924	-3.15361	-4.46381
H	-2.92908	-2.84256	-5.16667
H	-3.10916	-2.92024	-3.41750
H	-2.84718	1.62854	-1.66695
H	-2.03657	-0.63771	-3.22980
H	-1.84769	-0.55888	-4.98961
H	-2.65777	0.76247	-4.11642
H	1.10377	-0.71522	1.89988
H	-0.94246	0.60178	1.68405
H	-0.23931	-3.30531	-1.28383
H	-2.32605	-2.04218	-1.40505

INT3

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.092134 Eh

Thermal Gibb's Corr. = 2.019598 Eh

Gibb's Free Energy= -6648.072536 Eh

Lowest Frequency = 9.0648 cm^{-1}

Second Frequency = 11.3271 cm^{-1}

K	0.39174	0.97968	2.04432
Si	-3.11013	-0.54935	3.59133
Si	-4.69202	-3.17843	-1.05409
Al	-2.71141	-1.02848	0.44315
O	-3.12962	0.71637	-0.43912
N	-2.48742	0.10113	2.03591
N	-4.39382	-1.56129	-0.35365
C	-5.09771	-0.47656	-0.88454
C	-2.91192	1.80215	0.40525
C	-2.55154	1.45638	1.70738
C	-4.91105	1.93999	-1.44202
C	-4.41792	0.73807	-0.98471
C	-2.26250	2.56346	2.53234
H	-1.91958	2.38059	3.54122
C	-3.03788	4.11777	0.84890
H	-3.29655	5.12807	0.55317
C	-2.49425	3.87979	2.11963
C	-3.26268	3.06362	-0.03486
C	-6.43057	-0.41297	-1.31380
H	-7.04821	-1.29604	-1.22489
C	-6.23817	1.93739	-1.87971
H	-6.67848	2.85531	-2.24654
C	-7.00158	0.76665	-1.81218
C	-3.95580	3.13778	-1.39731
C	-4.85341	-1.21970	3.18432
H	-4.65163	-1.95690	2.38873
C	-3.10836	0.68999	5.06669
H	-2.15574	1.23676	5.02299
C	-1.97905	-1.99540	4.10923
H	-2.31395	-2.27021	5.11871
C	-6.50720	-3.77384	-0.85654
H	-7.07007	-3.15324	-1.56692
C	-8.47269	0.73227	-2.23499

