Electronic Supplementary Material (ESI) for Chemical Communications.

Electronic Supplementary Information for:

Alumination of Aryl Methyl Ethers: Switching Between sp^2 and sp^3 C–O Bond Functionalisation with Pd-Catalysis

Ryan K. Brown,†[a] Thomas N. Hooper,†[a] Feriel Rekhroukh,†[b] Andrew J. P. White,[a]

Paulo J. Costa,[b] and Mark R. Crimmin*

† these authors contributed equally and are listed in alphabetical order.

a) *Department of Chemistry, Molecular Sciences Research Hub, Imperial College London, 82 Wood Lane, Shepherds Bush, London, W12 0BZ, UK.*

b) *BioISI – Biosystems & Integrative Sciences Institute, Faculty of Sciences, University of Lisboa, 1749-016 Lisboa, Portugal.*

Table of contents

1. General Experimental, Preparation of Materials and Instruments

1.1 Materials

Dipp-*BDI*Al(I) (**1**) was synthesised by the literature procedures (Ar-*BDI* = $\{(ArNCMe)_2CH\}^-$, Ar = 2,6-$^i Pr_2C_6H_3$ (Dipp)).[1] $[Pd(PCy_3)_2]$ was synthesised as an analytically pure pale brown crystalline solid from $PdCl_2$ in a 3 step procedure (via intermediates $[Pd(\eta^3\text{-}C_3H_4Ph)(\mu\text{-}Cl)]_2$ and $[CpPd(\eta^3\text{-}C_3H_4Ph)]$) based on literature reactions.[2] C–O substrates were purchased from common suppliers (e.g. Sigma-Aldrich, Fluorochem, Merck, Alfa Aesar, TCI etc. unless otherwise stated below), liquid reagents were stored over activated 3 Å molecular sieves, degassed by the freeze-pump-thaw method (x 3) and stored in the glove box; solid reagents were dried under high vacuum and stored in the glove box. All other reagents were purchased from common suppliers and used without further purification.

Solvents for air sensitive procedures (toluene, *n*-hexane) were dried using a solvent purification system (SPS) and stored over activated 3 Å molecular sieves under an inert atmosphere of N_2 or argon before use. C_6H_6 (Sigma-Aldrich anhydrous grade), *n*-heptane, cyclohexane, hexamethyldisiloxane, C_6D_6 and toluene-D_8 were degassed by the freeze-pump-thaw method (x 3) and stored under inert atmosphere over activated 3 Å molecular sieves. Silica gel (technical grade, 230–400 mesh particle size) for column chromatography was purchased from Sigma-Aldrich.

1.2 Instruments

^{1}H NMR and ^{13}C NMR spectra were recorded and analysed using a Bruker 400 MHz Spectrometer at 298 K. The reported values for ^{1}H and ^{13}C NMR data are as follows: chemical shifts (δ ppm), multiplicity (where s = singlet, d = doublet, t = triplet, m = multiplet), integration (not ^{13}C) and coupling constant, *J* (Hz). AT-IR spectra were recorded on an Agilent Technologies Cary 630 FTIR spectrometer. Elemental analysis was carried out by Stephen Boyer, London Metropolitan University.

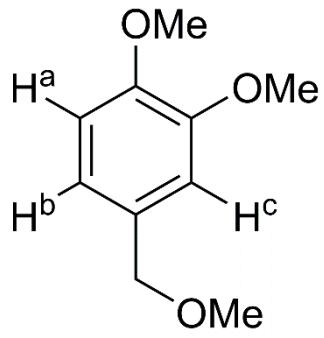
[1] (a) S. Yow, S. J. Gates, A. J. P. White, M. R. Crimmin, *Angew. Chem. Int. Ed.,* 2012, **51**, 12559. (b) C. Cui, H.W. Roesky, H.-G. Schmidt, M. Noltemeyer, H. Hao and F. Cimpoesu, *Angew. Chem. Int. Ed*., 2000, **39**, 4274.

[2] (a) P. R. Auburn, P. B. Mackenzie, B. Bosnich, *J. Am. Chem. Soc.*, 1985, **107**, 2033. (b) S. D. Robinson, B. L. Shaw, *J. Chem. Soc.*, 1963, 4806. (c) T. Yoshida, S. Otsuka, *Inorg. Synth*., 1990, **28**, 114.

2. Experimental Results

2.1 Synthesis of Protected C–O Substrates

2.1.1 Synthesis of 3,4-$(MeO)_2C_6H_3CH_2OMe$ (2c)

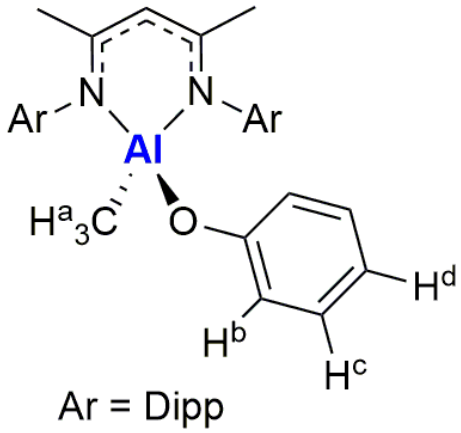


3,4-$(MeO)_2C_6H_3CH_2OMe$ was synthesised from 3,4-$(MeO)_2C_6H_3CH_2OH$ using the literature procedure.[3] The NMR spectra in C_6D_6 are presented here for completeness. **^{1}H NMR** (400 MHz, C_6D_6, 298 K): δ 6.87 (d, $^4J_{HH}$ = 1.9 Hz, 1H, H^c), 6.84 (dd, $^3J_{HH}$ = 8.0 Hz, $^4J_{HH}$ = 1.9 Hz, 1H, H^b), 6.60 (d, $^3J_{HH}$ = 8.0 Hz, 1H, H^a), 4.29 (s, 2H, CH_2), 3.41 (s, 3H, Ar-OCH_3), 3.40 (s, 3H, Ar-OCH_3), 3.18 (s, 3H, CH_2OCH_3) ppm. **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 149.94 (s, C^{ipso}-O), 149.38 (s, C^{ipso}-O), 131.19 (s, C^{ipso}-C), 119.93 (s, C-H^b), 111.70 (s, C-H^c), 111.64 (s, C-H^a), 74.33 (s, CH_2), 57.13 (s, 3H, $CH_2OC\mathbf{H_3}$), 55.25 (s, Ar-OCH_3), 55.10 (s, Ar-OCH_3) ppm.

[3] E. Napolitano, E. Giannone, R. Fiaschi, A. Marsili, *J. Org. Chem*., 1983, **48**, 3653.

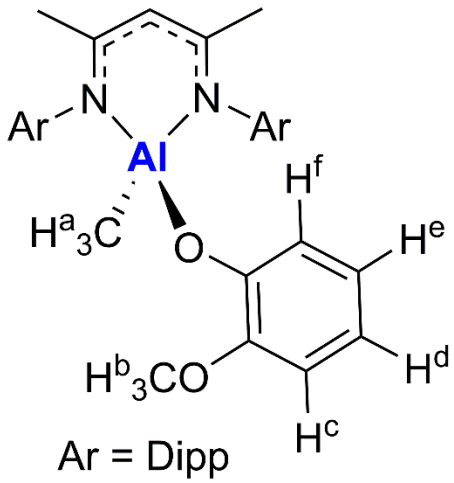
2.2 Aluminated Products from Uncatalysed Insertion into the C–O bonds of Anisole and Derivatives

2.2.1 Synthesis of Dipp-*BDI*Al(Me)(OPh) (3a)



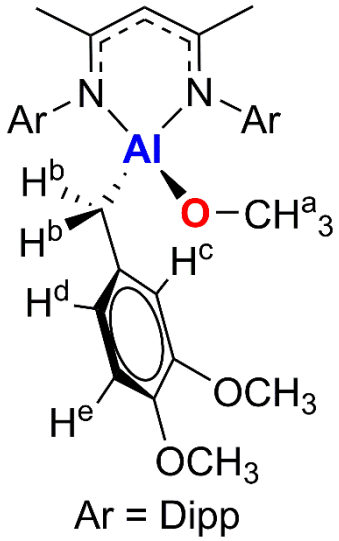
In a glovebox, Dipp-*BDI*Al(I) (**1**, 5.0 mg, 0.0113 mmol) was dissolved in cyclohexane (0.55 mL) and anisole (122 µL, 1.13 mmol, 100 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube and sealed. The tube was removed from the box and heated to 60 °C for 192 hours with monitoring by NMR spectroscopy. Once the reaction was complete (in situ yield 88%) the tube was returned to the glovebox and solution was transferred to a 4 mL vial. The solvent removed *in vacuo*. The oily product was dissolved in *n*-heptane (0.1 mL) and stored at -35 °C. Colourless crystals of the product formed, the mother liquor was decanted and the product **3a** dried *in vacuo*. An isolated yield was obtained from a scaled-up reaction using the same conditions and 20.0 mg (0.0450 mmol) of **1**. Isolated yield: 8 mg (32%). **^{1}H NMR** (400 MHz, C_6D_6, 298 K): δ 7.24 (t, $^3J_{HH}$ = 7.7 Hz, 2H, H^c), 7.14-7.04 (overlapping m, 6H, Dipp-Ar-H), 6.87 (d, $^3J_{HH}$ = 7.7 Hz, 2H, H^b), 6.83 (t, $^3J_{HH}$ = 7.7 Hz, 1H, H^d), 5.14 (s, 1H, C-H), 4.76 (dd, $^3J_{HH}$ = 7.3 Hz, $^3J_{HH}$ = 5.6 Hz, 1H, H^c), 3.32 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 3.22 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 1.55 (s, 6H, CH_3), 1.30 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.11 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.08 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.02 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), -0.68 (s, 3H, Al-CH^a_3) ppm; **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 169.95, 158.92 (s, C^{ipso}), 145.30, 142.96, 140.02, 128.86 (s, C-H^b), 127.19, 124.64, 123.75, 120.50 (s, C-H^c), 117.68 (s, C-H^d), 98.07, 28.59, 27.51, 25.12, 24.43, 24.06, 23.82, 23.03, -14.29 (Al-CH_3) ppm. The C–Al resonance was detected by the HMQC experiment.

2.2.2 Synthesis of Dipp-*BDI*Al(Me)(OC_6H_4OMe) (3b)



In a glovebox, Dipp-*BDI*Al(I) (**1**, 5.0 mg, 0.0113 mmol) was dissolved in cyclohexane (0.55 mL) and 1,2-dimethoxybenzene (143 µL, 1.13 mmol, 100 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube and sealed. The tube was removed from the box and heated to 60 °C for 18 hours with monitoring by NMR spectroscopy (in situ yield 79%). Once the reaction was complete the tube was placed under high vacuum to remove the cyclohexane and then gently heated to remove the excess 1,2-dimethoxybenzene to yield a colourless oily solid. The tube was returned to the glovebox and n-heptane (0.5 mL) added and solution was transferred to a 4 mL vial and stored at -35 °C. Colourless crystals of the product formed, the mother liquor was decanted and the product **3b** dried *in vacuo*. An isolated yield was obtained from a scaled-up reaction using the same conditions and 15.0 mg (0.0338 mmol) of **1**. Isolated yield: 11 mg (56%). **^{1}H NMR** (400 MHz, C_6D_6, 298 K): δ = 7.14-7.06 (overlapping m, 6H, Dipp-Ar-H), 6.90 (td, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 1.6 Hz, 1H, Ar-H), 6.80-6.74 (m, 2H, Ar-H), 6.71-6.67 (m, 1H, Ar-H), 5.10 (s, 1H, C-H), 3.43 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -CHMe$_2$), 3.32 (s, 3H, H^b), 3.26 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -CHMe$_2$), 1.58 (s, 6H, CH_3), 1.32 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.10 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.07 (overlapping d, $^3J_{HH}$ = 6.8 Hz, 12H, Dipp-CH_3), -0.65 (s, 3H, Al-$CH^a{}_3$) ppm; **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 169.75, 151.02 (s, C^{ipso}), 148.97 (s, C^{ipso}), 145.40, 143.13, 140.45, 127.02, 124.52, 123.68, 120.88 (s, C^{Ar}-H), 120.34 (s, C^{Ar}-H), 117.72 (s, C^{Ar}-H), 111.84 (s, C^{Ar}-H), 98.03, 54.76 (s, C-$H^a{}_3$), 28.49, 27.70, 24.80, 24.50, 24.13, 24.10, 23.17, -13.24 (Al-CH_3) ppm. The C–Al resonance was detected by the HMQC experiment. **Elemental analysis**: calc. for $C_{37}H_{51}AlN_2O_2$ – C 76.25%, H 8.82%, N 4.81%; found – C 76.32%, H 8.90%, N 4.84%.

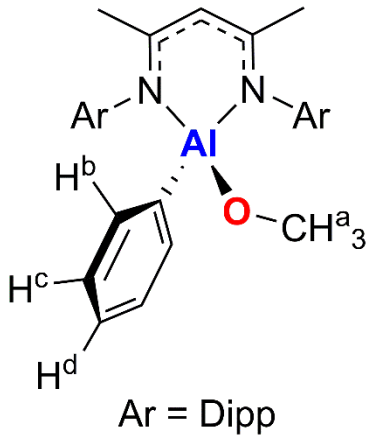
2.2.3 Synthesis of Dipp-*BDI*Al(OMe)($CH_2C_6H_3(OMe)_2$) (3c)



In a glove box, Dipp-*BDI*Al(I) (**1**, 5.0 mg, 0.0113 mmol) was dissolved in cyclohexane (0.55 mL) and 1-(methoxymethyl)-3,4-dimethoxybenzene (**2c,** 3.0 µL, 0.0225 mmol, 2 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube, sealed and removed from the glove box. The tube was left to stand at 25 °C for 10 minutes with monitoring by NMR spectroscopy. Once the reaction was complete (in situ yield 98%) the tube was returned to the glove box. The solution was transferred to a 4 mL vial and the solvent removed *in vacuo*. The oily product was dissolved in *n*-heptane (0.2 mL) and stored at -35 °C. Colourless crystals of the product formed, the mother liquor was decanted and the product **3c** dried *in vacuo*. An isolated yield was obtained from a scaled-up reaction using the same conditions and 15.0 mg (0.0338 mmol) of **1**. Isolated yield: 14 mg (66%). **^{1}H NMR** (400 MHz, C_6D_6, 298 K): δ 7.21-7.10 (overlapping m, 6H, Dipp-Ar-H), 6.43 (d, $^3J_{HH}$ = 8.1 Hz, 1H, H^e), 6.04 (d, $^4J_{HH}$ = 2.0 Hz, 1H, H^c), 6.01 (dd, $^3J_{HH}$ = 8.1 Hz, $^4J_{HH}$ = 2.0 Hz, 1H, H^d), 4.90 (s, 1H, C-H), 3.67 (s, 3H, O-CH_3), 3.55 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 3.43 (s, 3H, O-CH_3), 3.40 (s, 3H, O-CH_3), 3.20 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 1.54 (s, 6H, CH_3), 1.46 (s, 2H, CH^b_2), 1.34 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.29 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.23 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.07 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3) ppm; **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 169.63, 149.58, 145.22, 145.19, 142.89, 140.62, 137.91 (s, C-CH_2^b), 127.14, 124.77, 123.82, 119.07 (s, C-H^d), 113.40 (s, C-H^e), 112.40 (s, C-H^c), 97.69, 56.07, 55.23, 51.68, 28.65, 27.43, 24.95, 24.51, 24.27, 24.06, 22.89, 16.45 (br, Al-CH_2^b) ppm. The C-Al resonance was detected by the HMQC experiment.

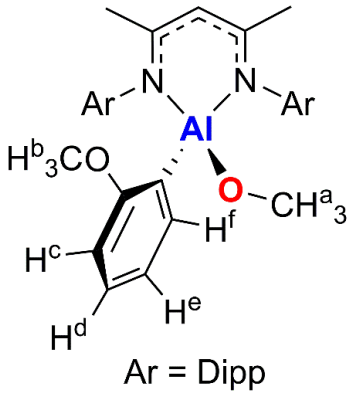
2.3 Aluminated Products from Catalysed Insertion into the C–O Bonds of Anisole and Derivatives

2.3.1 Synthesis of Dipp-*BDI*Al(OMe)(Ph) (4a)



In a glove box, Dipp-*BDI*Al(I) (**1**, 5.0 mg, 0.0113 mmol) and [Pd(PCy_3)$_2$] (50 µL, 0.0113 M solution in cyclohexane, 0.00056 mmol, 5 mol%) were dissolved in cyclohexane (0.50 mL) and ansiole (2.4 µL, 0.0225 mmol, 2 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube, sealed and removed from the glove box. The tube was heated to 40 °C for 24 hours with monitoring by NMR spectroscopy. Once the reaction was complete (in situ yield 85%) the tube was return to the glove box. The solution was transferred to a 4 mL vial and the solvent removed *in vacuo*. The oily product was dissolved in *n*-heptane (0.1 mL) and stored at -35 °C. Colourless crystals of the product formed, the mother liquor was decanted and the product **4a** dried *in vacuo*. An isolated yield was obtained from a scaled-up reaction using the same conditions and 15.0 mg (0.0338 mmol) of **1**. Isolated yield: 10 mg (54%). **^{1}H NMR** (400 MHz, C_6D_6, 298 K): δ 7.21-7.13 (overlapping m, 6H, Ar-H), 7.06-6.94 (overlapping m, 5H, Ar-H), 4.98 (s, 1H, C-H), 3.73 (overlapping sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 3.69 (overlapping s, 3H, O-CH^a_3), 3.08 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 1.61 (s, 6H, CH_3), 1.48 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.24 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.04 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 0.76 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3) ppm; **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 170.06, 144.64, 143.77, 140.55, 137.74, 127.35, 127.16, 126.57, 124.40, 124.13, 97.68, 51.59 (s, C-H^a), 28.47, 27.97, 24.96, 24.40, 24.29, 23.54, 22.94 ppm. The C-Al resonance could not be observed due to line-broadening associated with coupling to the quadrapolar *I* = 5/2 ^{27}Al nucleus.

2.3.2 Synthesis of Dipp-*BDI*Al(OMe)(C_6H_4OMe) (4b)

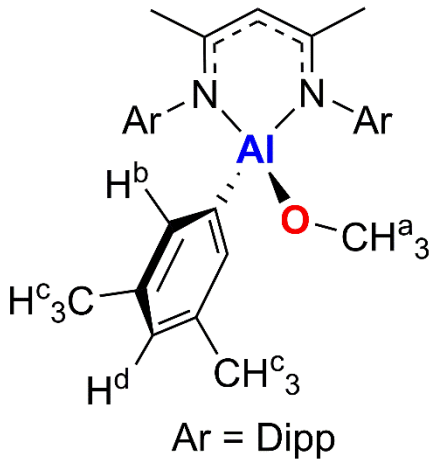


Ar = Dipp

In a glove box, Dipp-*BDI*Al(I) (**1**, 5.0 mg, 0.0113 mmol) and [$Pd(PCy_3)_2$] (50 µL, 0.0113 M solution in cyclohexane, 0.00056 mmol, 5 mol%) were dissolved in cyclohexane (0.50 mL) and 1,2-dimethoxybenzene (2.4 µL, 0.0225 mmol, 2 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube, sealed and removed from the glove box. The tube was heated to 40 °C for 40 hours with monitoring by NMR spectroscopy. Once the reaction was complete (in situ yield 93%) the tube was return to the glove box. The solution was transferred to a 4 mL vial and the solvent removed *in vacuo*. The oily product was dissolved in *n*-heptane (0.2 mL) and stored at -35 °C overnight. The solution was filtered through a glass fibre plug to remove any solid and the solution was evaporated to dryness in vacuo. The remaining product was dissolved in hexamethyldisiloxane (0.2 mL) and stored at -35 °C. Colourless crystals of the product formed, the mother liquor was decanted and the product **4b** dried *in vacuo*. An isolated yield was obtained from a scaled-up reaction using the same conditions and 20.0 mg (0.0450 mmol) of **1**. Isolated yield: 8 mg (31%). The ^{1}H NMR spectrum of **4b** at 298 K showed a more complex spectrum than anticipated suggesting desymmetrisation of the β-diketiminate ligand and several peaks were broadened suggesting a fluxional process in solution. Heating the sample to 333 K gave a simplified spectrum with the expected number of resonances for symmetrical diketiminate environments. Some of the peaks remained broad at this temperature and further heating to 353 K did not sharpen the peaks significantly. The ^{1}H NMR data is given at 333 K. **^{1}H NMR** (400 MHz, C_6D_6, 333 K): δ 7.60 (br, FWHM ≈ 50 Hz, 1H, Ar-H), 7.19-7.08 (overlapping m, 5H, Ar-H), 7.02-6.97 (m, 2H, Ar-H), 6.79 (br, FWHM ≈ 30 Hz, 1H, Ar-H), 6.61 (br, FWHM ≈ 35 Hz, 1H, Ar-H), 5.06 (s, 1H, C-H), 3.67 (overlapping br, FWHM ≈ 50 Hz, 2H, -$CHMe_2$), 3.56 (overlapping br, FWHM ≈ 65 Hz, 3H, O-CH_3), 3.38 (overlapping br, FWHM ≈ 50 Hz, 3H, O-CH_3), 3.11 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 1.61 (s, 6H, CH_3), 1.52 (br d, FWHM = 16 Hz, 6H, Dipp-CH_3), 1.21 (br d, FWHM = 16 Hz, 6H, Dipp-CH_3), 1.06 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 0.44 (br, FWHM ≈ 40 Hz, 6H, Dipp-CH_3) ppm; **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 169.43, 167.39, 144.75, 144.58, 140.22, 139.48, 129.27, 126.85, 124.09, 123.92, 120.30, 107.72, 97.33, 53.60 (s, O-CH_3), 51.76 (s, O-CH_3), 28.60, 26.99, 24.64, 24.49, 24.21, 23.86, 22.96 ppm. The C-Al resonance could not be observed due to line-broadening associated with coupling to the quadrapolar *I* = 5/2 ^{27}Al nucleus. A peak for the

solvent of crystallisation $(SiMe_3)_2O$ was observed in the ^1H NMR spectrum at δ 0.10 (s) ppm and the $^{13}C\{^1H\}$ NMR spectrum at δ 1.70 (s) ppm.

2.3.3 Synthesis of Dipp-*BDI*Al(OMe)(3,5-$Me_2C_6H_3$) (4d)



In a glove box, Dipp-*BDI*Al(I) (**1**, 5.0 mg, 0.0113 mmol) and [$Pd(PCy_3)_2$] (50 µL, 0.0113 M solution in cyclohexane, 0.00056 mmol, 5 mol%) were dissolved in cyclohexane (0.50 mL) and 3,5-dimethylansiole (3.2 µL, 0.0225 mmol, 2 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube, sealed and removed from the glove box. The tube was heated to 40 °C for 96 hours with monitoring by NMR spectroscopy. Once the reaction was complete (in situ yield 78%) the tube was returned to the glove box. The solution was transferred to a 4 mL vial and the solvent removed *in vacuo*. The oily product was dissolved in *n*-heptane (0.3 mL) and stored at -35 °C. Colourless crystals of the product formed, the mother liquor was decanted and the product **4d** dried *in vacuo*. An isolated yield was obtained from a scaled-up reaction using the same conditions and 15.0 mg (0.0338 mmol) of **1**. Isolated yield: 10 mg (51%). **^{1}H NMR** (400 MHz, C_6D_6, 298 K): δ 7.24-7.18 (m, 4H, Ar-H), 7.09-7.05 (m, 2H, Ar-H), 6.71 (s, 1H, H^d), 6.57 (s, 2H, H^b), 4.99 (s, 1H, C-H), 3.75 (overlapping sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 3.75 (overlapping s, 3H, O-CH^a_3), 3.07 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, -$CHMe_2$), 2.03 (s, 6H, CH^c_3), 1.63 (s, 6H, CH_3), 1.50 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.26 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 1.05 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3), 0.82 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-CH_3) ppm; **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 298 K): δ 169.84, 144.81, 143.74, 140.90, 135.75 (s, C-H^b), 134.60 (s, C-CH^c), 128.76 (s, C-H^d), 127.00, 124.45, 123.96, 97.67, 51.63 (s, C-H^a), 28.59, 27.84, 25.13, 24.40, 23.36, 22.97, 21.14 (s, C-H^c) ppm. The C–Al resonance could not be observed due to line-broadening associated with coupling to the quadrapolar *I* = 5/2 ^{27}Al nucleus.

3. X-ray Crystallographic Data

3.1 Tabulated X-ray Data

Compound	**3a**	**3c**	**4a**
CCDC No.	1973118	1973122	1973119
Formula	$C_{36}H_{49}AlN_2O$	$C_{39}H_{55}AlN_2O_3$	$C_{36}H_{49}AlN_2O$
M	552.75	626.83	552.75
Crystal System	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/c$ (14)	*P*-1 (2)	$C2/c$ (15)
T [K]	173(2)	173(2)	173(2)
a [Å]	9.1329(4)	14.1139(8)	17.6433(3)
b [Å]	36.3892(15)	14.5855(9)	20.3069(3)
c [Å]	10.2426(4)	18.1458(10)	18.5103(3)
α [°]	90	82.674(5)	90
β [°]	96.380(3)	80.349(5)	95.838(2)
γ [°]	90	88.508(5)	90
V [Å^3]	3382.9(2)	3652.5(4)	6597.49(18)
Z	4	4	8
Density [g cm^{-3}]	1.085	1.140	1.113
Radiation Used	Mo-Kα	Mo-Kα	Cu-Kα
μ (mm^{-1})	0.088	0.093	0.744
θ range [deg]	$2.508 \leq \theta \leq 28.364$	$2.304 \leq \theta \leq 28.346$	$3.328 \leq \theta \leq 73.345$
Reflns collected	11733	21313	10961
R_{int}	0.0355	0.0252	0.0211
Completeness	0.985	0.986	0.981
No. of data/restr/param	6749/0/372	14412/0/837	6280/0/372
R_1 [$I > 2\sigma(I)$]	0.0633	0.0482	0.0490
wR_2 [all data]	0.1620	0.1320	0.1438
GoF	1.088	1.020	1.050
Largest diff. pk and hole [eÅ^{-3}]	0.32/-0.30	0.32/-0.34	0.63/-0.32

Table S3.1: Crystal Data, Data Collection and Refinement Parameters for the structures of **3a**, **3c, 4a**.

Compound	**4b**	**4d**
CCDC No.	1973120	1973121
Formula	$C_{37}H_{51}AlN_2O_2$	$C_{38}H_{53}AlN_2O$
M	582.77	580.80
Crystal System	Orthorhombic	Monoclinic
Space group	*Pbca* (61)	$P2_1/c$ (14)
T [K]	173(2)	173(2)
a [Å]	8.8671(2)	11.4499(4)
b [Å]	22.1194(7)	18.5015(6)
c [Å]	38.8787(11)	17.1875(5)
α [°]	90	90
β [°]	90	104.408(3)
γ [°]	90	90
V [Å^3]	7625.5(4)	3526.5(2)
Z	8	4
Density [g cm^{-3}]	1.015	1.094
Radiation Used	Mo-Kα	Mo-Kα
μ (mm^{-1})	0.083	0.087
θ range [deg]	$2.530 \leq \theta \leq 28.172$	$2.519 \leq \theta \leq 28.158$
Reflns collected	17191	12722
R_{int}	0.0229	0.0221
Completeness	0.991	0.990
No. of data/restr/param	7744/0/391	7088/0/392
R_1 [$I > 2\sigma(I)$]	0.0552	0.0480
wR_2 [all data]	0.1434	0.1238
GoF	1.045	1.019
Largest diff. pk and hole [eÅ^{-3}]	0.30/-0.27	0.28/-0.23

Table S3.1 cont: Crystal Data, Data Collection and Refinement Parameters for the structures of **4b**, and **4d**.

Table S3.1 provides a summary of the crystallographic data for the structures of **3a**, **3c**, **4a**, **4b**, **4d**. Data were collected using Agilent Xcalibur 3 E (**3a**, **3c**, **4b**, **4d**) and Xcalibur PX Ultra A (**4a**) diffractometers, and the structures were refined using the SHELXTL and SHELX-2014 program systems.[4]

[4] SHELXTL v5.1, Bruker AXS, Madison, WI, 1998. SHELX-2014, G.M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.

3.2 X-ray crystal structures

3.2.1 The X-ray crystal structure of 3a

The crystal structure of **3a** presented no significant issues.

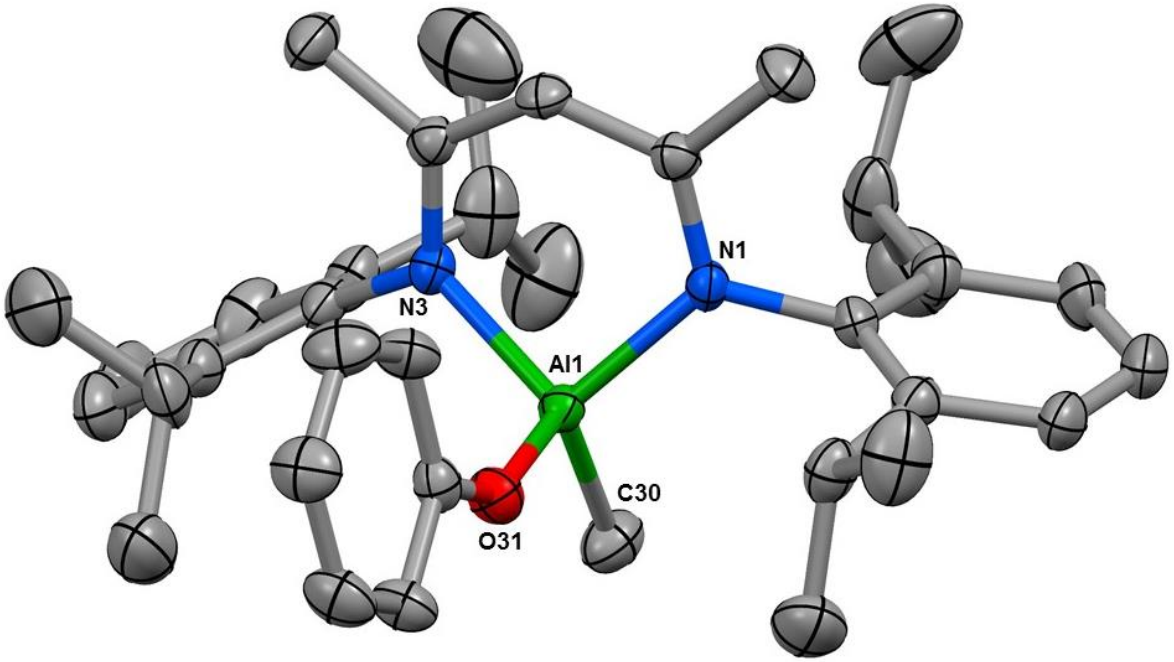


Figure S3.1: The crystal structure of **3a** (50% probability ellipsoids). Hydrogen atoms omitted for clarity.

3.2.2 The X-ray crystal structure of 3c

The crystal structure of **3c** contains two independent molecules in the asymmetric unit.

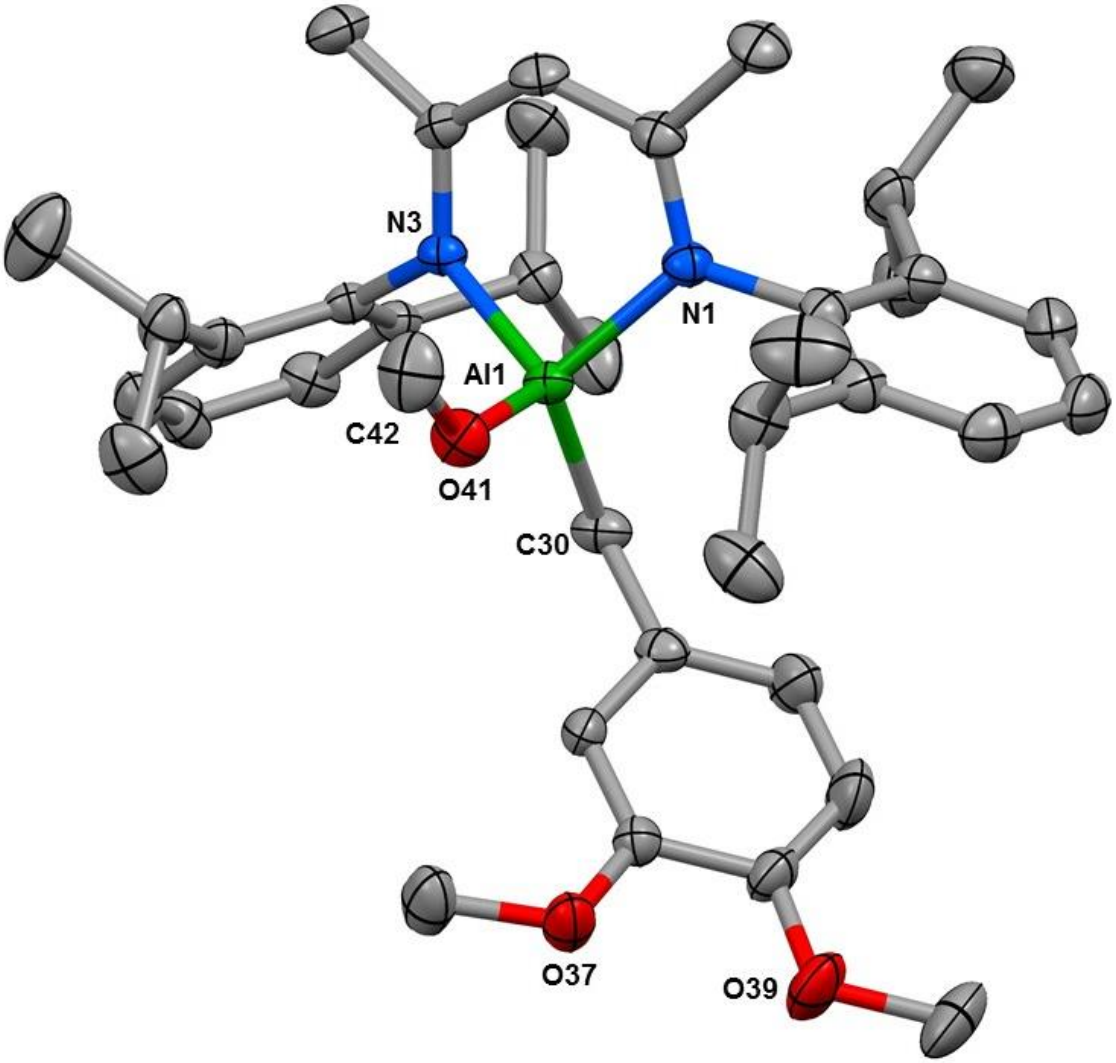


Figure S3.2: The crystal structure of **3c** (50% probability ellipsoids). Hydrogen atoms and second independent molecule omitted for clarity.

3.2.3 The X-ray crystal structure of 4a

The crystal structure of **4a** presented no significant issues.

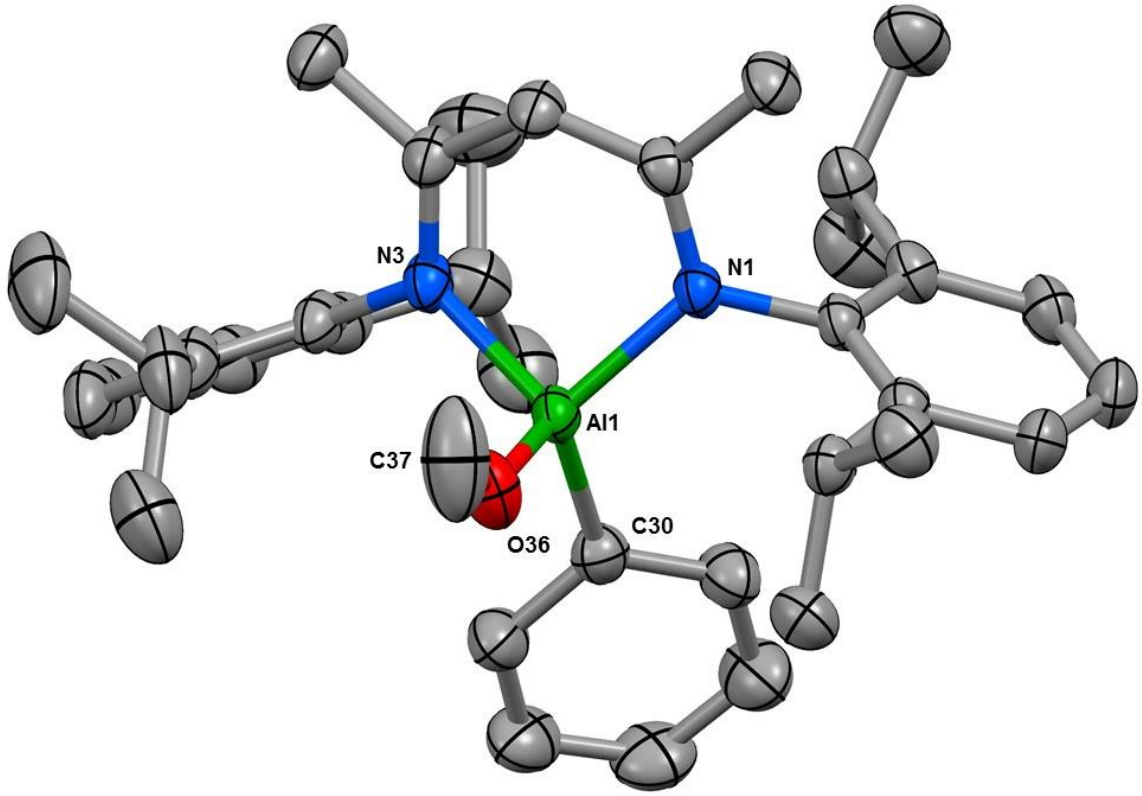


Figure S3.3: The crystal structure of **4a** (50% probability ellipsoids). Hydrogen atoms omitted for clarity.

3.2.4 The X-ray crystal structure of 4b

The crystal structure of **4b** contained a large void with disordered solvent of crystallization *n*-heptane within it. Attempts to model these molecules were unsuccessful so the SQUEEZE programme was used to remove this electron density.

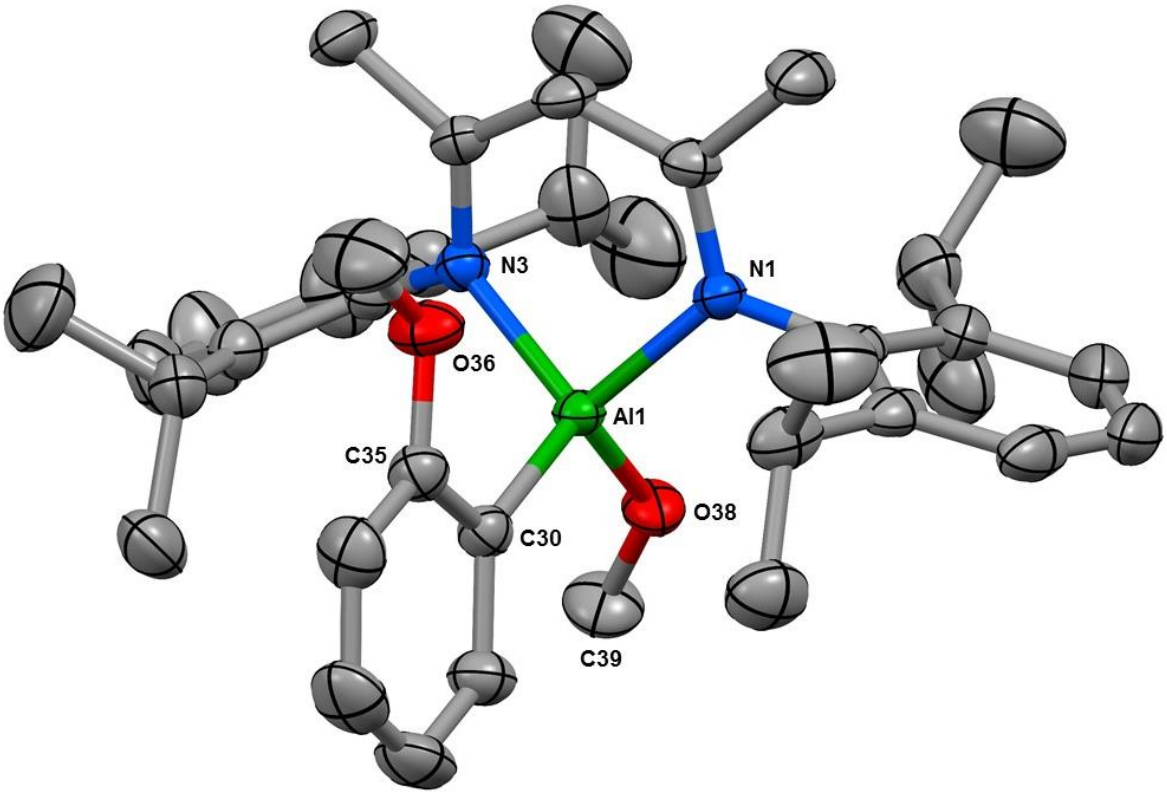


Figure S3.4: The crystal structure of **4b** (50% probability ellipsoids). Hydrogen atoms omitted for clarity.

3.2.5 The X-ray crystal structure of 4d

The crystal structure of **4d** presented no significant issues.

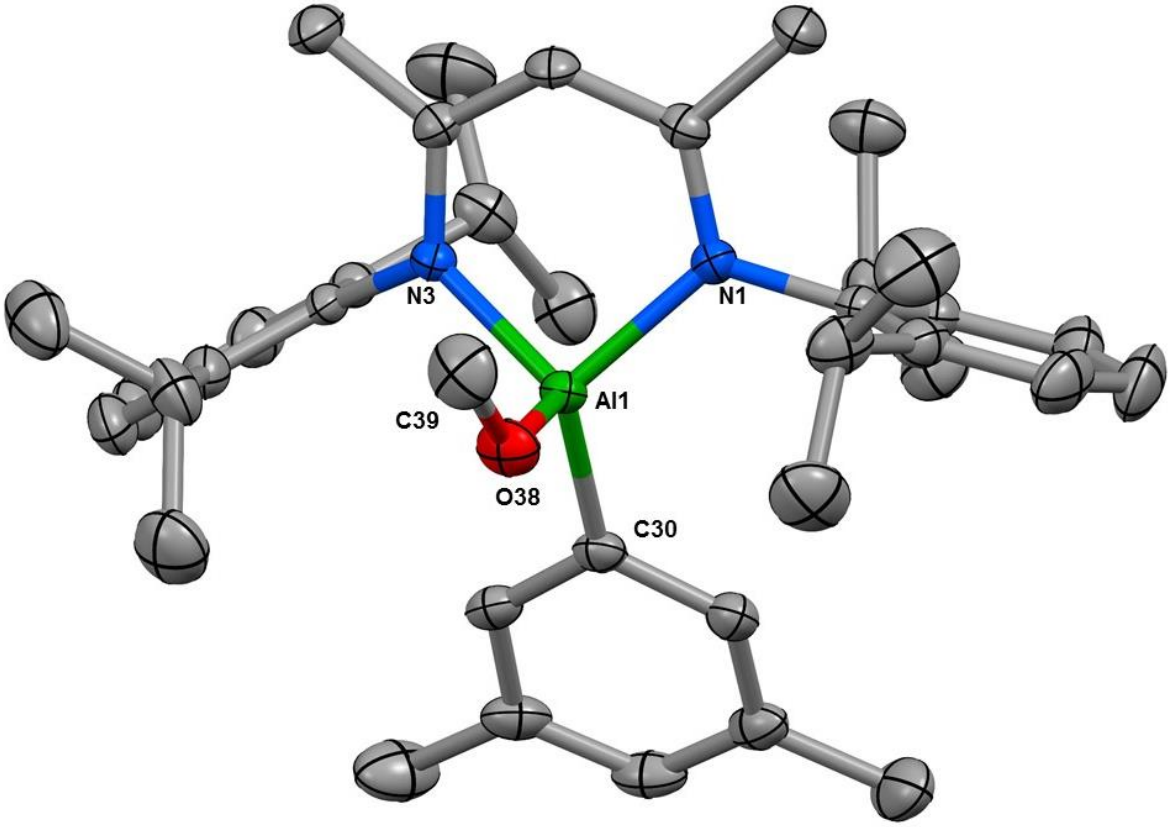


Figure S3.5: The crystal structure of **4d** (50% probability ellipsoids). Hydrogen atoms omitted for clarity.

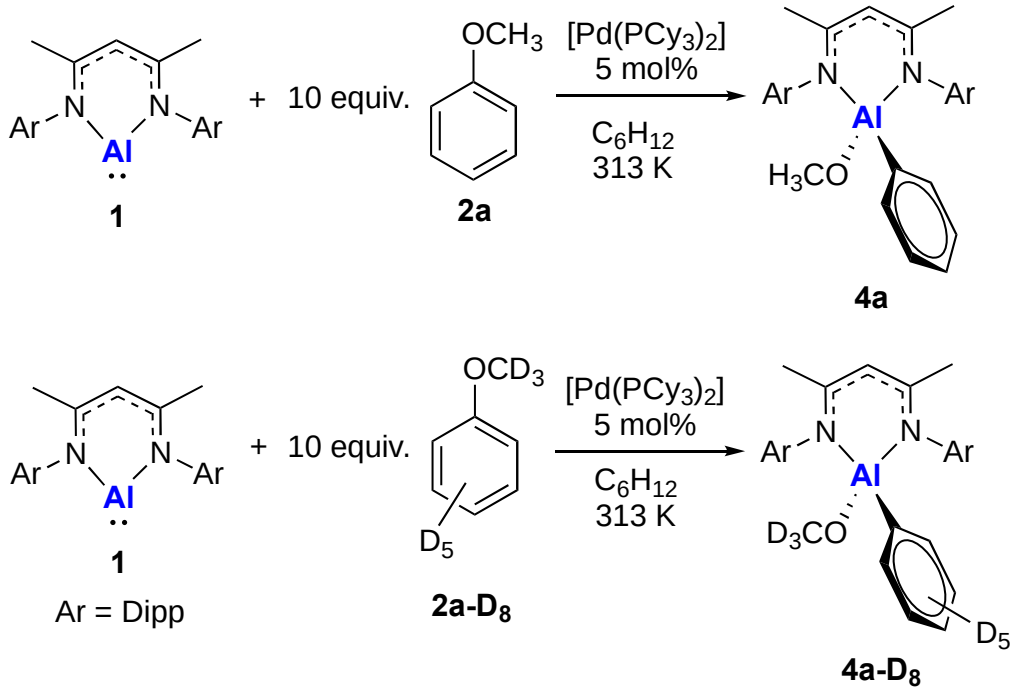
4. Kinetic Studies by NMR Spectroscopy

4.1 Kinetic Studies by NMR Spectroscopy

4.1.1 Kinetic Isotope Effect Measurement for the Palladium Catalysed Alumination of Anisole to form 4a through Measurement of Rate Constants

Experimental Procedure

1 (0.40 mL of 0.0225 M standard solution in C_6H_{12}, 0.0090 mmol) was added to a vial. A solution of anisole or anisole-D_8 (50.0 µL, 1.80 M standard solution in C_6H_{12}, 0.090 mmol, 10 equiv.) was added followed by a solution of [$Pd(PCy_3)_2$] (180.0 µL, 0.0025 M standard solution in C_6H_{12}, 0.00045 mmol, 0.05 equiv.). The solution was mixed and transferred to a Young's NMR tube containing a capillary insert standard (ferrocene in C_6D_6). The tube was sealed, removed from the glove box and frozen in liquid nitrogen while transported directly to the NMR spectrometer. The sample was warmed to room temperature and loaded into the spectrometer pre-set at 313 K. The sample was locked to the C_6D_6 standard and shimmed and the first ^1H NMR spectrum recorded ~5 min after mixing.



Scheme S4.1: Parallel reactions for KIE measurement for palladium catalysed C–O alumination of anisole by **1**.

A plot of ln[**1**] (determined from initial concentration and integration against internal standard) vs time for both reactions using anisole or anisole-D_8 indicated the reaction is (pseudo)-first order in [**1**]. The data was cut off after 3 half-lives, 87.5% conversion. Standard errors were calculated by use of the regression analysis calculation in Microsoft Excel software. The rate constant for the anisole reaction was found to be $k_{C\text{-}H}$ = 7.67 x 10^{-5} (± 2.16 x 10^{-6}) s^{-1} and $k_{C\text{-}D}$ = 6.12 x 10^{-5} (± 1.21 x 10^{-6}) s^{-1} for anisole-D_4 at 313 K. This gave a KIE of 1.3 (± 0.1) for the reaction.