C	-2.23536	5.06208	3.05753
C	-4.33910	-3.14896	-2.94858
H	-4.13256	-4.19824	-3.20835
C	-5.52902	-1.95858	4.33908
H	-4.88532	-2.73041	4.77544
H	-6.45160	-2.44953	4.00447
H	-5.80758	-1.26847	5.14370
C	-3.45804	-4.35548	-0.17069
H	-2.65199	-3.69366	0.17633
C	-2.12813	-3.22704	3.22503
H	-3.12638	-3.66188	3.30400
H	-1.40449	-4.00645	3.49729
H	-1.94680	-2.98900	2.16768
C	-1.35746	6.10988	2.35741
H	-0.37810	5.69463	2.10053
H	-1.20034	6.96959	3.01759
H	-1.81522	6.47875	1.43541
C	-4.69157	4.45911	-1.58436
H	-5.18485	4.48386	-2.56003
H	-3.98692	5.29522	-1.55890
H	-5.44696	4.61470	-0.80854
C	-0.51679	-1.55979	4.18609
H	-0.10340	-1.47548	3.17451
H	0.09898	-2.30340	4.70682
H	-0.38307	-0.60815	4.71731
C	-8.66379	-0.31226	-3.34463
H	-8.05064	-0.06938	-4.21845
H	-9.71251	-0.34498	-3.66023
H	-8.38416	-1.31581	-3.01070
C	-2.90638	2.97620	-2.51644
H	-2.32762	2.05713	-2.39321
H	-2.20985	3.81888	-2.50379
H	-3.40221	2.94450	-3.49146
C	-9.33644	0.35323	-1.02199
H	-9.07130	-0.63211	-0.62720
H	-10.39567	0.32832	-1.30133
H	-9.21109	1.08125	-0.21423
C	-7.11520	-3.54763	0.52700
H	-6.67743	-4.21447	1.27542
H	-8.19612	-3.73827	0.51926
H	-6.95603	-2.52089	0.87292
C	-6.68305	-5.21709	-1.33786
H	-6.30050	-5.35935	-2.35471
H	-7.74323	-5.49986	-1.34540
H	-6.16662	-5.93323	-0.69162
C	-3.58579	5.69245	3.43304
H	-4.12033	6.05041	2.54825
H	-3.43559	6.54463	4.10502
H	-4.22658	4.96404	3.94040
C	-3.09598	-2.32606	-3.28785
C	-2.82148	-5.38910	-1.10109
H	-3.57048	-6.06572	-1.52939
H	-2.10134	-6.01036	-0.55312
H	-2.28793	-4.92030	-1.93409
C	-5.77988	-0.16894	2.56994
H	-6.13529	0.54271	3.32095
H	-6.66408	-0.63844	2.12274
H	-5.29026	0.40492	1.77766
C	-4.25255	1.70628	5.03082
H	-4.32923	2.22953	4.07369
H	-4.12763	2.46050	5.81868
H	-5.21105	1.21037	5.21549
C	-8.95655	2.08385	-2.76349
H	-8.88330	2.86716	-2.00197
H	-10.00771	2.00749	-3.05890
H	-8.38693	2.40201	-3.64287
C	-4.03606	-5.04105	1.06800
H	-4.50873	-4.33079	1.75194
H	-3.24707	-5.56101	1.62534
H	-4.78841	-5.78960	0.80289
C	-3.11366	-0.04592	6.41252
H	-3.97045	-0.72139	6.50840
H	-3.17985	0.67570	7.23635
H	-2.20632	-0.63614	6.56781
C	-1.52633	4.64135	4.34732
H	-2.13088	3.95040	4.94403
H	-1.33546	5.52463	4.96439
H	-0.55847	4.17027	4.14036
C	-5.51478	-2.68718	-3.81394
H	-6.41460	-3.29081	-3.65883
H	-5.25777	-2.75747	-4.87889
H	-5.77520	-1.64400	-3.61008
H	-1.34739	-2.59861	-0.97728
H	-3.23504	-1.27405	-3.01458
H	-2.88552	-2.35810	-4.36502
H	-2.20317	-2.67899	-2.76245
C	-0.99828	-1.76697	-0.33874
C	1.68905	-0.33938	-0.04075
C	0.14574	-2.23006	0.53604
C	0.66849	0.05868	-0.96747
C	1.32744	-1.54553	0.66466
C	-0.51646	-0.60356	-1.19462
K	1.82531	-2.32017	-2.07179
Si	3.27599	3.77176	-1.02624
Si	5.28008	-0.61922	2.74929
Al	3.29839	0.71020	0.37579
O	4.85665	-0.12831	-1.35279
N	3.39386	2.01096	-1.11726
N	4.50884	-0.65322	1.16330
C	4.65135	-1.73574	0.31997
C	4.13625	0.19635	-2.47571
C	3.36651	1.36653	-2.33960
C	4.88714	-2.41278	-2.05741
C	4.82979	-1.46548	-1.05092
C	2.58466	1.67704	-3.46242
H	1.94046	2.54652	-3.40625
C	3.31100	-0.29856	-4.65617
H	3.28704	-0.93252	-5.53424
C	2.53709	0.86635	-4.60413
C	4.13361	-0.64688	-3.57299
C	4.56027	-3.09965	0.63675
H	4.38203	-3.36856	1.67202
C	4.78930	-3.76295	-1.68080
H	4.85062	-4.53351	-2.43984
C	4.63389	-4.11005	-0.33295
C	5.03856	-1.87836	-3.48319
C	4.17831	4.29961	0.57803
H	3.88121	3.51946	1.29195
C	4.02574	4.56504	-2.60645
H	3.30563	4.34974	-3.40835
C	1.47319	4.43466	-0.86059
H	1.59557	5.47128	-0.51411
C	6.72318	-1.88808	2.83301
H	6.23423	-2.87225	2.82163
C	4.50624	-5.56492	0.12563
C	1.58241	1.26448	-5.73243
C	4.08748	-1.07488	4.19184
H	4.63894	-0.82216	5.10931
C	3.75044	5.64852	1.15696
H	2.68590	5.67250	1.41323
H	4.30986	5.86696	2.07635
H	3.93883	6.47692	0.46444
C	5.86045	1.18322	3.03358
H	5.04879	1.77924	2.59254

C	0.72416	3.65441	0.21734
H	1.26619	3.67063	1.17184
H	-0.28570	4.04860	0.38278
H	0.62626	2.61104	-0.10488
C	1.65575	0.30584	-6.92210
H	1.36770	-0.71283	-6.64004
H	0.96801	0.63713	-7.70672
H	2.66209	0.27225	-7.35220
C	6.50000	-1.43300	-3.69040
H	7.17500	-2.28898	-3.58769
H	6.62508	-0.99971	-4.68805
H	6.78292	-0.68058	-2.95051
C	0.64129	4.47994	-2.13912
H	0.36769	3.47118	-2.46916
H	-0.29986	5.02147	-1.97235
H	1.16089	4.97645	-2.96563
C	3.14296	-5.76784	0.80592
H	2.32359	-5.54936	0.11147
H	3.03388	-6.80406	1.14556
H	3.02183	-5.11438	1.67446
C	4.69498	-2.92757	-4.53575
H	3.66191	-3.28665	-4.45270
H	4.82445	-2.51767	-5.54109
H	5.35908	-3.79183	-4.44848
C	5.62669	-5.88000	1.12855
H	5.57041	-5.23548	2.01064
H	5.55768	-6.92016	1.46665
H	6.60951	-5.73082	0.67051
C	7.69886	-1.86755	1.65511
H	8.27230	-0.93737	1.61957
H	8.42095	-2.69050	1.74225
H	7.18730	-1.97831	0.69549
C	7.47490	-1.77746	4.16246
H	6.80717	-1.84634	5.02838
H	8.22102	-2.57697	4.25920
H	8.01427	-0.82683	4.23899
C	1.93209	2.67485	-6.22968
H	2.95825	2.70906	-6.60904
H	1.25558	2.97480	-7.03804
H	1.84793	3.41688	-5.43025
C	2.81954	-0.22582	4.14723
C	6.00398	1.59662	4.49836
H	6.76488	1.00418	5.01924
H	6.30926	2.64852	4.57578
H	5.06798	1.48772	5.05559
C	5.69778	4.22823	0.43476
H	6.07813	5.01367	-0.22829
H	6.18769	4.36514	1.40729
H	6.02224	3.26365	0.03228
C	5.36566	3.97304	-3.04428
H	5.30213	2.89172	-3.19357
H	5.69440	4.42124	-3.99146
H	6.15189	4.15933	-2.30713
C	4.61271	-6.55434	-1.03607
H	5.57508	-6.47086	-1.55128
H	4.52453	-7.57801	-0.65851
H	3.81464	-6.40482	-1.77191
C	7.13961	1.49335	2.25578
H	7.05438	1.20422	1.20312
H	7.37092	2.56477	2.28843
H	8.00209	0.96705	2.67991
C	4.11094	6.08739	-2.47223
H	4.84205	6.38091	-1.71076
H	4.42842	6.54960	-3.41608
H	3.15049	6.53630	-2.19414
C	0.14057	1.25575	-5.19725
H	0.00932	1.96934	-4.37852
H	-0.56621	1.52212	-5.99155
H	-0.12877	0.26426	-4.81656
C	3.70955	-2.55334	4.25978
H	4.58465	-3.20855	4.32389
H	3.07959	-2.76348	5.13510
H	3.13104	-2.85001	3.37615
H	3.03590	1.69430	1.67954
H	2.24542	-0.51642	3.26035
H	2.18808	-0.39754	5.03001
H	3.03420	0.84545	4.07134
H	-1.18213	-0.22965	-1.97150
H	0.87167	0.91483	-1.61261
H	0.00891	-3.14715	1.10766
H	2.07322	-1.98227	1.33306

TS3-4

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.078614 Eh

Thermal Gibb's Corr. = 2.015894 Eh

Gibb's Free Energy= -6648.06272 Eh

Lowest Frequency = -383.2085 cm^{-1}

Second Frequency = 9.6016 cm^{-1}

K	0.18605	-0.45618	2.59942
Si	-4.59005	-3.42590	-0.65965
Si	-4.41017	2.32777	-2.22215
Al	-3.50459	-0.23338	-0.30450
O	-4.34454	0.16372	1.48971
N	-3.98514	-2.01353	0.21628
N	-4.12039	1.53985	-0.66236
C	-3.88813	2.22726	0.53249
C	-3.73311	-0.81615	2.25519
C	-3.55415	-2.01247	1.54135
C	-3.54412	1.87507	2.97272
C	-3.94229	1.47419	1.71765
C	-2.87953	-3.01875	2.25100
H	-2.66828	-3.94960	1.74082
C	-2.66202	-1.58965	4.20300
H	-2.34567	-1.44467	5.23012
C	-2.45769	-2.83101	3.57405
C	-3.29868	-0.53670	3.53391
C	-3.51398	3.56267	0.72102
H	-3.45327	4.21381	-0.14232
C	-3.14497	3.21208	3.09217
H	-2.82659	3.58751	4.05567
C	-3.15249	4.06226	1.98187
C	-3.60545	0.85080	4.11133
C	-5.95949	-2.69314	-1.77048
H	-5.49827	-1.76042	-2.13444
C	-5.20503	-4.77723	0.54949
H	-4.29327	-5.20765	0.98803
C	-3.28047	-4.20507	-1.81669
H	-3.85025	-4.90803	-2.44325
C	-5.65471	3.76569	-1.99124
H	-5.06443	4.58708	-1.56044
C	-2.75028	5.53530	2.09151
C	-1.81031	-3.97293	4.36415
C	-2.88251	3.05293	-3.13825
H	-3.29680	3.28718	-4.13167
C	-6.33219	-3.52214	-2.99879
H	-5.46951	-3.72982	-3.63911
H	-7.07663	-2.99674	-3.61120
H	-6.77210	-4.48525	-2.71837
C	-5.07418	0.89537	-3.30450
H	-4.42907	0.04078	-3.02070
C	-2.66670	-3.14844	-2.73822