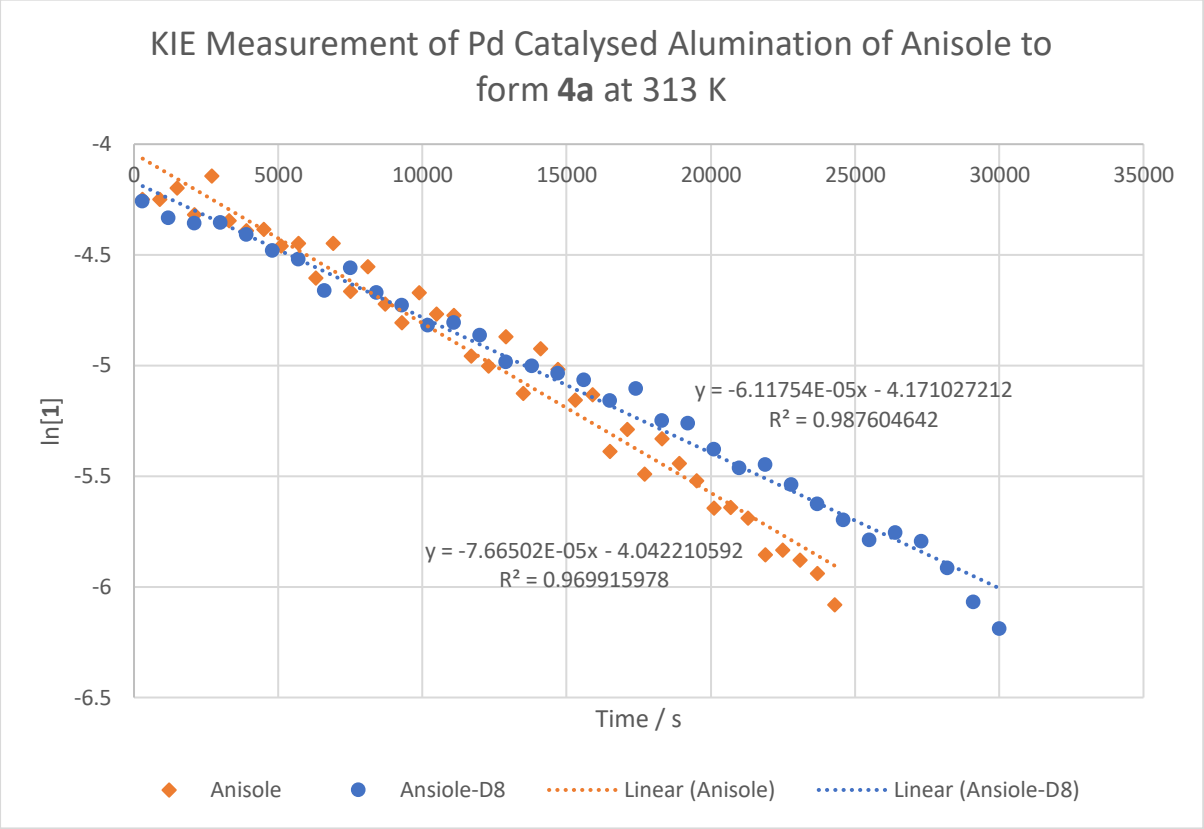
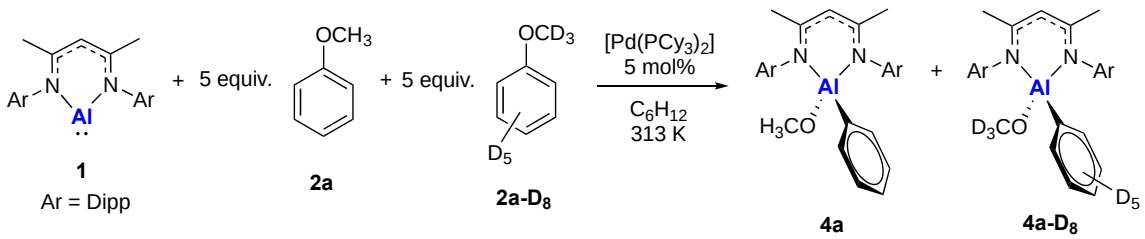


Figure S4.1: Kinetic study of the palladium catalysed C–O alumination of anisole to determine the kinetic isotope effect.

4.1.2 Kinetic Isotope Effect Measurement for the Palladium Catalysed Alumination of Anisole to form 4a through Measurement of Product Ratios from a Competition Experiment



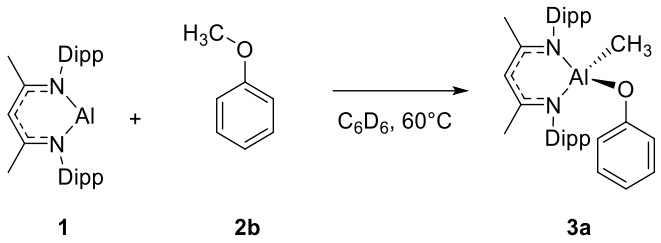
Scheme S4.2: Competition experiment for KIE measurement for palladium catalysed C–O alumination of ansiole by **1**.

Experimental Procedure

1 (0.40 mL of 0.0225 M standard solution in C_6H_{12}, 0.0090 mmol) was added to a vial. A solution of anisole (25.0 µL, 1.80 M standard solution in C_6H_{12}, 0.045 mmol, 5 equiv.) and anisole-D_8 (25.0 µL, 1.80 M standard solution in C_6H_{12}, 0.045 mmol, 5 equiv.) were added followed by a solution of $[Pd(PCy_3)_2]$ (180.0 µL, 0.0025 M standard solution in C_6H_{12}, 0.00045 mmol, 0.05 equiv.). The solution was mixed and transferred to a Young's NMR tube containing a capillary insert standard (ferrocene in C_6D_6). The tube was sealed, removed from the glove box and the ^{1}H NMR spectrum measured. The tube was then heated to 313 K for 18 h whereupon the reaction was complete and **1** had been consumed. The ^{1}H NMR spectrum was measured and the tube returned to the glove box. The solvent was removed in vacuo and the oily product redissolved in C_6D_6. The ^{1}H NMR spectrum was measured again and the relative ratio of **4a**:**4a-D$_8$** determined by integration of the diketiminate ligand signals versus signals for C–O aluminated anisole. The KIE was determined to be 1.2 (± 0.1).

4.1.2 Kinetic Analysis to determine the rate dependence in 1 for the non Catalysed Alumination reaction of Anisole

In order to verify the rate dependence in Al(I) in the reaction, reaction progression was monitored for four different initial concentrations of **1** (0.0093 M; 0.028 M; 0.037 M and 0.075 M).



1 **2b** **3a**

Scheme S4.3: Kinetic analysis for the non catalysed C–O alumination of **2b** to form **3a** for four different initial concentrations of **1**

In a glovebox, Dipp-BDIAl(I) (**1**) was dissolved in cyclohexane (0.6 mL) and anisole (122 µL) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube containing a capillary insert standard (ferrocene in C_6D_6) and sealed. The tube was removed from the box and heated to 60 °C for 361 hours with monitoring by NMR spectroscopy. Conversions were calculated from reagent and product concentrations, based on integration value, relative to the internal standard (ferrocene). Kinetics are plotted for one half-life (approx. 50% production of **3a**).

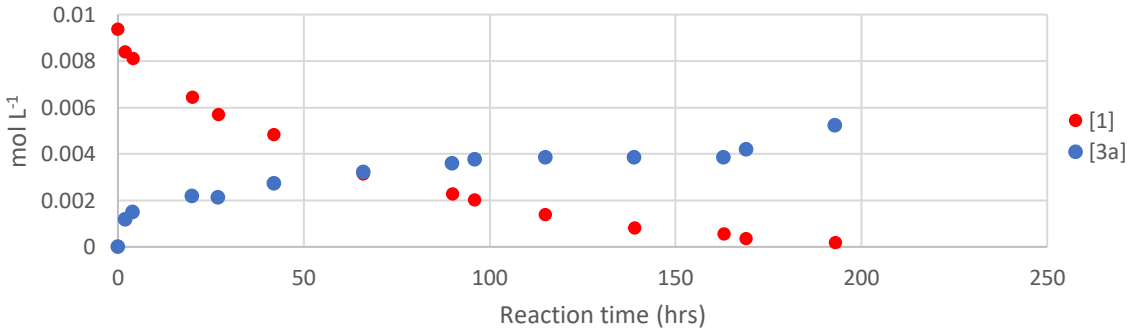


Figure S4.2. Plot of the concentration *vs* time for the reaction between the Al(I) complex (**1**) and Anisole to form **3a** with an initial concentration of **0.0093 M** in **1.**

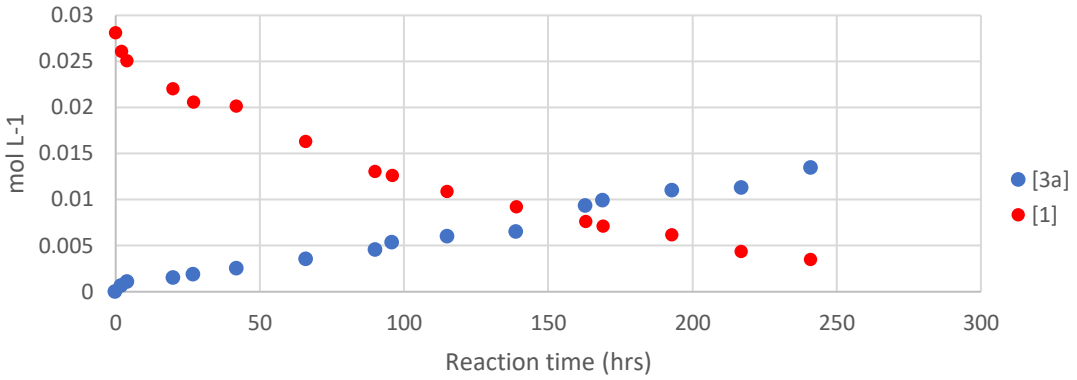


Figure S4.3. Plot of the concentration *vs* time for the reaction between the Al(I) complex (**1**) and Anisole to form **3a** with an initial concentration of **0.028 M** in **1**.

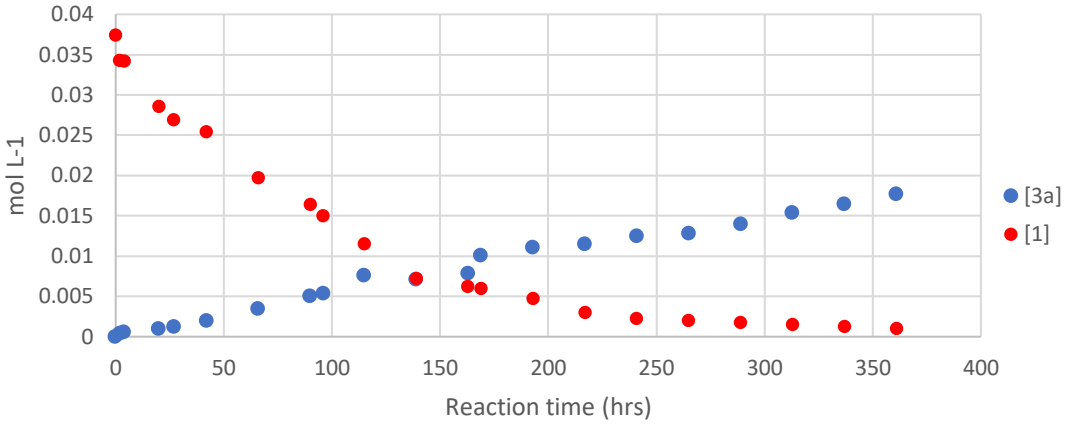


Figure S4.4. Plot of the concentration vs time for the reaction between the Al(I) complex (**1**) and Anisole to form **3a** with an initial concentration of **0.037 M** in **1**.

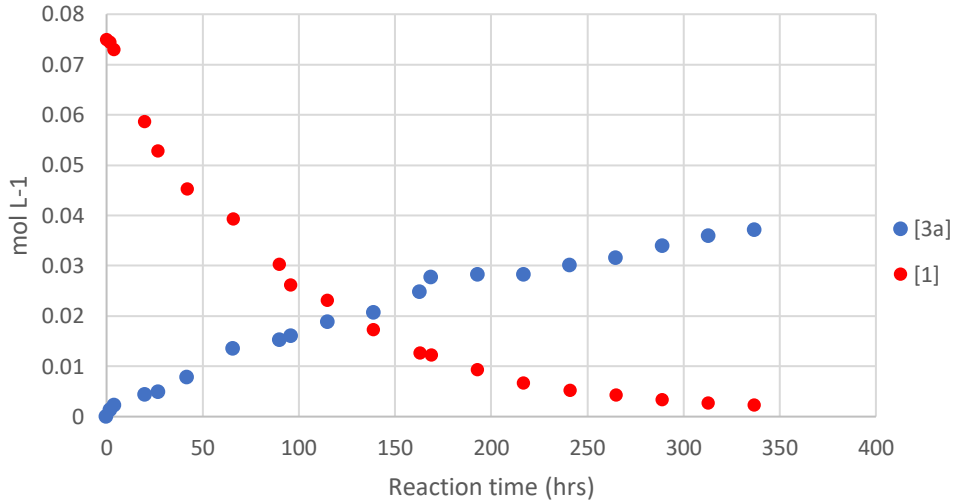


Figure S4.5 Plot of the concentration vs time for the reaction between the Al(I) complex (**1**) and Anisole to form **3a** with an initial concentration of **0.075 M** in **1.**

Data were fitted using standard approaches. A plot of ln[**1**] vs time showed linear fits for indicating the reaction is (pseudo)-first order under these conditions. These fits gave the better r^2-values compared to both 0^{th} order and 2^{nd} order fits. First order kinetics was confirmed across a series of initial concentrations of **1** (**Figure S4.6** - **Figure S4.9**). Similar linear fits could be plotted for production of **3a**.

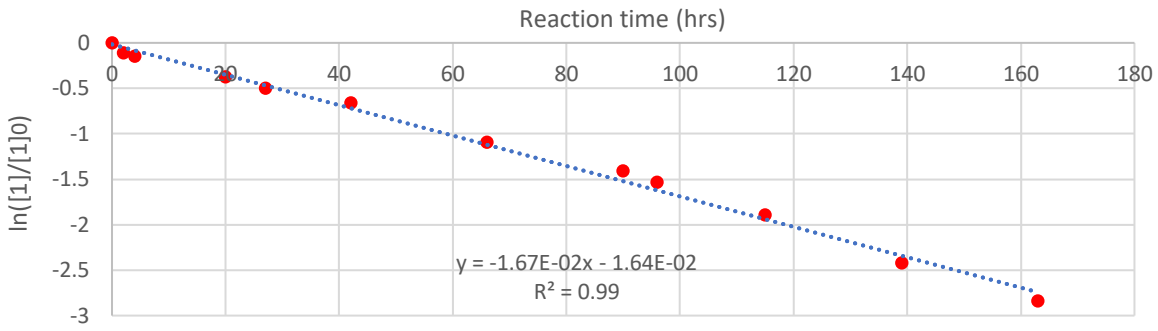


Figure S4.6. Ln plot of the concentration vs time for the reaction between the Al(I) complex (1) and Anisole to form **3a** with an initial concentration of **0.0093 M** in **1.**

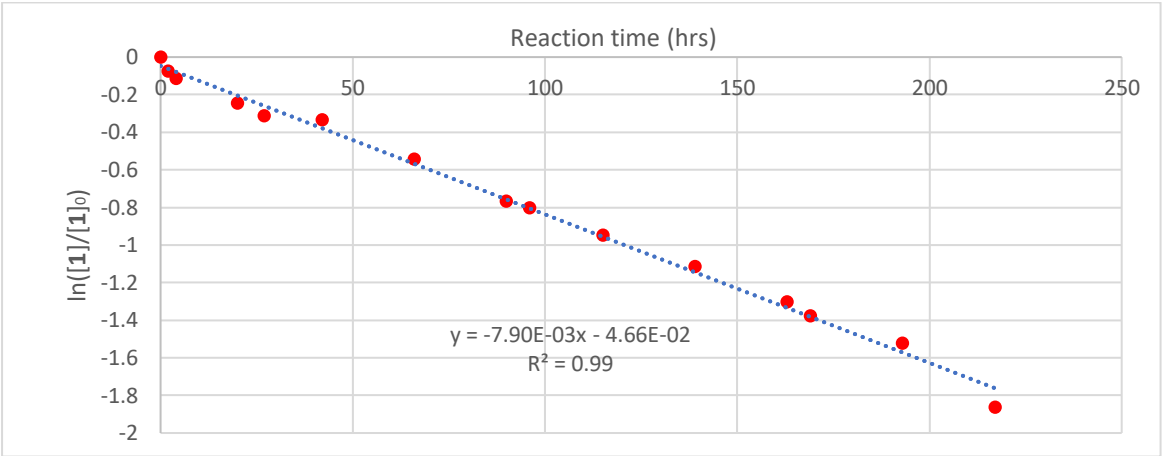


Figure S4.7. Ln plot of the concentration vs time for the reaction between the Al(I) complex (1) and Anisole to form **3a** with an initial concentration of **0.028 M** in **1.**

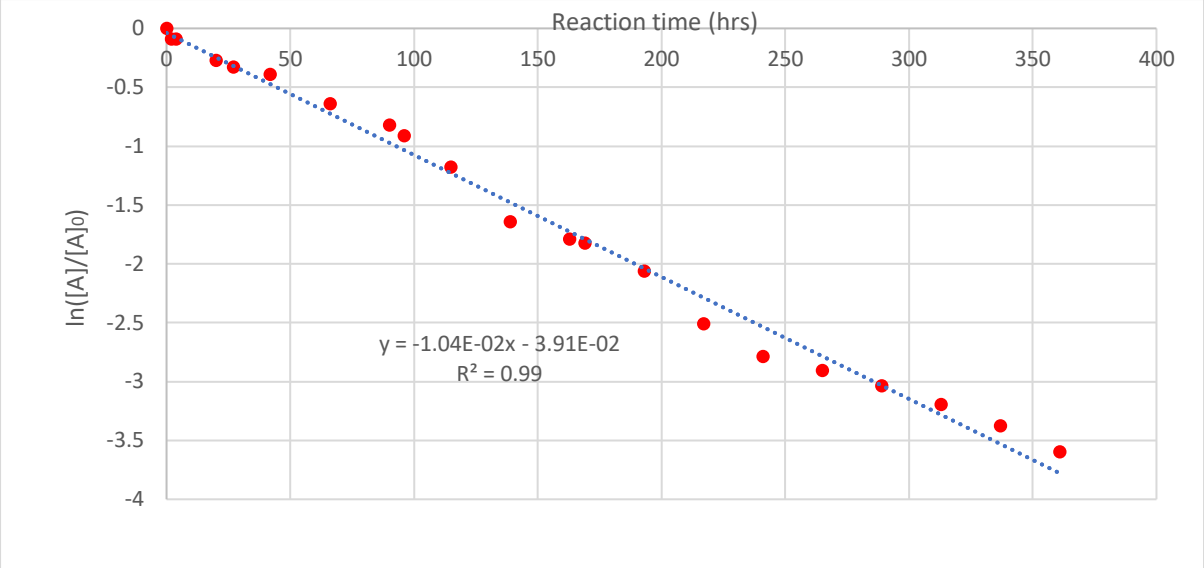


Figure S4.8. Ln plot of the concentration vs time for the reaction between the Al(I) complex (1) and Anisole to form **3a** with an initial concentration of **0.037 M** in **1.**

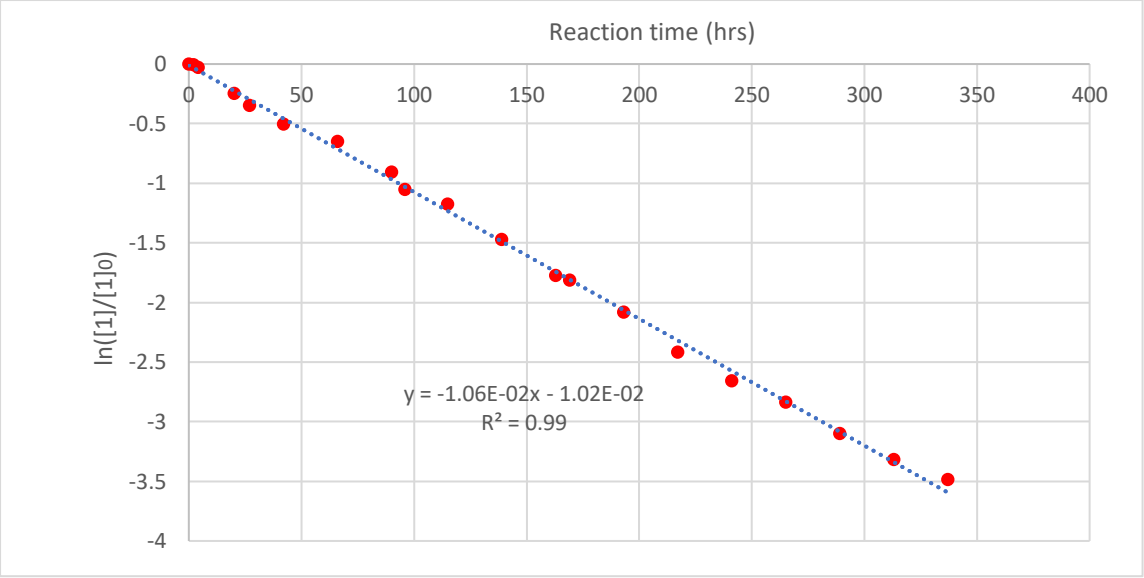


Figure S4.19. Ln plot of the concentration vs time for the reaction between the Al(I) complex (1) and Anisole to form **3a** with an initial concentration of **0.075 M** in **1.**

A plot of 1/[**1**] *vs* time shown for an initial concentration of **0.0093 M** and **0.037 M** in **1** (**Figure S4.10** and **Figure S4.11**, respectively) rules out an order 2 in **1**. This indicates that a bimolecular mechanism, such as an S_N2 mechanism, is feasible and rules out a termolecular reaction in which 2 equiv. of **1** are required to react with anisole.

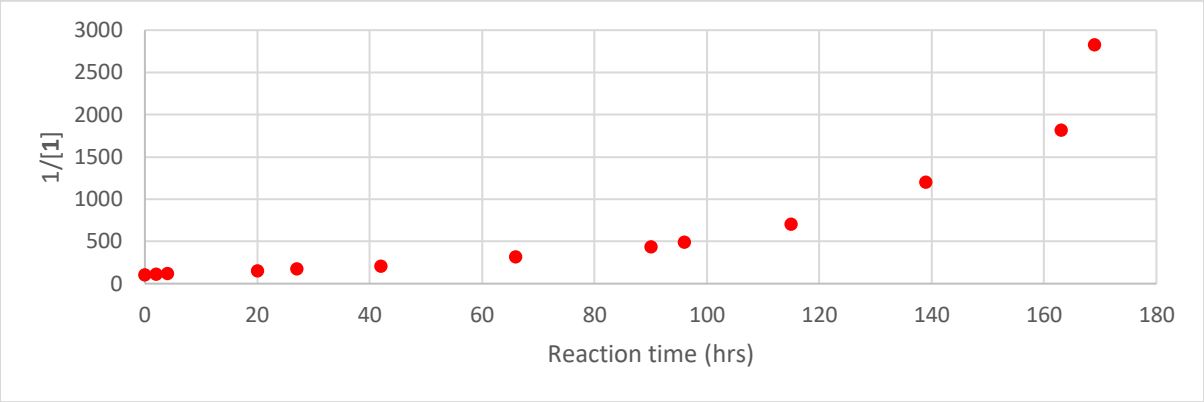


Figure S4.10. 1/[**1**] plot vs time for the reaction between the Al(I) complex (**1**) and Anisole to form **3a** with an initial concentration of **0.0093 M** in **1.**

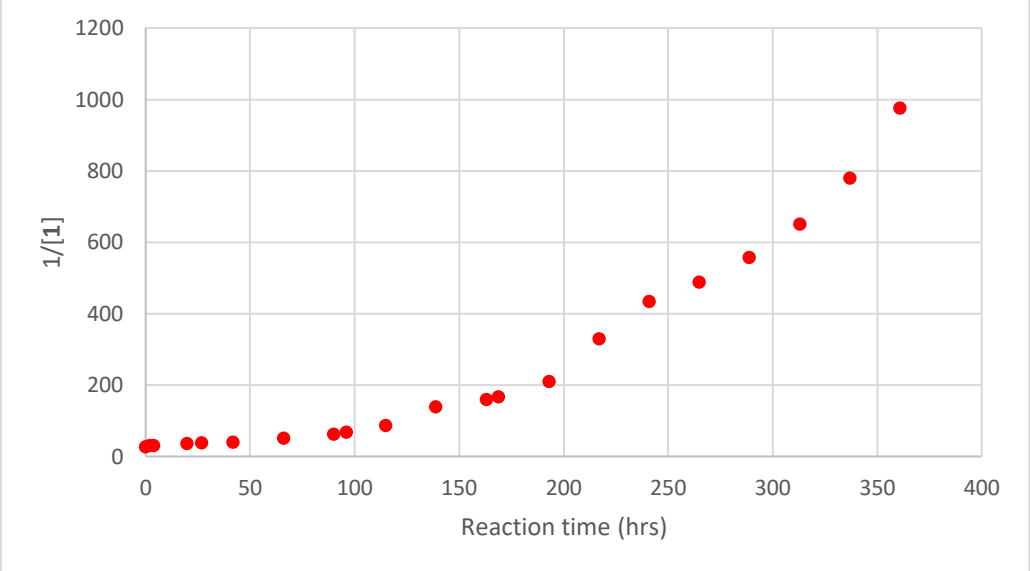


Figure S4.11. 1/[**1**] plot vs time for the reaction between the Al(I) complex (**1**) and Anisole to form **3a** with an initial concentration of **0.037 M** in **1.**

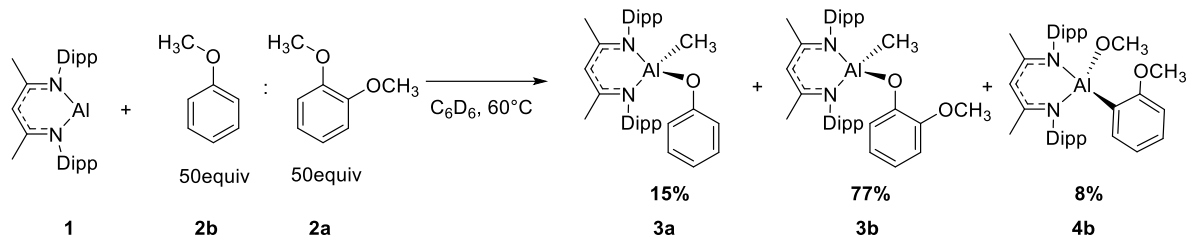
Consideration of the rate constants from the linear fits to first order reveals more complex behaviour.

$[\mathbf{1}]_{initial}$ **(M)**	K_{obs} / h^{-1}
0.0093	1.67×10^{-2}
0.028	7.90×10^{-3}
0.037	1.04×10^{-2}
0.075	1.06×10^{-2}

Table S4.1. Rate constants at different initial concentrations**.**

1st order rates constants at different initial concentrations that rate dependence on $[\mathbf{1}]_{initial}$ is complex. Fastest rates are observed at the lowest and highest concentrations and these data cannot be fitted to a linear dependence. These findings are consistent with more complex kinetic behaviour which is likely a consequence of either (i) side-reactions of **1** at different initial concentrations: one of the major side products is the sp^2 C–O bond activation of anisole (**4a**) which is formed alongside species tentatively assigned as productions from sp^2 C–H bond activation or (ii) **1** playing a more complex role in the reaction beyond a reagent.

5. Competition experiment between 2a and 2b



Scheme S4.3. Competition experiment between **2a** and **2b**

In a glovebox, Dipp-BDIAl(I) (**1**, 5.0 mg, 0.0113 mmol) was dissolved in benzene (0.6 mL) and mixtures of Anisole (61.1 µL, 0.56 mmol, 50 equiv.) and 1,2-dimethoxybenzene (71.6 µL, 0.56 mmol, 50 equiv.) was added by micropipette. The solution was mixed and transferred to a Young's NMR tube containing a capillary insert standard (ferrocene in C_6D_6) and sealed. The tube was removed from the box and heated to 60 °C and monitored by NMR spectroscopy. The reaction was complete after 18 hours at 60 °C.

The yields were determined by NMR spectroscopy using ferrocene as an internal standard (by comparison with the chemical shifts of the isolated C–O products **3a**, **3b** and **4b**). Formation of three species: **3b** (77%), **3a** (15%), and traces of **4b** (8%).

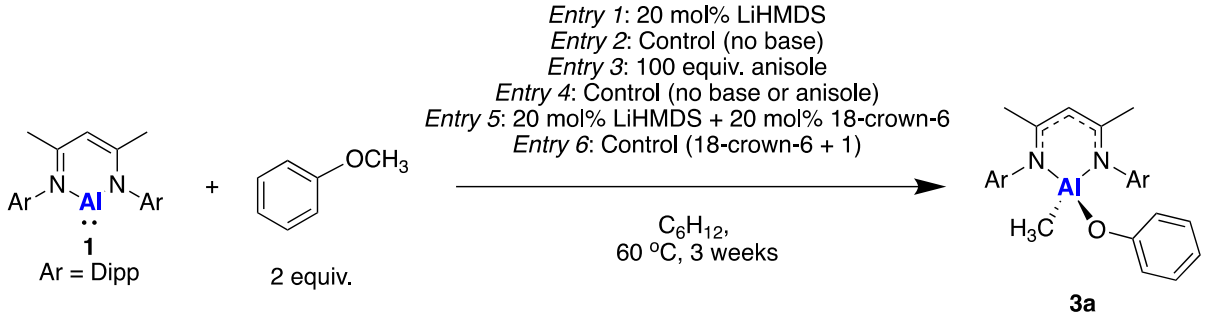
This competition experiment allows a clear conclusion that **2b** reacts fastest than **2a**.

6. Base catalysed reaction of 1 with anisole

Control reactions in which **1** was reacted with 2 equiv. of anisole in the presence and absence of 20 mol% [Li{N(SiMe$_3$)$_2$}] at 60 °C led to the formation of **3a** in 46% and 20% yield respectively. The minor product of these reactions was a known decomposition product of **1.**[35] Based on these findings it seems plausible that base catalysis may be operating in the reaction of **1** with anisole and the necessity for a vast excess of substrate may be to promote the formation of catalytic base *in situ* that can deprotonate **1** (see section 6.2.2 for relevant DFT calculations).

Experimental Procedure

In a glovebox, **1** (5.0 mg, 0.0113 mmol) was dissolved in cyclohexane (0.55 mL) and anisole (12.5 µL, 1.80 M in C_6H_{12}, 0.0225 mmol, 2 equiv.) was added by micropipette. In a separate vial, an aliquot of a Li[N(SiMe$_3$)$_2$] (LiHMDS) stock solution (45.0 µL, 0.1 M in toluene, 0.00225 mmol, 20 mol %) was dried *in-vacuo.* The solid Li[N(SiMe$_3$)$_2$] residue was then dissolved in prepared C_6H_{12} solution containing **1** and anisole. The solution was mixed and transferred to a Young's NMR tube loaded with a capillary tube containing a 0.01 M solution of ferrocene in C_6D_6, and sealed. The tube was removed from the glovebox and a ^{1}H NMR spectrum was recorded before heating at 60 °C for 3 weeks, unless otherwise stated.



Scheme S6.1: Parallel reactions for the base catalysed C–O alumination of anisole by **1**.

Entry	Anisole (mmol)	LiHMDS (mmol)	18-crown-6 (mmol)	**3a**
1	0.0225	0.00225	-	49.1% (46.1%)[a]
2	0.0225	-	-	13.7% (19.8%)[a]
3[b]	1.13	-	-	71% (73%)[a]
4	-	-	-	n/a
5[d]	0.0225	0.00225	0.00225	18.3%
6[d]	-	-	0.00225	n/a

Table S6.1: Reaction conditions and yields for the formation of **3a**. Yields derived by integrations of product peaks against a ferrocene internal standard. *a:* Value in brackets derived from a repeat experiment. *b:* reaction time of 3 days. *c:* 18-crown-6 added by micropipette (22.5 µL, 0.01 M in C_6H_{12}, 0.00225 mmol, 20 mol %).