H	-3.42648	-2.55870	-3.26415
H	-2.02930	-3.61474	-3.50039
H	-2.04253	-2.45623	-2.16097
C	-0.56707	-3.47996	5.11864
H	0.18873	-3.09445	4.42618
H	-0.10849	-4.30777	5.66935
H	-0.80208	-2.69901	5.84748
C	-5.04285	0.82772	4.67042
H	-5.31047	1.81341	5.06377
H	-5.12740	0.08979	5.47477
H	-5.76006	0.56548	3.88788
C	-2.19365	-5.00199	-1.09536
H	-1.60184	-4.36490	-0.42899
H	-1.49137	-5.44970	-1.81027
H	-2.61105	-5.81706	-0.49463
C	-1.57154	5.82215	1.14961
H	-0.72087	5.17495	1.38176
H	-1.24694	6.86342	1.25321
H	-1.83693	5.66406	0.10116
C	-2.63838	1.21748	5.23574
H	-1.60520	1.28712	4.87864
H	-2.68134	0.48120	6.04270
H	-2.90600	2.18266	5.67300
C	-3.94859	6.40991	1.69302
H	-4.27479	6.20138	0.66939
H	-3.68306	7.47127	1.75216
H	-4.80015	6.23118	2.35735
C	-6.78152	3.46199	-1.00371
H	-7.43506	2.66310	-1.36619
H	-7.40804	4.34968	-0.84901
H	-6.39228	3.15439	-0.02911
C	-6.19809	4.26582	-3.33225
H	-5.39851	4.53700	-4.03054
H	-6.82587	5.15483	-3.19326
H	-6.82065	3.50920	-3.82239
C	-2.84135	-4.49403	5.37809
H	-3.14595	-3.70584	6.07380
H	-2.42370	-5.32244	5.96113
H	-3.73903	-4.85264	4.86447
C	-1.75162	2.04138	-3.32516
C	-4.92715	1.09111	-4.81339
H	-5.50396	1.95508	-5.16162
H	-5.30262	0.21438	-5.35602
H	-3.88831	1.24674	-5.11853
C	-7.20228	-2.30341	-0.97107
H	-7.74903	-3.19244	-0.63820
H	-7.89569	-1.71059	-1.57989
H	-6.94702	-1.71554	-0.08303
C	-6.07922	-4.28424	1.70346
H	-5.58561	-3.50787	2.29367
H	-6.32153	-5.11310	2.38131
H	-7.02736	-3.87448	1.34412
C	-2.32401	5.91685	3.51033
H	-3.13153	5.76420	4.23400
H	-2.05139	6.97638	3.53781
H	-1.45045	5.34245	3.83724
C	-6.51776	0.53909	-2.95074
H	-6.65662	0.39818	-1.87466
H	-6.83433	-0.38265	-3.45498
H	-7.20266	1.33113	-3.27164
C	-5.90425	-5.90073	-0.22224
H	-6.84757	-5.55516	-0.65952
H	-6.14779	-6.73870	0.44272
H	-5.28803	-6.29690	-1.03673
C	-1.38325	-5.13306	3.46011
H	-2.24161	-5.61212	2.97856
H	-0.87901	-5.89794	4.05893
H	-0.68802	-4.80576	2.67986
C	-2.31234	4.34620	-2.56099
H	-3.07564	5.11674	-2.40839
H	-1.55184	4.77208	-3.22804
H	-1.82228	4.15713	-1.60056
H	-1.91174	-0.23514	-1.57874
H	-1.28421	1.84213	-2.35158
H	-0.97839	2.44412	-3.99648
H	-2.10987	1.09309	-3.74209
C	-1.58349	-0.21059	-0.36857
C	1.38511	-0.14499	-0.01938
C	-0.75574	-1.41863	-0.09868
C	0.56596	1.02687	0.01007
C	0.62196	-1.35711	-0.04824
C	-0.81108	1.03015	-0.07828
K	0.53691	-0.25243	-2.69679
Si	4.22989	2.65301	2.15579
Si	4.52315	-3.32526	0.76552
Al	3.22645	-0.20764	0.68236
O	4.29513	0.25475	-1.33931
N	3.78584	1.69912	0.73605
N	3.85675	-1.93425	-0.08799
C	3.60523	-1.95482	-1.44043
C	3.82305	1.51113	-1.63810
C	3.58584	2.29848	-0.49589
C	3.55601	-0.53126	-3.47868
C	3.82689	-0.75015	-2.14283
C	3.10334	3.58602	-0.77383
H	2.89208	4.24496	0.05884
C	3.04008	3.16324	-3.15478
H	2.82173	3.48954	-4.16373
C	2.83296	4.02805	-2.07636
C	3.55188	1.87451	-2.94253
C	3.08017	-2.99680	-2.21885
H	2.85150	-3.93595	-1.72775
C	3.03980	-1.61684	-4.21245
H	2.84926	-1.49667	-5.27200
C	2.81527	-2.85223	-3.58907
C	3.88347	0.85551	-4.03573
C	5.15197	1.46930	3.34443
H	4.57112	0.54047	3.26223
C	5.29551	4.17058	1.65031
H	4.59724	4.88100	1.18699
C	2.72452	3.33943	3.15450
H	3.15928	3.67209	4.10815
C	5.44435	-4.49665	-0.45493
H	4.64971	-4.98136	-1.03936
C	2.28484	-4.06574	-4.35768
C	2.33600	5.46257	-2.27096
C	3.20633	-4.41790	1.64653
H	3.80044	-5.15278	2.21098
C	5.15658	1.88712	4.81524
H	4.14563	1.98080	5.22545
H	5.68544	1.14190	5.42417
H	5.66350	2.84565	4.97326
C	5.68361	-2.61337	2.11085
H	5.12861	-1.74047	2.48498
C	1.72372	2.22297	3.44465
H	2.20748	1.34843	3.89712
H	0.91673	2.56363	4.11106
H	1.27361	1.91987	2.49114
C	1.89900	5.73435	-3.71185
H	1.09404	5.05809	-4.02090
H	1.52680	6.76034	-3.79776
H	2.72910	5.62584	-4.41727
C	5.39866	0.91551	-4.31700
H	5.67602	0.17268	-5.07239

H	5.67775	1.91108	-4.67727
H	5.96665	0.70851	-3.40642
C	1.99253	4.52783	2.53699
H	1.47556	4.23194	1.61705
H	1.22609	4.92130	3.21930
H	2.66530	5.35692	2.29265
C	0.97177	-4.54689	-3.72256
H	0.20817	-3.76296	-3.76936
H	0.58599	-5.42447	-4.25386
H	1.09976	-4.81966	-2.67130
C	3.13216	1.14637	-5.33266
H	2.04448	1.14498	-5.19313
H	3.41348	2.12640	-5.72688
H	3.38066	0.40810	-6.09991
C	3.32615	-5.19363	-4.28884
H	3.52267	-5.49488	-3.25576
H	2.97529	-6.07487	-4.83783
H	4.27594	-4.87010	-4.72598
C	6.37484	-3.80983	-1.45635
H	7.22810	-3.34024	-0.95946
H	6.77743	-4.54195	-2.16924
H	5.86071	-3.03650	-2.03260
C	6.18442	-5.60863	0.29380
H	5.53323	-6.15548	0.98451
H	6.60573	-6.34013	-0.40811
H	7.02069	-5.20887	0.87772
C	3.47646	6.42850	-1.91496
H	4.34274	6.26186	-2.56312
H	3.15318	7.46960	-2.03123
H	3.80410	6.28674	-0.88028
C	2.36813	-3.63122	2.65249
C	5.95791	-3.53971	3.29600
H	6.48392	-4.45065	2.98911
H	6.59252	-3.03935	4.03932
H	5.04079	-3.84945	3.80683
C	6.56958	1.16107	2.86465
H	7.22896	2.03057	2.96618
H	7.01363	0.35135	3.45784
H	6.58504	0.85086	1.81534
C	6.37405	3.86427	0.61056
H	5.94889	3.42388	-0.29531
H	6.90166	4.78236	0.31943
H	7.12369	3.16795	0.99752
C	2.01337	-3.75292	-5.83021
H	2.92267	-3.43749	-6.35164
H	1.63481	-4.64789	-6.33413
H	1.26003	-2.96530	-5.94626
C	6.99475	-2.10964	1.50636
H	6.82024	-1.44581	0.65311
H	7.58379	-1.55450	2.24591
H	7.61794	-2.94205	1.16111
C	5.88972	4.86749	2.87669
H	6.63349	4.23663	3.37534
H	6.39818	5.79780	2.59180
H	5.12689	5.12562	3.62009
C	1.13579	5.73803	-1.35365
H	1.40526	5.68103	-0.29586
H	0.73932	6.74334	-1.53636
H	0.33542	5.01523	-1.53416
C	2.28870	-5.19043	0.69912
H	2.84611	-5.82508	0.00176
H	1.60174	-5.84375	1.25467
H	1.66783	-4.50784	0.10585
H	3.15126	-0.59066	2.29109
H	1.70523	-2.94089	2.11848
H	1.74205	-4.30505	3.25217
H	2.97797	-3.02969	3.33364
H	-1.34374	1.96933	0.05864
H	1.05308	1.98829	0.18276
H	-1.25323	-2.37990	0.00258
H	1.16432	-2.29820	0.07042