7. NMR Spectra of complexes

Figure S7.1: ^{1}H NMR spectrum of complex **3a**

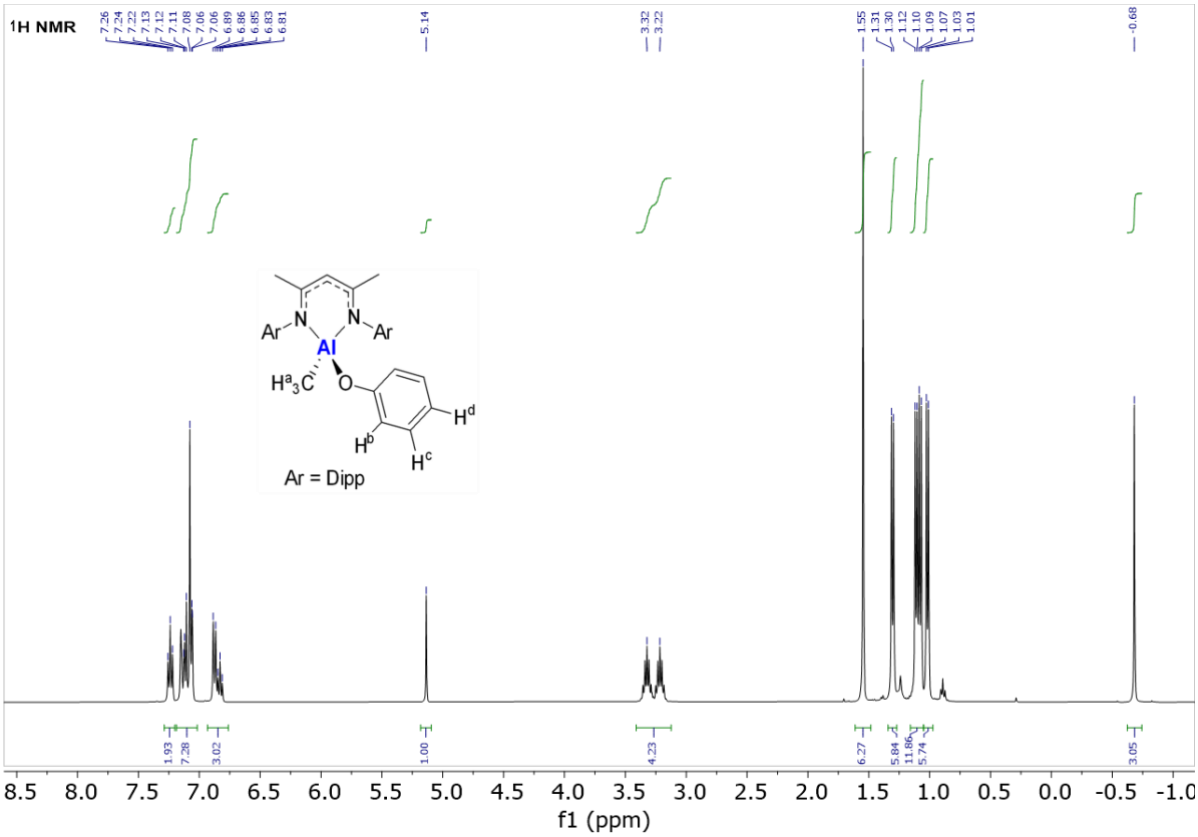


Figure S7.2: ^{13}C{^{1}H} NMR spectrum of complex **3a**

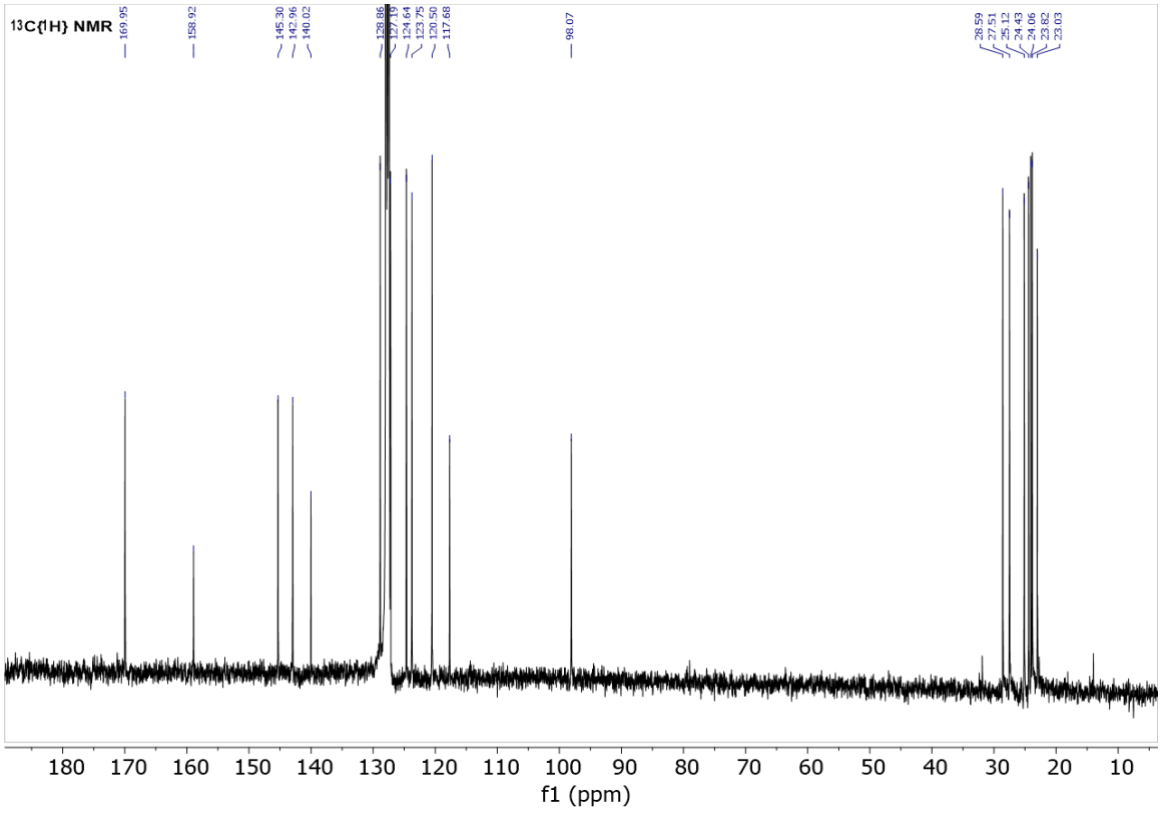


Figure S7.3: ^{1}H NMR spectrum of complex **3b**

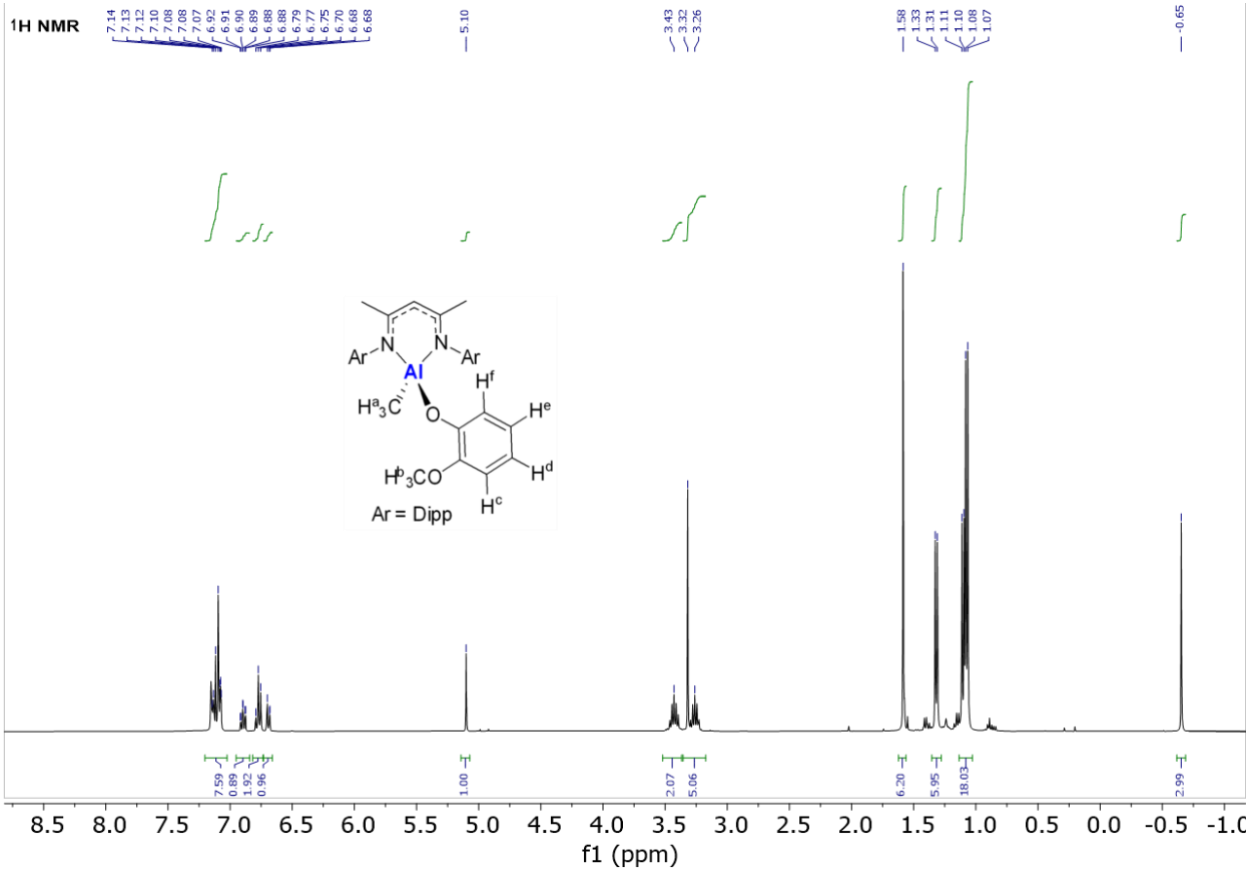


Figure S7.4: ^{13}C{^{1}H} NMR spectrum of complex **3b**

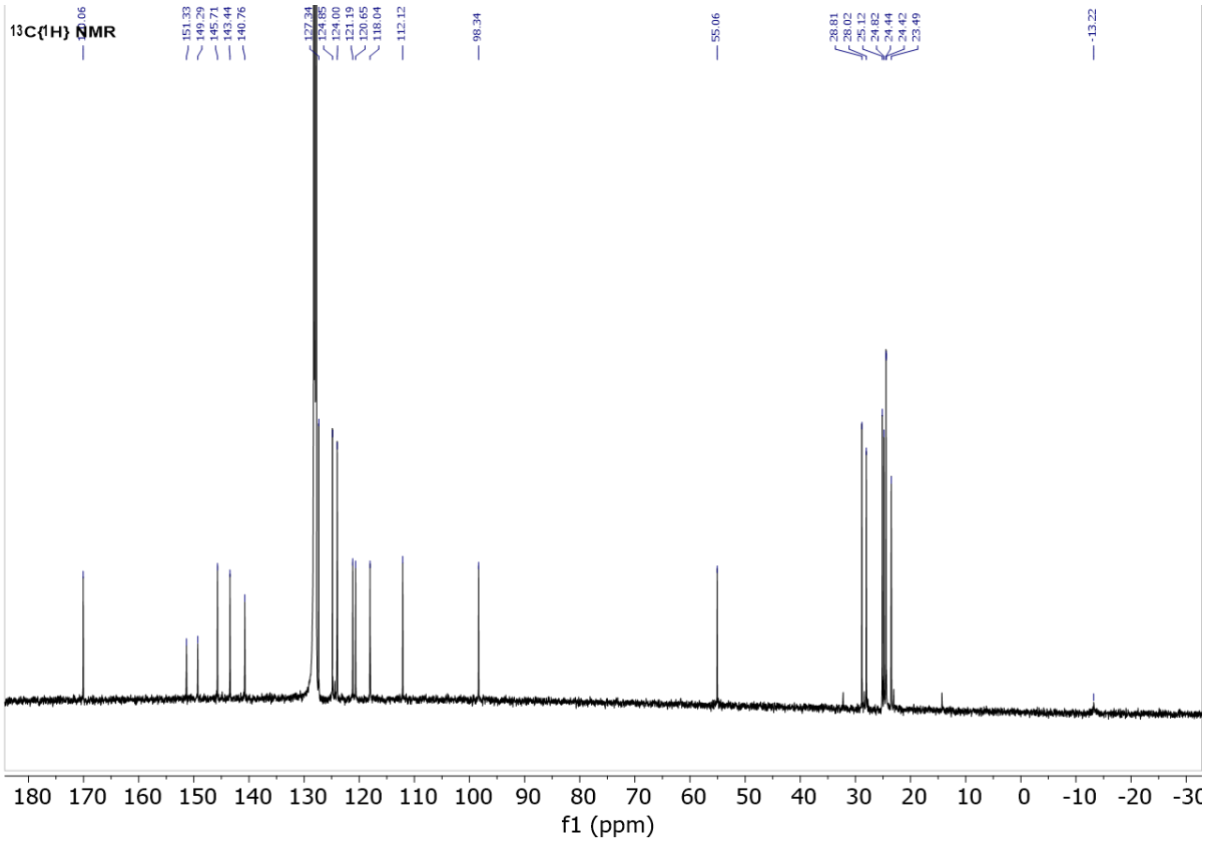


Figure S7.5: ^{1}H NMR spectrum of complex **3c**

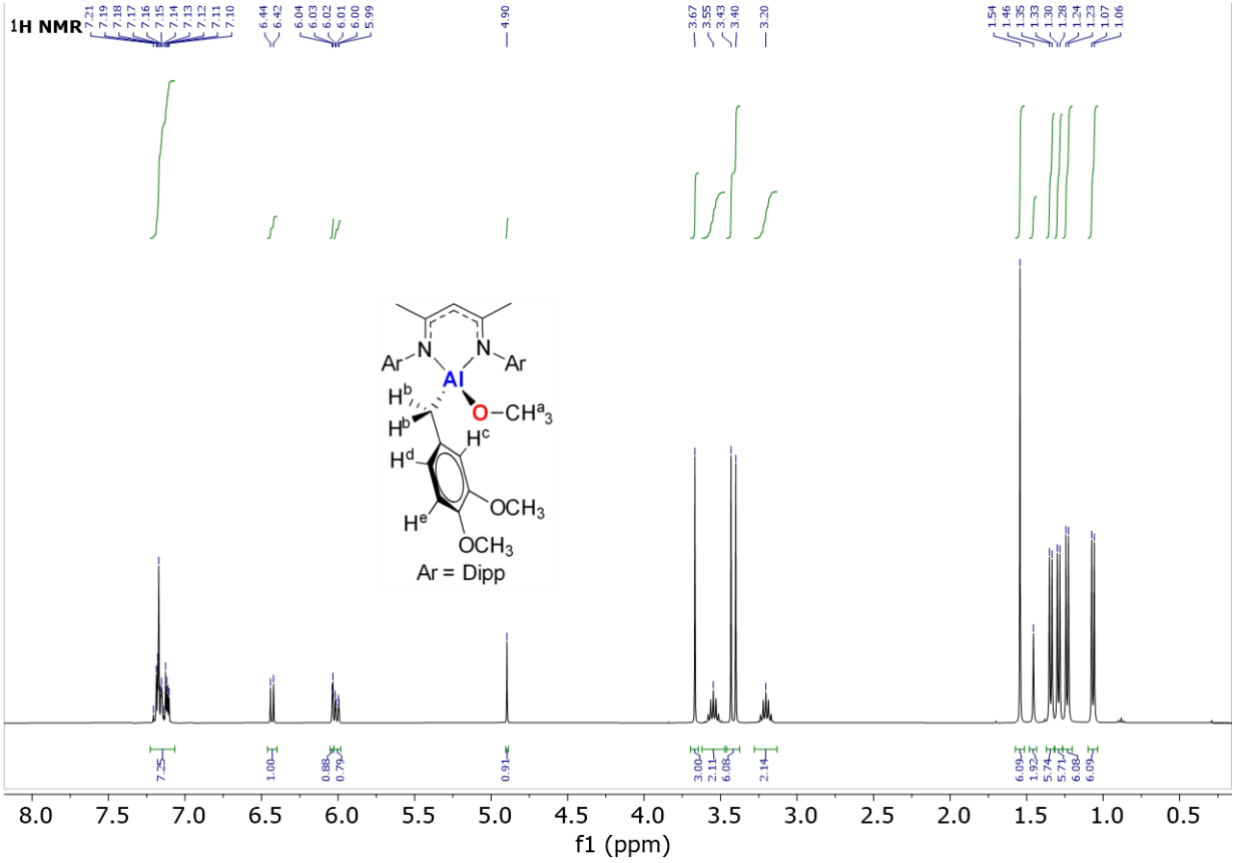


Figure S7.6: ^{13}C{^{1}H} NMR spectrum of complex **3c**

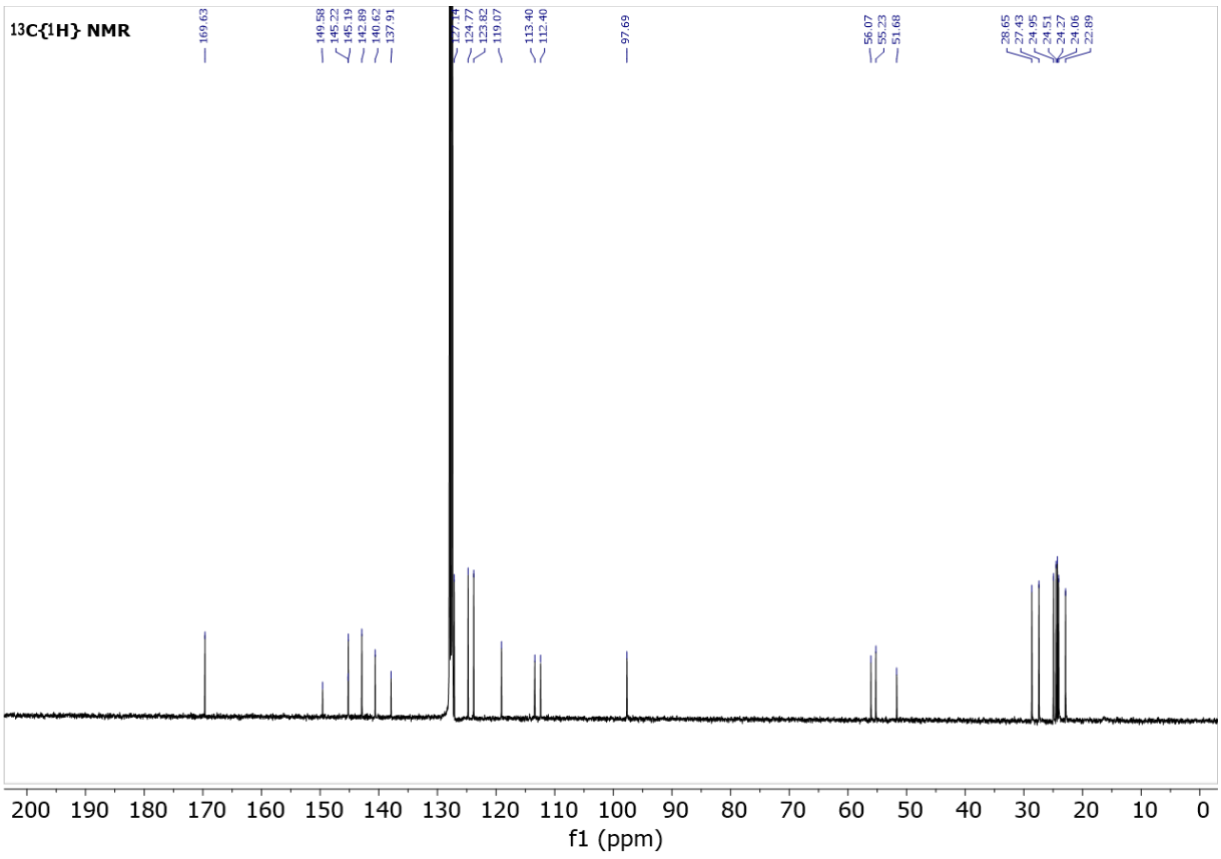


Figure S7.7: ^{1}H NMR spectrum of complex **4a**

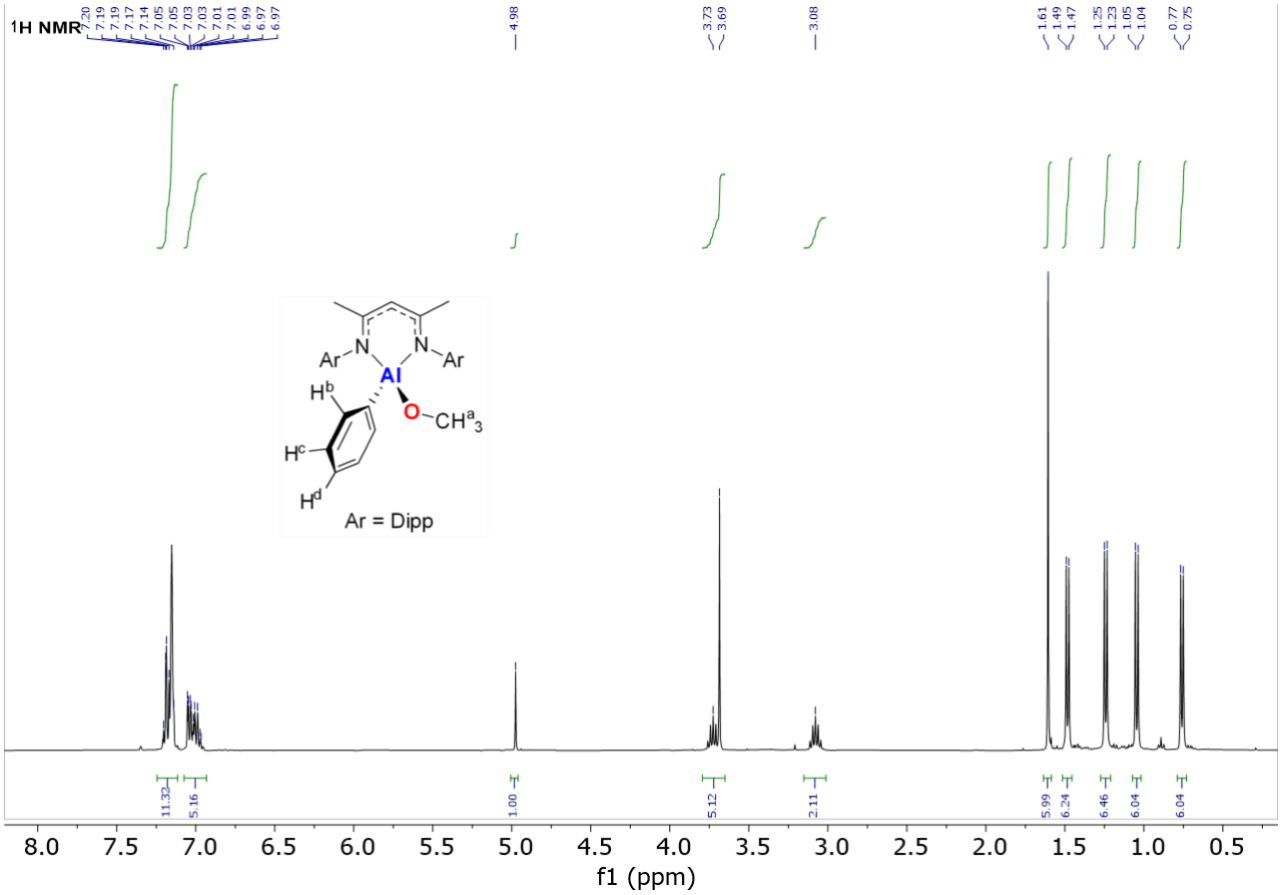


Figure S7.8: ^{13}C{^{1}H} NMR spectrum of complex **4a**

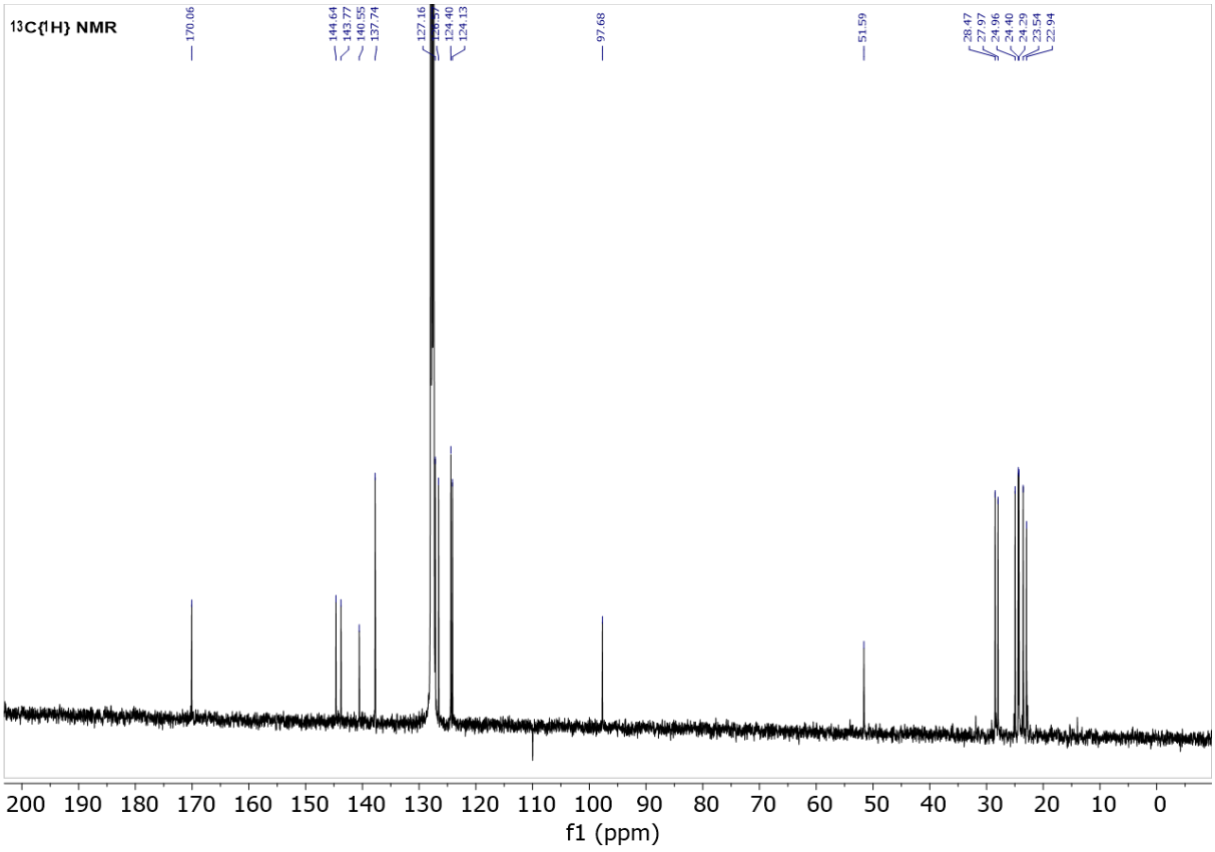


Figure S7.9: ^{1}H NMR spectrum of complex **4b**

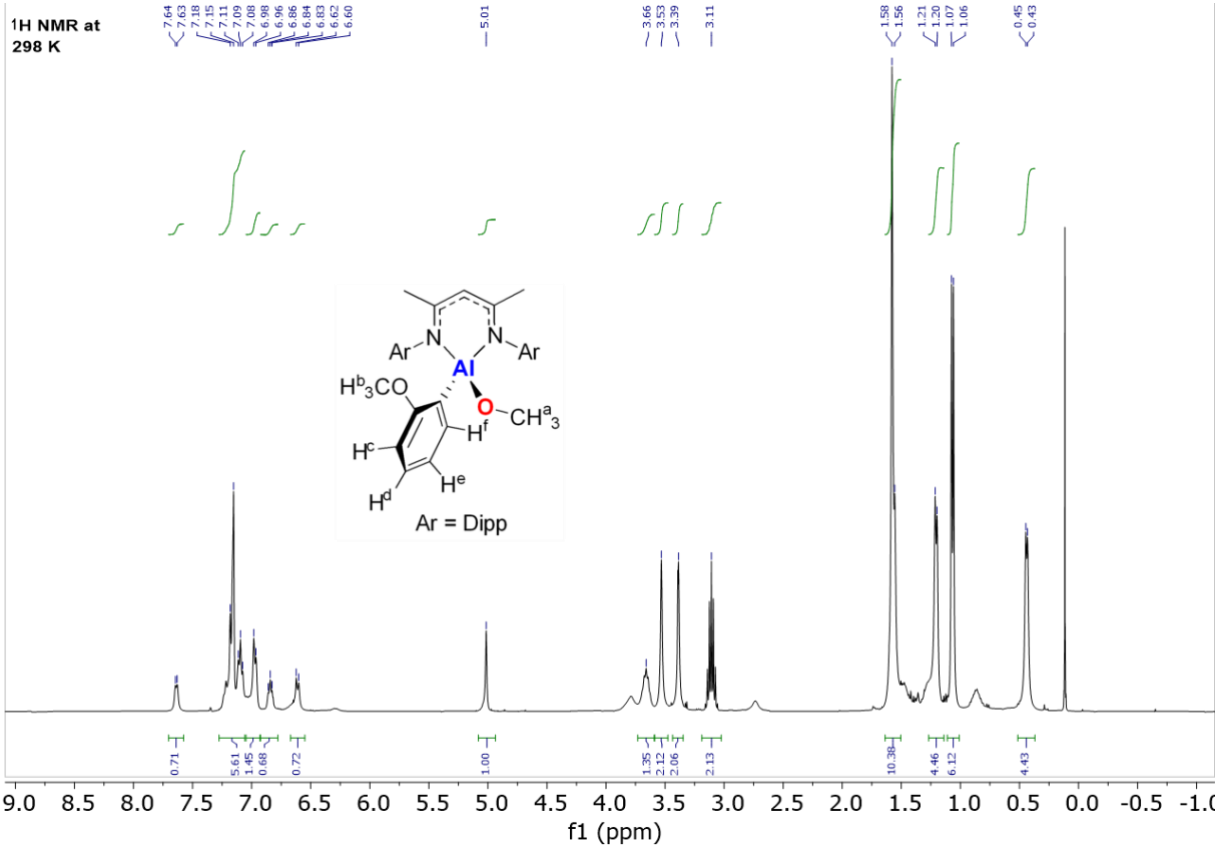


Figure S7.10: ^{13}C{^{1}H} NMR spectrum of complex **4b**

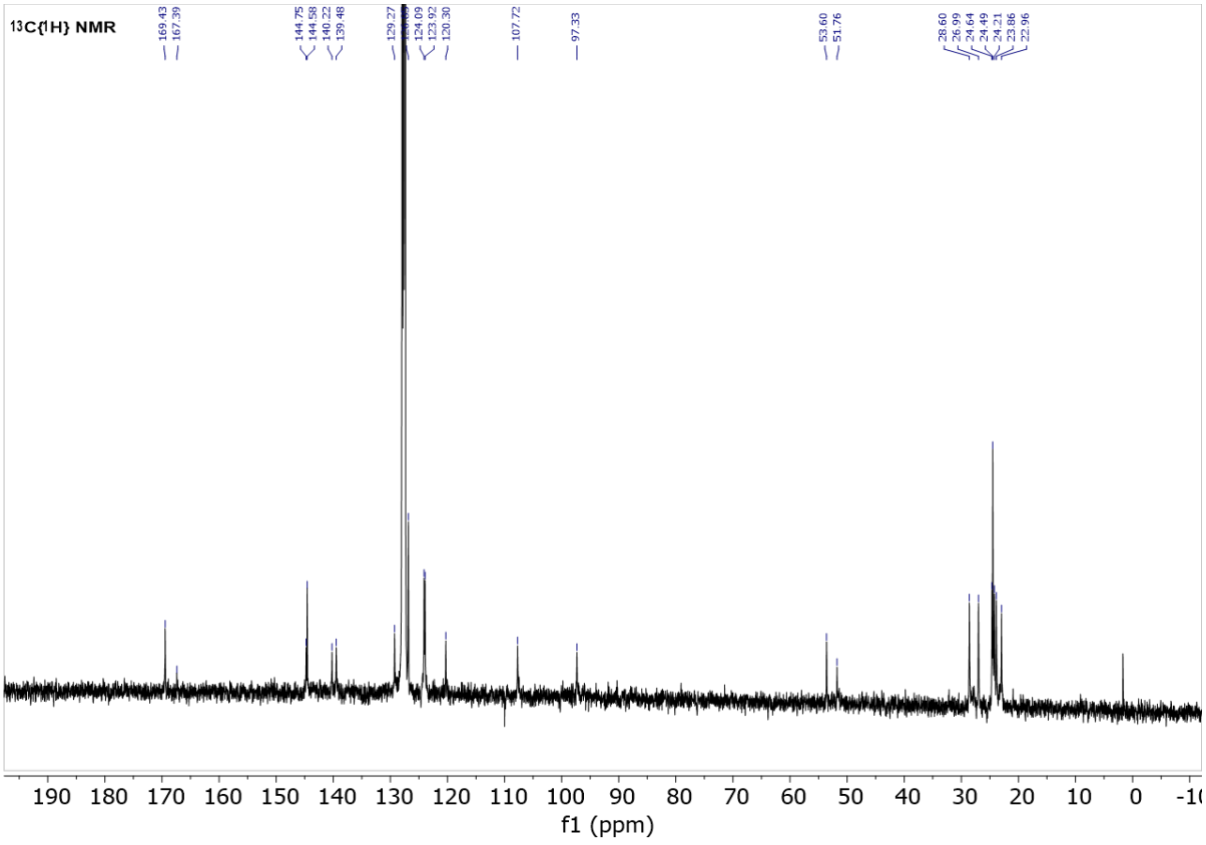


Figure S7.11: ^{1}H NMR spectrum of complex **4d**

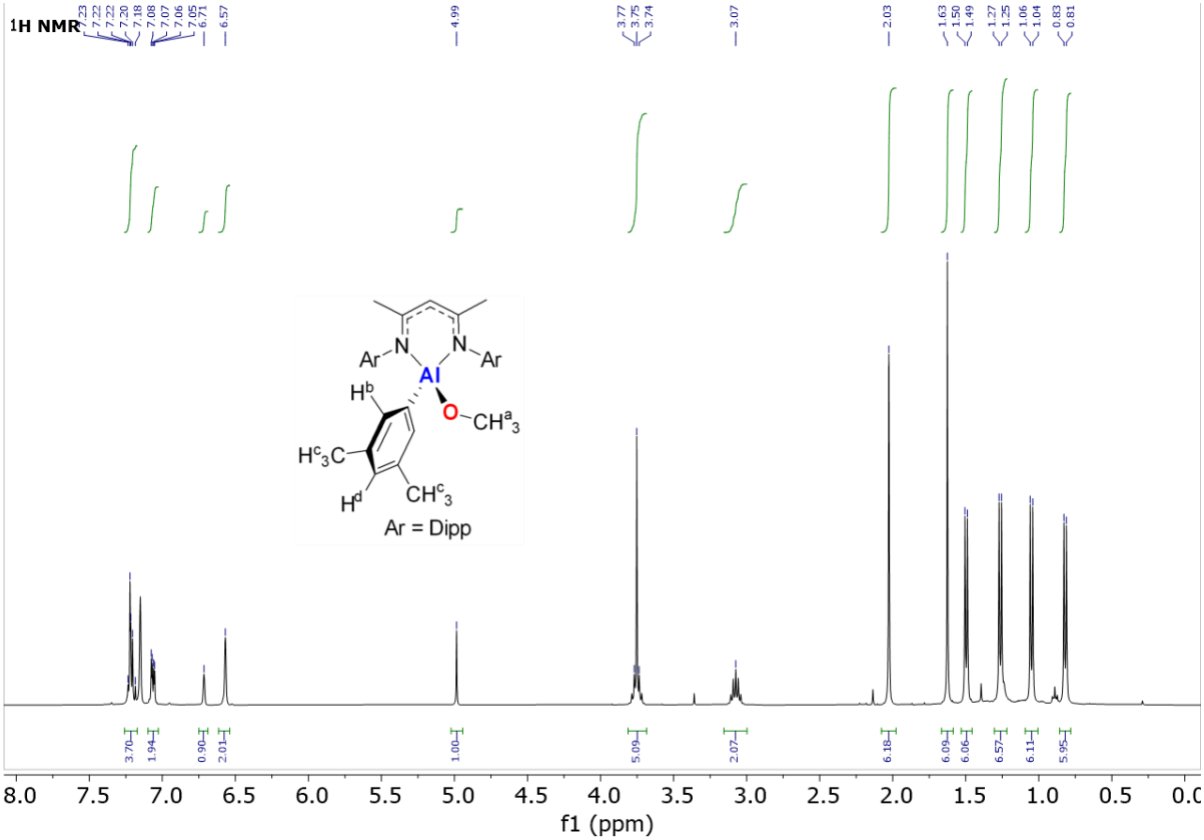
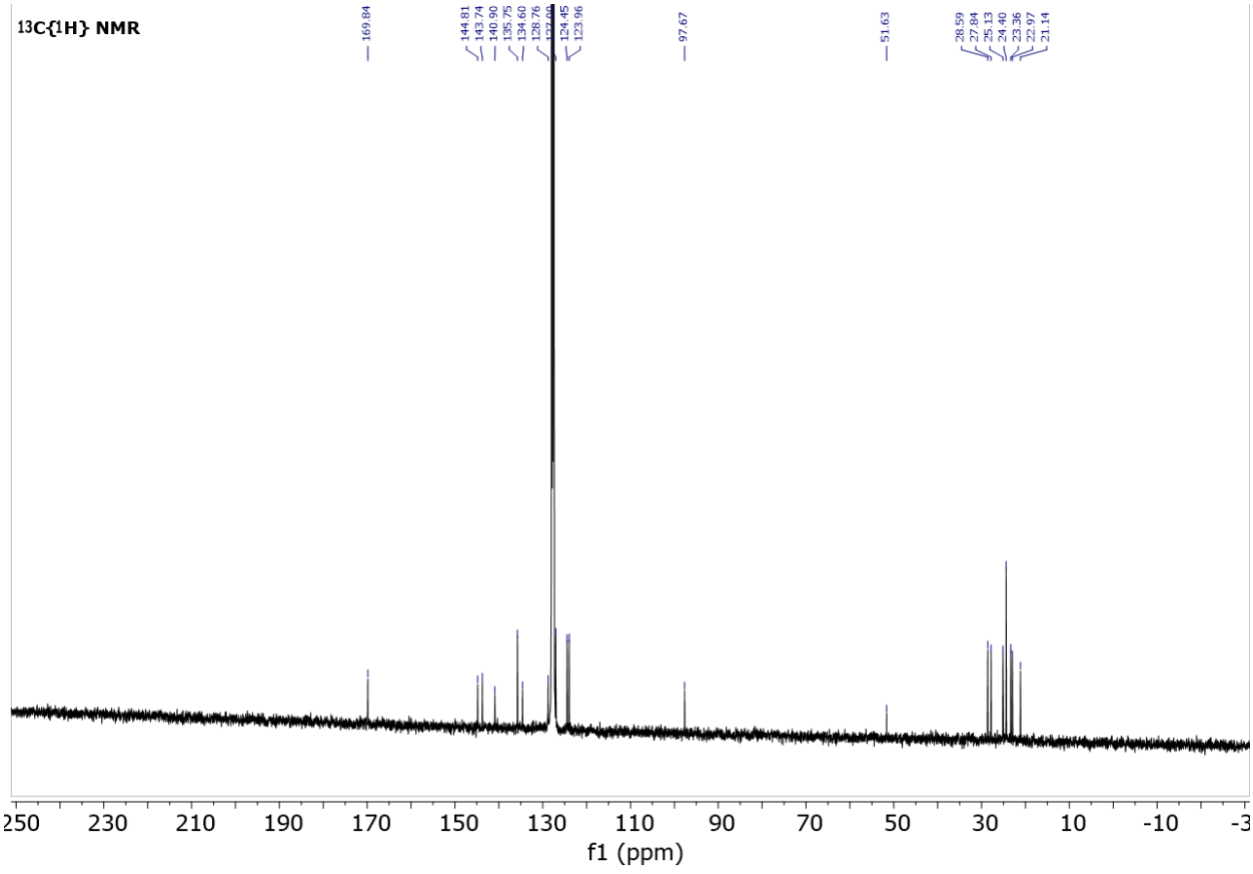


Figure S7.12: ^{13}C{^{1}H} NMR spectrum of complex **4d**



8. Computational details

8.1 Methods

The geometries of products were optimised with the M06L DFT functional using the Gaussian09 program package.[5] Stationary points were characterised depending on their imaginary frequencies (0 for minima and 1 for TSs). NBO analysis was performed using the NBO 6.0 version program.[6] The ωB97x hybrid exchange-correlation DFT functional, the B3PW91 functional and the M062X Minnesota DFT functional were also employed to assess differences in performance arising from the level of theory.

The SDD effective core potential was used for all Pd and Al (SDDAll). The split-valence 6-31G** basis set was used for C, H, N, P, Li and O atoms. The default numerical integration grid was also improved using a pruned grid with 99 radial shells and 590 angular points per shell (int=ultrafine). Intrinsic Reaction Coordinate (IRC) calculations were used to connect transition states and minima located on the potential energy surface to give a full energy profile.

Non-catalysed: For the uncatalysed route the pathways presented herein were calculated with the M06L functional and include dispersion and solvation corrections. ***Catalysed:*** For the catalysed route the pathways were calculated with M06L but do not include dispersion and solvent corrections unless otherwise stated.

Dispersion effects were included via single point energy corrections and were modelled using Grimme's D3 correction for M06L (EmpiricalDispersion=GD3)[7].

Solvent effects were included via single point energy corrections (benzene, ε = 2.2706, cyclohexane, ε = 2.0165) and were modelled using the polarizable continuum model (PCM) to free energies for M06L.

---

[5] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision D.01*; Gaussian, Inc., Wallingford, CT, 2009.

[6] *NBO 6.0*. Glendening, E. D.; Badenhoop, J. K.; Reed, A. E.; Carpenter, J. E.; Bohmann, J. A.; Morales, C. M.; Landis, C. R.; Weinhold, F. Theoretical Chemistry Institute, University of Wisconsin, Madison (2013).

[7] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J Chem. Phys.* 2010, **132**, 154104.

8.2 Catalysed C–H and C–O alumination of Anisole from [Pd(1)$_2$]

8.2.1 General Pathway

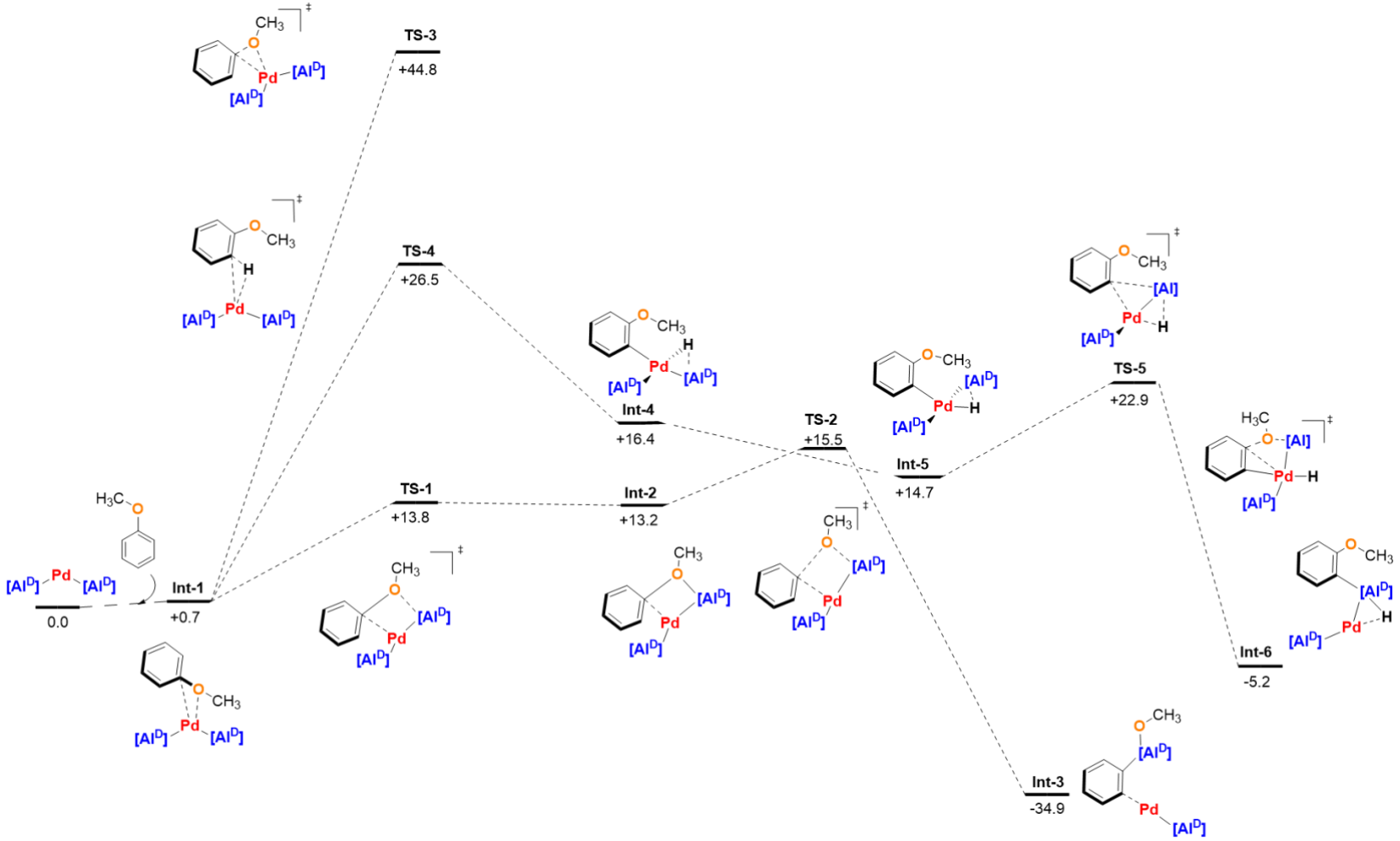


Figure S8.1: DFT calculated pathway for the palladium-catalysed C–H and C–O alumination reactions of [Pd(**1**)$_2$] with anisole.

When dispersion and solvent corrections were included into the calculations with M06L for the general pathway, no impact on the local barriers energies was observed (**Table S8.5**).

Functional	ΔTS-1	ΔTS-2	ΔTS-3	ΔTS-4	ΔTS-5
M06L	13.8	2.3	44.8	26.5	8.2
M06L (GD3)	12.6	2.2	43.1	25.7	8.2
M06L (pcm)	15.6	2.3	46.4	28.1	8.4

Table S8.1: Comparison of the calculated free-energy local barriers using M06L and including dispersion (GD3) and solvent (pcm) corrections. All energies provided in kcal mol^{-1}.

The performance of the three functionals was then inspected for **TS-1**, **TS-2, TS-3**, **TS-4** and **TS-5**.

Functional	ΔTS-1	ΔTS-2	ΔTS-3	ΔTS-4	ΔTS-5
M06L	13.8	2.3	44.8	26.5	8.2
ωB97X	26.8	-	62.9	28.5	7.6
B3PW91	39.3	3.0	77.7	45.9	7.1

Table S8.2: Comparison of the calculated free-energy local barriers of M06L with ωB97X and B3PW91. All energies provided in kcal mol^{-1}.

For ωB97X, the ligand oxidative addition step involves a one step process where **Int-1** evolves to **Int-3** by **TS-1**. **Int-2** neither **TS-2** were found for this functional. IRC calculations connect **TS-1** and both **Int-1** and **Int-3** on the potential energy surface.

8.2.2 Key geometrical parameters of intermediates, **Int-1** – **Int-6**

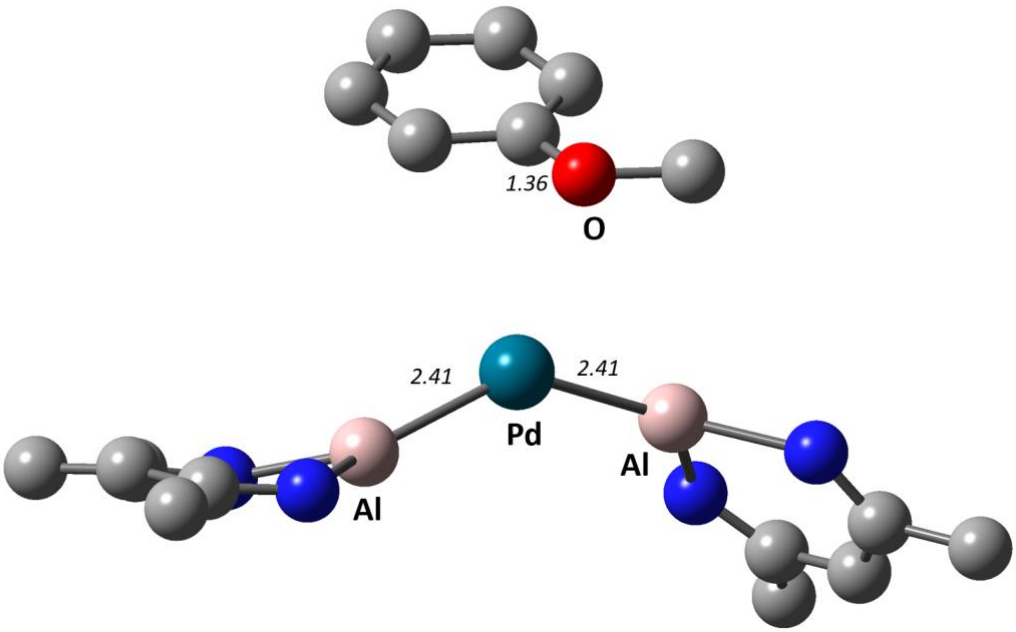


Figure S8.2: Selected bond lengths (in Å) for **Int-1**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

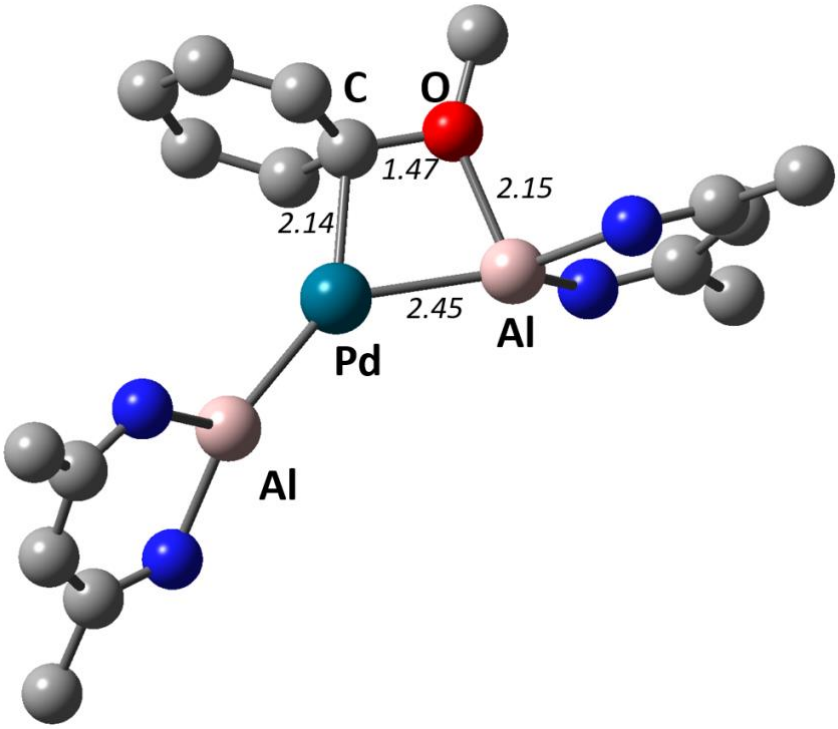


Figure S8.3: Selected bond lengths (in Å) for **Int-2**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

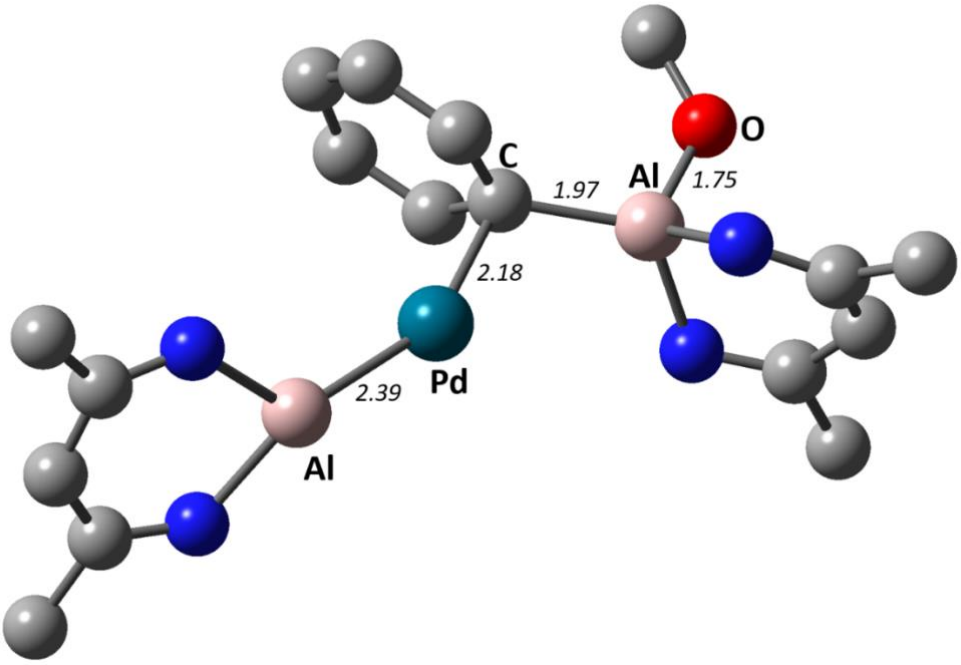


Figure S8.4: Selected bond lengths (in Å) for **Int-3**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

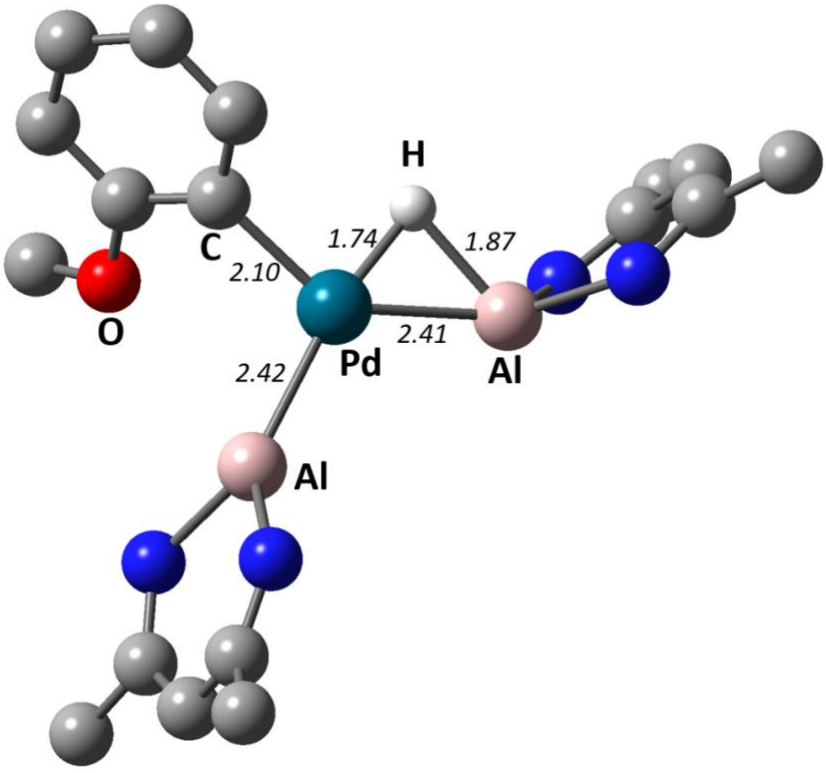


Figure S8.5: Selected bond lengths (in Å) for **Int-4**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

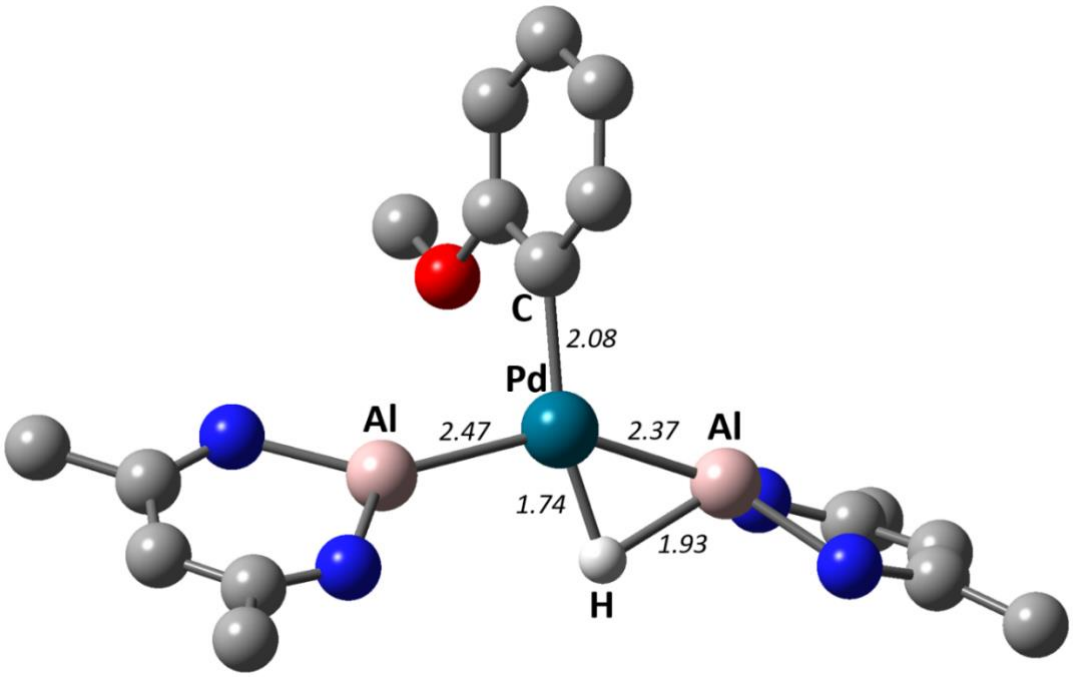


Figure S8.6: Selected bond lengths (in Å) for **Int-5**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

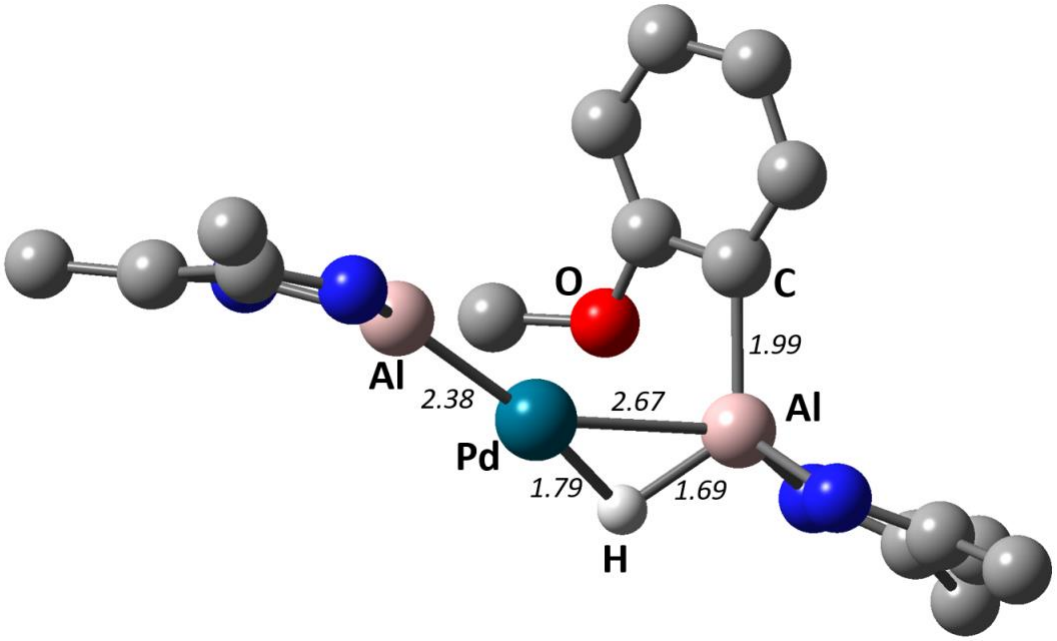


Figure S7.7: Selected bond lengths (in Å) for **Int-6**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

7.2.3 Key geometrical parameters of transition states, **TS-1** – **TS-5**

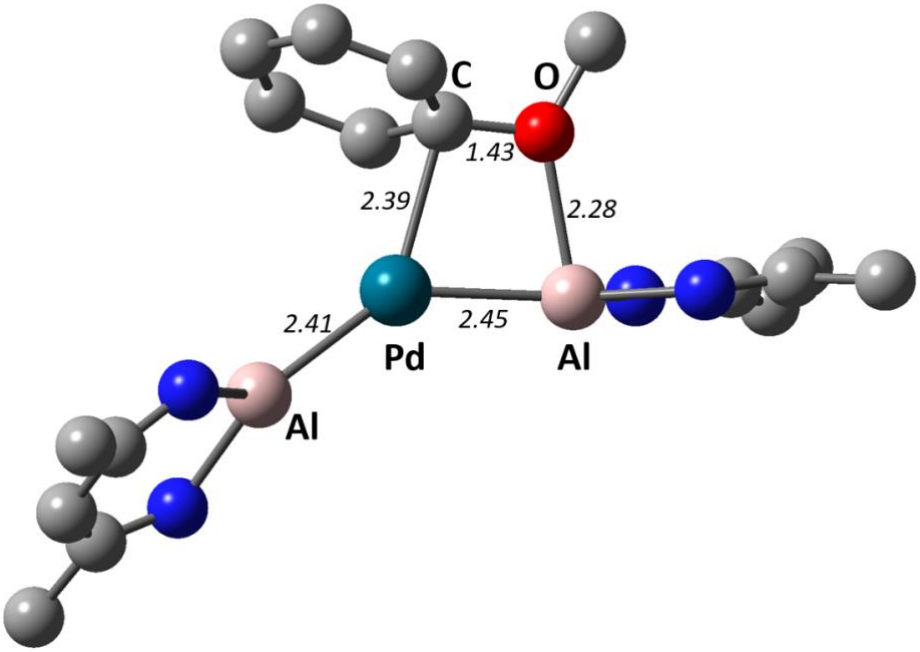


Figure S7.8: Selected bond lengths (in Å) for **TS-1**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

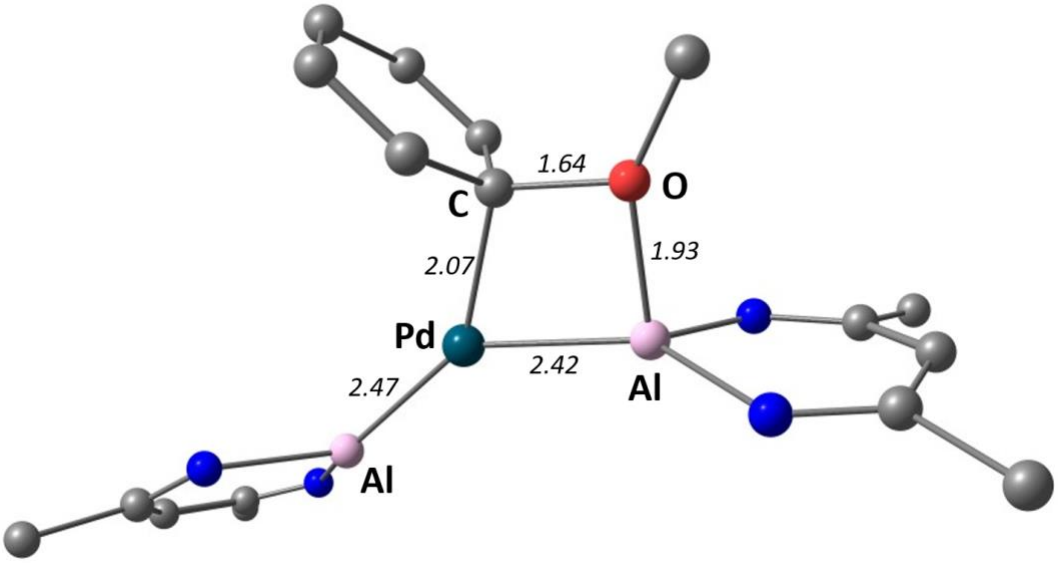


Figure S8.9: Selected bond lengths (in Å) for **TS-2**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

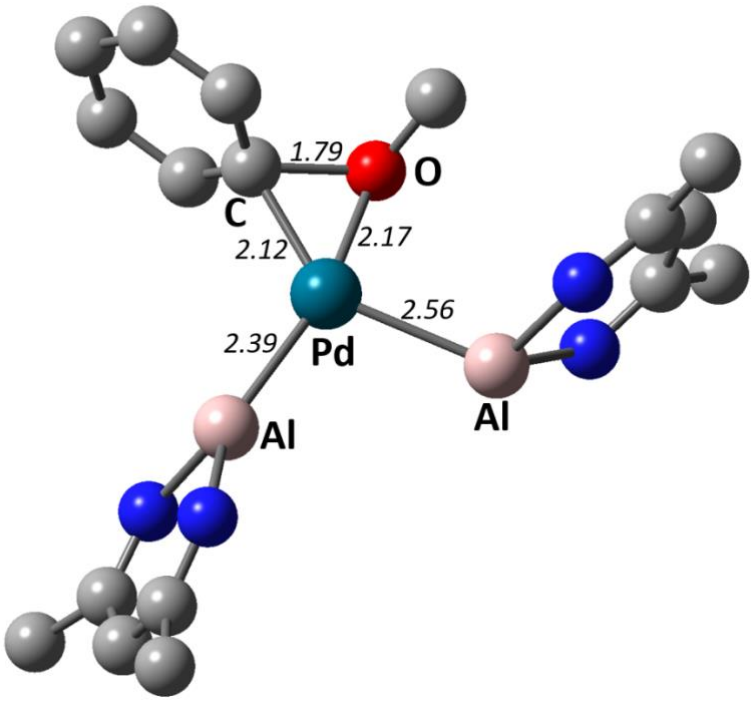


Figure S8.10: Selected bond lengths (in Å) for **TS-3**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

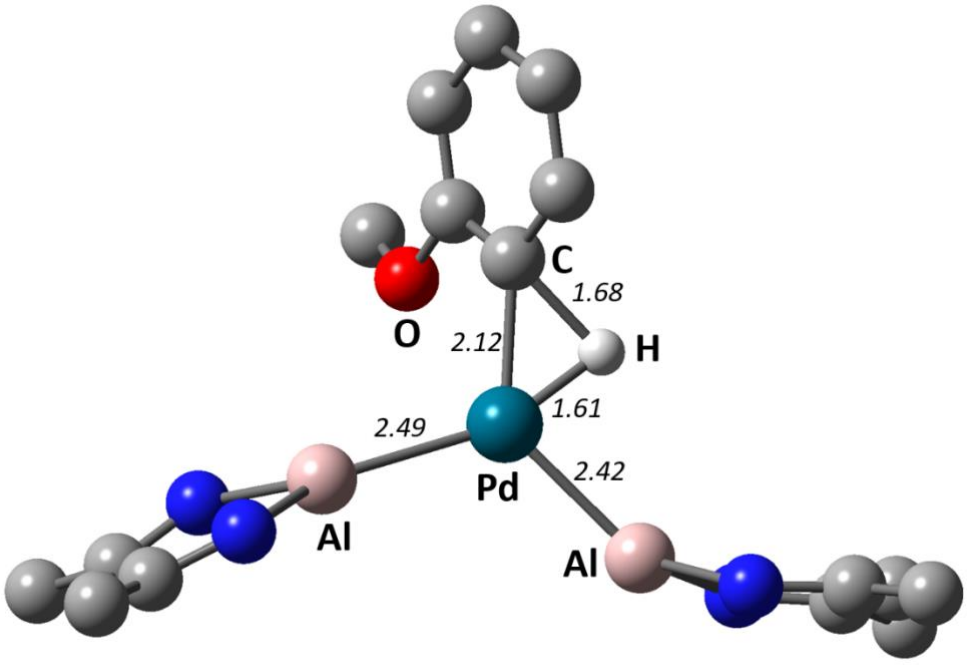


Figure S8.11: Selected bond lengths (in Å) for **TS-4**. 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

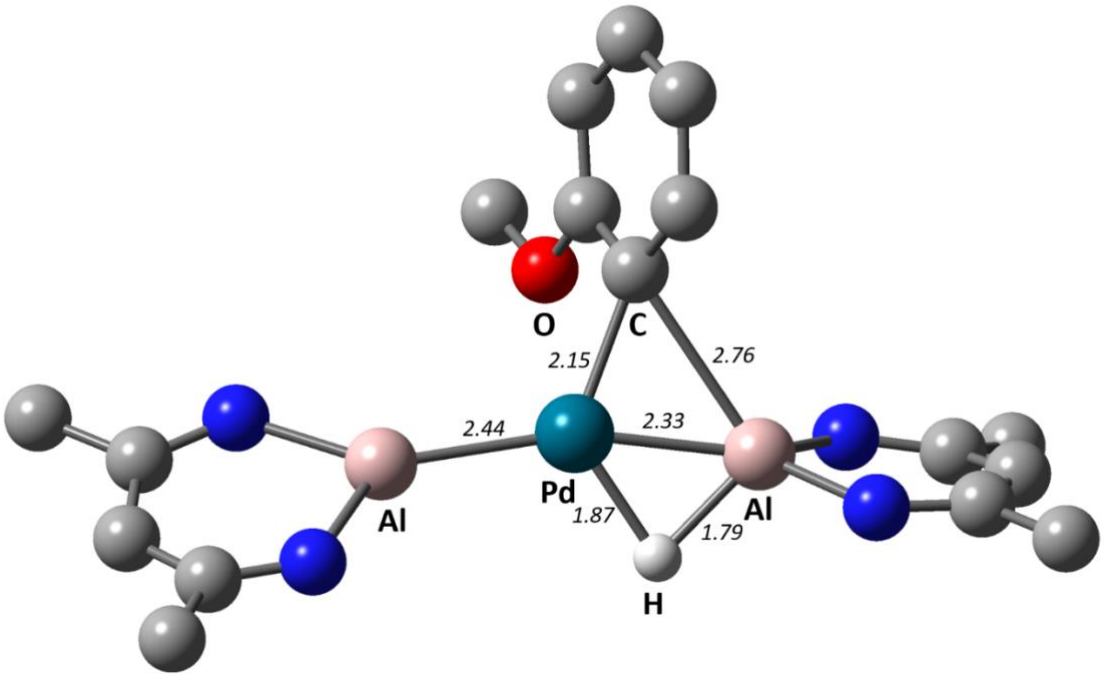
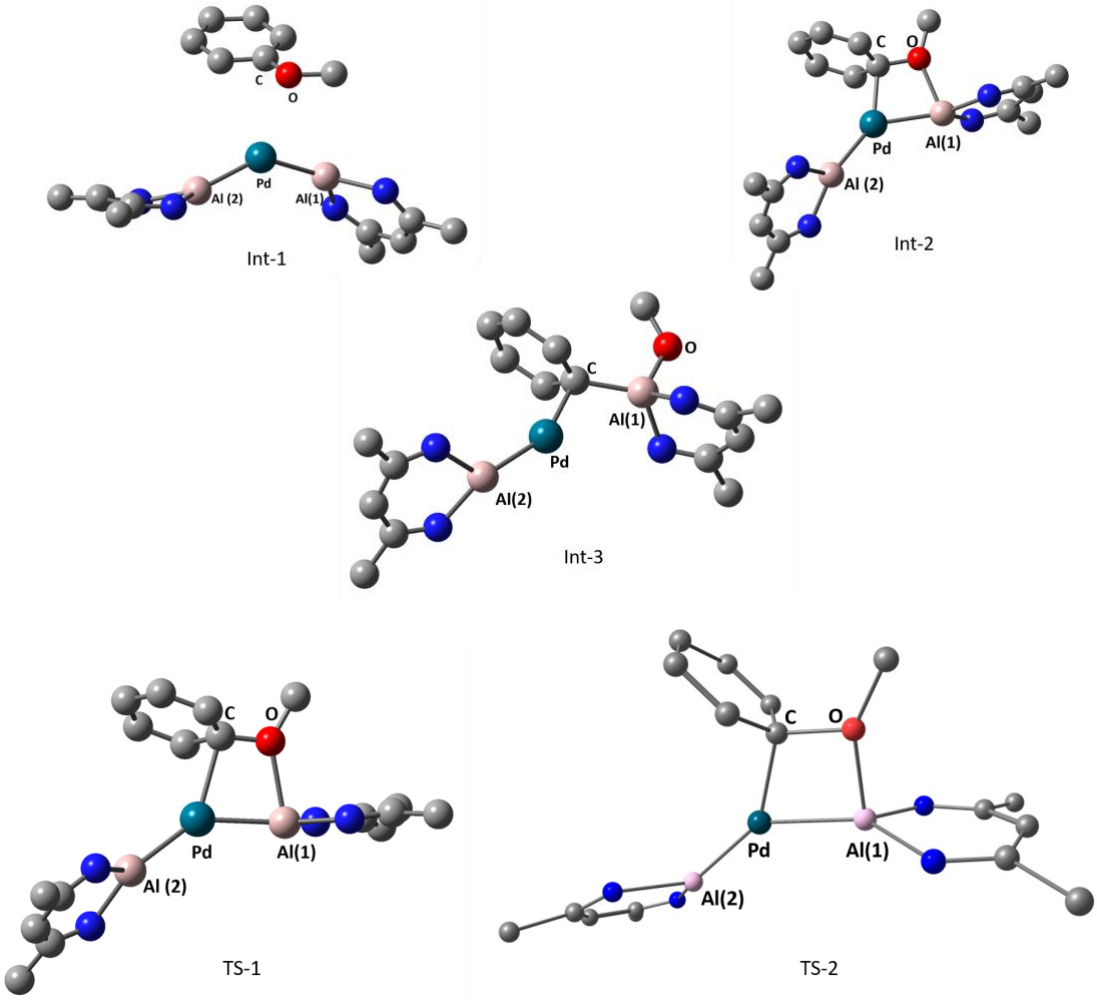


Figure S8.12: Selected bond lengths (in Å) for **TS-5.** 2,6-diisopropylphenyl groups and some hydrogens have been omitted for clarity.

8.3 Catalysed C–O Bond Alumination: NBO analysis

Wiberg Bond Indices (WBI) and NPA charges were inspected (M06L) for the pathway from [Pd(**1**)$_2$].



	Int-1	TS-1	Int-2	TS-2	Int-3
Pd-Al(1)	0.58	0.46	0.44	0.47	0.05
Pd-Al(2)	0.56	0.60	0.61	0.60	0.76
Pd-C	0.01	0.15	0.25	0.32	0.19
Al(1)-O	0	0.10	0.13	0.19	0.31
C-O	1.01	0.85	0.79	0.57	0.02
Al(1)-C	0.01	0.05	0.11	0.23	0.38

Table S8.3: Wiberg Bond Indices on stationary points on the pathway from [Pd(**1**)$_2$] of **Int-1**, **Int-2**, **Int-3**, **TS-1** and **TS-24**.

	Pd	C	O	Al(1)	Al(2)
Int-1	-0.55	0.34	-0.52	0.99	1.09
TS-1	-0.34	0.22	-0.64	1.09	1.01
Int-2	-0.39	0.11	-0.62	0.99	0.70
TS-2	-0.26	-0.01	-0.79	1.39	1.09
Int-3	-0.19	-0.79	-1.03	2.16	1.04

Table S8.4: NPA charges on stationary points on the pathway from [Pd(**1**)$_2$].

8.4 Catalysed C–O Bond Alumination: QTAIM analysis

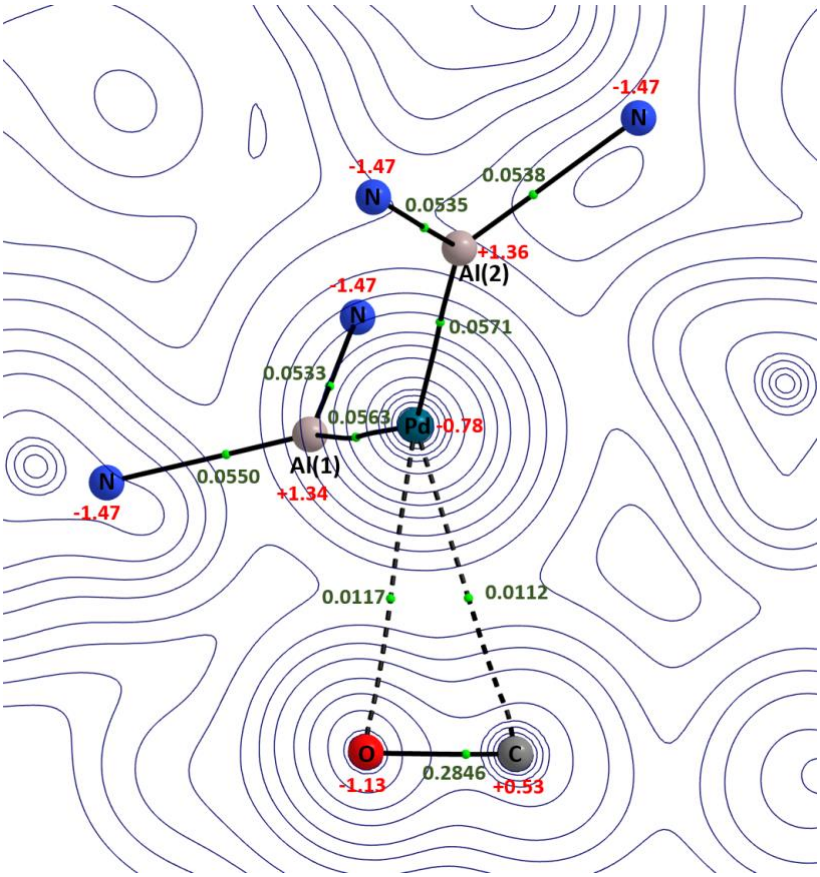


Figure S8.13: QTAIM contour plot of ρ for **Int-1**. Charges are depicted in red and electron density (ρ) in green.

	ρ	$\nabla^2\rho$	ε
Pd–Al(1)	0.0563	0.0027	0.1001
Pd–Al(2)	0.0571	0.0010	0.0887
Pd–O	0.0117	0.0380	0.6667
Pd–C	0.0112	0.0378	1.8912
C–O	0.2846	-0.2112	0.0095
Al(1)–O	-	-	-
Al(1)–C	-	-	-

Table S8.5: Electron density (ρ), Laplacian ($\nabla^2\rho$) and ellipticity (ε) computed at the bond critical points for **Int-1**.

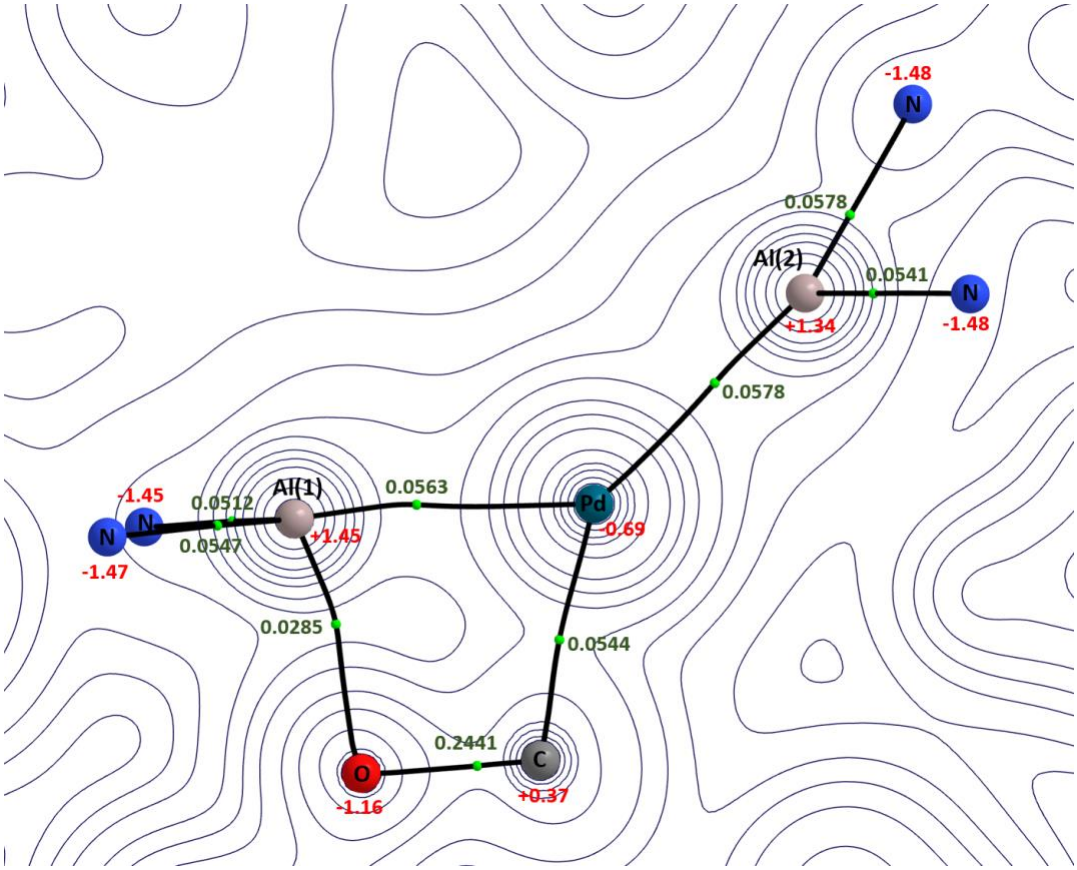


Figure S8.14: QTAIM contour plot of ρ for **TS-1**. Charges are depicted in red and electron density (ρ) in green.

	ρ	$\nabla^2\rho$	ε
Pd–Al(1)	0.0563	-0.0107	0.0154
Pd–Al(2)	0.0578	-0.00083	0.1783
Pd–O	-	-	-
Pd–C	0.0544	0.1435	0.5103
C–O	0.2441	-0.3700	0.0370
Al(1)–O	0.0285	0.0484	0.6437
Al(1)–C	-	-	-

Table S8.6: Electron density (ρ), Laplacian ($\nabla^2\rho$) and ellipticity (ε) computed at the bond critical points for **TS-1**.

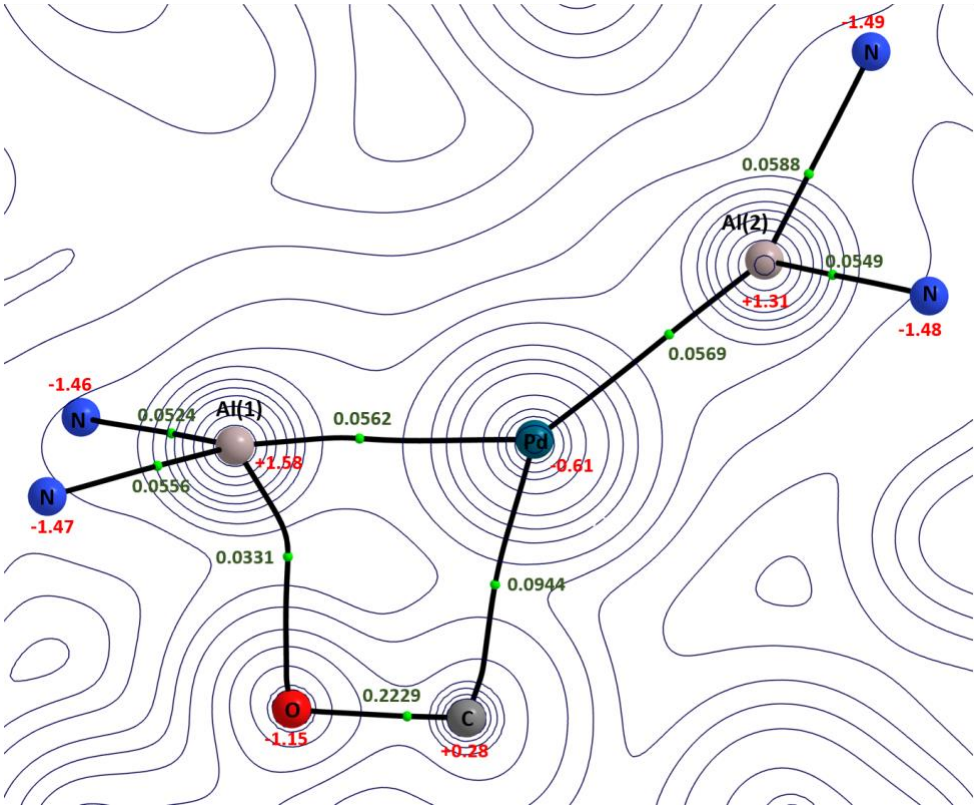


Figure S8.15: QTAIM contour plot of ρ for **Int-2**. Charges are depicted in red and electron density (ρ) in green.

	ρ	$\nabla^2\rho$	ε
Pd–Al(1)	0.0562	-0.0115	0.0252
Pd–Al(2)	0.0569	-0.0073	0.1413
Pd–O	-	-	-
Pd–C	0.0944	0.169642	0.0312
C–O	0.2229	-0.36925	0.0249
Al(1)–O	0.0331	0.119256	0.5384
Al(1)–C	-	-	-

Table S8.7: Electron density (ρ), Laplacian ($\nabla^2\rho$) and ellipticity (ε) computed at the bond critical points for **Int-2**.

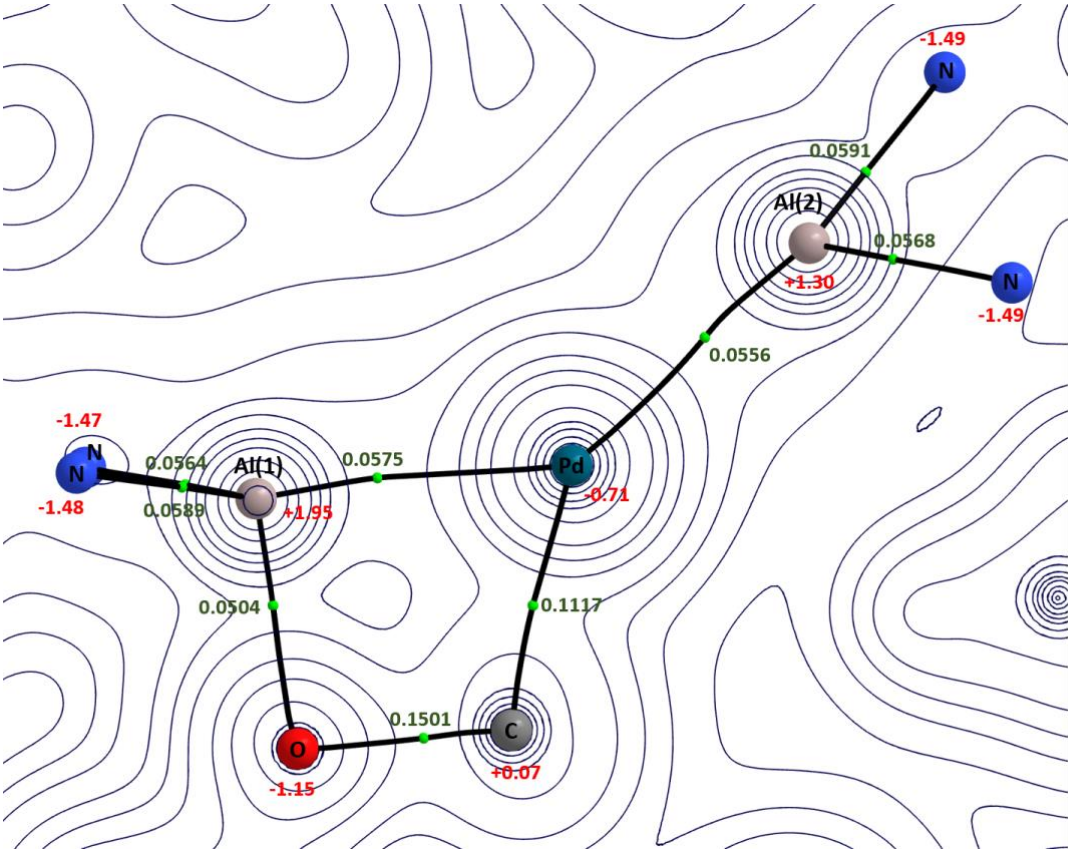


Figure S8.16: QTAIM contour plot of ρ for **TS-2**. Charges are depicted in red and electron density (ρ) in green.

	ρ	$\nabla^2\rho$	ε
Pd–Al(1)	0.0575	0.0153	0.0181
Pd–Al(2)	0.0556	-0.0128	0.0669
Pd–O	-	-	-
Pd–C	0.1117	0.1832	0.0444
C–O	0.1501	-0.0088	0.0439
Al(1)–O	0.0504	0.3582	0.0166
Al(1)–C	-	-	-

Table S8.8: Electron density (ρ), Laplacian ($\nabla^2\rho$) and ellipticity (ε) computed at the bond critical points for **TS-2**.

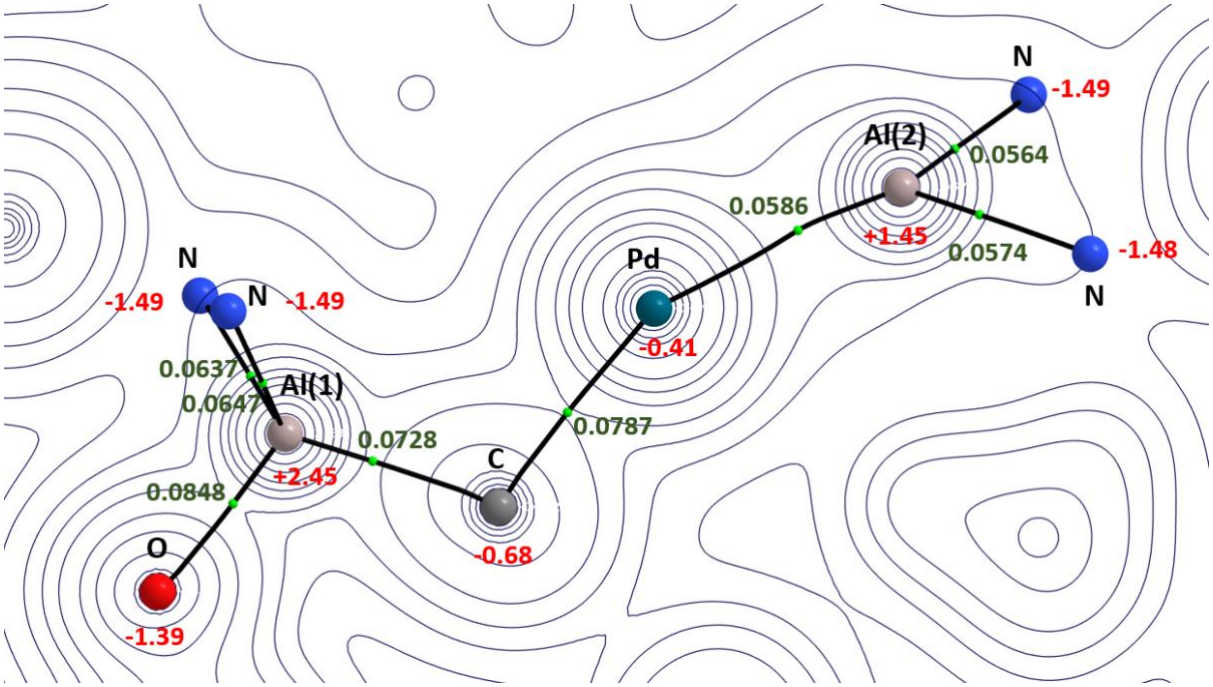


Figure S8.17: QTAIM contour plot of ρ for **Int-3**. Charges are depicted in red and electron density (ρ) in green.

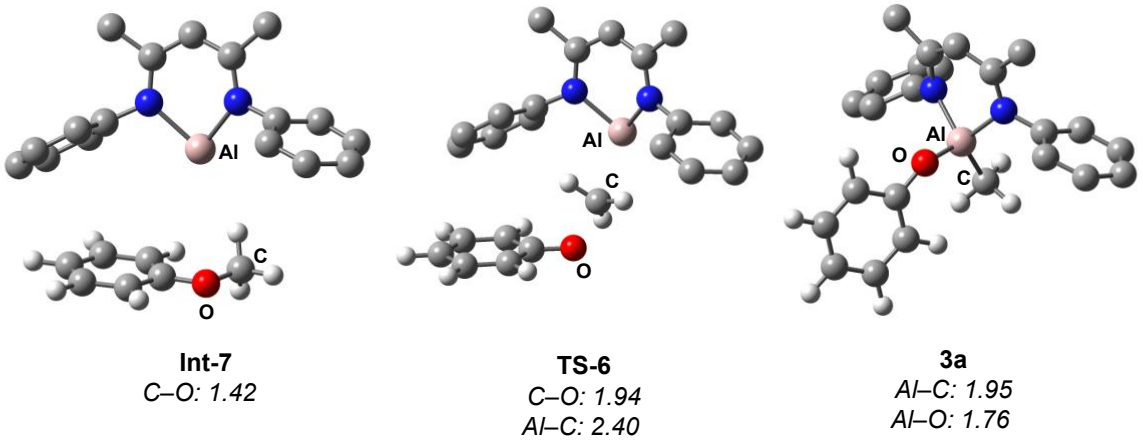
	ρ	$\nabla^2\rho$	ε
Pd–Al(1)	-	-	-
Pd–Al(2)	0.0586	0.0038	0.0394
Pd–O	-	-	-
Pd–C	0.0787	0.1767	0.0977
C–O	-	-	-
Al(1)–O	0.0848	0.7364	0.0513
Al(1)–C	0.0728	0.3343	0.0589

Table S8.9: Electron density (ρ), Laplacian ($\nabla^2\rho$) and ellipticity (ε) computed at the bond critical points for **Int-3.**

8.5 Non-catalysed C–O Bond Alumination of Anisole: Calculated Mechanisms

DFT calculations using the M06L functional and a hybrid basis-set reveal a number of pplausible pathways. S_N2 attack occurs via **TS-6** with a $\Delta G^{\ddagger}$ = 34.1 kcal mol^{-1}. This value is beyond that expected for a reaction occurring at 60 °C, nevertheless the reaction time is exhaustively long (> 1 week) and 100 equiv. of anisole are required for clean generation of the product.

8.5.1 S_N2 reaction of **1** and anisole



Int-7
C–O: 1.42

TS-6
C–O: 1.94
Al–C: 2.40

3a
Al–C: 1.95
Al–O: 1.76

Figure S8.18 Selected bond lengths (in Å) for **Int-7**, **TS-6** and **3a**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

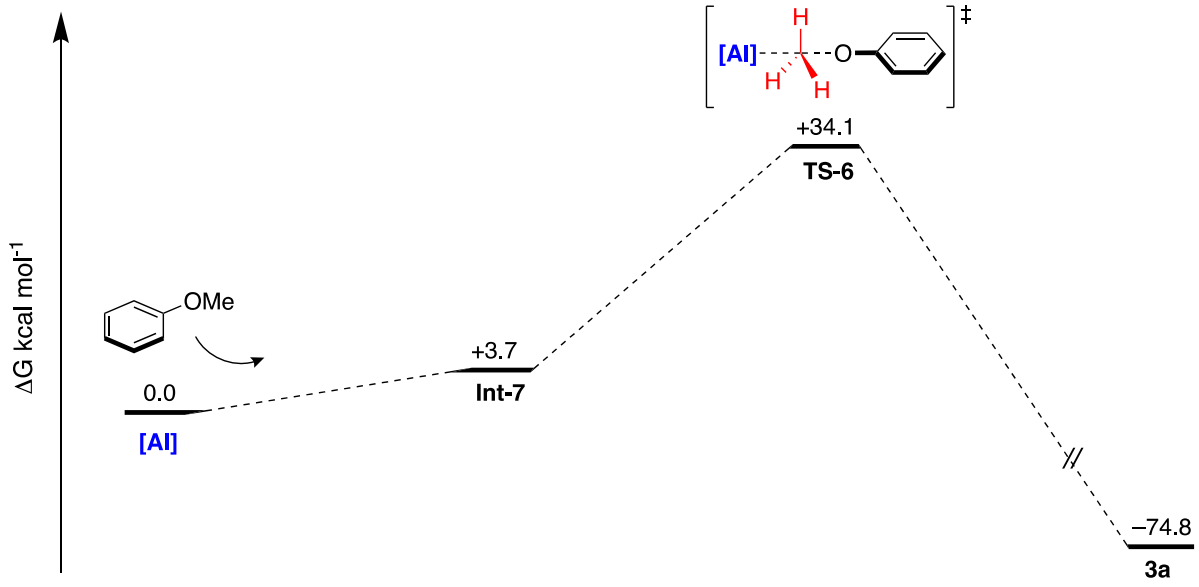
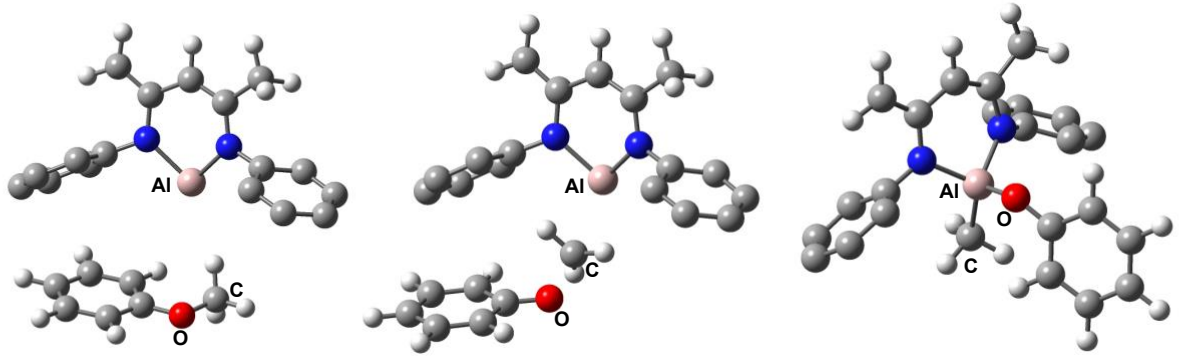


Figure S8.19 Calculated pathway for S_N2 reaction of **1** with anisole. [Al] represents **1**.

8.5.2 S_N2 reaction of **[1–H]**$^-$ and anisole

Recently Harder and coworkers have reported the synthesis of the aluminyl anion **[1–H]**$^-$ and its role in activating strong C–H bonds of arenes. Furthermore, organic bases such as DMAP have been shown to be competent for the deprotonation of **1**. Given the unusual reaction conditions to form **3a**, we hypothesised that **[1–H]**$^-$ may be generated in situ from deprotonation of **1** with adventitious base and acting as the true nucleophile in this case. In line with this hypothesis, the nucleophilic attack of **[1–H]**$^-$ on anisole by an S_N2 mechanism was calculated to occur by a lower energy transition state **TS-7** with $\Delta G^{\ddagger}$ = 23.3 kcal mol^{-1}. Following nucleophilic, attack protonation of **Int-9** would be required to form **3a**. Further analysis of both **TS-6** and **TS-7** revealed that **[1–H]**$^-$ leads to an earlier transition state resulting in a lower energy barrier for C–O bond cleavage.



Int-8
C–O: 1.42

TS-7
C–O: 1.90
Al–C: 2.55

Int-9
Al–C: 1.97
Al–O: 1.80

Figure S8.20 Selected bond lengths (in Å) for **Int-8**, **TS-7** and **Int-9**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

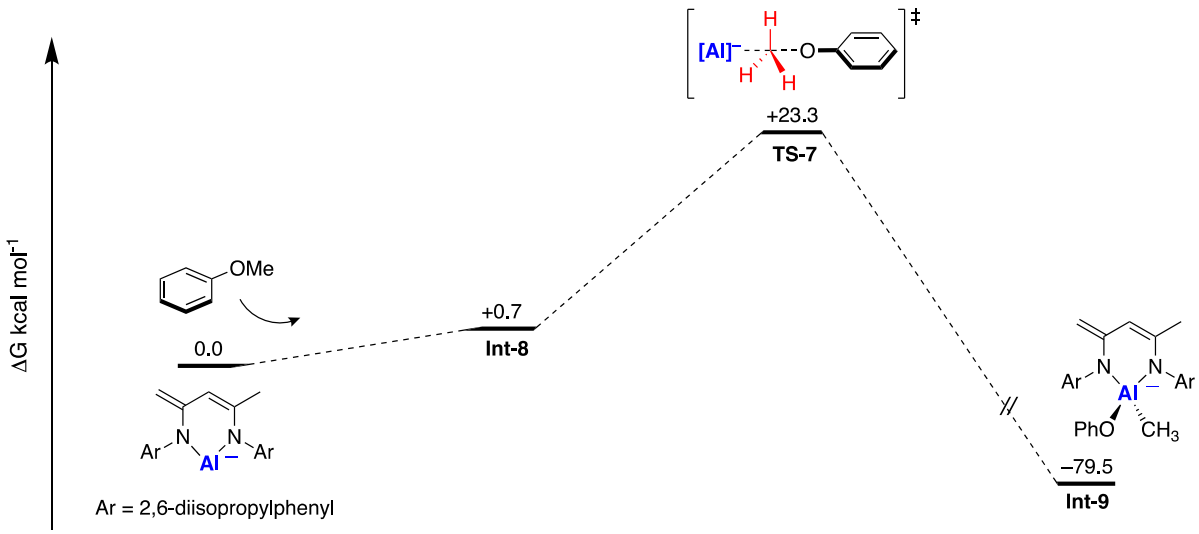
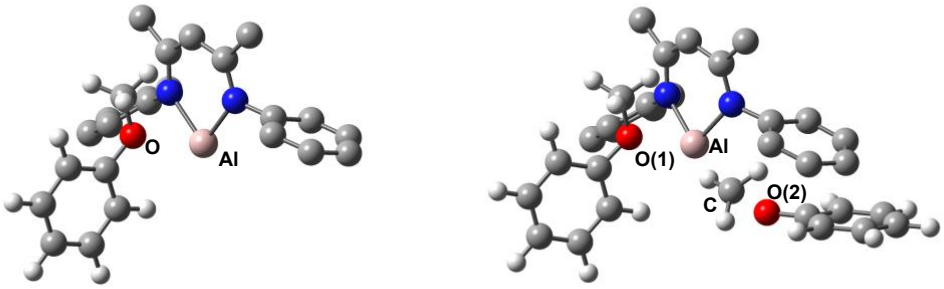


Figure S8.21 Calculated pathway for S_N2 reaction of **[1–H]**$^-$ with anisole.

A series of alternate mechanisms, including those involving the explicit solvation of **1** with anisole, were considered computationally and are detailed below.

8.5.3 S_N2 reaction of **1** and anisole using an explicit solvation model



Int7a
Al–O: 3.25

TS6a
C–O(2): 1.93
Al–C: 2.43
Al–O(1): 3.06

Figure S8.22 Selected bond lengths (in Å) for **Int7a** and **TS6a**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

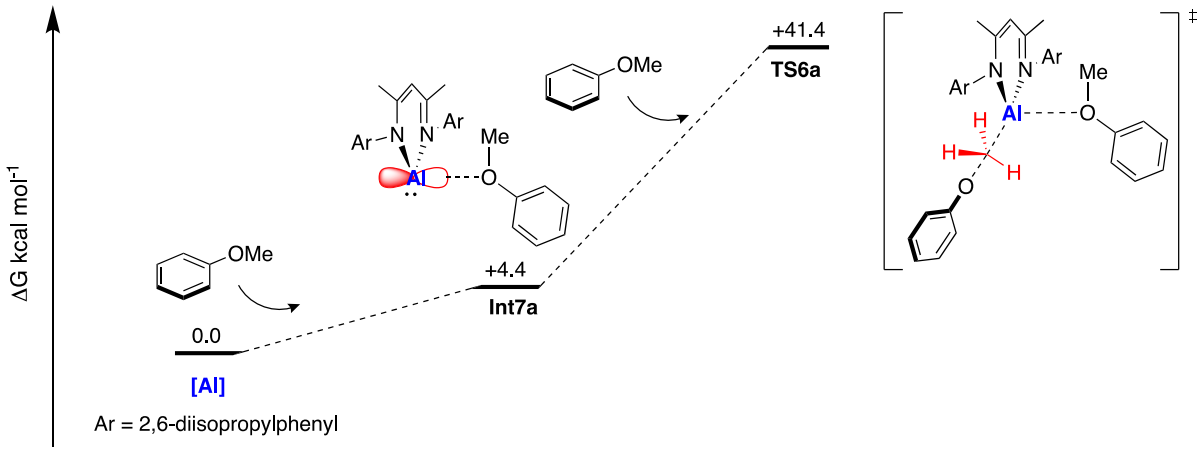
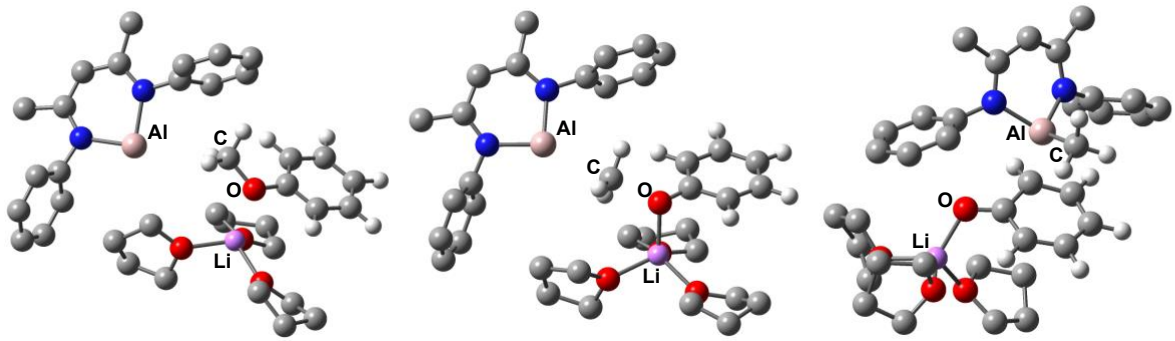


Figure S8.23 Calculated pathway for S_N2 reaction of **1** with anisole including explicit solvation model. **[Al]** represents **1**.

8.5.4 Lewis-acid assisted S_N2 reaction of **1** with anisole



Int7b
C–O: 1.44
Li–O: 2.05

TS6b
C–O: 1.89
Al–C: 2.66
Li–O: 1.92

Int8b
Al–C: 1.95
Li–O: 1.89

Figure S8.24 Selected bond lengths (in Å) for **Int7b**, **TS6b** and **Int8b**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

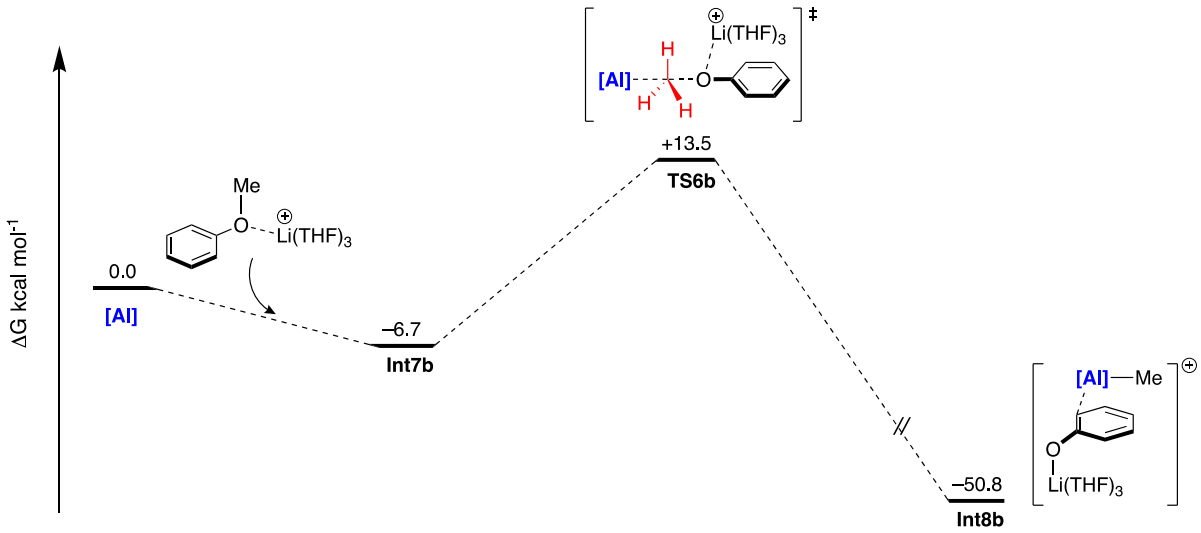
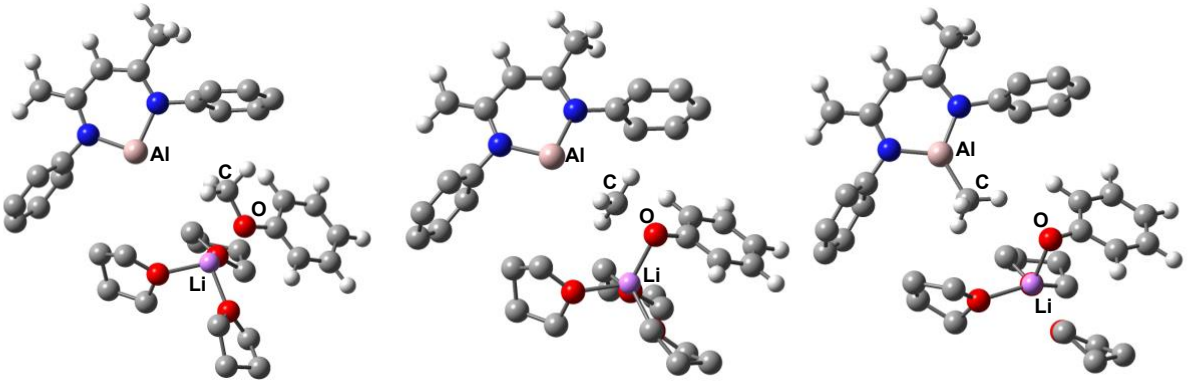


Figure S8.25 Calculated pathway for the Lewis acid assisted S_N2 reaction of **1** with anisole. **[Al]** represents **1**.

8.2.5 Lewis-acid assisted S_N2 reaction of **[1–H]$^-$** and anisole



Int8c
C–O: 1.44
Li–O: 2.06

TS7c
C–O: 1.82
Al–C: 2.88
Li–O: 1.93

Int9c
Al–C: 1.93
Li–O: 1.83

Figure S8.26 Selected bond lengths (in Å) for **Int8c**, **TS7c** and **Int9c**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

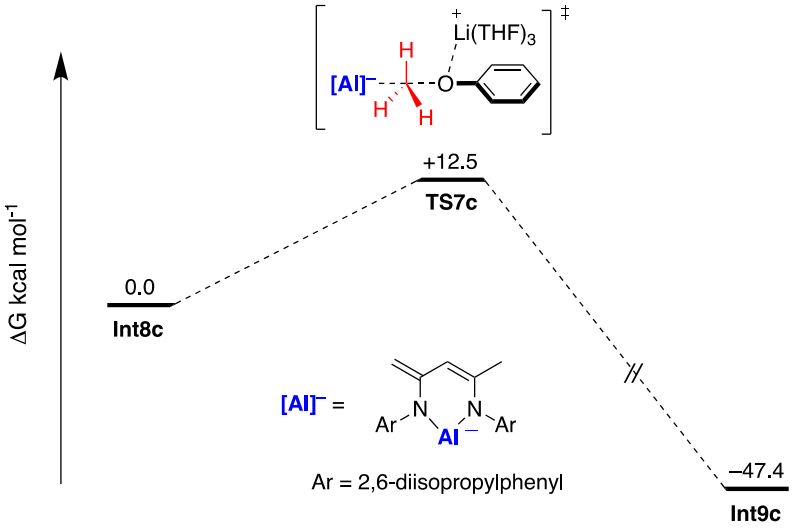
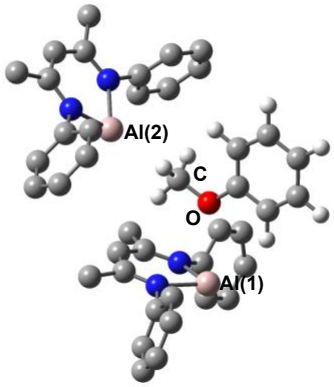
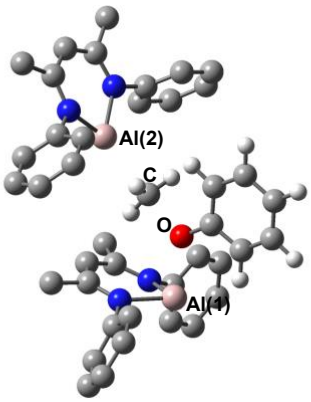


Figure S8.27 Calculated pathway for the Lewis acid assisted S_N2 reaction of **[1–H]$^-$** with anisole. **Int8c** represents an encounter complex.