compound 3

SCF (PBE0-D3BJ-(CPCM=BENZENE)/DEF2-TZVPP) Energy = -6650.159606 Eh

Thermal Gibb's Corr. = 2.016255 Eh

Gibb's Free Energy= -6648.143351 Eh

Lowest Frequency = 6.7622 cm^{-1}

Second Frequency = 12.1474 cm^{-1}

K	0.22243	-0.22923	2.78543
Si	4.44808	2.50128	-2.15377
Si	4.44749	-3.45203	-0.52577
Al	3.37955	-0.26753	-0.62881
O	4.20217	0.21520	1.43644
N	3.94435	1.62264	-0.69822
N	3.79624	-1.99961	0.24627
C	3.43830	-1.96322	1.57398
C	3.78250	1.50594	1.67283
C	3.68135	2.27169	0.49685
C	3.28917	-0.46408	3.55047
C	3.64583	-0.74440	2.24396
C	3.24855	3.59011	0.70598
H	3.13535	4.23794	-0.15404
C	2.99404	3.24075	3.08669
H	2.72593	3.60976	4.06824
C	2.91405	4.08354	1.97534
C	3.44009	1.91931	2.94476
C	2.79832	-2.95646	2.34114
H	2.56539	-3.89691	1.85921
C	2.67691	-1.49869	4.27350
H	2.42047	-1.34148	5.31602
C	2.42943	-2.74644	3.67519
C	3.63843	0.92332	4.08873
C	5.42731	1.25735	-3.22866
H	4.83497	0.33669	-3.14122
C	5.48383	4.05402	-1.69891
H	4.76515	4.79599	-1.32536
C	2.95677	3.09875	-3.22427
H	3.40212	3.42273	-4.17601
C	5.21682	-4.61888	0.79626
H	4.36067	-5.04239	1.34037
C	1.77637	-3.85502	4.50624
C	2.47244	5.54376	2.09599
C	3.13321	-4.48815	-1.47126
H	3.72101	-5.27281	-1.97185
C	5.51385	1.61041	-4.71418
H	4.52641	1.70726	-5.17725
H	6.05415	0.82829	-5.26331
H	6.04942	2.55000	-4.88718
C	5.72844	-2.82741	-1.80208
H	5.22615	-1.96207	-2.25902
C	2.00839	1.93484	-3.50841
H	2.52337	1.07970	-3.96046
H	1.18382	2.24300	-4.16988
H	1.58620	1.60627	-2.55114
C	2.07651	5.91604	3.52591
H	1.23723	5.30904	3.88300
H	1.76474	6.96472	3.55967
H	2.91171	5.79655	4.22377
C	5.12960	0.92233	4.48311
H	5.31281	0.19510	5.28095
H	5.42818	1.91609	4.83176

H	5.75484	0.65765	3.62652
C	2.16534	4.27251	-2.65235
H	1.64914	3.98479	-1.72933
H	1.39296	4.61159	-3.35617
H	2.79901	5.13680	-2.42637
C	1.39749	-5.07155	3.65774
H	0.70434	-4.80577	2.85238
H	0.90669	-5.82015	4.28775
H	2.27750	-5.54497	3.21091
C	2.80638	1.29132	5.31485
H	1.73411	1.34519	5.09121
H	3.10901	2.26649	5.70456
H	2.95524	0.56556	6.11880
C	2.77154	-4.30453	5.58717
H	3.69294	-4.67682	5.12859
H	2.34165	-5.10641	6.19788
H	3.03974	-3.47719	6.25132
C	6.11037	-3.93528	1.83309
H	7.01494	-3.52320	1.37756
H	6.43220	-4.65620	2.59641
H	5.59755	-3.11792	2.34662
C	5.95242	-5.79148	0.14129
H	5.32833	-6.32935	-0.58063
H	6.28072	-6.51782	0.89587
H	6.85041	-5.45339	-0.38736
C	3.63344	6.45166	1.66244
H	4.51025	6.29160	2.29795
H	3.34363	7.50614	1.73394
H	3.93224	6.25300	0.62862
C	2.42334	-3.68194	-2.55821
C	6.06617	-3.81455	-2.92009
H	6.54624	-4.72034	-2.53381
H	6.76487	-3.36278	-3.63616
H	5.18155	-4.12867	-3.48276
C	6.81323	0.96118	-2.65634
H	7.48565	1.82003	-2.76127
H	7.28148	0.12116	-3.18519
H	6.76846	0.70117	-1.59399
C	6.50852	3.82093	-0.58782
H	6.03888	3.44705	0.32584
H	7.02605	4.75645	-0.33797
H	7.27237	3.09773	-0.88834
C	0.49765	-3.33283	5.17889
H	0.69649	-2.49103	5.84915
H	0.03188	-4.12259	5.77796
H	-0.23901	-3.01839	4.43052
C	7.00241	-2.32118	-1.12431
H	6.78188	-1.62248	-0.31025
H	7.65165	-1.80416	-1.84073
H	7.58426	-3.14946	-0.70495
C	6.14308	4.66552	-2.93795
H	6.91831	4.00800	-3.34551
H	6.62861	5.61843	-2.69144
H	5.42328	4.86290	-3.74036
C	1.26129	5.79560	1.18758
H	1.49718	5.61960	0.13477
H	0.92128	6.83313	1.28074
H	0.42915	5.13879	1.45881
C	2.10653	-5.18198	-0.57593
H	2.57416	-5.82404	0.17812
H	1.42832	-5.81414	-1.16479
H	1.47866	-4.45472	-0.04714
H	3.34276	-0.70566	-2.20118
H	1.79208	-2.90964	-2.10322
H	1.77991	-4.33018	-3.16701
H	3.12044	-3.16716	-3.22620
C	1.43951	-0.12590	-0.09434
C	-1.45704	-0.12907	0.18026
C	0.68420	1.06299	-0.05719
C	-0.70039	-1.31886	0.13660
C	-0.71063	1.06181	0.08174
C	0.69262	-1.31759	0.01907
K	-0.08441	-0.44007	-2.71459
Si	-4.45048	-3.47196	0.54694
Si	-4.53683	2.50729	2.10332
Al	-3.41928	-0.27412	0.64139
O	-4.14019	0.17503	-1.44710
N	-3.78376	-2.02722	-0.22915
N	-3.99622	1.61871	0.66694
C	-3.69738	2.25537	-0.52585
C	-3.56186	-0.79060	-2.23035
C	-3.38315	-2.00611	-1.54332
C	-3.35760	1.86904	-2.95743
C	-3.73716	1.46943	-1.69244
C	-2.73695	-3.01325	-2.28717
H	-2.52769	-3.95288	-1.79320
C	-2.56378	-1.57723	-4.23256
H	-2.29305	-1.43537	-5.27339
C	-2.34892	-2.82343	-3.61978
C	-3.17167	-0.52519	-3.52957
C	-3.28362	3.57888	-0.74073
H	-3.21584	4.24307	0.11126
C	-2.93662	3.19820	-3.10464
H	-2.64075	3.55785	-4.08155
C	-2.91473	4.05936	-2.00544
C	-3.49582	0.85716	-4.09593
C	-5.78249	-2.83896	1.76524
H	-5.29686	-1.97180	2.23581
C	-5.16498	-4.67258	-0.77694
H	-4.28806	-5.10561	-1.27861
C	-3.15746	-4.47733	1.55425
H	-3.74916	-5.27273	2.03301
C	-5.54222	4.07345	1.62375
H	-4.80588	4.81216	1.27919
C	-2.50127	5.52714	-2.13323
C	-1.73530	-3.96326	-4.43855
C	-3.05802	3.08422	3.20236
H	-3.50920	3.45151	4.13539
C	-6.16537	-3.81815	2.87570
H	-5.30233	-4.13606	3.46892
H	-6.88378	-3.35717	3.56598
H	-6.63952	-4.72218	2.47853
C	-5.56016	1.28099	3.15600
H	-4.96921	0.35733	3.09745
C	-2.51028	-3.65354	2.66746
H	-3.24717	-3.16884	3.31482
H	-1.86601	-4.28343	3.29517
H	-1.89213	-2.85389	2.24393
C	-0.47502	-3.48457	-5.17433
H	0.29277	-3.15080	-4.46699
H	-0.04171	-4.30370	-5.75802
H	-0.68551	-2.66712	-5.87028
C	-4.96505	0.84805	-4.56515
H	-5.24833	1.83757	-4.93789
H	-5.10663	0.11257	-5.36399
H	-5.63174	0.58984	-3.73825
C	-2.08342	-5.15398	0.70183
H	-1.45646	-4.41745	0.18508
H	-1.41060	-5.76328	1.32034
H	-2.50944	-5.81545	-0.06025
C	-1.32250	5.81589	-1.19376
H	-0.46871	5.17658	-1.43747
H	-1.00436	6.86040	-1.28693
H	-1.58251	5.64166	-0.14618