8.5.6 Trimolecular S_N2 reaction of anisole with two equivalents of **1**



Int7d
Al(1)–O: 3.03
Al(2)–C: 3.58
C–O: 1.42



TS6d
Al(1)–O: 1.44
Al(2)–C: 2.42
C–O: 1.94

Figure S8.28 Selected bond lengths (in Å) for **Int7d** and **TS6d**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

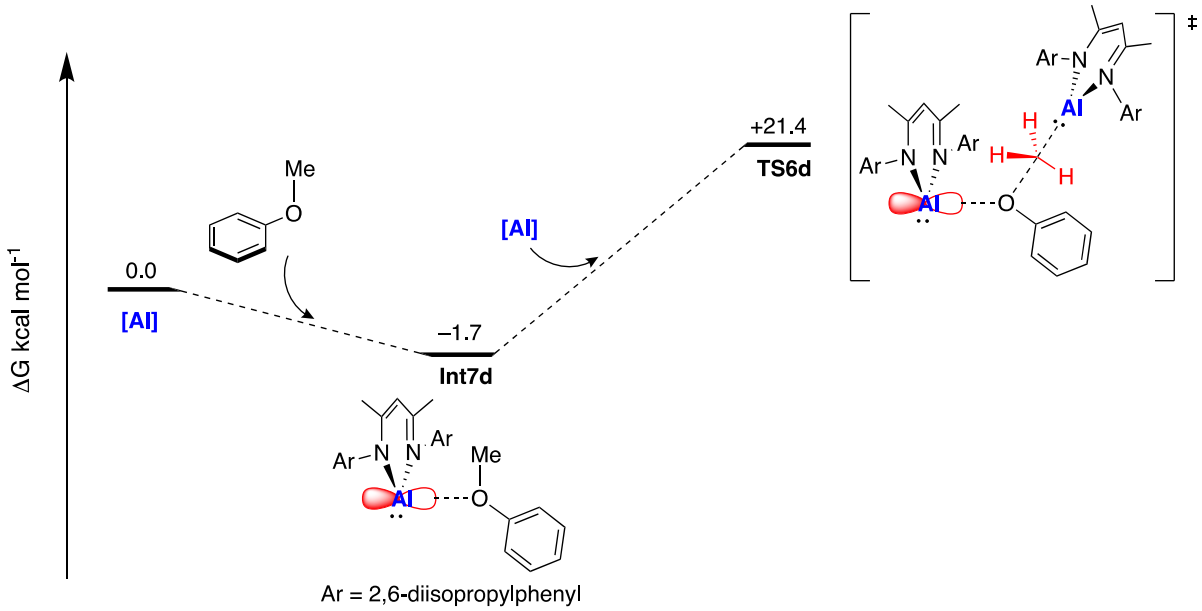
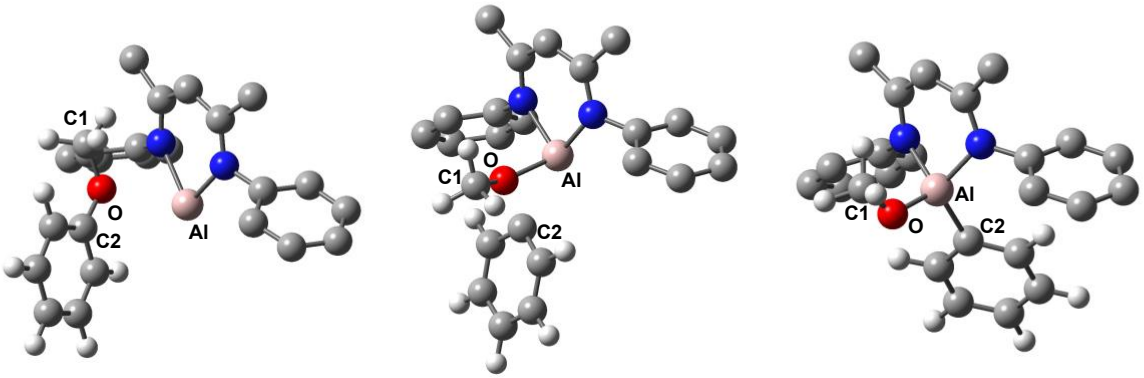


Figure S8.29 Calculated pathway for the trimolecular S_N2 reaction of 2 equivalents of **1** with anisole, where **1** acts as the nucleophile and a Lewis acidic coordination site. **[Al]** represents **1**.

8.5.7 Other Calculated Mechanisms

8.5.7.1 Oxidative Addition of sp^2C–O and sp^3C–O bonds to **1**



Int7e
C(1)–O: 1.42
C(2)–O: 1.37
Al–O: 3.26

TS6e
C(1)–O: 1.42
C(2)–O: 1.62
Al–O: 1.93
Al–C(2): 2.29

4a
C(1)–O: 1.39
C(2)–O: 3.09
Al–O: 1.74
Al–C(2): 1.97

Figure S8.30 Selected bond lengths (in Å) for **Int7e**, **TS6e** and **4a**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

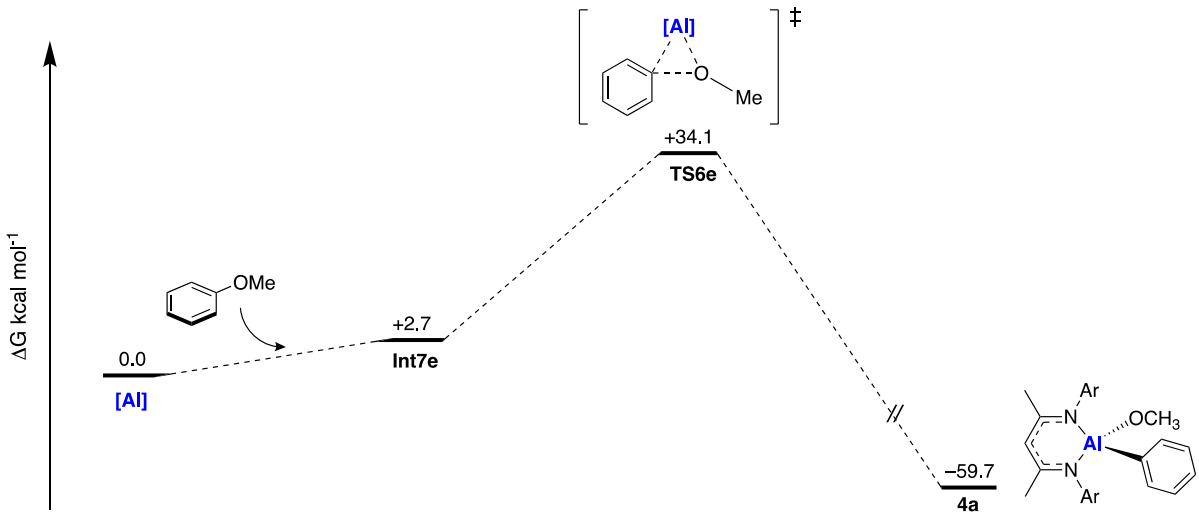
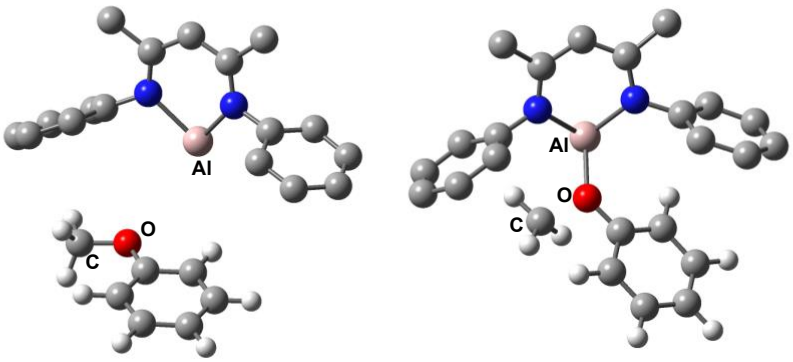


Figure S8.31 Calculated pathway for the oxidative addition of the sp^{2}C–O bond of anisole to **1**. **[Al]** represents **1.**



Int7f
C–O: 1.41

TS6f
C–O: 1.89
Al–O: 1.99
Al–C: 2.75

Figure S8.32 Selected bond lengths (in Å) for **Int7f** and **TS6f** . ^{i}Pr groups and some hydrogens have been omitted for clarity.

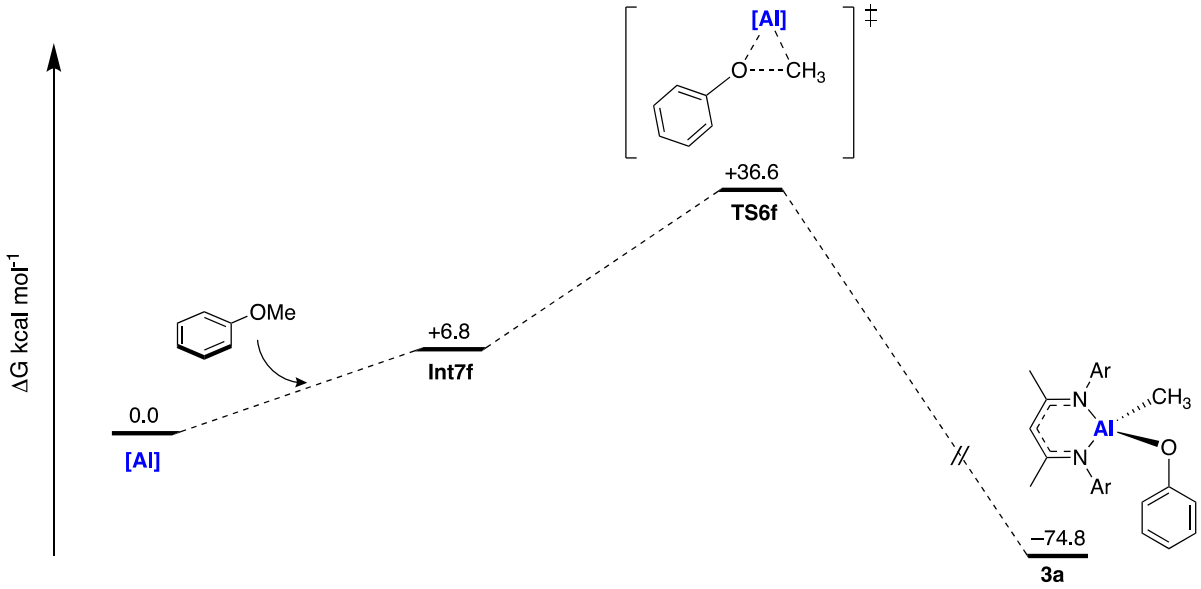
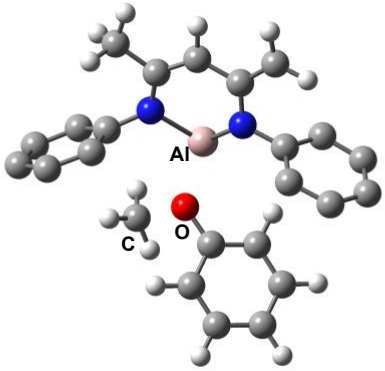


Figure S8.33 Calculated pathway for the oxidative addition of the sp^{3}C–O bond of anisole to **1**. **[Al]** represents **1.**

8.5.7.2 Oxidative addition of sp^3C–O to **[1–H]$^-$**



TS7g
C–O: 1.93
Al–O: 2.06
Al–C: 3.08

Figure S8.34 Selected bond lengths (in Å) for **TS7g**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

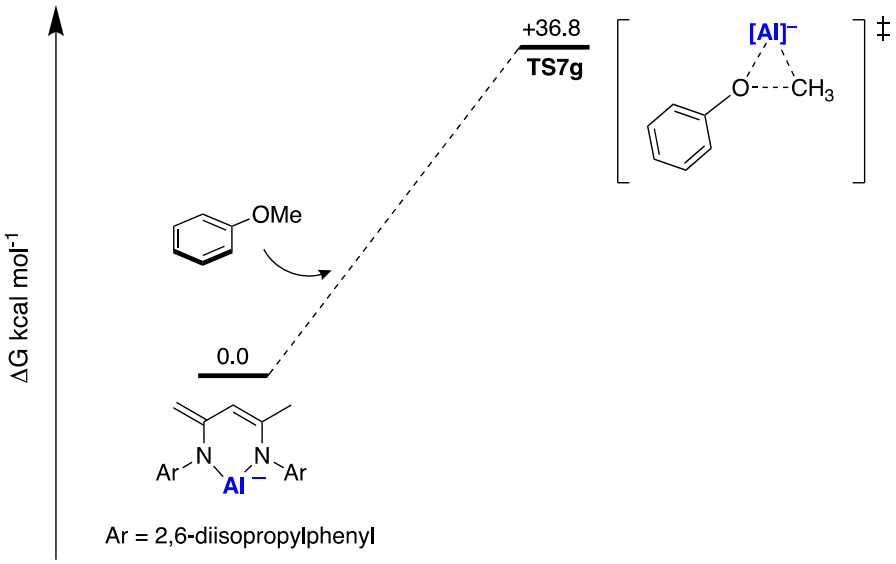
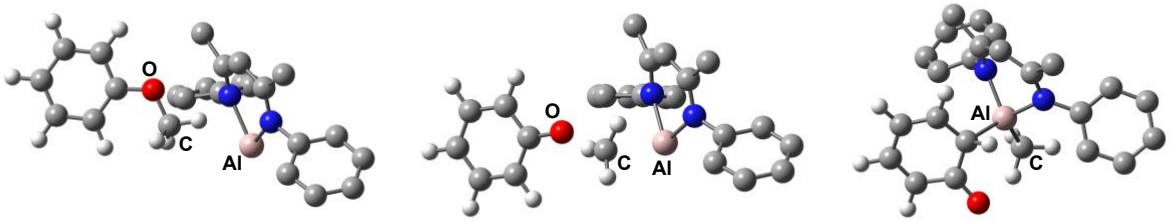


Figure S8.35 Calculated pathway for the oxidative addition of the sp^{3}C–O bond of anisole to **[1–H]$^-$**.

8.5.7.3 Abstraction of methyl group from anisole with **1**



Int7h
C–O: 1.41
Al–C: 3.75

TS6h
C–O: 1.98
Al–C: 2.34

Int8h
Al–C:1.95

Figure S8.36 Selected bond lengths (in Å) for **TS6h**. ^{i}Pr groups and some hydrogens have been omitted for clarity.

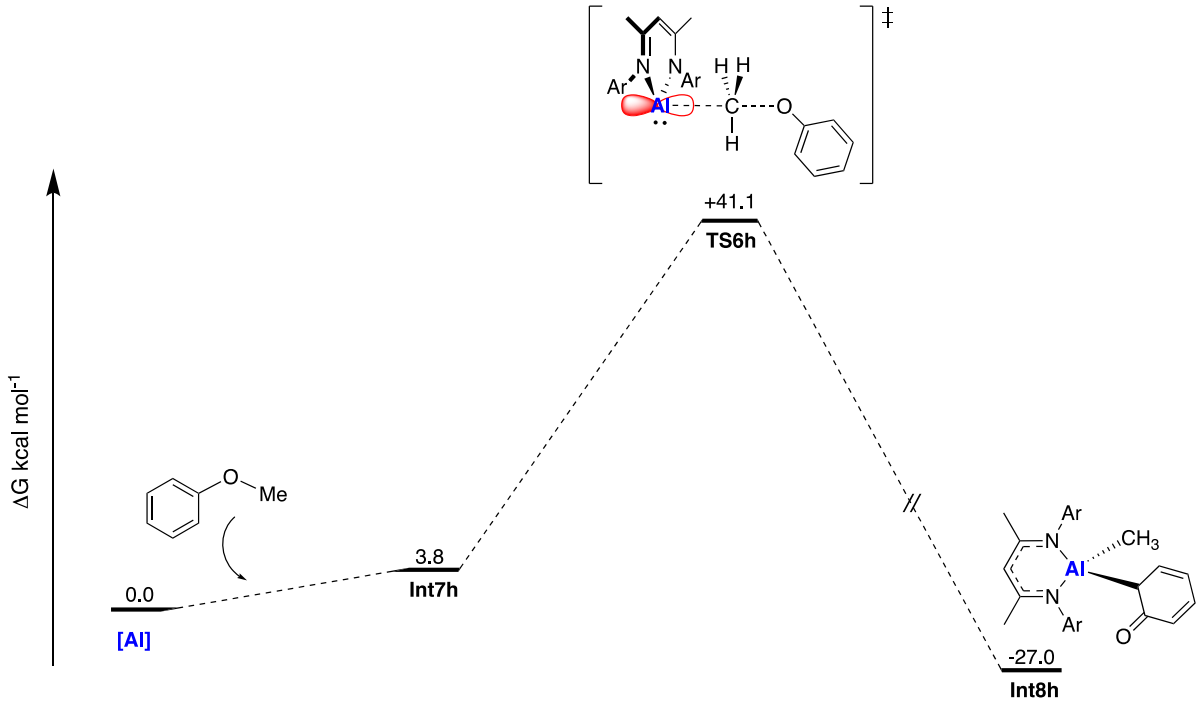
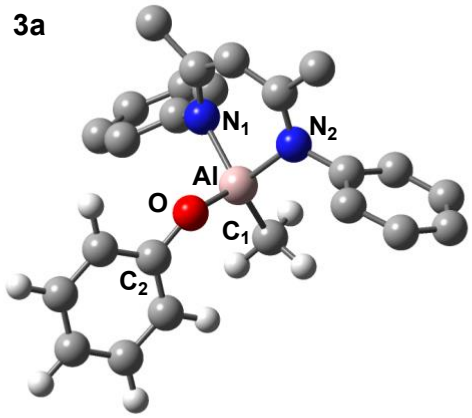


Figure S8.37 Calculated pathway for the abstraction of the methyl group in anisole to **1**.

8.6 Non-catalysed C–O Bond Alumination: NBO analysis

8.6.1 NBO analysis of the stationary points for the S_N2 pathway of **1** with anisole



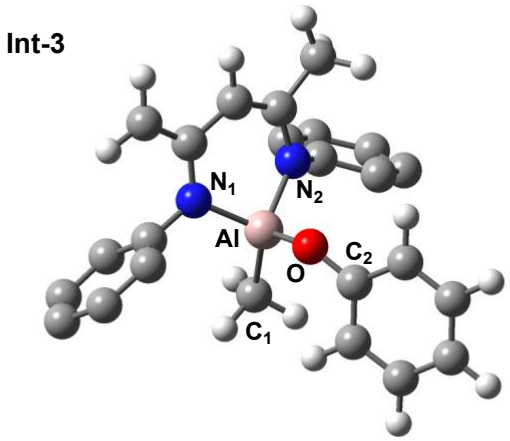
	1	2a	Int-7	TS-6	3a
Al–N₁	0.20		0.17	0.21	0.23
Al–N₂	0.20		0.18	0.21	0.23
Al–C₁			0.01	0.52	0.47
Al–O			0.01	0.21	0.33
C₁–O		0.91	0.90	0.42	0.02
C₂–O		1.01	1.01	1.18	1.05

Table S8.10 Wiberg bond indices on stationary points for the S_N2 pathway of **1** with anisole.

	1	9a	Int-7	TS-6	3a
Al	0.78		0.80	1.19	2.15
C₁		-0.33	-0.32	-0.76	-1.46
O		-0.55	-0.53	-0.59	-0.95
C₂		0.33	0.34	0.36	0.36

Table S8.11 NPA charges on stationary points for the S_N2 pathway of **1** with anisole.

8.6.2 NBO analysis of the stationary points for the S_N2 pathway of **[1–H]⁻** with anisole



	[1–H]⁻	**2a**	**Int-8**	**TS-7**	**Int-9**
Al–N₁	0.32		0.23	0.25	0.25
Al–N₂	0.26		0.28	0.29	0.28
Al–C₁			0.02	0.51	0.44
Al–O			0.00	0.18	0.31
C₁–O		0.91	0.90	0.43	0.02
C₂–O		1.01	1.00	1.20	1.10

Table S8.12 Wiberg bond indices on stationary points for the S_N2 pathway of **[1–H]⁻** with anisole.

	[1–H]⁻	**2a**	**Int-8**	**TS-7**	**Int-9**
Al	0.68		0.74	1.11	2.14
C₁		-0.33	-0.32	-0.67	-1.43
O		-0.55	-0.54	-0.60	-0.92
C₂		0.33	0.34	0.37	0.38

Table S8.13 NPA charges on stationary points for the S_N2 pathway of **[1–H]⁻** with anisole.

8.6 XYZ Coordinates

Anisole_M06L.log

SCF (M06L) = -346.731003883
E(SCF)+ZPE(0 K) = -346.597592
H(298 K) = -346.589878
G(298 K) = -346.628455
Lowest Frequency = 106.0301 cm^{-1}

C	0.496920	-1.303937	-0.000175
C	-0.455449	-0.278582	-0.000248
C	-0.043707	1.056173	-0.000339
C	1.319546	1.351246	-0.000038
C	2.270481	0.338169	0.000281
C	1.847867	-0.992232	0.000170
H	0.149566	-2.332310	-0.000246
H	-0.769071	1.862466	-0.000581
H	1.632773	2.391844	-0.000222
H	3.329030	0.578443	0.000480
H	2.578991	-1.796033	0.000253
O	-1.756917	-0.682649	-0.000192
C	-2.739930	0.329743	0.000390
H	-2.669253	0.966529	-0.891468
H	-3.703207	-0.180144	0.001203
H	-2.667861	0.966917	0.891861

1.log

SCF (M06L) = -1241.24018280
E(SCF)+ZPE(0 K)= -1240.602632
H(298 K)= -1240.566224
G(298 K)= -1240.669746
Lowest Frequency = 11.7804cm-1

Al	9.836661	1.454985	3.307972
N	8.896836	2.853496	4.439726
N	10.339142	2.953944	2.036225
C	8.738248	4.164690	4.223745
C	9.317739	4.830729	3.138075
H	9.151302	5.900694	3.082863
C	10.091303	4.266512	2.117625
C	7.914659	4.978450	5.180403
H	6.912136	4.551789	5.289522
H	7.823403	6.013839	4.849226
H	8.353752	4.971137	6.183959
C	10.649842	5.191858	1.074790
H	10.247866	4.957063	0.083151
H	11.735351	5.074608	0.992660
H	10.423417	6.234424	1.302449
C	8.292146	2.282863	5.608226
C	7.050699	1.630151	5.497468
C	6.526001	1.006949	6.633606
H	5.568337	0.494873	6.559347
C	7.203061	1.029398	7.844024
H	6.780770	0.537179	8.715680
C	8.425325	1.685998	7.938335
H	8.952477	1.701776	8.889101
C	8.991360	2.321803	6.832815
C	6.266766	1.585899	4.199398
H	6.815795	2.169697	3.448402
C	6.146168	0.155401	3.676382
H	7.132945	-0.292116	3.515017
H	5.600264	0.130894	2.727143
H	5.604894	-0.479331	4.387268
C	4.885750	2.220199	4.359034
H	4.947887	3.252590	4.718089
H	4.272240	1.662153	5.075151
H	4.348611	2.227584	3.405277
C	10.346890	2.996131	6.937863
H	10.404853	3.759703	6.151324
C	10.565241	3.700454	8.273073
H	9.749052	4.390153	8.511262
H	11.497312	4.273225	8.254004
H	10.647487	2.988752	9.101455
C	11.467518	1.990452	6.671380
H	11.347632	1.499096	5.696530
H	11.467666	1.200895	7.431137
H	12.448603	2.477822	6.687993
C	11.119350	2.480014	0.930176
C	12.495834	2.245654	1.104462
C	13.216022	1.702938	0.036164
H	14.280785	1.513551	0.159861
C	12.598417	1.401850	-1.168893
H	13.174002	0.977799	-1.986992
C	11.238356	1.645328	-1.326380
H	10.757819	1.407633	-2.272290
C	10.476078	2.185452	-0.290040
C	13.218820	2.565426	2.399293
H	12.495626	3.017079	3.091713
C	13.760212	1.297210	3.057168
H	12.956076	0.581620	3.260380
H	14.257704	1.530192	4.004684
H	14.492718	0.800031	2.411109
C	14.340852	3.578698	2.176780
H	13.972978	4.504548	1.722848
H	15.114702	3.175365	1.514047
H	14.824506	3.837712	3.124017
C	8.983950	2.403165	-0.460128
H	8.674328	3.181464	0.249320
C	8.603040	2.882429	-1.857284
H	9.180236	3.761798	-2.160858
H	7.541571	3.145373	-1.893921
H	8.763465	2.106133	-2.612987
C	8.212925	1.132956	-0.099049
H	8.444588	0.794017	0.919468
H	8.476667	0.314188	-0.777825
H	7.131356	1.294139	-0.165889

[Pd(1)$_2$].log

SCF (M06L) = -2610.58136399
E(SCF)+ZPE(0 K) = -2609.302627
H(298 K) = -2609.228276
G(298 K) = -2609.409952
Lowest Frequency = 16.2727 cm^{-1}

Pd	0.004121	-0.065181	-1.394658
Al	2.149727	-0.207636	-0.377820
N	3.392991	1.323921	-0.175072
N	2.874528	-1.038878	1.281248
C	4.061002	1.678612	0.926832
C	4.151536	0.851651	2.056292
H	4.740979	1.232170	2.882836
C	3.679530	-0.459255	2.183656
C	4.792716	2.987883	0.969405
H	5.453947	3.099514	0.104165
H	5.381933	3.085446	1.882304
H	4.086010	3.823445	0.922345
C	4.129424	-1.239795	3.384487

H	3.279127	-1.531263	4.010193
H	4.825910	-0.663393	3.994510
H	4.614776	-2.173467	3.082097
C	3.539710	2.130970	-1.358216
C	4.422756	1.671187	-2.361682
C	4.592887	2.456188	-3.503242
H	5.271887	2.124468	-4.283238
C	3.897502	3.648458	-3.668757
H	4.045565	4.245121	-4.564733
C	2.994894	4.055850	-2.698736
H	2.419203	4.967730	-2.844623
C	2.791258	3.309386	-1.534654
C	5.158760	0.351791	-2.209161
H	4.446602	-0.355556	-1.750987
C	5.584399	-0.259540	-3.537691
H	4.743288	-0.352264	-4.231201
H	6.000797	-1.258591	-3.374491
H	6.366230	0.330657	-4.028495
C	6.363530	0.456174	-1.272924
H	7.083227	1.192897	-1.648878
H	6.881185	-0.507461	-1.204355
H	6.081095	0.746993	-0.257440
C	1.726113	3.753166	-0.554874
H	1.803535	3.120611	0.335693
C	0.336866	3.531722	-1.154116
H	-0.443812	3.806097	-0.435849
H	0.182270	2.477753	-1.429139
H	0.199770	4.144884	-2.053769
C	1.882787	5.207976	-0.116128
H	2.874848	5.423025	0.296497
H	1.136299	5.452436	0.647737
H	1.724019	5.897788	-0.952691
C	2.572920	-2.435317	1.436406
C	1.543478	-2.860400	2.301077
C	1.259720	-4.226025	2.375544
H	0.460705	-4.561438	3.034165
C	1.964893	-5.157648	1.624612
H	1.721606	-6.214309	1.694932
C	2.978242	-4.725069	0.781615
H	3.533582	-5.449048	0.188414
C	3.301346	-3.370017	0.670752
C	0.721312	-1.897229	3.135358
H	1.205834	-0.914633	3.096321
C	-0.681573	-1.740471	2.550060
H	-1.172416	-2.715285	2.436074
H	-0.636043	-1.268728	1.558420
H	-1.318940	-1.127223	3.197971
C	0.639939	-2.321460	4.601216
H	0.060597	-3.242944	4.723620
H	0.141775	-1.548435	5.195593
H	1.628055	-2.499467	5.038758
C	4.421323	-2.964334	-0.268418
H	4.576407	-1.881513	-0.170778
C	4.044881	-3.256653	-1.720975
H	3.843524	-4.324154	-1.868299
H	4.857528	-2.974770	-2.399279
H	3.145701	-2.704309	-2.019604
C	5.740182	-3.642642	0.098771
H	6.038914	-3.422177	1.128545
H	6.544436	-3.306771	-0.564238
H	5.672223	-4.731884	0.001667
Al	-2.129338	0.166050	-0.362975
N	-3.394498	-1.339659	-0.085919
N	-2.845512	1.090910	1.246682
C	-4.169324	-1.572692	0.975232
C	-4.216871	-0.710423	2.080798
H	-4.850212	-1.021068	2.904291
C	-3.658801	0.568780	2.178743
C	-5.096726	-2.753248	0.987068
H	-5.994458	-2.531022	0.397918
H	-5.418223	-2.990611	2.002830
H	-4.642482	-3.636668	0.531854
C	-4.032424	1.385234	3.382943
H	-3.161276	1.557516	4.023560
H	-4.798617	0.884857	3.976534
H	-4.398732	2.375419	3.093724
C	-3.565838	-2.157081	-1.256114
C	-4.649562	-1.893305	-2.117751
C	-4.791674	-2.674488	-3.266191
H	-5.621053	-2.476156	-3.942289
C	-3.886098	-3.683639	-3.564846
H	-4.013920	-4.284961	-4.460836
C	-2.806544	-3.909236	-2.720959
H	-2.088201	-4.688523	-2.963703
C	-2.615223	-3.151015	-1.562958
C	-5.606315	-0.738460	-1.886366
H	-5.445965	-0.346706	-0.873363
C	-5.295395	0.391060	-2.869980
H	-5.450950	0.058851	-3.902684
H	-4.252642	0.721081	-2.787256
H	-5.946148	1.255977	-2.695631
C	-7.072698	-1.149158	-1.994273
H	-7.727379	-0.308879	-1.740450
H	-7.318960	-1.980989	-1.326182
H	-7.329850	-1.462801	-3.011846
C	-1.441971	-3.442959	-0.650255
H	-1.262458	-2.545268	-0.046613
C	-1.771709	-4.595635	0.298537
H	-2.627046	-4.365641	0.943753
H	-0.915321	-4.819069	0.943869
H	-2.015556	-5.506438	-0.261928
C	-0.144736	-3.714394	-1.403942
H	0.686874	-3.793995	-0.693876
H	0.088338	-2.891370	-2.090026
H	-0.179187	-4.651361	-1.973375
C	-2.495010	2.480869	1.355528
C	-1.481668	2.913973	2.232665
C	-1.198577	4.281107	2.301102
H	-0.412717	4.622993	2.972421
C	-1.891283	5.202214	1.528653
H	-1.660347	6.261677	1.600916
C	-2.865345	4.757932	0.642880
H	-3.387623	5.478224	0.019542
C	-3.175827	3.401339	0.527034
C	-0.653443	1.954076	3.062249
H	-1.118920	0.964006	3.001224
C	0.753758	1.838219	2.478729
H	1.251131	2.817145	2.466925
H	0.720616	1.462476	1.446131
H	1.380819	1.164981	3.073854
C	-0.575238	2.354932	4.534523
H	-0.061318	1.581112	5.114665
H	-1.562701	2.510962	4.981065
H	-0.010173	3.283915	4.668100
C	-4.235647	2.939202	-0.455557
H	-3.939717	1.938611	-0.809125
C	-4.325994	3.823691	-1.692228
H	-4.737030	4.813172	-1.463822
H	-4.986487	3.368355	-2.436059
H	-3.342837	3.962556	-2.153722
C	-5.600807	2.786757	0.215200
H	-5.937163	3.740957	0.637527
H	-5.578235	2.049348	1.024215
H	-6.355295	2.457402	-0.508714

Int-1_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.33159230
E(SCF)+ZPE(0 K) = -2955.919508

H(298 K) = -2955.836454
G(298 K) = -2956.037285
Lowest Frequency = 16.2722 cm^{-1}

Pd	0.141241	-0.289024	0.719378
Al	-2.250184	-0.276697	0.401112
N	-3.741521	-1.592830	0.155778
N	-3.590187	1.178069	0.698666
C	-4.990670	-1.449646	0.617315
C	-5.446786	-0.269085	1.218813
H	-6.449557	-0.295460	1.630564
C	-4.825031	0.985052	1.185170
C	-5.974095	-2.575748	0.478155
H	-6.052853	-2.892192	-0.567057
H	-6.963046	-2.283282	0.832968
H	-5.652123	-3.460867	1.036657
C	-5.635848	2.158180	1.658676
H	-6.446661	1.829293	2.311328
H	-6.085252	2.691881	0.813568
H	-5.015289	2.886378	2.187995
C	-3.403814	-2.828461	-0.496578
C	-3.319966	-2.863373	-1.902206
C	-2.979725	-4.068582	-2.524062
H	-2.911364	-4.099495	-3.610114
C	-2.717097	-5.212136	-1.784383
H	-2.448143	-6.138895	-2.284156
C	-2.781554	-5.156981	-0.397844
H	-2.548939	-6.044863	0.185986
C	-3.120139	-3.978642	0.269872
C	-3.543425	-1.637693	-2.763321
H	-3.873323	-0.819392	-2.110251
C	-2.231437	-1.215096	-3.427603
H	-1.457851	-0.992044	-2.680270
H	-2.372948	-0.324149	-4.049825
H	-1.848367	-2.013039	-4.074916
C	-4.637738	-1.859122	-3.804748
H	-4.367673	-2.653247	-4.509718
H	-4.804120	-0.949093	-4.390931
H	-5.588456	-2.140360	-3.340754
C	-3.089878	-3.949895	1.784872
H	-3.611365	-3.045440	2.123409
C	-1.641314	-3.842229	2.255934
H	-1.577683	-3.785897	3.348242
H	-1.149502	-2.954536	1.841218
H	-1.058334	-4.713943	1.932864
C	-3.786339	-5.150378	2.420283
H	-4.812430	-5.276398	2.057292
H	-3.825933	-5.036967	3.507847
H	-3.251614	-6.084273	2.216662
C	-3.223536	2.528018	0.369991
C	-2.251528	3.219226	1.119241
C	-1.935002	4.529316	0.743471
H	-1.184928	5.068692	1.317621
C	-2.543740	5.145635	-0.338913
H	-2.280368	6.165736	-0.608980
C	-3.485879	4.445094	-1.081540
H	-3.946097	4.915120	-1.947958
C	-3.840241	3.137318	-0.748647
C	-1.553988	2.638327	2.332149
H	-1.777234	1.564400	2.389301
C	-0.037048	2.775830	2.215430
H	0.285308	3.821800	2.291408
H	0.322908	2.375442	1.258216
H	0.458531	2.215156	3.014490
C	-2.063186	3.293783	3.615633
H	-1.898647	4.377838	3.594855
H	-1.531291	2.894802	4.485860
H	-3.135514	3.125472	3.767533
C	-4.790625	2.385542	-1.663824
H	-5.164360	1.496974	-1.141761
C	-4.016495	1.895610	-2.886752
H	-3.612278	2.741540	-3.457200
H	-4.653484	1.304671	-3.555504
H	-3.165658	1.275886	-2.585643
C	-6.003958	3.210125	-2.084683
H	-6.540081	3.622272	-1.223289
H	-6.706570	2.593942	-2.654079
H	-5.724121	4.051499	-2.727378
H	-1.117741	-1.416447	3.595067
C	-0.271584	-0.840000	3.957016
C	1.018827	-1.228321	3.563721
C	-0.437698	0.233950	4.820417
C	2.128143	-0.496221	3.998883
C	0.667138	0.946640	5.289536
C	1.940307	0.583389	4.861818
H	3.128479	-0.761969	3.671399
H	0.533178	1.784366	5.968167
H	2.808670	1.144292	5.198839
H	-1.441713	0.514841	5.129982
O	1.088719	-2.359582	2.812419
C	2.366807	-2.777986	2.375211
H	2.825181	-2.021073	1.723226
H	3.034250	-2.992192	3.221967
H	2.205088	-3.689310	1.797500
Al	2.173357	0.158061	-0.502054
N	2.802396	1.781963	-1.491382
N	3.426115	-0.969400	-1.556889
C	4.071385	-0.634090	-2.684632
C	4.124309	0.675506	-3.170645
C	3.617839	1.826523	-2.552059
C	4.060601	3.152126	-3.104784
H	3.215158	3.756348	-3.448035
H	4.553737	3.743562	-2.326179
H	4.754597	3.020378	-3.935873
C	4.836815	-1.679931	-3.444075
H	5.140315	-1.310099	-4.424639
H	4.244505	-2.591149	-3.570198
H	4.706716	0.829757	-4.072063
H	5.739110	-1.979021	-2.898800
C	3.686003	-2.279730	-1.026815
C	4.891657	-2.490535	-0.318553
C	5.159613	-3.765819	0.179490
C	4.270239	-4.816901	-0.019440
C	3.078744	-4.585852	-0.689323
C	2.752804	-3.319133	-1.188372
H	2.367739	-5.398899	-0.823527
H	4.502887	-5.808172	0.360286
H	6.082161	-3.940665	0.727461
C	5.841617	-1.343697	-0.023682
H	5.724472	-0.584963	-0.808038
H	4.404550	-0.350199	1.295121
H	7.598018	-2.286633	-0.917977
C	7.309938	-1.754926	-0.005454
H	7.542804	-2.406610	0.843440
H	5.557546	-1.400138	2.130390
H	7.950805	-0.873077	0.087607
C	5.451054	-0.687818	1.302420
H	6.083206	0.181134	1.519361
C	1.397675	-3.123400	-1.834387
C	0.295245	-3.431983	-0.824462
H	0.299624	-4.492240	-0.538537
H	-0.690075	-3.205246	-1.244483
H	0.411109	-2.820296	0.080851
H	1.297453	-2.066391	-2.114833
C	1.230210	-3.965886	-3.097062
H	1.983068	-3.729541	-3.856759
H	1.311029	-5.036456	-2.873451
H	0.241100	-3.801352	-3.537869
C	3.051341	3.503676	0.240899
C	2.399212	3.036779	-0.915082

C	1.351052	3.773916	-1.509023
C	0.991029	4.991116	-0.931378
C	1.634040	5.472332	0.203959
C	2.649825	4.728853	0.783097
H	3.147668	5.096869	1.678434
H	1.335645	6.424274	0.636630
H	0.186785	5.570148	-1.375781
C	0.604957	3.240333	-2.716156
C	0.012178	4.332814	-3.599717
H	0.750503	5.092227	-3.879628
H	-0.821032	4.841602	-3.099948
H	-1.256970	2.807028	-1.696192
H	-0.390743	3.896405	-4.518922
H	1.314501	2.667754	-3.328137
H	-0.112304	1.469644	-1.631353
C	-0.491661	2.274208	-2.274247
H	-0.978340	1.817309	-3.143932
C	4.168268	2.738491	0.923363
H	4.374747	1.833247	0.335163
H	2.855446	1.645977	2.275223
C	3.736949	2.297190	2.320842
H	3.477974	3.159824	2.947008
H	4.540345	1.748220	2.826730
H	6.267474	2.965877	1.433926
C	5.461823	3.549571	0.975764
H	5.339141	4.459597	1.573638
H	5.793431	3.854885	-0.021966

Int-2_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.31199191
E(SCF)+ZPE(0 K) = -2955.901240
H(298 K) = -2955.818427
G(298 K) = -2956.017352
Lowest Frequency = 20.0823 cm^{-1}

Pd	0.143128	-0.222231	-0.954626
Al	-2.152351	-0.083449	-0.101613
N	-3.378681	1.497166	-0.296485
N	-3.563105	-1.130321	0.821997
C	-4.671619	1.543795	0.032733
C	-5.385303	0.421302	0.486213
H	-6.444484	0.572607	0.664405
C	-4.852987	-0.782995	0.957742
C	-5.424933	2.848329	0.030514
H	-5.231213	3.387390	0.964577
H	-6.500964	2.673368	-0.030302
H	-5.124232	3.517337	-0.776218
C	-5.786994	-1.661976	1.744080
H	-5.598397	-2.725202	1.577391
H	-6.827448	-1.435580	1.503580
H	-5.649983	-1.490388	2.818067
C	-2.731510	2.748239	-0.589323
C	-2.078797	3.436907	0.451051
C	-1.550622	4.702523	0.177630
H	-1.051497	5.251639	0.973365
C	-1.645355	5.263151	-1.087254
C	-2.222390	4.535194	-2.121373
H	-2.243881	4.956999	-3.122607
C	-2.758394	3.263544	-1.904319
C	-3.101867	-2.223094	1.636812
C	-2.880132	-3.488828	1.057360
C	-2.496182	-4.541163	1.892404
H	-2.333168	-5.527001	1.465469
C	-2.310863	-4.349969	3.256597
C	-2.474718	-3.083998	3.800443
H	-2.285951	-2.923750	4.860128
C	-2.866999	-2.001606	3.008854
C	-1.079479	-0.872381	-2.590026
C	-0.523900	0.221267	-3.327030
C	-0.609952	-2.181065	-2.905416
C	0.409556	-0.005389	-4.340601
H	-0.891318	1.223596	-3.130802
C	0.324682	-2.372106	-3.913280
H	-0.996351	-3.027388	-2.344455
C	0.819972	-1.297808	-4.661735
H	0.671159	-3.382487	-4.119887
H	1.543211	-1.466773	-5.454402
H	-1.238496	6.253117	-1.278496
H	-2.013978	-5.182653	3.888684
C	-3.070588	-3.704650	-0.430859
C	-4.544406	-3.877369	-0.803656
C	-2.253311	-4.869927	-0.975265
H	-2.712917	-2.791734	-0.925133
H	-5.130624	-2.979253	-0.590501
H	-4.650372	-4.092133	-1.872776
H	-4.992585	-4.713429	-0.253255
H	-1.197195	-4.787607	-0.696054
H	-2.626851	-5.836911	-0.619103
H	-2.312000	-4.892635	-2.068993
C	-2.958206	-0.621953	3.635216
C	-1.551466	-0.071075	3.876304
C	-3.765381	-0.606823	4.931332
H	-3.459292	0.052530	2.928198
H	-0.976135	-0.006757	2.943134
H	-1.596237	0.929843	4.321436
H	-0.994904	-0.717799	4.565818
H	-4.765211	-1.034531	4.802530
H	-3.267950	-1.174503	5.725296
H	-3.884158	0.418976	5.295341
C	-3.302369	2.448083	-3.066803
C	-2.651493	2.823389	-4.397542
C	-4.823847	2.498585	-3.231236
H	-3.040550	1.407678	-2.844913
H	-1.563679	2.919309	-4.319584
H	-2.866125	2.058946	-5.151376
H	-3.039402	3.773295	-4.783264
H	-5.353615	1.992385	-2.421002
H	-5.185632	3.532557	-3.283306
H	-5.114819	2.003183	-4.164302
C	-1.918600	2.846286	1.839743
C	-2.898363	3.447407	2.846584
C	-0.482653	2.977935	2.332027
H	-2.135531	1.770612	1.777142
H	-3.940576	3.245385	2.578302
H	-2.731365	3.027693	3.845589
H	-2.776258	4.534483	2.919429
H	0.222823	2.508368	1.633594
H	-0.185670	4.023172	2.458909
H	-0.367694	2.491872	3.305959
Al	2.406831	0.077271	-0.092115
N	3.709992	-1.425505	-0.052654
N	3.781407	1.306143	0.572694
C	5.100648	1.075091	0.693036
C	5.663644	-0.198842	0.579586
C	4.983900	-1.404321	0.330964
H	6.728913	-0.274207	0.769601
C	6.024341	2.216799	1.009469
H	5.804181	3.082559	0.377480
H	7.067264	1.928163	0.869894
H	5.901329	2.557402	2.043435
H	5.552531	-3.018314	1.594461
H	6.812468	-2.537018	0.458585
C	5.735582	-2.683090	0.566272
H	5.413690	-3.490281	-0.093801
C	3.277542	2.585999	0.978984
C	3.194729	2.866037	2.363822
C	2.726614	4.117854	2.758827

C	2.310063	5.058765	1.821030
C	2.331270	4.741309	0.472367
C	2.812216	3.505947	0.021812
H	1.971338	5.462921	-0.259359
H	1.944252	6.028772	2.148906
H	2.666128	4.355673	3.817806
C	3.521871	1.797282	3.393372
H	4.319666	1.159958	2.992444
C	2.303813	0.895825	3.618106
H	1.898263	0.500001	2.676248
H	2.554713	0.045053	4.262595
H	1.493583	1.455986	4.099124
H	4.859596	3.046602	4.586609
C	4.019416	2.357331	4.720787
H	4.349793	1.545879	5.375988
H	3.231098	2.896625	5.257035
H	3.191431	2.203183	-1.624764
C	2.819868	3.224844	-1.468235
C	3.764221	4.172883	-2.206124
H	3.443540	5.215303	-2.096288
H	4.789615	4.103457	-1.828158
C	1.407832	3.291689	-2.049414
H	1.417092	3.015019	-3.110298
H	0.729928	2.601235	-1.528807
H	0.988188	4.301291	-1.970781
H	3.784340	3.945915	-3.276868
C	3.075908	-2.663590	-0.399251
C	2.303259	-3.333221	0.569860
C	1.620795	-4.493139	0.194526
C	1.707691	-4.987729	-1.099383
C	2.462868	-4.303360	-2.042929
C	3.139474	-3.119993	-1.732018
C	3.904808	-2.444119	-2.863463
H	2.520548	-4.677100	-3.064078
H	1.177678	-5.895595	-1.376745
H	1.012683	-5.011371	0.935338
C	2.198010	-2.846661	2.001820
H	2.787571	-1.923583	2.094445
C	2.786994	-3.867165	2.976180
H	3.821099	-4.128241	2.727372
H	2.771248	-3.479635	4.000532
H	2.205610	-4.796360	2.968408
H	0.695168	-2.147723	3.404975
C	0.754099	-2.520683	2.375616
H	0.326633	-1.763127	1.704522
H	0.117754	-3.410511	2.314590
H	3.463886	-2.874842	-3.774824
H	5.542821	-3.896334	-2.766709
C	5.388736	-2.817448	-2.873343
H	5.855617	-2.500628	-3.811959
H	5.929372	-2.314827	-2.063960
H	4.041220	-0.621278	-4.008244
C	3.745757	-0.930176	-2.999105
H	4.388477	-0.384629	-2.298559
H	2.707191	-0.612823	-2.846302
H	0.812004	0.849406	-4.881844
O	-2.468165	-0.759979	-2.124882
C	-3.471221	-1.132897	-3.080764
H	-3.373277	-0.533387	-3.994401
H	-3.383795	-2.196417	-3.333073
H	-4.436735	-0.937489	-2.606714

Int-3_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.39401279
E(SCF)+ZPE(0 K) = -2955.980514
H(298 K) = -2955.898488
G(298 K) = -2956.094106

Lowest Frequency = 17.0052 cm^{-1}

Pd	0.121247	-0.207137	-0.320982
Al	-3.248294	-0.289370	-0.547175
N	-3.603782	1.417334	0.245597
N	-3.518527	-1.305259	1.062905
C	-4.637621	1.474990	1.100961
C	-5.164732	0.332323	1.722445
H	-6.051629	0.482718	2.328298
C	-4.565307	-0.934812	1.816582
C	-5.241524	2.804142	1.456396
H	-4.546856	3.405657	2.050365
H	-6.157841	2.672689	2.033570
H	-5.461478	3.393869	0.562366
C	-5.134912	-1.867882	2.845198
H	-4.848592	-2.906626	2.669248
H	-6.225235	-1.792172	2.845251
H	-4.798722	-1.592353	3.849680
C	-2.961264	2.650757	-0.100854
C	-2.001083	3.178419	0.785876
C	-1.496628	4.454409	0.516782
H	-0.756334	4.886164	1.185120
C	-1.895519	5.161475	-0.610444
C	-2.757228	4.573932	-1.528461
H	-3.009041	5.104943	-2.442538
C	-3.296900	3.304232	-1.303788
C	-2.744111	-2.453211	1.431299
C	-2.751850	-3.591325	0.590947
C	-1.951802	-4.680269	0.939926
H	-1.942984	-5.559306	0.302296
C	-1.168673	-4.662575	2.087960
C	-1.174528	-3.541824	2.902612
H	-0.549764	-3.518888	3.793898
C	-1.946599	-2.418239	2.594311
C	-1.609432	-0.511336	-1.618217
C	-1.345593	0.486515	-2.604425
C	-1.007794	-1.781907	-1.874913
C	-0.704476	0.205559	-3.806748
H	-1.701892	1.501955	-2.434107
C	-0.366892	-2.067839	-3.089531
H	-1.140348	-2.596796	-1.164009
C	-0.252721	-1.090710	-4.070110
H	0.033230	-3.064305	-3.260111
H	0.220193	-1.322808	-5.022257
H	-1.494980	6.154822	-0.799099
H	-0.552686	-5.521778	2.342229
C	-3.622689	-3.638758	-0.650518
C	-5.102416	-3.799277	-0.302035
C	-3.197909	-4.695772	-1.661737
H	-3.528390	-2.672332	-1.160572
H	-5.475788	-2.956142	0.283677
H	-5.705745	-3.849373	-1.213927
H	-5.270687	-4.721913	0.266006
H	-2.132239	-4.627361	-1.906199
H	-3.396732	-5.711849	-1.301642
H	-3.762450	-4.565655	-2.590000
C	-1.843379	-1.210701	3.507299
C	-0.427792	-0.635613	3.480223
C	-2.222234	-1.547501	4.950830
H	-2.525465	-0.431864	3.143675
H	-0.099439	-0.383785	2.460322
H	-0.365670	0.266858	4.099325
H	0.290300	-1.356613	3.888312
H	-3.194884	-2.041519	5.031498
H	-1.482866	-2.219425	5.401384
H	-2.250242	-0.640050	5.563405
C	-4.169512	2.630439	-2.349630
C	-3.834645	3.087851	-3.765923
C	-5.667948	2.763768	-2.082534
H	-3.956094	1.555694	-2.301125

H	-2.756367	3.056599	-3.960239
H	-4.327867	2.439172	-4.496125
H	-4.177720	4.110396	-3.961047
H	-5.967290	2.218076	-1.184679
H	-5.963547	3.814646	-1.975495
H	-6.238269	2.338424	-2.914886
C	-1.471175	2.365474	1.957088
C	-2.304067	2.490862	3.236316
C	-0.018977	2.706907	2.265151
H	-1.496113	1.308335	1.639826
H	-3.282432	2.008321	3.162401
H	-1.777334	2.018917	4.073700
H	-2.458456	3.544087	3.502716
H	0.600551	2.679023	1.363251
H	0.084345	3.698158	2.722988
H	0.392327	1.980680	2.970412
Al	2.463849	0.013585	0.096379
N	3.859479	-1.278216	-0.448916
N	3.790288	1.469311	0.085309
C	5.102992	1.393465	-0.186524
C	5.757589	0.185149	-0.448924
C	5.178502	-1.088518	-0.530573
H	6.831774	0.238437	-0.586822
C	5.940140	2.641441	-0.176882
H	5.448509	3.454055	-0.719773
H	6.920692	2.458010	-0.618542
H	6.091118	3.007672	0.844676
H	6.195442	-2.767058	0.295472
H	7.096627	-1.956593	-0.992205
C	6.099024	-2.265705	-0.675542
H	5.715758	-3.013262	-1.373109
C	3.258726	2.746983	0.468853
C	3.491579	3.220159	1.777631
C	2.979634	4.470691	2.126469
C	2.244461	5.223689	1.218130
C	1.980382	4.717915	-0.047530
C	2.467349	3.469256	-0.445636
H	1.368139	5.292183	-0.738084
H	1.856180	6.197411	1.506852
H	3.150309	4.856332	3.128445
C	4.208801	2.362028	2.805186
H	4.913643	1.708634	2.276271
C	3.209158	1.449329	3.520751
H	2.617597	0.853345	2.811890
H	3.720587	0.759832	4.201550
H	2.498951	2.042311	4.109083
H	5.698914	3.871397	3.330104
C	5.013516	3.170030	3.817179
H	5.605835	2.504458	4.452046
H	4.366144	3.750198	4.483327
H	2.119080	1.825943	-1.738899
C	2.156242	2.921472	-1.824699
C	3.258021	3.263736	-2.825931
H	3.386540	4.349153	-2.915212
H	4.221992	2.834605	-2.531290
C	0.783999	3.342186	-2.333904
H	0.546556	2.797710	-3.254238
H	0.004454	3.110396	-1.598302
H	0.728305	4.413060	-2.563329
H	3.014366	2.872408	-3.819380
C	3.317435	-2.574163	-0.739535
C	3.086259	-3.482918	0.309466
C	2.449888	-4.691478	0.019221
C	2.073676	-5.007156	-1.278671
C	2.334666	-4.106495	-2.303383
C	2.938609	-2.867722	-2.065002
C	3.177698	-1.969691	-3.274026
H	2.048991	-4.353031	-3.325073
H	1.579109	-5.950843	-1.492783
H	2.247616	-5.391108	0.828354
C	3.489529	-3.180529	1.738573
H	4.022507	-2.220238	1.747335
C	4.434507	-4.243061	2.297497
H	5.324791	-4.372741	1.673294
H	4.764427	-3.978970	3.307388
H	3.939113	-5.218313	2.361610
H	2.528066	-2.707329	3.634696
C	2.255057	-3.035358	2.624565
H	1.546790	-2.313937	2.201300
H	1.728727	-3.992809	2.714296
H	2.481515	-2.355780	-4.033239
H	4.863266	-3.192406	-3.957299
C	4.588286	-2.138646	-3.843901
H	4.662186	-1.662203	-4.827108
H	5.334579	-1.658251	-3.201446
H	2.738554	-0.031826	-4.118983
C	2.853305	-0.483269	-3.126223
H	3.653167	0.069098	-2.617613
H	1.909680	-0.322789	-2.587635
H	-0.564849	0.993780	-4.544486
O	-4.658261	-0.596277	-1.545551
C	-4.657031	-1.018524	-2.869644
H	-4.647953	-0.170282	-3.579511
H	-3.785662	-1.649579	-3.131257
H	-5.560690	-1.607630	-3.085822

Int-4_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.30808291
E(SCF)+ZPE(0 K) = -2955.898422
H(298 K) = -2955.816639
G(298 K) = -2956.012313
Lowest Frequency = 18.0050 cm^{-1}

Pd	0.139802	-0.188228	1.077740
Al	-2.160870	-0.516899	0.431879
N	-3.227132	-2.162962	0.391484
N	-3.726333	0.603317	0.862991
C	-4.418080	-2.302853	0.987806
C	-5.104261	-1.239406	1.589521
H	-6.024971	-1.494281	2.101714
C	-4.824563	0.125995	1.470226
C	-5.088480	-3.644948	0.999330
H	-5.253225	-3.999388	-0.023848
H	-6.048431	-3.603062	1.514581
H	-4.462042	-4.402526	1.479289
C	-5.863258	1.078005	1.993001
H	-6.509938	0.581228	2.718120
H	-6.498083	1.450883	1.181186
H	-5.408145	1.957609	2.455733
C	-2.647418	-3.338879	-0.203168
C	-2.822737	-3.571916	-1.581545
C	-2.297614	-4.743638	-2.132452
H	-2.423254	-4.930312	-3.197324
C	-1.612539	-5.662448	-1.348131
H	-1.213488	-6.570568	-1.792424
C	-1.418791	-5.399631	0.001010
H	-0.853619	-6.101072	0.612023
C	-1.917759	-4.239300	0.599385
C	-3.491542	-2.558687	-2.487851
H	-3.996500	-1.818854	-1.853107
C	-2.426026	-1.826486	-3.308818
H	-1.704224	-1.312039	-2.660206
H	-2.876674	-1.080401	-3.972794
H	-1.864792	-2.534594	-3.930819
C	-4.546310	-3.179241	-3.399247
H	-4.103986	-3.883298	-4.112394
H	-5.051272	-2.404711	-3.986002

H	-5.308362	-3.721955	-2.831290
C	-1.621206	-3.982449	2.064814
H	-2.138187	-3.063969	2.368015
C	-0.123873	-3.750863	2.265527
H	0.097206	-3.513626	3.312080
H	0.244954	-2.914256	1.661912
H	0.447506	-4.647713	1.991767
C	-2.103350	-5.121214	2.962953
H	-3.175245	-5.319132	2.856306
H	-1.912331	-4.884467	4.013981
H	-1.575807	-6.055602	2.739977
C	-3.735410	1.996594	0.510542
C	-2.932232	2.915743	1.209785
C	-2.984523	4.261118	0.826684
H	-2.369830	4.982886	1.359420
C	-3.796520	4.688338	-0.213283
H	-3.822652	5.739657	-0.490556
C	-4.572375	3.764562	-0.905390
H	-5.192162	4.098363	-1.733725
C	-4.556945	2.412433	-0.562931
C	-2.054689	2.512270	2.377123
H	-1.914244	1.425043	2.346725
C	-0.671349	3.146124	2.283357
H	-0.706903	4.233490	2.410799
H	-0.205694	2.933292	1.314112
H	-0.007693	2.751768	3.058231
C	-2.725361	2.852598	3.707898
H	-2.911480	3.930295	3.790324
H	-2.087727	2.558315	4.547891
H	-3.685672	2.339356	3.826391
C	-5.325898	1.409881	-1.404403
H	-5.576992	0.542629	-0.781550
C	-4.423023	0.903419	-2.528047
H	-4.147389	1.723926	-3.201508
H	-4.919689	0.126095	-3.120785
H	-3.489734	0.484287	-2.130409
C	-6.633693	1.955028	-1.967390
H	-7.265697	2.391191	-1.187022
H	-7.200945	1.155453	-2.453045
H	-6.463980	2.727854	-2.724575
H	-1.208172	-0.751548	2.029362
C	1.378838	-0.340302	2.770048
C	2.440005	-1.255818	2.813996
C	1.114003	0.343312	3.961620
C	3.220690	-1.448063	3.956932
C	1.881715	0.177572	5.119229
C	2.945088	-0.715607	5.111972
H	4.039735	-2.163414	3.956131
H	1.635689	0.732649	6.022043
H	3.552951	-0.864224	6.001012
H	0.262531	1.021709	4.002530
O	2.665978	-1.976637	1.653235
C	3.332587	-3.208589	1.806116
H	4.409853	-3.088770	1.996739
H	2.896491	-3.795106	2.627107
H	3.211865	-3.744573	0.861853
Al	1.701661	0.563551	-0.615006
N	2.006231	2.315712	-1.501409
N	3.017251	-0.322517	-1.772138
C	3.434230	0.151585	-2.965023
C	3.226348	1.465770	-3.388172
C	2.697519	2.516583	-2.630303
C	3.010225	3.911554	-3.092992
H	2.121504	4.537831	-3.202093
H	3.638991	4.410558	-2.346814
H	3.549832	3.896051	-4.040483
C	4.249509	-0.719270	-3.879716
H	4.494118	-0.188895	-4.800668
H	3.712978	-1.638277	-4.134960
H	3.668773	1.735777	-4.339815
H	5.181440	-1.037161	-3.400056
C	3.668596	-1.551676	-1.376680
C	4.837254	-1.453943	-0.598525
C	5.630463	-2.595717	-0.460419
C	5.254294	-3.804879	-1.033626
C	4.029974	-3.908454	-1.683780
C	3.208667	-2.790724	-1.853342
H	3.705407	-4.870827	-2.071346
H	5.894415	-4.677333	-0.933736
H	6.551788	-2.537205	0.113643
C	5.218995	-0.147573	0.071930
H	4.276063	0.372994	0.304419
H	5.349159	-0.985117	2.078440
H	5.501071	1.032245	-1.756516
C	6.041232	0.759633	-0.844398
H	6.973777	0.264671	-1.140839
H	6.925059	-0.794160	1.277768
H	6.309300	1.689587	-0.330588
C	5.931423	-0.349780	1.403637
H	6.075521	0.614953	1.900960
C	1.813608	-2.917319	-2.422593
C	0.857752	-3.125643	-1.246320
H	1.063347	-4.086872	-0.758426
H	-0.184813	-3.134599	-1.578346
H	0.967119	-2.341793	-0.485454
H	1.550266	-1.965099	-2.905187
C	1.645024	-4.026533	-3.452526
H	2.352460	-3.937738	-4.284367
H	1.779445	-5.017576	-3.004429
H	0.630940	-4.006079	-3.864249
C	2.271508	3.966200	0.298143
C	1.547780	3.493955	-0.810938
C	0.397014	4.165894	-1.282751
C	-0.014060	5.312992	-0.602929
C	0.685832	5.789965	0.500862
C	1.815411	5.120228	0.943240
H	2.361291	5.490044	1.809036
H	0.344114	6.684809	1.015155
H	-0.896954	5.845060	-0.946075
C	-0.357394	3.664643	-2.501314
C	-1.173247	4.747147	-3.198379
H	-0.579276	5.639652	-3.422912
H	-2.029301	5.055018	-2.586689
H	-2.064130	2.793986	-1.490464
H	-1.577950	4.363894	-4.139937
H	0.383561	3.299814	-3.225067
H	-0.711972	1.678983	-1.641761
C	-1.253053	2.479719	-2.155560
H	-1.702033	2.056881	-3.061807
C	3.514995	3.275424	0.822299
H	3.759997	2.451319	0.138309
H	2.400898	1.992902	2.191572
C	3.253483	2.679311	2.204259
H	3.035664	3.466565	2.936225
H	4.122590	2.119167	2.568081
H	5.609266	3.680187	1.213177
C	4.723780	4.208873	0.844072
H	4.557814	5.063888	1.508561
H	4.958231	4.603945	-0.150250

Int-5_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.30953555
E(SCF)+ZPE(0 K) = -2955.900996
H(298 K) = -2955.818985
G(298 K) = -2956.014957

Lowest Frequency = 17.4625 cm^{-1}

Pd	0.010643	0.218218	0.566573
Al	2.310946	0.801247	0.520227
N	3.062393	2.427920	-0.276611
N	4.053786	-0.058275	0.547625
C	4.343661	2.801088	-0.226814
C	5.349782	1.959729	0.271729
H	6.347639	2.379250	0.328608
C	5.228132	0.599701	0.566009
C	4.754898	4.156430	-0.724081
H	5.837982	4.220487	-0.836941
H	4.438871	4.941221	-0.028304
H	4.279827	4.388533	-1.681496
C	6.491836	-0.153201	0.866454
H	7.320800	0.533563	1.042318
H	6.767501	-0.816295	0.039776
H	6.366896	-0.799466	1.740688
C	2.093231	3.327222	-0.833498
C	1.571787	3.034690	-2.109794
C	0.602011	3.891882	-2.633600
H	0.182722	3.689327	-3.615419
C	0.159272	4.996805	-1.917161
H	-0.598982	5.650820	-2.341425
C	0.674549	5.256479	-0.654498
H	0.306458	6.109788	-0.088804
C	1.641615	4.428379	-0.081412
C	2.086864	1.853295	-2.911652
H	2.317193	1.044618	-2.203718
C	1.059281	1.294738	-3.885814
H	0.119118	1.056648	-3.377204
H	1.437374	0.374715	-4.343006
H	0.839644	1.992638	-4.702253
C	3.389174	2.198135	-3.636275
H	3.246412	3.042498	-4.320862
H	3.741770	1.345448	-4.228495
H	4.189260	2.463785	-2.937798
C	2.123214	4.698777	1.332038
H	3.043821	4.126581	1.498939
C	1.097331	4.200189	2.348175
H	1.450201	4.356406	3.373256
H	0.877785	3.135107	2.218663
H	0.147633	4.737560	2.240180
C	2.448404	6.171987	1.568185
H	3.144655	6.570697	0.821749
H	2.895762	6.311112	2.557041
H	1.547151	6.793539	1.536406
C	4.136528	-1.492221	0.509402
C	3.915761	-2.257751	1.667606
C	4.136239	-3.635901	1.597224
H	3.977909	-4.239424	2.489374
C	4.545486	-4.244224	0.418661
H	4.724582	-5.316354	0.390281
C	4.688095	-3.481975	-0.734060
H	4.961855	-3.964214	-1.670974
C	4.479659	-2.102240	-0.715592
C	3.426254	-1.647369	2.964119
H	3.430637	-0.555300	2.851522
C	1.982878	-2.077540	3.228909
H	1.911955	-3.168743	3.322152
H	1.315537	-1.766737	2.412611
H	1.609457	-1.632957	4.157764
C	4.327538	-1.993672	4.146955
H	4.330689	-3.070819	4.348034
H	3.977024	-1.495792	5.056072
H	5.365087	-1.688979	3.975235
C	4.564454	-1.316577	-2.011879
H	4.511712	-0.246679	-1.776122
C	3.352937	-1.650084	-2.883181
H	3.357917	-2.710588	-3.165631
H	3.353006	-1.059692	-3.807497
H	2.417396	-1.451436	-2.347994
C	5.863721	-1.556199	-2.775721
H	6.746309	-1.321109	-2.171967
H	5.900634	-0.932282	-3.674749
H	5.956446	-2.598361	-3.100813
C	-0.953644	1.087000	2.198034
C	-1.643979	2.302790	2.016665
C	-0.837422	0.649433	3.523536
C	-2.168460	3.035686	3.085356
C	-1.345107	1.366888	4.612972
C	-2.007226	2.567309	4.391782
H	-2.687743	3.975146	2.917264
H	-1.212622	0.989798	5.625145
H	-2.406758	3.144592	5.222141
H	1.180607	-0.263732	-0.634269
H	-0.299934	-0.277340	3.724409
O	-1.721359	2.751384	0.712115
C	-2.269367	4.031479	0.515961
H	-3.310030	4.095672	0.858881
H	-1.681448	4.808776	1.029199
H	-2.237242	4.219800	-0.559510
Al	-1.933175	-0.897108	-0.476590
N	-2.105525	-2.815664	-0.935251
N	-3.805257	-0.599859	-0.946302
C	-4.638626	-1.442275	-1.584930
C	-4.322924	-2.778644	-1.839187
C	-3.175445	-3.457967	-1.407754
C	-3.222684	-4.958337	-1.412501
H	-2.256748	-5.414196	-1.635265
H	-3.512457	-5.307281	-0.413397
H	-3.969539	-5.326731	-2.118423
C	-6.011514	-0.977152	-1.976054
H	-6.583683	-1.786068	-2.432001
H	-5.963004	-0.143106	-2.683655
H	-5.099741	-3.380390	-2.297114
H	-6.559716	-0.603542	-1.104594
C	-4.361339	0.656159	-0.515888
C	-4.759855	0.774747	0.831185
C	-5.397230	1.956528	1.218129
C	-5.622765	2.983721	0.309432
C	-5.155136	2.873641	-0.994045
C	-4.502948	1.718089	-1.426920
H	-5.286220	3.703316	-1.685436
H	-6.133806	3.888098	0.629665
H	-5.714588	2.076269	2.249849
C	-4.507682	-0.343391	1.830347
H	-3.491030	-0.728191	1.631145
H	-3.849019	0.994794	3.419585
H	-5.432603	-1.991109	0.694070
C	-5.488429	-1.507952	1.673513
H	-6.519217	-1.164745	1.823406
H	-5.515991	0.404222	3.609723
H	-5.285891	-2.275985	2.429204
C	-4.506719	0.134517	3.275371
H	-4.155028	-0.665819	3.933510
C	-3.906576	1.643486	-2.818588
C	-2.531363	2.316024	-2.827046
H	-2.631475	3.395164	-2.654618
H	-2.033909	2.180879	-3.794710
H	-1.873623	1.926233	-2.038922
H	-3.753585	0.584961	-3.065799
C	-4.805016	2.242059	-3.896118
H	-5.809360	1.804799	-3.886071
H	-4.919115	3.324527	-3.773731
H	-4.376193	2.076996	-4.889255
C	-0.966960	-4.036411	0.853089
C	-0.984995	-3.588287	-0.481099
C	0.092759	-3.822247	-1.357961
C	1.194809	-4.516888	-0.851768

C	1.228425	-4.978463	0.458451
C	0.153897	-4.738260	1.300816
H	0.182616	-5.089918	2.330620
H	2.097653	-5.518096	0.821573
H	2.045172	-4.696547	-1.508612
C	0.116405	-3.451112	-2.835441
C	-0.239686	-2.011258	-3.202174
H	0.206328	-1.287376	-2.512635
H	-1.324318	-1.843937	-3.218245
H	-1.775575	-4.257345	-3.564793
H	0.127451	-1.788272	-4.210688
H	1.166444	-3.588561	-3.129139
H	-0.481376	-5.465977	-3.454987
C	-0.700236	-4.420020	-3.693533
H	-0.480603	-4.263696	-4.754976
C	-2.105103	-3.758750	1.817332
H	-2.945680	-3.336678	1.249226
H	-1.335076	-1.792704	2.379928
C	-1.685354	-2.717998	2.854760
H	-0.864992	-3.096105	3.477419
H	-2.518764	-2.460725	3.519090
H	-3.482352	-4.813530	3.120174
C	-2.607970	-5.030180	2.498031
H	-1.844161	-5.461958	3.154026
H	-2.889976	-5.802462	1.774468

Int-6_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.34262900
E(SCF)+ZPE(0 K) = -2955.932371
H(298 K) = -2955.850519
G(298 K) = -2956.046764
Lowest Frequency = 16.1446 cm^{-1}

Pd	0.021566	0.003765	-0.646496
Al	-2.323836	0.630562	0.478421
N	-4.240365	0.259762	0.286486
N	-2.502777	2.552472	0.286151
C	-5.174353	1.207867	0.398397
C	-4.884943	2.562243	0.650875
H	-5.742446	3.205477	0.812818
C	-3.652389	3.207618	0.509206
C	-6.619989	0.872701	0.157437
H	-6.801802	0.824758	-0.922910
H	-7.273802	1.644010	0.567772
H	-6.908813	-0.099220	0.560673
C	-3.644357	4.708602	0.550125
H	-4.630732	5.103869	0.796106
H	-3.327844	5.131034	-0.409246
H	-2.921298	5.069428	1.289855
C	-4.680333	-1.084671	0.017386
C	-4.760836	-1.550681	-1.305316
C	-5.240441	-2.847008	-1.523956
H	-5.315497	-3.214127	-2.546092
C	-5.617047	-3.664203	-0.468865
H	-5.997835	-4.664141	-0.659177
C	-5.481827	-3.203489	0.836171
H	-5.742276	-3.855788	1.666557
C	-5.001301	-1.922066	1.107304
C	-4.312709	-0.727778	-2.496668
H	-3.954520	0.240890	-2.126748
C	-3.139511	-1.413531	-3.195668
H	-2.287164	-1.512131	-2.515961
H	-2.804141	-0.838104	-4.064919
H	-3.417309	-2.414238	-3.548355
C	-5.451729	-0.464890	-3.479512
H	-5.828111	-1.398620	-3.913104
H	-5.110239	0.165927	-4.307552
H	-6.299693	0.038112	-3.003075
C	-4.803048	-1.474746	2.543517
H	-4.067889	-0.662565	2.532766
C	-4.231001	-2.588460	3.418419
H	-3.864961	-2.173607	4.363206
H	-3.392527	-3.093282	2.931119
H	-4.986120	-3.344694	3.663545
C	-6.084931	-0.929111	3.175671
H	-6.429548	-0.008141	2.697645
H	-5.921917	-0.703755	4.234713
H	-6.897101	-1.663812	3.114474
C	-1.426375	3.309152	-0.298804
C	-0.456211	3.930795	0.505132
C	0.505952	4.735740	-0.109622
H	1.260618	5.217353	0.508264
C	0.513588	4.927347	-1.484342
H	1.254875	5.578399	-1.942920
C	-0.421789	4.267889	-2.271642
H	-0.401013	4.390605	-3.353133
C	-1.392019	3.439775	-1.703504
C	-0.384910	3.694628	1.995715
H	-1.319347	3.205691	2.300651
C	0.777094	2.744915	2.284161
H	1.721730	3.202368	1.970493
H	0.665872	1.801145	1.732909
H	0.849169	2.510947	3.352817
C	-0.241804	4.981892	2.803182
H	0.719965	5.471355	2.610160
H	-0.281861	4.767458	3.876033
H	-1.031023	5.706501	2.574934
C	-2.375981	2.723623	-2.606335
H	-2.938998	2.015010	-1.988658
C	-1.653141	1.912027	-3.678371
H	-1.072689	2.553719	-4.351639
H	-2.375629	1.364133	-4.294230
H	-0.967466	1.185702	-3.220497
C	-3.383245	3.688356	-3.230161
H	-3.963797	4.220288	-2.468815
H	-4.091913	3.150096	-3.869661
H	-2.881955	4.440598	-3.850724
C	-1.619678	-0.074289	2.207306
C	-1.353816	-1.443995	2.038642
C	-1.201464	0.482939	3.417529
C	-0.627415	-2.208984	2.944052
C	-0.498362	-0.260309	4.371278
C	-0.193537	-1.594392	4.121170
H	-0.420233	-3.259311	2.750979
H	-0.170751	0.207650	5.296754
H	0.373726	-2.171591	4.848608
H	-1.719709	0.189078	-1.029016
H	-1.397434	1.534796	3.623249
O	-1.937691	-1.953187	0.901245
C	-1.379341	-3.120247	0.325294
H	-0.297058	-2.996846	0.176357
H	-1.575265	-4.007309	0.944349
H	-1.870866	-3.247641	-0.642781
Al	2.352281	-0.457581	-0.466735
N	4.071529	0.522190	-0.516452
N	3.272557	-2.138566	-0.902270
C	4.490707	-2.272888	-1.446689
C	5.410357	-1.220663	-1.496552
C	5.256075	0.049583	-0.923381
C	6.506192	0.852757	-0.705680
H	6.366455	1.916760	-0.905809
H	6.809407	0.772904	0.345463
H	7.326359	0.474212	-1.317974
C	4.933693	-3.611428	-1.958645
H	5.959683	-3.575591	-2.327106
H	4.283349	-3.952856	-2.770563
H	6.390893	-1.455277	-1.894938

H	4.865813	-4.372610	-1.174329
C	2.493248	-3.323930	-0.675552
C	2.481029	-3.870495	0.628951
C	1.729516	-5.027443	0.847395
C	0.997393	-5.617819	-0.177666
C	0.984803	-5.038508	-1.437902
C	1.723728	-3.883249	-1.711723
H	0.382016	-5.479588	-2.229279
H	0.420033	-6.517913	0.016058
H	1.705938	-5.469713	1.839162
C	3.243305	-3.206568	1.765354
H	3.040615	-2.123788	1.690168
H	1.699456	-3.556204	3.269608
H	5.197727	-2.943809	0.780100
C	4.759267	-3.399627	1.670253
H	5.012416	-4.466432	1.668257
H	3.059493	-4.692202	3.349099
H	5.250256	-2.948072	2.539787
C	2.780300	-3.651665	3.146825
H	3.258722	-3.038225	3.916905
C	1.620554	-3.243028	-3.082450
C	0.255324	-2.573590	-3.242195
H	-0.549416	-3.317666	-3.187584
H	0.173830	-2.063739	-4.209068
H	0.080003	-1.827237	-2.449538
H	2.384380	-2.457585	-3.151590
C	1.864262	-4.238536	-4.215124
H	2.820646	-4.763097	-4.113670
H	1.079058	-5.001433	-4.253278
H	1.862412	-3.727174	-5.182518
C	4.315543	1.819752	1.543462
C	4.067363	1.794118	0.155031
C	3.824480	2.977588	-0.570969
C	3.898717	4.188095	0.126748
C	4.181224	4.239274	1.485677
C	4.373674	3.057418	2.187910
H	4.559019	3.089709	3.259422
H	4.229543	5.196422	1.998443
H	3.725530	5.111125	-0.424804
C	3.541923	3.055103	-2.065407
C	2.420609	2.163081	-2.592834
H	1.551394	2.126689	-1.924944
H	2.759802	1.132442	-2.756223
H	5.142591	1.836079	-2.910418
H	2.077884	2.536997	-3.564687
H	3.204221	4.089956	-2.218699
H	5.623513	3.512460	-2.578006
C	4.799420	2.876322	-2.918283
H	4.587304	3.133134	-3.961327
C	4.470914	0.548092	2.359299
H	4.617911	-0.292093	1.666196
H	2.310417	0.179281	2.512539
C	3.193759	0.271875	3.158048
H	2.992241	1.087138	3.863301
H	3.282582	-0.656113	3.735381
H	5.811862	-0.376742	3.789813
C	5.684158	0.586413	3.285337
H	5.573000	1.344896	4.067658
H	6.609333	0.808255	2.743298

TS1_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.31098646
E(SCF)+ZPE(0 K) = -2955.899994
H(298 K) = -2955.817843
G(298 K) = -2956.016399

Lowest Frequency = -89.7392 cm^{-1}

Pd	0.167439	-0.188963	-0.902704
Al	-2.136941	-0.091053	-0.072046
N	-3.407180	1.451233	-0.373238
N	-3.585538	-1.157084	0.786698
C	-4.709850	1.482984	-0.084471
C	-5.420517	0.356703	0.365095
H	-6.486895	0.494639	0.508465
C	-4.884826	-0.831170	0.873263
C	-5.483730	2.774746	-0.129008
H	-5.351500	3.314096	0.815661
H	-6.552048	2.582050	-0.247667
H	-5.151097	3.449944	-0.917882
C	-5.830279	-1.714917	1.640579
H	-5.619326	-2.776990	1.494558
H	-6.866164	-1.509124	1.364232
H	-5.730416	-1.527034	2.716025
C	-2.768203	2.706119	-0.666892
C	-2.166475	3.427517	0.381972
C	-1.637110	4.690714	0.099674
H	-1.177756	5.263376	0.903023
C	-1.680465	5.219271	-1.181475
C	-2.209059	4.461436	-2.220056
H	-2.192368	4.858326	-3.231595
C	-2.745141	3.191666	-1.993469
C	-3.131710	-2.234645	1.625062
C	-2.863507	-3.500069	1.064093
C	-2.474648	-4.534372	1.919151
H	-2.274301	-5.519625	1.507595
C	-2.327746	-4.326180	3.285433
C	-2.539002	-3.060610	3.812687
H	-2.381750	-2.885810	4.875164
C	-2.938982	-1.996139	3.000845
C	-1.138055	-1.000707	-2.739220
C	-0.435851	0.127141	-3.227642
C	-0.714179	-2.293115	-3.096748
C	0.664725	-0.066901	-4.073400
H	-0.814523	1.125022	-3.027452
C	0.377294	-2.456646	-3.942078
H	-1.247973	-3.153299	-2.704206
C	1.057869	-1.348256	-4.452068
H	0.696682	-3.461735	-4.205497
H	1.908680	-1.484479	-5.113975
H	-1.272525	6.207340	-1.380034
H	-2.024442	-5.145057	3.932275
C	-3.010143	-3.735151	-0.426685
C	-4.471781	-3.932557	-0.834543
C	-2.164825	-4.896846	-0.933837
H	-2.648841	-2.823204	-0.921623
H	-5.074544	-3.038594	-0.652363
H	-4.548115	-4.168199	-1.902024
H	-4.923806	-4.764710	-0.281410
H	-1.111346	-4.778288	-0.659370
H	-2.515867	-5.861111	-0.549057
H	-2.224060	-4.959634	-2.026052
C	-3.077258	-0.613982	3.612524
C	-1.688532	-0.029809	3.878588
C	-3.912619	-0.607297	4.890628
H	-3.578986	0.042943	2.889215
H	-1.094938	0.040313	2.957176
H	-1.764345	0.972962	4.315090
H	-1.132050	-0.659487	4.583802
H	-4.899614	-1.058261	4.743259
H	-3.420167	-1.157691	5.699691
H	-4.061908	0.418258	5.243819
C	-3.244982	2.349635	-3.156210
C	-2.540253	2.687907	-4.469171
C	-4.758929	2.408931	-3.378113
H	-2.999736	1.313585	-2.898868

H	-1.455160	2.774389	-4.351918
H	-2.735123	1.909299	-5.213937
H	-2.902229	3.632584	-4.891017
H	-5.322434	1.928066	-2.575113
H	-5.107572	3.444878	-3.466594
H	-5.022368	1.894830	-4.309294
C	-2.055552	2.878545	1.792292
C	-3.021118	3.561462	2.759463
C	-0.620704	2.969254	2.298478
H	-2.321097	1.812302	1.766542
H	-4.066655	3.421849	2.465371
H	-2.907238	3.154482	3.771052
H	-2.832280	4.640052	2.813494
H	0.068025	2.423431	1.639453
H	-0.275415	4.005160	2.361250
H	-0.540294	2.542061	3.303236
Al	2.444620	0.112179	-0.164765
N	3.766747	-1.376241	-0.002751
N	3.762447	1.364396	0.587889
C	5.077913	1.155457	0.773181
C	5.667299	-0.109754	0.701010
C	5.016414	-1.330502	0.448617
H	6.723246	-0.164674	0.943544
C	5.967581	2.314115	1.125854
H	5.750683	3.179342	0.492096
H	7.020152	2.046773	1.019003
H	5.805286	2.645182	2.157582
H	5.576526	-2.872262	1.802620
H	6.847659	-2.447033	0.659067
C	5.769702	-2.592135	0.759936
H	5.459421	-3.434361	0.139094
C	3.219421	2.629331	0.988522
C	3.078799	2.889009	2.373253
C	2.579773	4.128992	2.767427
C	2.185259	5.077690	1.827972
C	2.261489	4.779171	0.477193
C	2.778026	3.557614	0.028169
H	1.918534	5.506026	-0.257550
H	1.794052	6.038062	2.155035
H	2.476084	4.350669	3.826568
C	3.380837	1.811315	3.401312
H	4.204751	1.191782	3.026180
C	2.169055	0.888452	3.563665
H	1.810841	0.496216	2.601330
H	2.406287	0.034987	4.210015
H	1.330047	1.430637	4.015117
H	4.647528	3.065530	4.665435
C	3.814147	2.360882	4.755427
H	4.130919	1.545610	5.412659
H	2.995511	2.879605	5.266085
H	3.260206	2.296176	-1.623257
C	2.847536	3.301914	-1.464807
C	3.780573	4.294828	-2.156557
H	3.417087	5.323141	-2.047604
H	4.793356	4.259362	-1.741850
C	1.452714	3.328476	-2.089595
H	1.506714	3.095038	-3.159736
H	0.793150	2.590057	-1.612192
H	0.985187	4.314632	-1.988704
H	3.848449	4.082708	-3.228487
C	3.156894	-2.623893	-0.352805
C	2.339650	-3.277494	0.590899
C	1.662096	-4.434564	0.198686
C	1.789261	-4.937954	-1.088458
C	2.593293	-4.273489	-2.005491
C	3.276793	-3.099265	-1.675140
C	4.124213	-2.466544	-2.773122
H	2.689503	-4.658370	-3.019776
H	1.256306	-5.839623	-1.380362
H	1.022444	-4.941761	0.920406
C	2.191383	-2.782912	2.016681
H	2.773212	-1.856103	2.119706
C	2.760946	-3.797931	3.008775
H	3.800901	-4.058240	2.784559
H	2.720904	-3.406004	4.030871
H	2.181443	-4.728290	2.991626
H	0.650599	-2.101560	3.387132
C	0.737521	-2.462739	2.355409
H	0.328195	-1.697764	1.681426
H	0.103351	-3.352199	2.268090
H	3.698817	-2.873575	-3.702674
H	5.658227	-4.021607	-2.611429
C	5.580111	-2.934526	-2.715941
H	6.113126	-2.642223	-3.626964
H	6.109272	-2.473920	-1.874861
H	4.426222	-0.663941	-3.917005
C	4.072929	-0.945735	-2.918177
H	4.722032	-0.438343	-2.195932
H	3.053596	-0.559113	-2.804461
H	1.203613	0.805443	-4.437356
O	-2.454550	-0.837376	-2.206624
C	-3.515229	-1.206075	-3.098136
H	-3.445584	-0.643533	-4.037823
H	-3.489845	-2.280630	-3.314300
H	-4.444640	-0.953574	-2.580670

TS2_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.31034379
E(SCF)+ZPE(0 K) = -2955.899693
H(298 K) = -2955.817770
G(298 K) = -2956.013692
Lowest Frequency = -217.6975 cm^{-1}

Pd	0.053467	-0.254851	-0.769111
Al	-2.279786	-0.070973	-0.163851
N	-3.364305	1.579609	-0.103156
N	-3.519972	-1.064910	0.981374
C	-4.613190	1.667733	0.361923
C	-5.306482	0.564210	0.888350
H	-6.334344	0.746065	1.182611
C	-4.768288	-0.667834	1.279013
C	-5.317303	2.996802	0.428694
H	-4.985810	3.551506	1.313262
H	-6.397123	2.858371	0.509915
H	-5.101169	3.634531	-0.429019
C	-5.636196	-1.531874	2.151029
H	-5.522196	-2.594503	1.921413
H	-6.686005	-1.249649	2.053965
H	-5.355193	-1.413754	3.203682
C	-2.692654	2.802759	-0.451670
C	-1.896226	3.432792	0.524794
C	-1.336602	4.675693	0.214661
H	-0.718202	5.180779	0.952348
C	-1.542778	5.266224	-1.024420
C	-2.257508	4.587383	-2.003607
H	-2.359277	5.027958	-2.991654
C	-2.827164	3.336141	-1.751581
C	-3.003497	-2.187888	1.719589
C	-2.886340	-3.447611	1.098012
C	-2.468568	-4.531228	1.874749
H	-2.386809	-5.512843	1.415786
C	-2.150750	-4.376874	3.218851
C	-2.199070	-3.115279	3.794475
H	-1.894762	-2.982916	4.830980
C	-2.614863	-2.001344	3.061346
C	-1.096948	-0.722776	-2.429907
C	-0.782840	0.335081	-3.345612
C	-0.685712	-2.042103	-2.807566

C	-0.116089	0.081589	-4.536648
H	-1.057813	1.350636	-3.076135
C	-0.023331	-2.260998	-4.008663
H	-0.884871	-2.872563	-2.134371
C	0.259726	-1.216582	-4.894433
H	0.285852	-3.275934	-4.253981
H	0.778588	-1.408075	-5.829249
H	-1.109586	6.239334	-1.243195
H	-1.833932	-5.234450	3.806656
C	-3.216503	-3.624827	-0.370502
C	-4.723626	-3.729454	-0.610736
C	-2.496348	-4.806553	-1.009211
H	-2.865622	-2.719965	-0.882005
H	-5.249887	-2.815972	-0.318529
H	-4.935769	-3.905228	-1.670997
H	-5.153738	-4.564496	-0.044400
H	-1.422669	-4.790249	-0.792181
H	-2.896650	-5.768311	-0.667520
H	-2.618376	-4.776424	-2.097132
C	-2.554749	-0.628726	3.705601
C	-1.096326	-0.174802	3.801336
C	-3.219086	-0.583490	5.079545
H	-3.080548	0.086470	3.059496
H	-0.618855	-0.134528	2.812453
H	-1.027302	0.819879	4.257334
H	-0.515218	-0.866035	4.424210
H	-4.255060	-0.937396	5.051955
H	-2.683022	-1.201311	5.808391
H	-3.226185	0.439869	5.468579
C	-3.500989	2.553457	-2.868325
C	-2.969086	2.936606	-4.248273
C	-5.029433	2.633463	-2.886730
H	-3.237899	1.504412	-2.692230
H	-1.876441	3.000633	-4.270343
H	-3.273856	2.190292	-4.988835
H	-3.365267	3.903098	-4.581284
H	-5.490028	2.130070	-2.033426
H	-5.376209	3.673920	-2.898863
H	-5.415174	2.149509	-3.790902
C	-1.619326	2.774658	1.864749
C	-2.669386	3.108230	2.925153
C	-0.219005	3.083130	2.374047
H	-1.651164	1.686689	1.699331
H	-3.648264	2.678929	2.688913
H	-2.368846	2.706189	3.899796
H	-2.790411	4.192296	3.039187
H	0.540094	2.834521	1.622783
H	-0.093009	4.136203	2.648951
H	-0.008446	2.492539	3.270482
Al	2.343879	-0.044544	0.144639
N	3.638854	-1.504286	-0.154722
N	3.800900	1.203374	0.536001
C	5.123241	0.967036	0.493807
C	5.660501	-0.311246	0.313066
C	4.954078	-1.498690	0.064168
H	6.739391	-0.395587	0.383084
C	6.086265	2.105789	0.673708
H	5.809620	2.953613	0.039456
H	7.105239	1.799147	0.433699
H	6.076512	2.482877	1.702083
H	5.526245	-3.308125	1.028681
H	6.796067	-2.616815	0.009289
C	5.720761	-2.788826	0.082309
H	5.410304	-3.468569	-0.713702
C	3.354426	2.525338	0.871583
C	3.417743	2.944532	2.219731
C	3.002217	4.239485	2.527307
C	2.506700	5.088559	1.541829
C	2.389253	4.636661	0.236103
C	2.800991	3.349050	-0.126640
H	1.965637	5.287692	-0.526440
H	2.187441	6.094809	1.801887
H	3.050742	4.585528	3.556640
C	3.843079	1.978082	3.311716
H	4.589668	1.291866	2.893309
C	2.650651	1.122399	3.749976
H	2.149084	0.641950	2.898525
H	2.961405	0.335882	4.446853
H	1.898210	1.740662	4.252973
H	5.307888	3.315366	4.227003
C	4.481258	2.658455	4.516916
H	4.872327	1.911151	5.213624
H	3.757703	3.263329	5.073929
H	2.839459	1.816938	-1.603897
C	2.658656	2.898223	-1.566926
C	3.708201	3.554885	-2.461520
H	3.595859	4.645457	-2.469716
H	4.726274	3.329500	-2.124847
C	1.246760	3.119249	-2.101413
H	1.151472	2.682555	-3.102413
H	0.499042	2.635112	-1.457105
H	0.994153	4.183343	-2.174765
H	3.612341	3.201166	-3.493590
C	2.987165	-2.716695	-0.563109
C	2.363174	-3.521775	0.409246
C	1.664296	-4.656327	-0.010716
C	1.604923	-5.002855	-1.353047
C	2.219266	-4.189442	-2.296273
C	2.892899	-3.017917	-1.938436
C	3.477175	-2.182289	-3.071908
H	2.158914	-4.446107	-3.352162
H	1.068554	-5.894808	-1.666761
H	1.162394	-5.274314	0.732682
C	2.412964	-3.193616	1.888424
H	3.035353	-2.297828	2.021818
C	3.058182	-4.322986	2.691428
H	4.060033	-4.570489	2.324833
H	3.142001	-4.050414	3.748452
H	2.457253	-5.237681	2.637020
H	1.061901	-2.585878	3.480229
C	1.017229	-2.883735	2.425753
H	0.532249	-2.078838	1.857362
H	0.368520	-3.763603	2.359786
H	2.986024	-2.578045	-3.972769
H	5.251922	-3.453689	-3.261351
C	4.981120	-2.392516	-3.258147
H	5.309111	-1.959846	-4.209148
H	5.555602	-1.895117	-2.468830
H	3.345259	-0.257676	-4.043004
C	3.155835	-0.688383	-3.053090
H	3.790831	-0.142432	-2.343677
H	2.102412	-0.496575	-2.809012
H	0.124174	0.919401	-5.191148
O	-2.668278	-0.674120	-1.958154
C	-3.666248	-1.021273	-2.909829
H	-3.517070	-0.448371	-3.834395
H	-3.616932	-2.092592	-3.143436
H	-4.646281	-0.781965	-2.483993

TS-3_Direct_CO_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.26513548
E(SCF)+ZPE(0 K) = -2955.854471
H(298 K) = -2955.772909
G(298 K) = 2955.966992

Lowest Frequency = -414.0677 cm^{-1}

Pd	0.486220	-0.392176	1.170236
Al	-1.839179	-0.453768	0.092111
N	-2.766876	-2.236261	0.231882
N	-3.277617	0.376747	1.202437
C	-3.724672	-2.571756	1.102391
C	-4.323083	-1.650192	1.974244
H	-5.070107	-2.048694	2.651636
C	-4.186350	-0.259044	1.956021
C	-4.239152	-3.981403	1.151827
H	-4.433729	-4.370428	0.147806
H	-5.154000	-4.046978	1.742391
H	-3.496145	-4.646461	1.602345
C	-5.167757	0.532892	2.772942
H	-5.641614	-0.094418	3.529838
H	-5.958882	0.940443	2.133389
H	-4.697009	1.392470	3.257258
C	-2.332984	-3.216878	-0.724339
C	-2.795672	-3.094404	-2.054979
C	-2.388009	-4.043840	-2.994254
H	-2.744689	-3.967574	-4.017554
C	-1.521508	-5.074316	-2.648051
C	-1.046761	-5.157617	-1.347911
H	-0.350132	-5.949384	-1.077493
C	-1.437065	-4.242679	-0.364060
C	-3.437879	1.793716	1.039134
C	-2.623639	2.689857	1.760219
C	-2.863883	4.058922	1.619075
H	-2.255102	4.760706	2.184265
C	-3.842199	4.539472	0.758865
C	-4.584230	3.645797	-0.002121
H	-5.324596	4.020068	-0.707276
C	-4.403903	2.266076	0.124914
C	1.559429	-0.867673	2.938481
C	2.635646	-1.772604	2.813070
C	1.588908	0.088491	3.971243
C	3.720265	-1.677377	3.670329
H	2.628247	-2.515127	2.020262
C	2.697885	0.173070	4.811714
H	0.760874	0.782920	4.090737
C	3.768753	-0.708031	4.679569
H	2.714347	0.939975	5.584088
H	4.622230	-0.645915	5.348071
H	-1.210391	-5.801004	-3.393969
H	-4.006730	5.610039	0.662776
C	-1.513447	2.213663	2.675092
C	-1.948587	2.199880	4.139298
C	-0.239266	3.028115	2.481431
H	-1.264754	1.180722	2.386255
H	-2.795657	1.526836	4.309824
H	-1.129839	1.864069	4.785882
H	-2.245259	3.202344	4.470870
H	0.046171	3.050810	1.425677
H	-0.345085	4.063946	2.826621
H	0.589728	2.576893	3.036524
C	-5.215180	1.335313	-0.758920
C	-4.761157	1.466734	-2.213307
C	-6.718334	1.585542	-0.653821
H	-5.024130	0.300366	-0.446565
H	-3.704275	1.194535	-2.328030
H	-5.352462	0.817965	-2.869982
H	-4.878646	2.497715	-2.568730
H	-7.076954	1.525026	0.378471
H	-6.987915	2.577021	-1.034247
H	-7.273824	0.849406	-1.244086
C	-0.836428	-4.375499	1.020736
C	0.658727	-4.076649	0.973006
C	-1.052614	-5.766799	1.618836
H	-1.290220	-3.627406	1.681182
H	0.855221	-3.061507	0.603852
H	1.096752	-4.146621	1.972605
H	1.175156	-4.789223	0.316885
H	-2.100945	-6.082224	1.607473
H	-0.485539	-6.526064	1.068052
H	-0.703120	-5.793061	2.655520
C	-3.727093	-1.967373	-2.460421
C	-5.179756	-2.269176	-2.091757
C	-3.606388	-1.596424	-3.933068
H	-3.425157	-1.076199	-1.883583
H	-5.310070	-2.398021	-1.012539
H	-5.839295	-1.452304	-2.407982
H	-5.524693	-3.185434	-2.585264
H	-2.561706	-1.438432	-4.221605
H	-4.022583	-2.369946	-4.588059
H	-4.157463	-0.673748	-4.139854
H	4.552436	-2.367889	3.536506
O	0.007837	-1.743916	2.799378
C	-0.949914	-1.400178	3.766044
H	-0.477078	-1.052454	4.699138
H	-1.658320	-0.623838	3.434902
H	-1.531157	-2.305838	3.993111
Al	1.741078	0.648337	-0.585543
N	3.073248	-0.258888	-1.708827
N	1.723003	2.195387	-1.765661
C	2.319987	2.319159	-2.960235
C	3.169011	1.344624	-3.492000
C	3.613615	0.180334	-2.848131
H	5.707838	-0.196820	-2.915996
H	4.750195	-1.605643	-3.330504
C	4.800567	-0.521098	-3.440606
H	4.921593	-0.267859	-4.495365
H	3.625131	1.572047	-4.448832
C	2.113433	3.573426	-3.758675
H	2.406985	4.457711	-3.183249
H	1.054750	3.711812	-4.002545
H	2.685395	3.550101	-4.687027
C	2.035172	-3.059409	-2.237462
H	1.664152	-4.027695	-1.868384
H	3.450841	-3.957401	-3.650667
C	2.567976	-3.309500	-3.650125
H	1.796207	-3.787059	-4.263778
H	2.834544	-2.369517	-4.146290
C	0.815361	-2.146733	-2.299470
H	0.460161	-1.865896	-1.301054
H	3.359063	-4.746331	-0.715829
C	3.744657	-3.740090	-0.559826
C	3.147239	-2.687349	-1.263696
C	3.666531	-1.393861	-1.054502
C	4.734229	-1.161461	-0.162485
C	5.280059	-2.248595	0.521521
C	4.794236	-3.533863	0.325427
H	5.224759	-4.371692	0.867168
H	6.092785	-2.076703	1.224586
C	5.295746	0.226761	0.087868
H	4.840193	0.921055	-0.631698
C	4.947948	0.719414	1.492628
H	3.866552	0.711891	1.680857
H	5.401752	0.080716	2.258060
H	5.320489	1.739375	1.643479
H	7.338225	-0.330989	0.609337
C	6.807407	0.277020	-0.131309
H	7.177287	1.302875	-0.032693
C	-1.860547	3.706352	-3.555019
H	-2.359167	4.598633	-3.168433
H	-2.603400	3.130451	-4.116811
H	-1.099013	4.040100	-4.270571
C	-1.244080	2.836238	-2.453621
C	-0.289697	3.647185	-1.572698
C	1.043259	3.343811	-1.233226

H	-2.064037	2.563648	-1.765718
C	1.772086	4.136965	-0.311524
C	1.178791	5.294649	0.188319
H	1.726495	5.919219	0.888015
C	-0.123301	5.631038	-0.158777
C	-0.842800	4.802849	-1.002378
H	-1.882759	5.037370	-1.211896
H	-0.590298	6.520515	0.257269
C	-0.777070	1.528609	-3.085204
H	-0.417132	0.805965	-2.348928
H	-1.637202	1.061643	-3.580964
H	-0.007047	1.670363	-3.851487
H	2.681325	3.933472	2.278509
H	3.168479	2.620642	0.211704
C	3.469952	4.210758	1.572128
H	4.405497	3.766795	1.924151
H	3.598445	5.298013	1.612976
C	3.156717	3.723129	0.162268
C	4.265049	4.140213	-0.804601
H	4.156370	3.675986	-1.789233
H	5.246194	3.848951	-0.412240
H	4.271593	5.228000	-0.941756
H	7.094803	-0.092250	-1.121453
H	1.006594	-1.227594	-2.865732
H	-0.007743	-2.668043	-2.800848

TS-4_CH_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.29041843
E(SCF)+ZPE(0 K)= -2955.882111
H(298 K) = -2955.800210
G(298 K) = -2955.996107
Lowest Frequency = -696.3137 cm^{-1}