C	-2.60187	1.21453	-5.28168
H	-1.54398	1.27730	-5.00008
H	-2.70444	0.47935	-6.08430
H	-2.88786	2.18317	-5.69922
C	-3.69319	6.41584	-1.74637
H	-4.01835	6.22527	-0.71902
H	-3.42370	7.47524	-1.82478
H	-4.54736	6.22816	-2.40474
C	-6.53359	3.85507	0.47978
H	-7.31098	3.13524	0.75264
H	-7.03715	4.79567	0.22046
H	-6.03900	3.48358	-0.42150
C	-6.23688	4.68478	2.84350
H	-5.54418	4.86484	3.67335
H	-6.69880	5.64680	2.58716
H	-7.03636	4.03596	3.21655
C	-2.77628	-4.42726	-5.46956
H	-3.05326	-3.61409	-6.14752
H	-2.38265	-5.25484	-6.07052
H	-3.68691	-4.76833	-4.96719
C	-2.16089	1.89312	3.53516
C	-5.69497	1.64952	4.63411
H	-6.24253	2.58649	4.78034
H	-6.24591	0.86909	5.17504
H	-4.72311	1.75933	5.12636
C	-7.02696	-2.33385	1.03415
H	-7.59525	-3.16282	0.59774
H	-7.70196	-1.80915	1.72069
H	-6.77166	-1.64163	0.22465
C	-6.02294	-4.01803	-1.86164
H	-5.49601	-3.21007	-2.37558
H	-6.31411	-4.75838	-2.61884
H	-6.94542	-3.60052	-1.44876
C	-2.07145	5.88898	-3.55600
H	-2.88319	5.74145	-4.27585
H	-1.78142	6.94372	-3.59564
H	-1.20946	5.29544	-3.87989
C	-6.92674	0.98502	2.53885
H	-6.84551	0.71311	1.48161
H	-7.41760	0.15287	3.05967
H	-7.59834	1.84801	2.61065
C	-5.92112	-5.83335	-0.12429
H	-6.84320	-5.48774	0.35556
H	-6.21202	-6.58083	-0.87360
H	-5.32627	-6.34832	0.63782
C	-1.34768	-5.16101	-3.56709
H	-2.22210	-5.61798	-3.09322
H	-0.87350	-5.92861	-4.18695
H	-0.63965	-4.88008	-2.78020
C	-2.21358	4.21005	2.60997
H	-2.80968	5.09335	2.35676
H	-1.43514	4.53582	3.31386
H	-1.70240	3.87948	1.69854
H	-3.47550	-0.69738	2.21086
H	-1.77611	1.48828	2.59135
H	-1.31342	2.19928	4.16975
H	-2.70364	1.08699	4.03980
H	1.22718	-2.26583	0.00507
H	-1.22929	-2.26830	0.19524
H	1.19966	2.01886	-0.13426
H	-1.23224	2.01699	0.10427