Pd	0.145362	-0.270620	1.020305
Al	-2.186048	-0.361462	0.355455
N	-3.467546	-1.874100	0.346382
N	-3.630916	0.905890	0.889021
C	-4.673048	-1.889145	0.930734
C	-5.229508	-0.769653	1.561419
H	-6.178806	-0.923977	2.061878
C	-4.782990	0.553894	1.480668
C	-5.503394	-3.138229	0.892460
H	-5.706604	-3.430576	-0.143357
H	-6.453334	-2.998825	1.409443
H	-4.976871	-3.984640	1.342335
C	-5.703403	1.610718	2.024413
H	-6.396461	1.181344	2.750107
H	-6.299793	2.059512	1.221723
H	-5.150129	2.429575	2.491270
C	-3.040776	-3.076442	-0.321187
C	-3.213911	-3.185691	-1.715691
C	-2.821551	-4.368309	-2.348696
H	-2.948714	-4.457315	-3.426097
C	-2.263439	-5.417705	-1.632004
H	-1.964823	-6.330799	-2.140111
C	-2.070037	-5.281644	-0.264109
H	-1.605732	-6.089988	0.297831
C	-2.442463	-4.119203	0.415789
C	-3.750014	-2.047147	-2.560139
H	-4.115035	-1.263503	-1.883358
C	-2.620677	-1.453365	-3.406585
H	-1.809696	-1.064194	-2.776422
H	-2.984001	-0.633082	-4.035379
H	-2.189847	-2.215999	-4.066440
C	-4.921933	-2.472641	-3.440951
H	-4.620368	-3.222087	-4.180901
H	-5.319829	-1.615580	-3.994771
H	-5.739104	-2.901995	-2.852905
C	-2.144136	-4.014217	1.899046
H	-2.540792	-3.058767	2.264078
C	-0.633027	-4.003927	2.125040
H	-0.395918	-3.844104	3.182993
H	-0.143044	-3.209241	1.554866
H	-0.189562	-4.961551	1.822382
C	-2.786998	-5.141104	2.707131
H	-3.874230	-5.185937	2.585703
H	-2.577446	-5.013772	3.773628
H	-2.386465	-6.117691	2.412393
C	-3.468403	2.299369	0.572702
C	-2.549835	3.095421	1.282407
C	-2.447038	4.448428	0.939211
H	-1.742128	5.074809	1.479857
C	-3.214430	5.001684	-0.075061
H	-3.118374	6.056901	-0.320354
C	-4.097587	4.196724	-0.785066
H	-4.678220	4.624152	-1.598834
C	-4.239004	2.842402	-0.481725
C	-1.705993	2.554058	2.418129
H	-1.641514	1.462736	2.306398
C	-0.278843	3.086788	2.360795
H	-0.225827	4.158451	2.583116
H	0.161146	2.923109	1.370306
H	0.357458	2.574198	3.087800
C	-2.352732	2.847474	3.771440
H	-2.471282	3.927012	3.924551
H	-1.734003	2.461506	4.588713
H	-3.342639	2.387370	3.861468
C	-5.118304	1.967744	-1.356515
H	-5.429107	1.086200	-0.782919
C	-4.288700	1.464066	-2.536706
H	-3.959429	2.302147	-3.163030
H	-4.861321	0.770642	-3.164235
H	-3.385013	0.945756	-2.191172
C	-6.386671	2.661276	-1.841777
H	-6.958871	3.094484	-1.014892
H	-7.033935	1.949697	-2.363127
H	-6.168453	3.468364	-2.549064
H	-0.478019	-0.944319	2.350204
C	1.085656	-0.654091	2.887417
C	2.067239	-1.662604	2.913806
C	0.935522	0.101007	4.055689
C	2.890126	-1.859690	4.024059
C	1.758301	-0.070224	5.171637
C	2.740888	-1.051489	5.152414
H	3.654863	-2.631946	4.013701
H	1.612975	0.546797	6.055100
H	3.383830	-1.209732	6.014311
H	0.135205	0.837389	4.101376
O	2.182970	-2.415874	1.768812
C	2.858255	-3.647522	1.888728
H	3.942073	-3.519337	2.024239
H	2.464956	-4.237442	2.728895
H	2.692201	-4.179457	0.949680
Al	1.837007	0.489381	-0.639820
N	2.351562	2.216208	-1.492170
N	3.095104	-0.488097	-1.803541
C	3.618741	-0.038188	-2.958772
C	3.569238	1.302827	-3.350118
C	3.097992	2.380880	-2.590497
C	3.519152	3.757954	-3.018895
H	2.669847	4.430151	-3.169450
H	4.130940	4.218621	-2.235297
H	4.105911	3.721129	-3.937496
C	4.365003	-0.980613	-3.860601
H	4.718389	-0.467417	-4.755837
H	3.730606	-1.820169	-4.162544
H	4.075984	1.550372	-4.275785
H	5.225191	-1.423329	-3.346726

C	3.544842	-1.798118	-1.401858
C	4.680745	-1.876415	-0.571738
C	5.278553	-3.125817	-0.390340
C	4.739933	-4.269612	-0.968430
C	3.541124	-4.188127	-1.666216
C	2.913070	-2.958256	-1.881876
H	3.079239	-5.093955	-2.052284
H	5.229001	-5.230717	-0.833238
H	6.174050	-3.203969	0.221366
C	5.234109	-0.637909	0.108250
H	4.379160	0.035578	0.278217
H	5.107978	-1.446785	2.127847
H	5.802291	0.444231	-1.710593
C	6.242205	0.107415	-0.766777
H	7.098288	-0.535558	-1.004045
H	6.735322	-1.539495	1.420227
H	6.626129	0.993375	-0.248730
C	5.826258	-0.930870	1.481721
H	6.104197	0.005334	1.977014
C	1.531917	-2.894096	-2.495492
C	0.518268	-3.131365	-1.373181
H	0.627980	-4.147329	-0.971696
H	-0.509102	-3.025127	-1.736149
H	0.660592	-2.426658	-0.542509
H	1.374687	-1.877759	-2.882733
C	1.303602	-3.873906	-3.640512
H	2.049810	-3.770719	-4.435848
H	1.327909	-4.913395	-3.293989
H	0.314343	-3.714563	-4.081682
C	2.682363	3.767056	0.383861
C	1.967682	3.400463	-0.771933
C	0.874546	4.165922	-1.236121
C	0.527083	5.312790	-0.521357
C	1.231089	5.697257	0.615174
C	2.293588	4.926922	1.061685
H	2.833781	5.218041	1.960522
H	0.941442	6.594858	1.156114
H	-0.311503	5.915557	-0.858908
C	0.095454	3.747560	-2.470036
C	-0.616257	4.905318	-3.160758
H	0.054156	5.747736	-3.362332
H	-1.452459	5.275822	-2.556030
H	-1.687386	3.021353	-1.471136
H	-1.038161	4.572447	-4.113885
H	0.810022	3.326167	-3.189690
H	-0.444123	1.788260	-1.638996
C	-0.907368	2.643798	-2.141662
H	-1.392497	2.277441	-3.054078
C	3.833157	2.943975	0.930615
H	4.062287	2.155752	0.200221
H	2.544765	1.640751	2.127075
C	3.435725	2.268992	2.245071
H	3.214107	3.016582	3.016621
H	4.244628	1.632552	2.622293
H	5.924219	3.141390	1.468233
C	5.105164	3.771058	1.104432
H	4.966208	4.573925	1.836746
H	5.426793	4.233069	0.165207

TS-5_Db_migr_Anisole_AlPdAl_M06L.log

SCF (M06L) = -2957.29338656
E(SCF)+ZPE(0 K)= -2955.886347
H(298 K) = -2955.804575
G(298 K) = -2956.001819
Lowest Frequency = -124.2558 cm^{-1}

Pd	-0.036982	0.000139	0.180768
Al	-2.354625	-0.222789	0.141702
N	-3.523361	-1.677205	-0.389880
N	-3.783939	1.014957	0.450262
C	-4.859159	-1.648845	-0.338527
C	-5.579841	-0.570081	0.199495
H	-6.654607	-0.702311	0.263121
C	-5.089954	0.694169	0.523183
C	-5.683265	-2.781742	-0.882996
H	-6.484820	-2.384449	-1.511054
H	-6.163425	-3.334948	-0.069201
H	-5.093315	-3.489754	-1.466162
C	-6.084285	1.749885	0.909778
H	-7.085853	1.329359	1.007506
H	-6.116340	2.560913	0.174904
H	-5.799462	2.216679	1.858576
C	-2.837807	-2.848711	-0.863372
C	-2.115159	-2.765259	-2.070868
C	-1.366089	-3.874652	-2.469196
H	-0.806149	-3.828276	-3.400426
C	-1.337475	-5.033308	-1.706135
H	-0.741892	-5.884303	-2.027505
C	-2.076388	-5.104266	-0.532816
H	-2.058710	-6.016834	0.060011
C	-2.842096	-4.025669	-0.085399
C	-2.229780	-1.567773	-2.995295
H	-2.588104	-0.710985	-2.413329
C	-0.896704	-1.145704	-3.597343
H	-0.167614	-0.931545	-2.806068
H	-1.022220	-0.234912	-4.192706
H	-0.479116	-1.912401	-4.259929
C	-3.280832	-1.835975	-4.073635
H	-2.995621	-2.688248	-4.701276
H	-3.400537	-0.964435	-4.727124
H	-4.259383	-2.062368	-3.635249
C	-3.655837	-4.185993	1.187996
H	-4.324074	-3.325041	1.289727
C	-2.778727	-4.198683	2.436286
H	-3.382219	-4.408458	3.326034
H	-2.274558	-3.241135	2.586046
H	-2.001698	-4.969452	2.370393
C	-4.528395	-5.441015	1.131315
H	-5.132953	-5.485957	0.219421
H	-5.204895	-5.477143	1.991271
H	-3.920894	-6.351740	1.163633
C	-3.495560	2.420532	0.313911
C	-3.184864	3.210983	1.431070
C	-3.075695	4.592469	1.253911
H	-2.841801	5.217362	2.114132
C	-3.249349	5.175076	0.006011
H	-3.176604	6.253881	-0.109042
C	-3.476676	4.368659	-1.101768
H	-3.568858	4.818753	-2.088787
C	-3.590153	2.982859	-0.976042
C	-2.898726	2.606594	2.787804
H	-3.159691	1.540309	2.746021
C	-1.398969	2.717062	3.065348
H	-1.088617	3.769282	3.081302
H	-0.810663	2.212166	2.286470
H	-1.136508	2.273072	4.032077
C	-3.712040	3.245573	3.909885
H	-3.454636	4.302572	4.040311
H	-3.513993	2.744871	4.862561
H	-4.789518	3.192730	3.720916
C	-3.806384	2.142685	-2.221438
H	-3.750750	1.084423	-1.935467
C	-2.694003	2.388647	-3.239019
H	-2.698078	3.423489	-3.601730
H	-2.815443	1.735803	-4.110982
H	-1.714617	2.185454	-2.792930

C	-5.184254	2.374693	-2.838753
H	-5.991119	2.128653	-2.140189
H	-5.318219	1.754235	-3.731574
H	-5.313778	3.420871	-3.139525
C	-0.476428	-1.215174	1.906241
C	0.124447	-2.494139	1.824668
C	-0.866779	-0.814108	3.192434
C	0.409837	-3.258286	2.958731
C	-0.636047	-1.584103	4.339588
C	0.017894	-2.801517	4.220234
H	0.920430	-4.213504	2.875422
H	-0.960889	-1.225281	5.313814
H	0.224972	-3.409567	5.097572
H	-1.303570	0.616275	-1.046888
H	-1.351607	0.152615	3.316156
O	0.430053	-2.924211	0.556962
C	1.054504	-4.181511	0.449627
H	2.010896	-4.206237	0.985600
H	0.409031	-4.989956	0.827107
H	1.236691	-4.344049	-0.614408
Al	2.286315	0.478605	-0.383432
N	3.052249	2.271928	-0.773866
N	4.076082	-0.324581	-0.572503
C	5.205497	0.260013	-1.011587
C	5.302405	1.628094	-1.278072
C	4.314266	2.597747	-1.048222
C	4.751586	4.034094	-1.042024
H	3.969180	4.713618	-1.383891
H	5.002796	4.329847	-0.016107
H	5.646978	4.175576	-1.650963
C	6.454373	-0.559721	-1.174808
H	7.302666	0.068204	-1.450433
H	6.327018	-1.326444	-1.946595
H	6.278010	1.993588	-1.578636
H	6.696521	-1.097166	-0.251878
C	4.179044	-1.687110	-0.127389
C	4.270763	-1.929337	1.258590
C	4.502045	-3.241790	1.679990
C	4.617770	-4.281510	0.764456
C	4.433646	-4.034634	-0.590882
C	4.195177	-2.741490	-1.060291
H	4.469685	-4.860510	-1.297826
H	4.815039	-5.292260	1.111980
H	4.590767	-3.450613	2.742867
C	4.151080	-0.795540	2.261545
H	3.432884	-0.070189	1.843560
H	2.630758	-1.777150	3.474470
H	5.844736	0.382464	1.520229
C	5.479140	-0.062048	2.451760
H	6.251429	-0.745007	2.825590
H	4.269467	-1.879934	4.154823
H	5.370767	0.748053	3.182268
C	3.575060	-1.238074	3.600071
H	3.377236	-0.365085	4.229713
C	3.891416	-2.487902	-2.523774
C	2.393690	-2.682521	-2.778187
H	2.117684	-3.738414	-2.660337
H	2.124231	-2.378843	-3.796183
H	1.778623	-2.106415	-2.074111
H	4.121002	-1.436387	-2.738534
C	4.717670	-3.344040	-3.477043
H	5.792349	-3.254113	-3.285281
H	4.458414	-4.405458	-3.398810
H	4.534793	-3.048038	-4.514445
C	2.029235	3.715798	0.907763
C	2.114813	3.303329	-0.436681
C	1.234464	3.801227	-1.419602
C	0.280687	4.739443	-1.015365
C	0.197787	5.179868	0.300041
C	1.067435	4.668383	1.250661
H	0.995423	4.998400	2.285896
H	-0.554334	5.910570	0.582546
H	-0.415927	5.126035	-1.758303
C	1.280044	3.442783	-2.899784
C	1.181466	1.958628	-3.249836
H	0.429805	1.439975	-2.646051
H	2.138192	1.438251	-3.108205
H	3.409221	3.571064	-3.353844
H	0.914797	1.847034	-4.307676
H	0.378631	3.913832	-3.318178
H	2.576450	5.137277	-3.397622
C	2.472588	4.070735	-3.623069
H	2.356312	3.966557	-4.707069
C	2.924031	3.147446	1.995294
H	3.653241	2.470612	1.528787
H	1.559529	1.514280	2.520540
C	2.115637	2.329264	3.004024
H	1.387859	2.963922	3.523487
H	2.774705	1.892167	3.763258
H	4.408592	3.809811	3.436597
C	3.710468	4.243826	2.713201
H	3.042261	4.912572	3.267322
H	4.285704	4.863865	2.017685

Int-7.log

SCF (M06L) = -1587.98870326
E(SCF)+ZPE(0 K)= -1587.216225
H(298 K)= -1587.171673
G(298 K)= -1587.291713
Lowest Frequency = 20.3001cm-1

Al	-0.484831	-0.718066	-0.757618
N	-2.053074	-0.404375	0.478856
N	0.364323	-1.776594	0.736626
C	-2.407484	-1.112666	1.556331
C	-1.584944	-2.105276	2.107239
H	-1.985264	-2.651920	2.953678
C	-0.247671	-2.357063	1.775681
C	-3.716765	-0.832969	2.237149
H	-3.805079	0.228765	2.489585
H	-3.826182	-1.422119	3.148741
H	-4.560303	-1.058482	1.575941
C	0.524960	-3.299049	2.652319
H	1.307229	-2.768458	3.204946
H	1.042769	-4.052975	2.050255
H	-0.124511	-3.800139	3.371537
C	-2.876307	0.689467	0.056055
C	-2.443167	2.003816	0.346322
C	-3.223083	3.069113	-0.108858
H	-2.910473	4.086977	0.105402
C	-4.380443	2.852655	-0.847891
H	-4.969549	3.696891	-1.195437
C	-4.769132	1.557043	-1.155981
H	-5.659116	1.390597	-1.759189
C	-4.029532	0.455816	-0.717058
C	-1.162548	2.253362	1.126178
H	-0.407784	1.545925	0.737263
C	-0.599627	3.657000	0.939772
H	-0.492659	3.930184	-0.113285
H	0.392472	3.725020	1.396294
H	-1.229924	4.410068	1.426878
C	-1.330866	1.958948	2.618499
H	-1.578765	0.912614	2.815814
H	-2.123914	2.583260	3.046868
H	-0.404676	2.183192	3.159951
C	-4.439867	-0.939327	-1.146441
H	-3.883078	-1.662696	-0.538545
C	-5.928778	-1.206839	-0.940577

H	-6.245804	-1.006887	0.088532
H	-6.168084	-2.249599	-1.170492
H	-6.545970	-0.584183	-1.597018
C	-4.046010	-1.173438	-2.605370
H	-2.970231	-1.026241	-2.754525
H	-4.570935	-0.472997	-3.264976
H	-4.300226	-2.189614	-2.924610
C	1.792303	-1.871907	0.644778
C	2.390235	-2.794610	-0.235158
C	3.784171	-2.807488	-0.339762
H	4.254211	-3.517964	-1.017411
C	4.572672	-1.936521	0.400156
H	5.654962	-1.962437	0.305050
C	3.966890	-1.024123	1.254586
H	4.580209	-0.324471	1.820001
C	2.578636	-0.966773	1.389693
C	1.579982	-3.763012	-1.072944
H	0.520555	-3.619335	-0.825347
C	1.754642	-3.470861	-2.562649
H	1.460933	-2.442901	-2.801089
H	1.143850	-4.147746	-3.168941
H	2.798939	-3.602091	-2.869127
C	1.939622	-5.215288	-0.762224
H	1.811005	-5.451986	0.298946
H	2.982787	-5.430172	-1.019856
H	1.312791	-5.903131	-1.338504
C	1.970212	0.085699	2.298611
H	0.879318	-0.033014	2.283044
C	2.435662	-0.066677	3.746070
H	2.213783	-1.058288	4.153304
H	1.947197	0.673684	4.388431
H	3.517044	0.087898	3.833422
C	2.290418	1.490192	1.789173
H	1.940637	1.645518	0.762335
H	3.370210	1.675707	1.786930
H	1.827055	2.248934	2.430613
C	2.976104	3.699204	-1.211293
C	4.153498	3.068099	-0.833640
C	4.332508	1.701826	-1.058122
C	3.318463	0.976360	-1.673504
C	2.137079	1.598418	-2.077787
C	1.963393	2.965210	-1.840156
H	2.816111	4.758852	-1.035279
H	4.934621	3.647912	-0.348390
H	5.246996	1.205953	-0.744552
H	3.431945	-0.094387	-1.835294
H	1.357562	1.010042	-2.549184
O	0.846649	3.665467	-2.185819
C	-0.230429	2.921206	-2.727186
H	-0.559814	2.123941	-2.042644
H	-1.045781	3.630302	-2.876559
H	0.036090	2.462793	-3.688303

TS-6.log

SCF (M06L) = -1587.93596359
E(SCF)+ZPE(0 K)= -1587.166913
H(298 K)= -1587.122661
G(298 K)= -1587.241251
Lowest Frequency = -577.8938cm-1

Al	-0.817262	-0.874051	-0.859075
N	-2.218914	-0.404600	0.435141
N	0.239313	-1.708941	0.574209
C	-2.472985	-1.054701	1.579027
C	-1.585029	-1.994813	2.117427
H	-1.904753	-2.503239	3.019847
C	-0.269934	-2.235751	1.696327
C	-3.749525	-0.781810	2.317879
H	-3.913411	0.291605	2.449496
H	-3.755462	-1.264883	3.295634
H	-4.607525	-1.152595	1.745252
C	0.596052	-3.093674	2.567510
H	1.298893	-2.478843	3.139548
H	1.203582	-3.779522	1.970046
H	-0.003389	-3.664442	3.278202
C	-3.060905	0.687367	0.033580
C	-2.607828	1.999897	0.297669
C	-3.399004	3.063909	-0.140902
H	-3.072564	4.082038	0.048824
C	-4.587578	2.844345	-0.827311
H	-5.183853	3.687948	-1.163261
C	-5.002290	1.547964	-1.095920
H	-5.922777	1.380100	-1.650991
C	-4.251384	0.446846	-0.675987
C	-1.316691	2.253434	1.059606
H	-0.619162	1.439075	0.809959
C	-0.637200	3.565840	0.684823
H	-0.421722	3.632265	-0.386212
H	0.321778	3.649179	1.205331
H	-1.236408	4.432803	0.983931
C	-1.539062	2.178920	2.571931
H	-1.892366	1.194089	2.892435
H	-2.275809	2.923373	2.895071
H	-0.604112	2.381325	3.105768
C	-4.707532	-0.952250	-1.040394
H	-4.101018	-1.668630	-0.471706
C	-6.172652	-1.197375	-0.686488
H	-6.385112	-0.976791	0.364870
H	-6.446546	-2.239749	-0.875675
H	-6.841341	-0.574320	-1.289747
C	-4.461358	-1.221559	-2.525351
H	-3.404291	-1.095605	-2.785043
H	-5.038316	-0.527375	-3.146581
H	-4.758950	-2.239953	-2.795730
C	1.653844	-1.795053	0.334823
C	2.140439	-2.670757	-0.657102
C	3.511079	-2.669615	-0.929994
H	3.896098	-3.347873	-1.688957
C	4.381011	-1.828073	-0.252612
H	5.442323	-1.834307	-0.485382
C	3.885737	-0.971128	0.720738
H	4.563150	-0.292207	1.234348
C	2.526864	-0.934474	1.038368
C	1.251333	-3.638730	-1.413427
H	0.214669	-3.483081	-1.086261
C	1.305043	-3.385803	-2.918701
H	1.027769	-2.353960	-3.159325
H	0.619747	-4.052861	-3.451320
H	2.311079	-3.561139	-3.315211
C	1.617966	-5.088067	-1.094826
H	1.553073	-5.299100	-0.022802
H	2.642318	-5.313871	-1.411315
H	0.951700	-5.782594	-1.616197
C	2.061741	0.040408	2.107292
H	0.995136	-0.132001	2.305064
C	2.820485	-0.160335	3.420660
H	2.795190	-1.197684	3.770250
H	2.397597	0.471507	4.207982
H	3.874263	0.117785	3.313480
C	2.221897	1.488763	1.644119
H	1.604254	1.720533	0.772431
H	3.257395	1.709750	1.359247
H	1.938119	2.182313	2.444291
C	3.016930	3.885152	-0.929776
C	4.332467	3.939432	-0.493495
C	5.180715	2.837918	-0.630719
C	4.681659	1.682894	-1.230690
C	3.368142	1.615637	-1.682087

C	2.496647	2.721566	-1.548887
H	2.351793	4.737559	-0.815946
H	4.700063	4.851236	-0.026545
H	6.208902	2.882967	-0.283562
H	5.324757	0.812548	-1.350079
H	3.001303	0.699700	-2.143489
O	1.243789	2.725840	-1.956306
C	0.340873	1.019955	-1.769972
H	1.006419	0.768652	-0.950018
H	-0.567010	1.585356	-1.611179
H	0.566035	0.655980	-2.758638

3a.log

SCF (M06L) = -1588.11239744
E(SCF)+ZPE(0 K)= -1587.341598
H(298 K)= -1587.297148
G(298 K)= -1587.416622
Lowest Frequency = 13.5585cm-1

Al	0.159703	0.359143	-0.087260
N	-1.675926	0.258752	0.459375
N	0.684783	-1.266822	0.775471
C	-1.997116	-0.291058	1.637610
C	-1.108533	-1.095263	2.371389
H	-1.459452	-1.432162	3.339935
C	0.115176	-1.621518	1.937545
C	-3.368924	-0.076016	2.202498
H	-3.508793	0.972341	2.487065
H	-3.538134	-0.697921	3.081927
H	-4.140176	-0.293812	1.457098
C	0.796370	-2.635988	2.806601
H	1.786416	-2.269696	3.101220
H	0.972294	-3.574271	2.272723
H	0.217281	-2.845928	3.706320
C	-2.677367	0.973026	-0.282712
C	-3.001734	2.300057	0.057387
C	-3.986104	2.950351	-0.692543
H	-4.244936	3.977210	-0.442865
C	-4.621340	2.318291	-1.750995
H	-5.386860	2.839549	-2.319120
C	-4.257185	1.022794	-2.099735
H	-4.736892	0.544249	-2.948735
C	-3.277376	0.330273	-1.386049
C	-2.267881	3.066163	1.140045
H	-1.634141	2.365987	1.696178
C	-1.339476	4.098393	0.498061
H	-0.665622	3.635423	-0.228358
H	-0.717048	4.590302	1.252315
H	-1.918118	4.870084	-0.023451
C	-3.214558	3.750080	2.124274
H	-3.918424	3.049000	2.585335
H	-3.809460	4.529258	1.634953
H	-2.649022	4.233317	2.926634
C	-2.871270	-1.076819	-1.783671
H	-1.793356	-1.167721	-1.589874
C	-3.569238	-2.134775	-0.927054
H	-3.293090	-2.057632	0.129584
H	-3.297964	-3.142794	-1.262131
H	-4.658991	-2.042480	-1.001318
C	-3.087999	-1.362377	-3.264872
H	-2.628848	-0.594986	-3.895751
H	-4.151817	-1.416400	-3.521065
H	-2.647457	-2.326919	-3.533290
C	1.722342	-2.100084	0.239085
C	1.341538	-3.234989	-0.507362
C	2.344879	-4.071793	-0.998839
H	2.065016	-4.958906	-1.563827
C	3.688062	-3.787265	-0.784382
H	4.455435	-4.451384	-1.172385
C	4.043711	-2.640250	-0.088630
H	5.095391	-2.401404	0.058060
C	3.076911	-1.775393	0.432626
C	-0.113611	-3.560578	-0.790523
H	-0.718575	-2.703788	-0.469159
C	-0.362184	-3.763802	-2.283385
H	-0.065774	-2.885984	-2.867014
H	-1.424895	-3.953297	-2.471922
H	0.192502	-4.623567	-2.674558
C	-0.590113	-4.781181	-0.003322
H	-0.515665	-4.628027	1.077563
H	0.003105	-5.668110	-0.254507
H	-1.637172	-5.007191	-0.232037
C	3.515535	-0.510344	1.141617
H	2.620498	0.009362	1.505772
C	4.405379	-0.798012	2.348770
H	3.919543	-1.461441	3.072002
H	4.660044	0.133800	2.864173
H	5.345531	-1.274789	2.048596
C	4.234938	0.418498	0.162121
H	3.609407	0.652184	-0.705548
H	5.154703	-0.047841	-0.210425
H	4.500524	1.366999	0.639954
C	2.470424	2.851114	2.052739
C	3.527400	3.753808	2.027660
C	3.905035	4.374140	0.836956
C	3.200100	4.084639	-0.329858
C	2.140499	3.183845	-0.315803
C	1.767534	2.542905	0.877010
H	2.172232	2.355258	2.973101
H	4.063344	3.973597	2.948209
H	4.732095	5.077544	0.820169
H	3.477077	4.565395	-1.265002
H	1.592078	2.958824	-1.228544
O	0.764137	1.661627	0.932197
C	0.487799	0.396137	-2.013322
H	-0.135483	1.140418	-2.524669
H	0.273639	-0.569125	-2.488623
H	1.527336	0.635933	-2.263822

[1-H]-.log

SCF (M06L) = -1240.66170127
E(SCF)+ZPE(0 K)= -1240.037603
H(298 K)= -1240.001980
G(298 K)= -1240.102537
Lowest Frequency = 21.3847cm-1

Al	10.303936	1.570361	3.578568
N	9.109917	2.766340	4.540053
N	10.646373	2.932866	2.180536
C	8.802924	4.110962	4.329720
C	9.484152	4.786444	3.243242
H	9.311178	5.858762	3.196803
C	10.280798	4.263701	2.265501
C	7.904843	4.816061	5.089445
H	7.353692	4.372530	5.910304
H	7.712338	5.858489	4.857189
C	10.827659	5.201951	1.222419
H	10.438999	4.978672	0.220310
H	11.919209	5.112165	1.144069
H	10.578883	6.239527	1.458442
C	8.396302	2.159470	5.605804
C	7.185239	1.483627	5.345362
C	6.515444	0.850468	6.395390
H	5.585467	0.320914	6.186508
C	7.011825	0.887975	7.692483
H	6.479623	0.389318	8.500013

C	8.194346	1.572451	7.947595
H	8.588051	1.612292	8.963647
C	8.893912	2.217176	6.925057
C	6.591376	1.443116	3.952735
H	7.265909	2.006455	3.296785
C	6.511091	0.012493	3.426357
H	7.507225	-0.444330	3.393140
H	6.091020	-0.015345	2.413710
H	5.876544	-0.613662	4.066528
C	5.229748	2.132128	3.911979
H	5.312671	3.165352	4.263586
H	4.496769	1.614053	4.544270
H	4.830143	2.148220	2.890560
C	10.163194	2.973999	7.254035
H	10.542934	3.389509	6.314421
C	9.878421	4.139966	8.198265
H	9.142365	4.817576	7.754435
H	10.791572	4.711376	8.403559
H	9.486744	3.787943	9.161777
C	11.232045	2.047102	7.828446
H	11.462275	1.232231	7.134778
H	10.902901	1.596864	8.773790
H	12.159924	2.594821	8.032070
C	11.197938	2.477762	0.959035
C	12.566461	2.143726	0.859647
C	13.060190	1.635741	-0.346396
H	14.117600	1.379445	-0.415392
C	12.238801	1.466902	-1.451186
H	12.641202	1.074697	-2.382655
C	10.891515	1.803870	-1.354578
H	10.242853	1.665677	-2.217765
C	10.354014	2.299366	-0.167269
C	13.527151	2.357408	2.011019
H	12.946899	2.776727	2.841742
C	14.139541	1.042326	2.485073
H	13.357784	0.347749	2.809095
H	14.819283	1.208322	3.329165
H	14.716655	0.561470	1.684659
C	14.619425	3.360086	1.640924
H	14.197084	4.318330	1.320150
H	15.242354	2.985585	0.818768
H	15.281710	3.551328	2.493098
C	8.866296	2.575160	-0.050009
H	8.724941	3.366401	0.696253
C	8.226989	3.051500	-1.349463
H	8.758470	3.909610	-1.775492
H	7.187919	3.350110	-1.175406
H	8.207601	2.263442	-2.112053
C	8.145559	1.335042	0.478607
H	8.582790	0.996161	1.427743
H	8.224694	0.504738	-0.234304
H	7.081287	1.537714	0.651209

Int-8.log

SCF (M06L) = -1587.41327498
E(SCF)+ZPE(0 K)= -1586.655581
H(298 K)= -1586.611447
G(298 K)= -1586.730795
Lowest Frequency = 22.0443cm-1

Al	0.371270	0.773655	-0.893613
N	1.882657	0.954460	0.353742
N	-0.815200	1.719619	0.310061
C	1.956408	1.906844	1.350626
C	0.902993	2.688727	1.737085
H	1.112557	3.429412	2.504757
C	-0.487441	2.615200	1.330412
C	3.272352	2.084106	2.058661
H	3.596374	1.146728	2.529456
H	3.198664	2.849680	2.834822
H	4.079365	2.367547	1.371234
C	-1.413049	3.397348	1.969698
H	-2.467133	3.373999	1.716606
H	-1.099613	4.056799	2.772340
C	2.945234	0.033165	0.190294
C	2.808904	-1.276822	0.719468
C	3.838702	-2.198492	0.515545
H	3.742577	-3.203844	0.918899
C	4.978258	-1.862517	-0.207775
H	5.767234	-2.596457	-0.357132
C	5.090842	-0.591171	-0.753328
H	5.968242	-0.335028	-1.346339
C	4.088607	0.364892	-0.570504
C	1.559299	-1.668497	1.490795
H	0.700817	-1.246492	0.939132
C	1.342157	-3.174089	1.588108
H	1.382623	-3.670357	0.613991
H	0.356539	-3.380051	2.018331
H	2.086048	-3.647867	2.241638
C	1.538339	-1.052669	2.891559
H	1.509831	0.039540	2.861502
H	2.424363	-1.363315	3.460615
H	0.653170	-1.389545	3.444312
C	4.205913	1.712045	-1.254983
H	3.450626	2.371968	-0.812891
C	5.574584	2.359594	-1.064903
H	5.843082	2.443981	-0.006089
H	5.590492	3.365640	-1.498342
H	6.367851	1.785068	-1.558230
C	3.875095	1.573882	-2.740848
H	2.868208	1.162030	-2.876951
H	4.585895	0.900182	-3.235994
H	3.920879	2.544150	-3.249492
C	-2.194920	1.427020	0.174829
C	-2.966281	1.994091	-0.862502
C	-4.314686	1.640090	-0.986118
H	-4.903440	2.082140	-1.790230
C	-4.914888	0.757244	-0.098068
H	-5.965833	0.495956	-0.205331
C	-4.152936	0.206529	0.927459
H	-4.610691	-0.498622	1.621621
C	-2.801677	0.518163	1.076504
C	-2.382840	3.011759	-1.819368
H	-1.313053	3.089402	-1.594646
C	-2.524845	2.569616	-3.272733
H	-2.045410	1.597607	-3.431687
H	-2.057166	3.292967	-3.950904
H	-3.578768	2.479613	-3.565599
C	-3.007645	4.387498	-1.592749
H	-2.854769	4.716065	-0.559954
H	-4.088277	4.369471	-1.785794
H	-2.565166	5.136962	-2.259830
C	-2.015761	-0.127902	2.200355
H	-0.973432	0.197571	2.102462
C	-2.519895	0.338121	3.564655
H	-2.475186	1.429335	3.634633
H	-1.908481	-0.084947	4.371137
H	-3.557130	0.019378	3.734213
C	-2.044763	-1.651864	2.100650
H	-1.621446	-2.006599	1.154150
H	-3.068073	-2.043107	2.160466
H	-1.474143	-2.104612	2.921564
C	-1.983092	-4.548544	-0.715391
C	-3.297949	-4.176895	-0.463487
C	-3.757137	-2.906033	-0.812229
C	-2.882394	-2.010754	-1.419444
C	-1.564184	-2.371878	-1.693099
C	-1.111256	-3.644266	-1.333104

H	-1.605121	-5.528815	-0.438280
H	-3.965474	-4.884049	0.024308
H	-4.777571	-2.604948	-0.589702
H	-3.211227	-1.001909	-1.665357
H	-0.895098	-1.634929	-2.130426
O	0.161337	-4.087197	-1.543972
C	1.076754	-3.139724	-2.073474
H	1.130268	-2.226916	-1.461043
H	2.052271	-3.629129	-2.080410
H	0.803522	-2.843036	-3.094990

TS-7.log

SCF (M06L) = -1587.37546921
E(SCF)+ZPE(0 K)= -1586.620518
H(298 K)= -1586.576637
G(298 K)= -1586.695425
Lowest Frequency = -544.4458cm-1

Al	0.813158	0.842234	-0.853644
N	2.281909	0.414584	0.313923
N	-0.162043	1.774109	0.478316
C	2.557674	1.134055	1.465142
C	1.712215	2.061861	2.004371
H	2.083253	2.599484	2.873073
C	0.356883	2.404209	1.614064
C	3.885468	0.896238	2.129948
H	4.017487	-0.158508	2.401729
H	3.981393	1.498387	3.036331
H	4.722946	1.140925	1.463591
C	-0.358029	3.295887	2.363467
H	-1.377006	3.571749	2.115894
H	0.083618	3.730345	3.253709
C	3.067624	-0.725273	-0.000213
C	2.605752	-2.007560	0.391376
C	3.362589	-3.128310	0.040038
H	3.017372	-4.116492	0.333340
C	4.539955	-3.007369	-0.689267
H	5.110661	-3.894251	-0.954964
C	4.971166	-1.750999	-1.091874
H	5.880177	-1.656883	-1.684729
C	4.250434	-0.601099	-0.760520
C	1.324154	-2.164732	1.193924
H	0.637859	-1.367037	0.873680
C	0.620762	-3.498376	0.964677
H	0.394458	-3.673776	-0.091650
H	-0.334642	-3.511886	1.498461
H	1.210647	-4.341186	1.345673
C	1.568910	-1.936918	2.687115
H	1.925062	-0.922873	2.889673
H	2.307868	-2.649434	3.075503
H	0.639073	-2.076189	3.251422
C	4.714685	0.747418	-1.272310
H	4.147740	1.514936	-0.732496
C	6.200820	0.992844	-1.026556
H	6.464614	0.869617	0.029422
H	6.481395	2.007704	-1.328873
H	6.826877	0.300963	-1.602443
C	4.382560	0.892461	-2.757054
H	3.306716	0.776024	-2.930627
H	4.901350	0.127904	-3.348501
H	4.685050	1.875042	-3.137577
C	-1.567714	1.857393	0.294731
C	-2.125597	2.744024	-0.650629
C	-3.508459	2.733767	-0.860812
H	-3.935569	3.416607	-1.595264
C	-4.339569	1.883758	-0.145161
H	-5.412885	1.884047	-0.322881
C	-3.786835	1.027932	0.801487
H	-4.433631	0.349337	1.356236
C	-2.412474	0.996356	1.037937
C	-1.275661	3.742567	-1.408603
H	-0.232363	3.568551	-1.120935
C	-1.385696	3.551575	-2.918877
H	-1.093452	2.536267	-3.208177
H	-0.737889	4.256139	-3.453406
H	-2.411958	3.717175	-3.269549
C	-1.631838	5.173167	-1.007114
H	-1.502949	5.318373	0.069820
H	-2.674211	5.408216	-1.257042
H	-0.995744	5.898398	-1.528141
C	-1.866458	0.065074	2.104570
H	-0.771810	0.131420	2.074533
C	-2.316036	0.517007	3.494093
H	-2.014403	1.552344	3.679991
H	-1.869087	-0.116025	4.270150
H	-3.406731	0.446356	3.596428
C	-2.260215	-1.391430	1.865269
H	-1.866653	-1.782565	0.922168
H	-3.348026	-1.525063	1.828573
H	-1.878334	-2.027094	2.674034
C	-3.341571	-4.004915	-0.968040
C	-4.690834	-4.019028	-0.649071
C	-5.461805	-2.856524	-0.729791
C	-4.841475	-1.679327	-1.144561
C	-3.491921	-1.649118	-1.477904
C	-2.695376	-2.817798	-1.400530
H	-2.736333	-4.905297	-0.890054
H	-5.148460	-4.951493	-0.319627
H	-6.517300	-2.868916	-0.470712
H	-5.413049	-0.753996	-1.204520
H	-3.040942	-0.708110	-1.786236
O	-1.414326	-2.870011	-1.688322
C	-0.497548	-1.210121	-1.620810
H	-1.039962	-0.855154	-0.751270
H	0.444326	-1.727335	-1.509753
H	-0.771308	-0.828734	-2.590813

Int-9.log

SCF (M06L) = -1587.54212322
E(SCF)+ZPE(0 K)= -1586.785693
H(298 K)= -1586.741835
G(298 K)= -1586.859412
Lowest Frequency = 16.4479cm-1

Al	-0.022161	-0.307973	-0.211853
N	1.222565	0.732532	0.739992
N	-1.592264	0.314247	0.596651
C	0.908818	1.055652	2.052691
C	-0.347187	0.981540	2.583863
H	-0.425352	1.180645	3.649691
C	-1.622807	0.708995	1.933609
C	2.058569	1.430160	2.947288
H	2.784274	0.607537	3.003943
H	1.715916	1.662613	3.958526
H	2.614653	2.295318	2.566187
C	-2.774838	0.886435	2.650046
H	-3.756095	0.741502	2.212434
H	-2.722758	1.232390	3.676204
C	2.332010	1.370897	0.141301
C	3.513506	0.651107	-0.140341
C	4.601430	1.324991	-0.701222
H	5.514327	0.767746	-0.911750
C	4.543371	2.684302	-0.981683
H	5.406230	3.196432	-1.401853
C	3.362268	3.379280	-0.743343
H	3.300505	4.437795	-0.994839

C	2.242376	2.740223	-0.208507
C	3.615073	-0.834516	0.134576
H	2.678780	-1.142766	0.615031
C	3.762514	-1.620155	-1.167850
H	2.934494	-1.413906	-1.853577
H	3.771557	-2.699648	-0.980357
H	4.694593	-1.351865	-1.682470
C	4.757547	-1.169947	1.089805
H	4.668860	-0.624541	2.035371
H	5.732870	-0.916923	0.654699
H	4.765865	-2.242706	1.314923
C	0.938230	3.499401	-0.046830
H	0.153219	2.758987	0.153842
C	0.967329	4.461244	1.139743
H	1.131648	3.929800	2.081376
H	0.016000	4.998576	1.227492
H	1.765148	5.206825	1.024573
C	0.561450	4.241423	-1.327467
H	0.515739	3.561973	-2.185358
H	1.280600	5.033660	-1.569240
H	-0.421087	4.716103	-1.222211
C	-2.834533	0.074696	-0.047019
C	-3.335387	1.030019	-0.962838
C	-4.537907	0.772907	-1.624430
H	-4.924290	1.502587	-2.332988
C	-5.248987	-0.400371	-1.395825
H	-6.185219	-0.583712	-1.919082
C	-4.747347	-1.339174	-0.505050
H	-5.289927	-2.269180	-0.334594
C	-3.543912	-1.126222	0.173667
C	-2.584708	2.326646	-1.190514
H	-1.515168	2.092627	-1.115210
C	-2.826192	2.942881	-2.562572
H	-2.642053	2.224786	-3.368952
H	-2.160709	3.799634	-2.715105
H	-3.852979	3.313576	-2.672891
C	-2.904019	3.330123	-0.081148
H	-2.674288	2.917240	0.906537
H	-3.970461	3.590268	-0.096652
H	-2.333584	4.258283	-0.214244
C	-3.015840	-2.205163	1.096665
H	-2.075766	-1.846888	1.526487
C	-3.982055	-2.489849	2.243749
H	-4.157596	-1.585602	2.834298
H	-3.575113	-3.258289	2.911101
H	-4.949285	-2.855880	1.874447
C	-2.710699	-3.481598	0.314181
H	-2.033567	-3.285016	-0.522291
H	-3.627906	-3.929941	-0.090241
H	-2.227677	-4.227503	0.955657
C	1.657709	-3.840848	0.667446
C	2.335976	-4.949332	0.176324
C	2.219604	-5.323092	-1.163436
C	1.399482	-4.567869	-2.001125
C	0.714732	-3.457281	-1.521114
C	0.839087	-3.060047	-0.173912
H	1.750909	-3.536333	1.707100
H	2.968620	-5.527754	0.847920
H	2.753710	-6.189125	-1.545497
H	1.290056	-4.847351	-3.047578
H	0.075606	-2.870812	-2.177492
O	0.208019	-2.007937	0.320146
C	0.058502	-0.049146	-2.166514
H	0.896479	-0.567642	-2.648191
H	0.166841	1.013440	-2.422832
H	-0.853755	-0.397142	-2.669187

Int7a.log

SCF (M06L) = -1587.99204944

E(SCF)+ZPE(0 K)= -1587.219120
H(298 K)= -1587.174851
G(298 K)= -1587.293297
Lowest Frequency = 26.6650cm-1

Al	10.788728	1.549013	3.858992
N	9.650983	2.898707	4.880569
N	11.096545	2.991370	2.461227
C	9.512742	4.209767	4.659311
C	10.169751	4.883510	3.619624
H	10.028445	5.958099	3.577881
C	10.865587	4.305962	2.549606
C	8.577403	5.024244	5.509646
H	7.539709	4.857515	5.197735
H	8.785771	6.091209	5.409734
H	8.630500	4.741416	6.564346
C	11.340324	5.226395	1.459686
H	11.010091	4.881089	0.475024
H	12.435560	5.249063	1.421158
H	10.981375	6.245046	1.615376
C	8.788485	2.295211	5.855522
C	7.444885	2.035351	5.520673
C	6.624322	1.439292	6.481049
H	5.585907	1.228140	6.234328
C	7.116117	1.100319	7.733707
H	6.463144	0.640501	8.470440
C	8.453292	1.329878	8.035470
H	8.838838	1.036324	9.007631
C	9.315899	1.918798	7.108606
C	6.898619	2.300935	4.130033
H	7.595458	2.963556	3.600862
C	6.833439	0.990069	3.344400
H	7.814821	0.501895	3.294215
H	6.483993	1.161935	2.319708
H	6.142504	0.285738	3.821395
C	5.533981	2.984251	4.141983
H	5.538940	3.905597	4.733791
H	4.757960	2.333574	4.559329
H	5.224674	3.240386	3.123464
C	10.779172	2.149536	7.430788
H	11.343238	1.915822	6.515353
C	11.073678	3.610429	7.770530
H	10.840720	4.282221	6.939275
H	12.136660	3.734081	8.011502
H	10.493905	3.934989	8.643045
C	11.314132	1.243504	8.531179
H	11.116810	0.187749	8.320235
H	10.874462	1.481454	9.506793
H	12.397102	1.370597	8.623873
C	11.630279	2.477890	1.232527
C	13.011945	2.524699	0.969966
C	13.477140	1.995877	-0.236386
H	14.543711	2.022022	-0.449429
C	12.605893	1.431013	-1.156992
H	12.985017	1.028175	-2.092136
C	11.247865	1.363481	-0.869768
H	10.574389	0.897724	-1.583877
C	10.734652	1.870443	0.325763
C	13.996193	3.064740	1.986763
H	13.429175	3.633385	2.731729
C	14.670005	1.909930	2.726701
H	13.926679	1.266394	3.210616
H	15.349846	2.278203	3.503238
H	15.249226	1.289587	2.033053
C	15.036099	3.997540	1.372463
H	14.575256	4.812787	0.804013
H	15.706893	3.464551	0.690053
H	15.663352	4.441861	2.152274
C	9.251569	1.779360	0.636979

H	9.158881	1.632681	1.724852
C	8.515814	3.077135	0.301104
H	8.893488	3.925491	0.879641
H	7.445306	2.982882	0.518137
H	8.619733	3.320286	-0.762917
C	8.571108	0.591066	-0.029832
H	9.102207	-0.343640	0.173005
H	8.504418	0.713133	-1.116621
H	7.547197	0.484261	0.341038
O	13.214011	3.148940	5.311797
C	13.389366	4.552579	5.272369
H	14.417444	4.817595	4.988244
H	12.688149	4.925854	4.523610
H	13.155172	5.016402	6.239701
C	14.006355	2.455094	6.187106
C	13.887765	1.061717	6.144539
C	14.884914	3.056776	7.090605
C	14.640276	0.279707	7.007591
H	13.184293	0.622926	5.438148
C	15.633323	2.253615	7.952614
H	14.989881	4.135433	7.133492
C	15.518428	0.869257	7.919016
H	14.536102	-0.801058	6.969308
H	16.313132	2.727454	8.655587
H	16.105350	0.253579	8.593575

TS6a.log

SCF (M06L) = -1934.68394779
E(SCF)+ZPE(0 K)= -1933.780119
H(298 K)= -1933.727590
G(298 K)= -1933.864819
Lowest Frequency = -574.9567cm-1

Al	10.930462	1.288866	4.163102
N	9.545050	2.418243	5.012070
N	10.874152	2.422735	2.563652
C	9.252757	3.680714	4.685467
C	9.849729	4.334731	3.595756
H	9.622192	5.388640	3.478102
C	10.554854	3.725021	2.551513
C	8.222994	4.447085	5.461592
H	7.229819	4.280852	5.030513
H	8.420699	5.519908	5.409301
H	8.174474	4.136733	6.507717
C	10.953485	4.571317	1.378393
H	10.644596	4.117547	0.432528
H	12.045863	4.658871	1.331993
H	10.529020	5.574091	1.445866
C	8.769915	1.746581	6.017544
C	7.493489	1.241587	5.697198
C	6.797207	0.542986	6.688373
H	5.812759	0.142397	6.455192
C	7.342403	0.340001	7.946980
H	6.784519	-0.207838	8.701025
C	8.614485	0.821848	8.235836
H	9.044181	0.639550	9.216313
C	9.355461	1.522749	7.283584
C	6.857676	1.391384	4.326319
H	7.527893	1.990783	3.694927
C	6.657272	0.033495	3.646972
H	7.577421	-0.547682	3.528940
H	6.215110	0.168507	2.653709
H	5.965971	-0.589174	4.226076
C	5.511436	2.114346	4.407287
H	5.575208	3.071834	4.933433
H	4.772843	1.504512	4.939263
H	5.113836	2.303874	3.405134
C	10.752014	2.031448	7.587927
H	11.362730	1.831801	6.692145
C	10.786314	3.542619	7.817903
H	10.455063	4.104838	6.940559
H	11.808140	3.863416	8.053102
H	10.145511	3.824716	8.661550
C	11.428192	1.317666	8.749825
H	11.429475	0.231317	8.617089
H	10.939048	1.541203	9.704860
H	12.468743	1.646905	8.832727
C	11.352955	1.802346	1.357100
C	12.728105	1.799894	1.061664
C	13.159575	1.111072	-0.074941
H	14.221790	1.092089	-0.310885
C	12.257931	0.446329	-0.892694
H	12.609607	-0.094922	-1.766843
C	10.901877	0.458552	-0.586329
H	10.210829	-0.092798	-1.216359
C	10.416116	1.129606	0.538493
C	13.741482	2.488266	1.953345
H	13.190621	3.088430	2.686391
C	14.559826	1.466495	2.740426
H	13.907998	0.806745	3.324809
H	15.245430	1.962325	3.436549
H	15.152918	0.836405	2.067809
C	14.660166	3.425969	1.173278
H	14.098415	4.156614	0.581553
H	15.302717	2.873753	0.479008
H	15.319210	3.975393	1.853907
C	8.927720	1.121925	0.861419
H	8.828778	0.985475	1.951444
C	8.242785	2.450162	0.524235
H	8.598876	3.286113	1.130611
H	7.163247	2.366600	0.693591
H	8.390516	2.705146	-0.531711
C	8.172040	-0.012123	0.178305
H	8.640826	-0.985915	0.335758
H	8.095043	0.158538	-0.901794
H	7.150080	-0.067464	0.564067
O	13.104462	3.134391	5.267851
C	13.118727	4.536508	5.062717
H	14.141154	4.899312	4.893912
H	12.508799	4.721649	4.177064
H	12.678859	5.075216	5.912302
C	13.894851	2.654022	6.282684
C	14.023348	1.263522	6.355392
C	14.538406	3.468123	7.216389
C	14.789752	0.693920	7.361681
H	13.498967	0.655319	5.621703
C	15.305108	2.877920	8.222278
H	14.447182	4.548043	7.173051
C	15.436545	1.496719	8.302479
H	14.880295	-0.387457	7.411081
H	15.802695	3.516104	8.947227
H	16.036200	1.047676	9.087938
C	8.159062	-3.848238	0.162133
C	8.093517	-3.474509	1.495994
C	9.201989	-2.879505	2.149320
C	10.370608	-2.677729	1.374386
C	10.417183	-3.049388	0.034059
C	9.317374	-3.634156	-0.589976
H	7.286642	-4.300845	-0.305632
H	7.187535	-3.624268	2.078077
H	11.244920	-2.219538	1.833031
H	11.330957	-2.870312	-0.530606
H	9.359831	-3.920413	-1.636822
O	9.085460	-2.541950	3.416140
C	10.143931	-0.990123	3.866014
H	9.934227	-0.596879	2.878416
H	9.476920	-0.815200	4.699278
H	11.070431	-1.510700	4.037335