References

[S1] W. L. F. Armarego, C. L. L. Chai, *Purification of Laboratory Chemicals*, Elsevier/Butterworth-Heinemann, Amsterdam; Boston, **2009**

[S2] H.-S. Lin, L. A. Paquette, *Synthetic Communications* **1994**, *24*, 2503–2506

[S3] a) F. Kallmeier, A. J. R. Matthews, G. R. Nelmes, N. R. Lawson, J. Hicks, *Dalton Trans.* **2024**, *53*, 12450–12454; b) J. Hicks, P. Vasko, J. M. Goicoechea and S. Aldridge, *Nature*, 2018, **557**, 92–95.

[S4] C. A. Cruz, D. J. H. Emslie, L. E. Harrington, J. F. Britten, C. M. Robertson, *Organometallics* **2007**, *26*, 692–701

[S5] A. Nicolay, M. S. Ziegler, L. Rochlitz, T. D. Tilley, *Polyhedron* **2020**, *180*, 114420.

[S6] G. M. Sheldrick, *Acta Crystallogr. C Struct. Chem.* **2015**, *71*, 3–8

[S7] G. M. Sheldrick, *Acta Crystallogr. A Found. Adv.* **2015**, *71*, 3–8

[S8] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst*., **2009**, *42*, 339–341

[S9] C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. Van De Streek, *J. Appl. Cryst.,* **2006**, *39*, 453–457

[S10] R. O. Piltz, *J. Appl. Cryst.,* **2018**, *51*, 635

[S11] R. O. Piltz*, J. Appl. Cryst.*, **2018**, *51*, 963

[S12] P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout, D. J. Watkin, *J. Appl. Cryst.* **2003**, *36*, 1487.

[S13] J. S. McMullen, A. J. Edwards, J. Hicks, *Dalton Trans.*, **2021**, *50*, 8685.

[S14] R. I. Cooper, R. O. Gould, S. Parsons, D. J. Watkin, *J. Appl. Crystallogr.*, **2002**, *35*, 168.

[S15] Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J., *Gaussian Inc.*, Wallingford CT, **2016**

[S16] Ernzerhof, M.; Scuseria, G. E., *J. Chem. Phys.*, **1999**, *110*, 5029-36

[S17] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.*, **2011**, *32*, 1456-1465

[S18] a) Bergner, A., Dolg, M., Küchle, W., Stoll, H., Preuß, H., *Mol. Phys.*, **1993**, *80*, 1431-1441, b) Fuentealba, P., Preuß, H., Stoll, H., Szentpály, L. V., *Chem. Phys. Lett.*, **1982**, *89*, 418-422

[S19] (a) Hariharan, P. C., Pople, J. A., *Theor. Chim. Acta.*, **1973**, *28*, 213-222; (b) Hehre, W. J., Ditchfield, R., Pople, J. A., *J. Chem. Phys.*, **1972**, *56*, 2257-2261

[S20] Huo, R., Armstrong, A. J., Nelmes, G. R., Lawes, D. J., Edwards, A. J., McMullin, C. L., Hicks, J., *Chem. Eur. J.* **2024**, *30*, e202400662

[S21] Weigend, F., Ahlrichs, R., *Phys. Chem. Chem. Phys.*, **2005**, *7*, 3297

[S22] a) Klamt, A., Schüürmann, G., J. Chem. Soc., *Perkin Trans.* **1993**, 2, 799; b) Andzelm, J., Kölmel, C., Klamt, A. J., *Chem. Phys.*, **1995**, *103*, 9312; c) Barone V., Cossi, M., *J. Phys. Chem. A*, **1998**, *102*, 1995; d) Cossi, M., Rega, N., Scalmani G., Barone, V., *J. Comput. Chem.*, **2003**, *24*, 669

[S23] Grams, S., Eyselein, J., Langer, J., Färber, C., Harder, S., *Angew. Chem. Int. Ed.*, **2020**, *59*, 15982-15986

[S24] Chai, J.-D., Head-Gordon, M., *Phys. Chem. Chem. Phys.*, **2008**, 10 6615-20

[S25] Cui, C., Roesky, H. W., Schmidt, H.-G., Noltemeyer, M., Hao, H., Cimpoesu, F., *Angew. Chem. Int. Ed.,* **2000**, *39*, 4274-4276

[S26] Gentner, T. X., Evans, M. J., Kennedy, A. R., Neale, S. A., McMullin, C. L., Coles, M. P., Mulvey, R. E., *Chem. Commun.*, **2022**, *58*, 1390-1393