AnisoleLi(THF)3.log

SCF (M06L) = -1051.49434585
E(SCF)+ZPE(0 K)= -1051.001965
H(298 K)= -1050.973677
G(298 K)= -1051.064457
Lowest Frequency = 17.9171cm-1

C	2.261423	3.755300	-0.456440
C	1.606516	4.700091	-1.245069
C	0.294683	4.487487	-1.653586
C	-0.363866	3.322947	-1.261413
C	0.280254	2.362668	-0.486396
C	1.597002	2.590543	-0.087269
H	3.287618	3.920095	-0.146014
H	2.126302	5.599574	-1.562910
H	-0.225969	5.204370	-2.283454
H	-0.224527	1.447977	-0.194315
H	2.102530	1.843125	0.516120
C	-2.223925	1.888398	-1.751942
H	-3.209697	1.990219	-2.208295
H	-1.586246	1.259116	-2.379303
H	-2.331694	1.425957	-0.765078
O	-1.688228	3.209282	-1.662556
O	-3.989413	4.103465	0.441187
C	-4.815172	5.096541	1.097669
C	-3.728061	3.011718	1.352467
C	-4.776341	4.746539	2.571318
H	-4.400557	6.082441	0.858296
H	-5.830990	5.030901	0.686774
C	-4.657847	3.227648	2.530547
H	-3.907097	2.072208	0.821022
H	-2.668862	3.051680	1.649249
H	-5.658073	5.099747	3.108705
H	-3.895024	5.187471	3.051121
H	-5.634204	2.773647	2.333400
H	-4.269320	2.796027	3.454463
O	-2.076203	6.255440	-0.333394
C	-1.680045	7.449324	-1.040973
C	-1.359484	6.172293	0.923624
C	-0.379222	7.880126	-0.398470
H	-1.601377	7.197848	-2.104756
H	-2.466046	8.209272	-0.924011
C	-0.603362	7.481763	1.056490
H	-2.091202	5.999181	1.721104
H	-0.683765	5.306962	0.873325
H	-0.174879	8.943903	-0.531520
H	0.457741	7.315684	-0.823050
H	-1.216040	8.231455	1.567669
H	0.324066	7.368360	1.620636
O	-3.804082	5.241639	-2.697782
C	-3.277910	5.110054	-4.039812
C	-4.873864	6.216199	-2.687234
C	-4.264655	5.833708	-4.933305
H	-2.281232	5.574124	-4.071501
H	-3.165362	4.044936	-4.259896
C	-4.772772	6.939473	-4.014475
H	-5.828253	5.684554	-2.579573
H	-4.734225	6.860851	-1.812070
H	-5.084515	5.166298	-5.217880
H	-3.803615	6.206288	-5.849518
H	-5.724979	7.367278	-4.332439
H	-4.042677	7.754467	-3.953569
Li	-2.925193	4.686851	-1.081465

Int7b.log

SCF (M06L) = -2292.77447689
E(SCF)+ZPE(0 K)= -2291.643120
H(298 K)= -2291.578341
G(298 K)= -2291.745038
Lowest Frequency = 19.7836cm-1

C	4.458119	3.835867	-2.582713
C	3.435588	4.781251	-2.666923
C	2.104512	4.390031	-2.566558
C	1.797464	3.042619	-2.374017
C	2.805684	2.084296	-2.301513
C	4.134744	2.492917	-2.407762
H	5.495285	4.142872	-2.667857
H	3.672123	5.830190	-2.824587
H	1.293312	5.107957	-2.645714
H	2.564373	1.033164	-2.171261
H	4.921799	1.744455	-2.351403
C	0.069228	1.380588	-2.460515
H	-1.014165	1.397095	-2.583033
H	0.538169	1.000466	-3.374146
H	0.326920	0.720188	-1.617093
O	0.457039	2.740687	-2.220921
O	-1.523688	2.775945	0.473813
C	-1.594051	3.044534	1.889735
C	-2.450303	1.708365	0.144939
C	-2.068530	1.745924	2.501409
H	-0.596154	3.365585	2.209284
H	-2.301990	3.867585	2.068311
C	-3.063360	1.247047	1.459810
H	-3.187100	2.093507	-0.569624
H	-1.868293	0.903048	-0.325974
H	-2.505994	1.870689	3.494706
H	-1.237388	1.033864	2.583730
H	-4.051009	1.693647	1.616525
H	-3.175031	0.159143	1.494214
O	1.544055	3.054175	0.736634
C	2.847409	3.646714	0.953438
C	1.604744	1.650628	1.059795
C	3.738341	2.527702	1.474212
H	3.204079	4.073960	0.008242
H	2.722521	4.456180	1.683423
C	2.734676	1.536742	2.055054
H	0.617450	1.344978	1.420286
H	1.816154	1.065934	0.146703
H	4.472589	2.884120	2.199275
H	4.285463	2.065934	0.643933
H	2.398973	1.851995	3.050011
H	3.122667	0.518026	2.135619
O	-0.170514	5.471391	-0.418436
C	-1.280114	6.099326	-1.101481
C	0.826226	6.462486	-0.087764
C	-1.060008	7.591284	-0.946740
H	-1.258221	5.788744	-2.156164
H	-2.207122	5.731577	-0.651132
C	0.461322	7.685150	-0.904119
H	0.780154	6.658524	0.992119
H	1.810031	6.042886	-0.326432
H	-1.489899	7.946464	-0.004443
H	-1.509857	8.166920	-1.757570
H	0.828821	8.612326	-0.460720
H	0.879618	7.608577	-1.914998
Li	0.023938	3.553029	-0.389633
Al	-0.360699	-1.631818	0.494458
N	-1.231383	-3.062080	1.553592
N	0.438635	-3.011900	-0.693602
C	-1.063649	-4.389901	1.468011
C	-0.313588	-4.988686	0.449429
H	-0.270706	-6.071752	0.456686
C	0.340985	-4.348071	-0.609332
C	-1.717961	-5.280279	2.481114

H	-1.469549	-4.957269	3.497263
H	-1.415337	-6.320306	2.356749
H	-2.809591	-5.227653	2.406635
C	0.928807	-5.209825	-1.687834
H	1.933024	-4.881374	-1.970410
H	0.319248	-5.146780	-2.596917
H	0.966631	-6.256250	-1.383053
C	-2.140180	-2.532728	2.531711
C	-1.639079	-1.974749	3.723028
C	-2.538333	-1.335941	4.583150
H	-2.164106	-0.895756	5.505719
C	-3.892545	-1.266307	4.288323
H	-4.575531	-0.769399	4.971415
C	-4.375866	-1.852742	3.123235
H	-5.439344	-1.808095	2.902620
C	-3.517975	-2.490442	2.225433
C	-0.179771	-2.084439	4.124180
H	0.339392	-2.672065	3.355710
C	0.496243	-0.716149	4.194873
H	0.483811	-0.218856	3.217152
H	1.539967	-0.811278	4.513223
H	-0.010215	-0.058902	4.911843
C	-0.029407	-2.823713	5.453920
H	-0.505586	-3.808435	5.429940
H	-0.485704	-2.262050	6.275969
H	1.026574	-2.966399	5.702044
C	-4.054893	-3.065858	0.927106
H	-3.359787	-3.842823	0.584546
C	-5.426062	-3.716038	1.079309
H	-5.440984	-4.453658	1.887250
H	-5.711857	-4.224046	0.154031
H	-6.207728	-2.979253	1.290798
C	-4.087403	-1.990029	-0.158929
H	-3.096593	-1.536065	-0.306463
H	-4.779279	-1.183194	0.112173
H	-4.414546	-2.405630	-1.117846
C	1.095015	-2.445783	-1.836693
C	0.401426	-2.335657	-3.057595
C	1.065758	-1.773872	-4.152114
H	0.543409	-1.685926	-5.102216
C	2.375178	-1.326332	-4.044736
H	2.882649	-0.904691	-4.907786
C	3.031523	-1.404434	-2.820773
H	4.049332	-1.031561	-2.741283
C	2.407385	-1.943348	-1.692416
C	-1.059266	-2.723774	-3.190827
H	-1.339864	-3.333481	-2.321679
C	-1.920480	-1.459177	-3.156205
H	-1.757056	-0.896626	-2.225833
H	-2.986390	-1.698187	-3.224117
H	-1.671252	-0.798975	-3.995942
C	-1.349761	-3.539637	-4.447244
H	-0.710304	-4.424939	-4.518943
H	-1.195782	-2.952439	-5.358378
H	-2.390436	-3.875717	-4.455349
C	3.123069	-1.999356	-0.354537
H	2.368901	-1.765807	0.418325
C	3.669818	-3.395213	-0.053430
H	2.875224	-4.141872	0.019051
H	4.213909	-3.401979	0.896046
H	4.365104	-3.716244	-0.837071
C	4.231817	-0.961538	-0.223998
H	3.877403	0.048060	-0.466650
H	5.081516	-1.182951	-0.879131
H	4.620245	-0.946593	0.799000

TS6b.log

SCF (M06L) = -2292.73817761

E(SCF)+ZPE(0 K)= -2291.610092
H(298 K)= -2291.545508
G(298 K)= -2291.712138
Lowest Frequency = -506.6370cm-1

C	0.774286	3.521155	-4.330004
C	-0.306681	4.379843	-4.536280
C	-1.577333	4.041971	-4.086305
C	-1.805497	2.836513	-3.391096
C	-0.712356	1.969717	-3.202744
C	0.552457	2.312353	-3.675012
H	1.764256	3.782621	-4.689081
H	-0.162358	5.320440	-5.063545
H	-2.426863	4.699112	-4.258132
H	-0.850022	1.021707	-2.687846
H	1.377947	1.619469	-3.518112
C	-3.382783	0.843651	-2.318353
H	-4.446428	0.961479	-2.444427
H	-2.819849	0.332701	-3.089431
H	-2.958167	0.964779	-1.333293
O	-3.034675	2.608856	-2.908859
O	-4.531674	3.291308	-0.183013
C	-4.451754	3.461488	1.238507
C	-5.761340	2.587923	-0.391405
C	-4.930958	2.131533	1.820830
H	-3.420116	3.734006	1.475899
H	-5.107910	4.293892	1.534347
C	-5.771084	1.511546	0.685871
H	-6.599065	3.292551	-0.269956
H	-5.767708	2.222835	-1.421105
H	-5.505337	2.276804	2.739148
H	-4.086794	1.480946	2.071796
H	-6.783897	1.250472	1.000925
H	-5.303247	0.588857	0.316636
O	-1.435100	3.463115	-0.272299
C	-0.183892	4.134275	-0.577763
C	-1.156343	2.232458	0.410170
C	0.915825	3.210492	-0.082761
H	-0.138401	4.314856	-1.658905
H	-0.191647	5.097088	-0.051529
C	0.217206	2.418058	1.016458
H	-1.960561	2.059472	1.134910
H	-1.155384	1.398798	-0.313486
H	1.795654	3.756330	0.263055
H	1.230004	2.540307	-0.891282
H	0.151100	3.003265	1.940074
H	0.708859	1.470454	1.249391
O	-3.272082	5.696827	-1.666553
C	-4.589642	6.060914	-2.138753
C	-2.318812	6.707370	-2.058582
C	-4.463627	7.478834	-2.663513
H	-4.879019	5.352791	-2.929628
H	-5.292179	5.954156	-1.305823
C	-3.013028	7.520849	-3.130516
H	-2.071403	7.317145	-1.178840
H	-1.412702	6.198317	-2.404067
H	-4.623643	8.201370	-1.856315
H	-5.183461	7.697528	-3.454501
H	-2.612501	8.532738	-3.217108
H	-2.907975	7.033358	-4.107040
Li	-3.049933	3.773480	-1.380932
Al	-3.858141	-1.644976	-1.516988
N	-4.656827	-2.952106	-0.330396
N	-2.814853	-2.992622	-2.434081
C	-4.562185	-4.290673	-0.418366
C	-3.796518	-4.927840	-1.400791
H	-3.816946	-6.011278	-1.397576
C	-2.929233	-4.326561	-2.322005
C	-5.275971	-5.140229	0.587045

H	-4.929053	-4.915864	1.601004
H	-5.124416	-6.201979	0.393519
H	-6.351266	-4.932661	0.584664
C	-2.082773	-5.216789	-3.180050
H	-1.025816	-4.942962	-3.103465
H	-2.346924	-5.110993	-4.237575
H	-2.197792	-6.264253	-2.901305
C	-5.305975	-2.370160	0.815716
C	-4.505949	-1.967407	1.903365
C	-5.129478	-1.334532	2.982814
H	-4.525936	-1.015268	3.830549
C	-6.500303	-1.114284	2.991478
H	-6.968929	-0.628595	3.842822
C	-7.272013	-1.515726	1.906730
H	-8.343867	-1.333796	1.915405
C	-6.695373	-2.141237	0.799562
C	-3.002486	-2.176732	1.929244
H	-2.720680	-2.764006	1.044553
C	-2.273780	-0.835507	1.837663
H	-2.585036	-0.276421	0.943717
H	-1.187246	-0.975017	1.788021
H	-2.487346	-0.208816	2.712497
C	-2.547603	-2.957306	3.159954
H	-3.049712	-3.925857	3.235015
H	-2.755134	-2.407923	4.084148
H	-1.469283	-3.140619	3.125013
C	-7.535741	-2.489135	-0.412691
H	-6.999401	-3.255927	-0.986114
C	-8.906676	-3.053619	-0.055577
H	-8.833192	-3.903616	0.629451
H	-9.427136	-3.390983	-0.956008
H	-9.546810	-2.302807	0.418633
C	-7.674228	-1.259204	-1.313285
H	-6.692678	-0.857138	-1.601968
H	-8.213130	-0.458586	-0.792954
H	-8.226071	-1.495568	-2.228244
C	-1.824631	-2.442514	-3.322905
C	-2.099561	-2.342893	-4.699905
C	-1.130649	-1.763633	-5.523738
H	-1.324498	-1.671342	-6.588814
C	0.071140	-1.303936	-5.004934
H	0.814016	-0.859902	-5.660988
C	0.313758	-1.387007	-3.639337
H	1.248597	-1.001147	-3.243680
C	-0.629688	-1.933873	-2.766167
C	-3.435550	-2.771929	-5.277060
H	-3.874406	-3.521306	-4.606672
C	-4.395689	-1.580923	-5.310106
H	-4.562425	-1.167992	-4.306268
H	-5.368971	-1.869278	-5.718923
H	-3.993912	-0.773011	-5.931392
C	-3.317356	-3.407150	-6.658769
H	-2.584817	-4.220075	-6.674508
H	-3.017497	-2.679191	-7.419096
H	-4.281393	-3.815505	-6.973903
C	-0.384289	-1.954137	-1.265422
H	-1.330012	-1.639957	-0.781951
C	-0.049894	-3.348550	-0.733056
H	-0.859765	-4.064740	-0.891758
H	0.147674	-3.312160	0.343962
H	0.849212	-3.741427	-1.220075
C	0.686184	-0.965892	-0.815610
H	0.508524	0.046090	-1.198627
H	1.684522	-1.273783	-1.143993
H	0.715207	-0.916152	0.277512

Int8b.log

SCF (M06L) = -2292.84822428

E(SCF)+ZPE(0 K)= -2291.716772
H(298 K)= -2291.652763
G(298 K)= -2291.814094
Lowest Frequency = 21.0796cm-1

C	-0.398668	1.338074	-3.315529
C	-1.435075	1.999308	-2.611156
C	-1.515660	1.967486	-1.240249
C	-0.527273	1.280103	-0.447749
C	0.375011	0.399908	-1.186505
C	0.514474	0.596436	-2.610631
H	-0.318094	1.439332	-4.392753
H	-2.165302	2.580789	-3.170458
H	-2.262899	2.557998	-0.713857
H	1.270492	0.106488	-0.631503
H	1.336908	0.107344	-3.129267
C	-2.203678	-1.504425	-2.449453
H	-2.702168	-2.481749	-2.412332
H	-1.983440	-1.305212	-3.501485
H	-2.948359	-0.761839	-2.145967
O	-0.440771	1.433290	0.806676
O	-2.359207	3.899572	1.503141
C	-2.586127	5.071767	2.306418
C	-3.337442	2.935514	1.928684
C	-3.073508	4.570940	3.670367
H	-1.642061	5.623605	2.343833
H	-3.336297	5.700303	1.808756
C	-3.374597	3.080169	3.439341
H	-4.305814	3.172256	1.462074
H	-2.999760	1.954754	1.577915
H	-3.960196	5.121797	3.992856
H	-2.309239	4.704984	4.439926
H	-4.328829	2.762753	3.866964
H	-2.594174	2.451149	3.880224
O	0.145108	3.571626	3.325451
C	1.212025	4.505454	3.568367
C	0.290956	2.460123	4.239660
C	2.360931	3.637141	4.032077
H	1.379764	5.050127	2.636117
H	0.904068	5.219199	4.347821
C	1.636729	2.643254	4.936014
H	-0.552946	2.460070	4.942263
H	0.235222	1.545463	3.639242
H	3.146434	4.195890	4.544734
H	2.810221	3.121942	3.174095
H	1.500657	3.071150	5.934143
H	2.173698	1.699123	5.057463
O	0.617335	4.302466	0.402374
C	0.157098	5.124944	-0.696374
C	1.877689	3.691617	0.057759
C	1.268537	5.100032	-1.732355
H	-0.775685	4.688128	-1.075213
H	-0.060649	6.125766	-0.309969
C	1.956572	3.768696	-1.451156
H	2.691724	4.253341	0.540221
H	1.869869	2.669551	0.458647
H	1.963587	5.931065	-1.573365
H	0.884796	5.178680	-2.751950
H	2.982132	3.722364	-1.823979
H	1.394113	2.944088	-1.903463
Li	-0.541541	3.171728	1.527448
Al	-0.614076	-1.519897	-1.314440
N	-0.940651	-2.315553	0.402044
N	0.770727	-2.746142	-1.857849
C	-0.868016	-3.659069	0.485520
C	-0.197963	-4.453449	-0.452480
H	-0.241711	-5.522581	-0.284751
C	0.674406	-4.027862	-1.465972
C	-1.503835	-4.356119	1.649722

H	-2.554500	-4.063923	1.744974
H	-1.030618	-4.075975	2.595289
H	-1.444651	-5.438653	1.541044
C	1.534070	-5.066889	-2.116961
H	2.589110	-4.778764	-2.103382
H	1.267736	-5.176310	-3.173088
H	1.424598	-6.035114	-1.629578
C	-1.355923	-1.615823	1.589793
C	-0.390123	-1.375308	2.588153
C	-0.802754	-0.769147	3.774657
H	-0.072808	-0.610014	4.567710
C	-2.120146	-0.366430	3.960024
H	-2.424394	0.100650	4.893655
C	-3.049950	-0.583308	2.952585
H	-4.085295	-0.279026	3.099328
C	-2.696759	-1.228066	1.762369
C	1.072083	-1.740807	2.414868
H	1.201445	-2.163519	1.410936
C	1.954675	-0.495757	2.510997
H	1.626713	0.282324	1.811191
H	3.001133	-0.746895	2.306690
H	1.920572	-0.070287	3.521742
C	1.530890	-2.793049	3.423338
H	0.966611	-3.725950	3.335056
H	1.414763	-2.434426	4.452104
H	2.588625	-3.034187	3.278079
C	-3.772685	-1.507718	0.732215
H	-3.319431	-2.074226	-0.089688
C	-4.908339	-2.352122	1.310977
H	-4.550535	-3.294803	1.735987
H	-5.642747	-2.593055	0.536997
H	-5.436783	-1.817449	2.107532
C	-4.332304	-0.208166	0.155770
H	-3.542506	0.423658	-0.266936
H	-4.844800	0.373356	0.931930
H	-5.060699	-0.412251	-0.635306
C	1.808751	-2.410983	-2.799794
C	1.587493	-2.567332	-4.182780
C	2.627569	-2.242397	-5.058459
H	2.468765	-2.358124	-6.128346
C	3.848651	-1.779133	-4.591516
H	4.647147	-1.543031	-5.288511
C	4.040374	-1.607742	-3.226500
H	4.993430	-1.231445	-2.864818
C	3.031572	-1.907277	-2.307540
C	0.262437	-3.016292	-4.768596
H	-0.415887	-3.270365	-3.943580
C	-0.368888	-1.872368	-5.565174
H	-0.448878	-0.958537	-4.967762
H	-1.371451	-2.141206	-5.911880
H	0.234748	-1.635965	-6.448390
C	0.405090	-4.244786	-5.667193
H	0.865738	-5.094368	-5.154612
H	1.023072	-4.023853	-6.543802
H	-0.573350	-4.568087	-6.033594
C	3.276614	-1.679930	-0.826591
H	2.298058	-1.599247	-0.336357
C	3.990974	-2.863025	-0.172799
H	3.383987	-3.773626	-0.205013
H	4.207369	-2.651311	0.880109
H	4.942921	-3.075040	-0.671409
C	4.036385	-0.379052	-0.569873
H	3.573865	0.470297	-1.086842
H	5.075959	-0.439427	-0.906420
H	4.062724	-0.151005	0.499685

Int8c.log

SCF (M06L) = -2292.27195211

E(SCF)+ZPE(0 K)= -2291.154076
H(298 K)= -2291.090104
G(298 K)= -2291.254156
Lowest Frequency = 18.8869cm-1

C	4.503544	3.833454	-2.514364
C	3.445446	4.717485	-2.726345
C	2.130911	4.262282	-2.710144
C	1.874147	2.910282	-2.474475
C	2.921158	2.013370	-2.267980
C	4.231902	2.485553	-2.291471
H	5.528220	4.191190	-2.533163
H	3.642320	5.769152	-2.918275
H	1.294240	4.932516	-2.883547
H	2.722440	0.959834	-2.093481
H	5.044929	1.781583	-2.128892
C	0.269182	1.132368	-2.588618
H	-0.805085	1.062652	-2.761359
H	0.816377	0.730821	-3.448323
H	0.512138	0.550943	-1.685894
O	0.547360	2.538556	-2.419620
O	-1.547735	2.824791	0.614422
C	-1.448497	3.467695	1.897897
C	-2.586861	1.826222	0.709240
C	-1.979066	2.468158	2.933288
H	-0.394542	3.736243	2.037116
H	-2.036947	4.398260	1.879939
C	-2.434929	1.264407	2.101531
H	-3.563311	2.308383	0.544357
H	-2.391789	1.081387	-0.072964
H	-2.806667	2.905175	3.499608
H	-1.210334	2.184269	3.659716
H	-3.348501	0.800254	2.478454
H	-1.667547	0.477004	2.078861
O	1.473700	2.788024	0.613860
C	2.667628	3.540860	0.897021
C	1.466749	1.563573	1.388149
C	3.550835	2.613804	1.709323
H	3.108892	3.860719	-0.054109
H	2.385048	4.435038	1.474479
C	2.523769	1.765496	2.451408
H	0.448185	1.410156	1.760942
H	1.695644	0.718702	0.720443
H	4.233432	3.155870	2.367596
H	4.151811	1.984359	1.042671
H	2.109105	2.316868	3.305199
H	2.921108	0.819701	2.825543
O	-0.215982	5.093233	-0.687484
C	-1.443157	5.591220	-1.258942
C	0.591933	6.187389	-0.223787
C	-1.505446	7.053896	-0.865034
H	-1.396420	5.462160	-2.350061
H	-2.264722	4.980491	-0.870671
C	-0.028082	7.429730	-0.832567
H	0.556591	6.213113	0.875870
H	1.626113	6.000433	-0.535204
H	-1.947742	7.162811	0.131730
H	-2.095300	7.653043	-1.561540
H	0.182792	8.332912	-0.256362
H	0.348699	7.583653	-1.850569
Li	-0.029351	3.143511	-0.540654
Al	-0.733625	-1.652539	0.083725
N	-1.483379	-2.940255	1.276442
N	0.250864	-2.971040	-0.941940
C	-1.413326	-4.339969	1.234835
C	-0.645004	-4.940173	0.160944
H	-0.652406	-6.026461	0.158649
C	0.114478	-4.346991	-0.804580
C	-2.013705	-5.147064	2.159110

H	-1.912455	-6.223269	2.075644
H	-2.591583	-4.759438	2.989445
C	0.882461	-5.230463	-1.749568
H	1.955041	-4.998521	-1.729165
H	0.570359	-5.103000	-2.793605
H	0.754128	-6.282194	-1.486380
C	-2.160156	-2.405499	2.405946
C	-1.424289	-2.088287	3.567713
C	-2.071927	-1.454338	4.631890
H	-1.500096	-1.183600	5.518877
C	-3.434646	-1.182335	4.582317
H	-3.927431	-0.696127	5.421139
C	-4.166037	-1.555350	3.459790
H	-5.237208	-1.359541	3.425691
C	-3.549833	-2.170865	2.366273
C	0.052044	-2.417377	3.664219
H	0.287962	-3.092181	2.832697
C	0.898988	-1.159516	3.485186
H	0.694441	-0.707960	2.504595
H	1.971892	-1.386860	3.541115
H	0.672407	-0.408271	4.255070
C	0.397746	-3.140621	4.961454
H	-0.207721	-4.044214	5.076178
H	0.230999	-2.509558	5.842595
H	1.452371	-3.436686	4.969440
C	-4.363826	-2.548172	1.146959
H	-3.737726	-3.207483	0.536013
C	-5.631287	-3.314888	1.509728
H	-5.395802	-4.205116	2.100157
H	-6.158379	-3.638815	0.606112
H	-6.332076	-2.702069	2.089347
C	-4.687855	-1.306626	0.316760
H	-3.765533	-0.803254	-0.001803
H	-5.280649	-0.587023	0.897899
H	-5.261259	-1.562867	-0.581523
C	1.126551	-2.474193	-1.935728
C	0.733175	-2.436043	-3.293363
C	1.617408	-1.922982	-4.246724
H	1.317832	-1.895456	-5.292797
C	2.870449	-1.446987	-3.881305
H	3.552725	-1.059069	-4.633751
C	3.244268	-1.461638	-2.540703
H	4.224925	-1.080480	-2.262342
C	2.388083	-1.952590	-1.550725
C	-0.657580	-2.881481	-3.703361
H	-1.028926	-3.565232	-2.932033
C	-1.603807	-1.680798	-3.723777
H	-1.636198	-1.194981	-2.738719
H	-2.624036	-1.982758	-3.984883
H	-1.273990	-0.937278	-4.461557
C	-0.688233	-3.618233	-5.037867
H	0.019668	-4.453512	-5.057426
H	-0.442107	-2.958694	-5.878035
H	-1.687781	-4.019806	-5.231044
C	2.794308	-1.941735	-0.086882
H	1.909517	-1.594948	0.475802
C	3.132188	-3.336524	0.440590
H	2.273261	-4.009490	0.385566
H	3.443568	-3.284597	1.490292
H	3.957609	-3.779403	-0.129864
C	3.935117	-0.978501	0.218628
H	3.744156	0.027562	-0.176380
H	4.886963	-1.321671	-0.204398
H	4.081227	-0.894485	1.301522

TS7c.log

SCF (M06L) = -2292.25117942
E(SCF)+ZPE(0 K)= -2291.136036
H(298 K)= -2291.072361
G(298 K)= -2291.236371
Lowest Frequency = -498.5641cm-1

C	1.002576	3.613902	-4.108155
C	-0.029278	4.512778	-4.380231
C	-1.354474	4.162179	-4.148002
C	-1.690380	2.899635	-3.620241
C	-0.645192	1.994992	-3.359713
C	0.676266	2.353722	-3.609871
H	2.036764	3.885007	-4.296069
H	0.196593	5.497363	-4.785738
H	-2.164284	4.853018	-4.373178
H	-0.860396	1.003595	-2.971004
H	1.461239	1.626776	-3.405617
C	-3.386382	1.002253	-2.701820
H	-4.442301	1.047551	-2.924535
H	-2.786355	0.348812	-3.325611
H	-3.090197	1.126575	-1.670417
O	-2.984208	2.654678	-3.357598
O	-4.660611	3.128844	-0.405432
C	-4.495850	3.636915	0.932144
C	-5.662450	2.098212	-0.324775
C	-4.855539	2.484034	1.882374
H	-3.460043	3.982439	1.013757
H	-5.159561	4.502876	1.067597
C	-5.325054	1.362104	0.949049
H	-6.659885	2.563985	-0.289726
H	-5.586581	1.480305	-1.223030
H	-5.647779	2.786072	2.573596
H	-4.003046	2.172320	2.494841
H	-6.161812	0.785575	1.348299
H	-4.519149	0.644120	0.744635
O	-1.665766	3.184875	-0.511626
C	-0.403111	3.886711	-0.494973
C	-1.530246	1.939709	0.195689
C	0.566174	2.978029	0.243835
H	-0.102638	4.096610	-1.529116
H	-0.560854	4.838280	0.032480
C	-0.361891	2.152911	1.130207
H	-2.490623	1.731234	0.679285
H	-1.319860	1.125874	-0.518677
H	1.324220	3.536017	0.797630
H	1.081959	2.323493	-0.468894
H	-0.677295	2.725451	2.011496
H	0.079530	1.214493	1.473212
O	-3.352887	5.535088	-1.820482
C	-4.523715	5.960903	-2.549623
C	-2.323180	6.539033	-1.919932
C	-4.315742	7.437280	-2.821711
H	-4.587797	5.378811	-3.480783
H	-5.401219	5.731782	-1.937149
C	-2.801169	7.513374	-2.979061
H	-2.214256	7.021764	-0.938543
H	-1.382424	6.039878	-2.176862
H	-4.641215	8.035207	-1.963334
H	-4.864103	7.783682	-3.700161
H	-2.395977	8.517908	-2.839808
H	-2.502880	7.166539	-3.975618
Li	-3.214324	3.574227	-1.672382
Al	-3.918770	-1.573920	-1.523919
N	-4.627486	-2.800525	-0.284761
N	-2.839389	-2.816899	-2.475940
C	-4.528132	-4.203792	-0.323807
C	-3.728865	-4.794114	-1.381167
H	-3.725671	-5.880171	-1.382261
C	-2.945504	-4.196089	-2.323697
C	-5.124020	-5.015645	0.596577
H	-4.997727	-6.089443	0.520356
H	-5.722707	-4.637283	1.415956

C	-2.123530	-5.065452	-3.232750
H	-1.055361	-4.828375	-3.148732
H	-2.378608	-4.924970	-4.290206
H	-2.260582	-6.120139	-2.987440
C	-5.273674	-2.281816	0.873059
C	-4.506745	-2.020675	2.029506
C	-5.131285	-1.460765	3.146812
H	-4.538713	-1.237717	4.033054
C	-6.497929	-1.202146	3.150351
H	-6.972715	-0.777687	4.031741
C	-7.253974	-1.500329	2.022456
H	-8.325834	-1.307960	2.026652
C	-6.662580	-2.043800	0.877217
C	-3.021221	-2.320725	2.060130
H	-2.801939	-2.963780	1.200178
C	-2.212918	-1.035403	1.889458
H	-2.465706	-0.549992	0.936255
H	-1.133483	-1.235447	1.890036
H	-2.422971	-0.318314	2.695457
C	-2.602387	-3.075516	3.316669
H	-3.185597	-3.993546	3.431049
H	-2.736125	-2.475383	4.224413
H	-1.543644	-3.351694	3.264035
C	-7.505980	-2.344057	-0.342961
H	-6.899314	-2.971892	-1.004801
C	-8.773854	-3.119270	0.000104
H	-8.537363	-4.041723	0.538196
H	-9.318330	-3.389634	-0.910478
H	-9.459636	-2.532830	0.622887
C	-7.835962	-1.051655	-1.089950
H	-6.918226	-0.535240	-1.401570
H	-8.405709	-0.363238	-0.451568
H	-8.433957	-1.247738	-1.986856
C	-1.872933	-2.304313	-3.382932
C	-2.152651	-2.233573	-4.765337
C	-1.188962	-1.701467	-5.626427
H	-1.402402	-1.637480	-6.691210
C	0.034628	-1.255349	-5.146597
H	0.776591	-0.848747	-5.828900
C	0.298470	-1.309492	-3.782857
H	1.252506	-0.940195	-3.414275
C	-0.644680	-1.806918	-2.879653
C	-3.501581	-2.667651	-5.306096
H	-3.936923	-3.370696	-4.586742
C	-4.445300	-1.467401	-5.386689
H	-4.599507	-1.024372	-4.395100
H	-5.424721	-1.758760	-5.781327
H	-4.034697	-0.688299	-6.040350
C	-3.409717	-3.375137	-6.653881
H	-2.697067	-4.206156	-6.629056
H	-3.095452	-2.695857	-7.454234
H	-4.386039	-3.776706	-6.942343
C	-0.372651	-1.795566	-1.384907
H	-1.300437	-1.437678	-0.903267
C	-0.089094	-3.188980	-0.821950
H	-0.937141	-3.865304	-0.952539
H	0.126758	-3.133976	0.251758
H	0.785603	-3.631686	-1.313249
C	0.742951	-0.839049	-0.978049
H	0.599275	0.168388	-1.389010
H	1.725340	-1.192449	-1.312516
H	0.789903	-0.758012	0.113809

Int9c.log

SCF (M06L) = -2292.34755459
E(SCF)+ZPE(0 K)= -2291.231531
H(298 K)= -2291.167400
G(298 K)= -2291.332308

Lowest Frequency = 14.6122cm-1

C	4.072582	3.344073	-2.713153
C	3.116795	4.347474	-2.889629
C	1.779585	4.122128	-2.586248
C	1.318415	2.880641	-2.059887
C	2.307258	1.859717	-1.946447
C	3.640140	2.094253	-2.261417
H	5.117281	3.520036	-2.951486
H	3.419739	5.322316	-3.272505
H	1.036336	4.902926	-2.743931
H	1.987102	0.870295	-1.615927
H	4.360112	1.281618	-2.151789
C	-0.833590	-0.038122	-0.178422
H	-1.821252	0.196758	-0.591949
H	-0.127423	0.474907	-0.842625
H	-0.781141	0.466641	0.792951
O	0.087604	2.706865	-1.679539
O	-1.571293	3.155865	1.142904
C	-1.504098	3.238614	2.566740
C	-2.833959	2.548344	0.847258
C	-2.032756	1.893421	3.036400
H	-0.465580	3.457240	2.829973
H	-2.138009	4.068648	2.919233
C	-3.094758	1.545001	1.978247
H	-3.608053	3.330670	0.819922
H	-2.751043	2.107571	-0.149528
H	-2.433632	1.921011	4.052871
H	-1.230690	1.144554	3.027917
H	-4.110678	1.647306	2.371269
H	-2.988366	0.509144	1.644082
O	1.514895	3.247774	1.145231
C	2.828992	3.814618	0.917331
C	1.671644	1.897306	1.596280
C	3.831453	2.780845	1.417580
H	2.948465	4.029774	-0.151618
H	2.872453	4.754141	1.482728
C	2.990843	1.899935	2.336209
H	0.797327	1.653507	2.210306
H	1.694345	1.211845	0.731064
H	4.689974	3.237288	1.915615
H	4.204970	2.193524	0.570943
H	2.868656	2.360924	3.323593
H	3.404874	0.898696	2.476786
O	-0.183365	5.581243	-0.202506
C	-1.263334	5.867837	-1.111563
C	0.868082	6.550176	-0.382152
C	-1.097876	7.329160	-1.473113
H	-1.174251	5.207644	-1.988209
H	-2.198428	5.633290	-0.593149
C	0.420613	7.463008	-1.513808
H	0.990263	7.092418	0.565114
H	1.800124	6.020273	-0.611028
H	-1.520742	7.966914	-0.688563
H	-1.581494	7.589037	-2.417556
H	0.771852	8.489705	-1.386601
H	0.806828	7.095553	-2.471303
Li	-0.045217	3.571063	-0.073736
Al	-0.617634	-1.950983	-0.039558
N	-1.430414	-3.036967	1.147068
N	0.342214	-3.058602	-1.103165
C	-1.313785	-4.445132	1.115269
C	-0.502965	-5.029320	0.058537
H	-0.476579	-6.114300	0.078542
C	0.251734	-4.443328	-0.915071
C	-1.915205	-5.242122	2.036518
H	-1.796292	-6.316799	1.975406
H	-2.514433	-4.844337	2.846686
C	1.069221	-5.307197	-1.827963
H	2.132633	-5.044869	-1.770708

H	0.786828	-5.185315	-2.880108
H	0.958483	-6.359570	-1.563429
C	-2.142667	-2.462446	2.243972
C	-1.430108	-2.074699	3.396646
C	-2.118691	-1.413988	4.417484
H	-1.575662	-1.084949	5.301880
C	-3.485170	-1.177645	4.322059
H	-4.006022	-0.660049	5.123975
C	-4.187587	-1.622506	3.207928
H	-5.260693	-1.452768	3.146100
C	-3.536405	-2.276497	2.158863
C	0.052635	-2.364631	3.529089
H	0.303759	-3.120383	2.775235
C	0.888141	-1.118165	3.237189
H	0.669889	-0.703102	2.243739
H	1.962134	-1.336966	3.275413
H	0.683733	-0.323218	3.966948
C	0.409662	-2.949774	4.891324
H	-0.183787	-3.843972	5.101709
H	0.240355	-2.234801	5.704274
H	1.467207	-3.230769	4.922848
C	-4.305454	-2.745888	0.941242
H	-3.687153	-3.499782	0.441343
C	-5.629611	-3.409173	1.304233
H	-5.481718	-4.227550	2.014856
H	-6.108641	-3.821226	0.410751
H	-6.337696	-2.701382	1.749815
C	-4.527244	-1.590137	-0.035185
H	-3.579424	-1.133956	-0.345570
H	-5.131041	-0.797690	0.424995
H	-5.047229	-1.924718	-0.939103
C	1.263476	-2.527951	-2.057686
C	0.907976	-2.478560	-3.419909
C	1.831617	-1.963598	-4.331543
H	1.575470	-1.919529	-5.386809
C	3.069168	-1.496819	-3.908269
H	3.775958	-1.094058	-4.628272
C	3.390369	-1.509830	-2.557071
H	4.347681	-1.108686	-2.237100
C	2.494665	-2.005181	-1.606636
C	-0.479956	-2.902276	-3.860783
H	-0.806127	-3.719823	-3.205716
C	-1.464243	-1.747791	-3.660296
H	-1.492639	-1.415855	-2.616004
H	-2.481138	-2.038782	-3.944853
H	-1.176470	-0.877428	-4.259557
C	-0.538138	-3.408641	-5.296519
H	0.198052	-4.197892	-5.479740
H	-0.352451	-2.607625	-6.020207
H	-1.529789	-3.813873	-5.518377
C	2.818500	-1.950595	-0.122931
H	1.903855	-1.600539	0.394240
C	3.160895	-3.320997	0.462933
H	2.335188	-4.031073	0.371713
H	3.407080	-3.234730	1.527408
H	4.034488	-3.745097	-0.045159
C	3.911093	-0.945934	0.218991
H	3.692203	0.051356	-0.180903
H	4.885069	-1.258633	-0.173491
H	4.020187	-0.866853	1.305580

Int7d.log

SCF (M06L) = -2829.25739547
E(SCF)+ZPE(0 K)= -2827.844851
H(298 K)= -2827.764203
G(298 K)= -2827.960281
Lowest Frequency = 10.6982cm-1

Al	-1.473640	-3.587488	-0.080135
N	-2.416357	-2.386037	1.277396
N	-1.610112	-2.042807	-1.413148
C	-2.701763	-1.080533	1.179133
C	-2.406582	-0.308925	0.048490
H	-2.638655	0.747557	0.115817
C	-1.958086	-0.768771	-1.197890
C	-3.432337	-0.381922	2.293452
H	-4.504318	-0.608364	2.248793
H	-3.309761	0.700957	2.214582
H	-3.087111	-0.709100	3.278463
C	-1.889391	0.231798	-2.317650
H	-2.363638	-0.149739	-3.227580
H	-0.844297	0.450780	-2.567566
H	-2.360770	1.175474	-2.032806
C	-2.999890	-3.098904	2.377587
C	-4.370026	-3.427327	2.330650
C	-4.928032	-4.115102	3.410785
H	-5.983321	-4.378997	3.383780
C	-4.156526	-4.479357	4.505295
H	-4.607451	-5.009947	5.339549
C	-2.797995	-4.186295	4.518215
H	-2.192235	-4.502369	5.362825
C	-2.191548	-3.505876	3.460187
C	-5.222831	-3.140375	1.108036
H	-4.697562	-2.413037	0.476261
C	-5.386641	-4.421265	0.287502
H	-4.414429	-4.841402	0.000986
H	-5.960988	-4.233396	-0.627318
H	-5.916452	-5.187005	0.865669
C	-6.586970	-2.548436	1.451247
H	-6.502402	-1.652966	2.075943
H	-7.216794	-3.264213	1.990688
H	-7.124789	-2.271818	0.538528
C	-0.703309	-3.220407	3.458674
H	-0.358326	-3.391522	2.429705
C	-0.385961	-1.762956	3.792757
H	-0.834593	-1.061087	3.083385
H	0.699811	-1.599942	3.773182
H	-0.743164	-1.503161	4.797867
C	0.099844	-4.146805	4.361855
H	-0.106495	-5.200623	4.149488
H	-0.109756	-3.969240	5.423356
H	1.170691	-3.977643	4.209786
C	-1.327002	-2.444445	-2.761181
C	-0.065592	-2.199155	-3.336762
C	0.160734	-2.628119	-4.646762
H	1.133431	-2.447936	-5.100032
C	-0.825586	-3.283745	-5.370332
H	-0.631878	-3.607949	-6.389309
C	-2.058113	-3.538874	-4.781031
H	-2.820547	-4.068745	-5.345618
C	-2.331628	-3.136353	-3.472238
C	1.053127	-1.543513	-2.554090
H	0.610318	-1.071844	-1.671137
C	2.045378	-2.599692	-2.067120
H	1.546103	-3.381744	-1.485135
H	2.820392	-2.150755	-1.432573
H	2.544704	-3.081289	-2.916148
C	1.770965	-0.448183	-3.335159
H	1.073742	0.303424	-3.722503
H	2.332593	-0.846072	-4.188662
H	2.488647	0.079683	-2.693908
C	-3.682289	-3.417240	-2.838919
H	-3.504353	-3.601434	-1.767721
C	-4.617204	-2.210728	-2.931521
H	-4.214149	-1.337917	-2.409230
H	-5.591487	-2.440371	-2.483821
H	-4.788958	-1.929113	-3.977242
C	-4.359886	-4.663737	-3.392414

H	-3.694409	-5.531514	-3.360466
H	-4.688954	-4.527325	-4.428715
H	-5.251711	-4.901165	-2.804108
O	1.023258	-2.184600	0.903757
C	1.059721	-0.770478	0.816650
H	1.847960	-0.431435	0.130310
H	0.092538	-0.454697	0.426246
H	1.211874	-0.305245	1.800925
C	2.145724	-2.808086	1.367775
C	2.089005	-4.204330	1.437036
C	3.302119	-2.130670	1.760987
C	3.179225	-4.911773	1.921662
H	1.178685	-4.701335	1.104521
C	4.387122	-2.859234	2.248609
H	3.363437	-1.050546	1.685848
C	4.333750	-4.245321	2.337524
H	3.125546	-5.995676	1.976098
H	5.282312	-2.325557	2.558916
H	5.182579	-4.803902	2.720000
Al	0.942528	2.546457	-0.530873
N	0.897515	3.834993	1.015265
N	2.220941	3.803552	-1.448710
C	1.317796	5.105985	1.062547
C	2.099616	5.677232	0.051839
H	2.418056	6.701758	0.208305
C	2.599796	5.035312	-1.089486
C	0.990623	5.954765	2.257315
H	-0.088963	6.123048	2.334746
H	1.485485	6.925579	2.204300
H	1.287931	5.455816	3.185091
C	3.626139	5.771373	-1.903063
H	3.438569	5.676191	-2.976354
H	4.622873	5.349328	-1.728301
H	3.658577	6.828680	-1.634948
C	0.214285	3.278631	2.146349
C	-1.165402	3.503753	2.313787
C	-1.823259	2.851766	3.360233
H	-2.892327	3.006650	3.493922
C	-1.140131	2.003336	4.218475
H	-1.668543	1.494140	5.020278
C	0.223101	1.793167	4.043082
H	0.741252	1.117187	4.716416
C	0.929101	2.414172	3.009387
C	-1.959046	4.386425	1.368308
H	-1.250742	4.972890	0.771029
C	-2.771335	3.537957	0.390750
H	-2.116235	2.885239	-0.199706
H	-3.341880	4.166996	-0.300667
H	-3.484049	2.898112	0.926236
C	-2.862646	5.368980	2.109854
H	-2.307929	5.962961	2.843853
H	-3.665130	4.854310	2.648706
H	-3.339454	6.059420	1.407478
C	2.413447	2.139798	2.803948
H	2.537542	1.861214	1.740370
C	3.300993	3.361715	3.059672
H	3.126574	4.175907	2.354833
H	4.356825	3.082484	2.973738
H	3.146273	3.745363	4.074871
C	2.940476	0.985357	3.649734
H	2.352962	0.068220	3.544417
H	2.954191	1.248661	4.713577
H	3.971307	0.751103	3.364757
C	2.858722	3.198607	-2.582276
C	4.139210	2.629146	-2.436044
C	4.731191	2.037259	-3.554020
H	5.717989	1.590016	-3.459981
C	4.073511	1.996859	-4.776538
H	4.550518	1.535131	-5.636540
C	2.791479	2.520441	-4.890473
H	2.268086	2.448432	-5.839854
C	2.153421	3.116611	-3.800517
C	4.824089	2.558521	-1.083193
H	4.383917	3.325121	-0.431695
C	4.535328	1.200970	-0.436657
H	3.453223	1.026352	-0.355763
H	4.967278	1.135875	0.569296
H	4.949646	0.381689	-1.036587
C	6.325192	2.819115	-1.148882
H	6.554451	3.764258	-1.651811
H	6.854339	2.024899	-1.685812
H	6.750507	2.861218	-0.141505
C	0.737499	3.649361	-3.913991
H	0.235478	3.411118	-2.960235
C	0.708859	5.169204	-4.076740
H	1.146121	5.683379	-3.216441
H	-0.319450	5.528432	-4.187467
H	1.265377	5.473764	-4.970838
C	-0.073774	2.982932	-5.018112
H	-0.026857	1.890537	-4.960254
H	0.270749	3.279567	-6.015179
H	-1.124815	3.277180	-4.942425

TS6d.log

SCF (M06L) = -2829.21635939
E(SCF)+ZPE(0 K)= -2827.807564
H(298 K)= -2827.727065
G(298 K)= -2827.921470
Lowest Frequency = -509.0459cm-1

Al	11.136282	2.770524	4.113303
N	9.883184	3.855425	5.335330
N	10.664746	4.059505	2.598228
C	9.473383	5.109644	5.127006
C	9.699490	5.813279	3.932702
H	9.368217	6.845321	3.917607
C	10.188850	5.301562	2.721748
C	8.690732	5.837099	6.188080
H	7.625747	5.583830	6.135064
H	8.784296	6.917971	6.054181
H	9.028596	5.572030	7.194266
C	10.214172	6.234506	1.541707
H	9.744373	5.792334	0.657527
H	11.255105	6.448092	1.264563
H	9.724103	7.184143	1.772641
C	9.310591	3.162360	6.452465
C	7.952309	2.785372	6.412561
C	7.407293	2.133424	7.521858
H	6.361599	1.833122	7.497218
C	8.177852	1.845318	8.639011
H	7.735103	1.342170	9.494463
C	9.527763	2.176394	8.644626
H	10.139302	1.917573	9.504592
C	10.118950	2.824061	7.559115
C	7.100099	2.959656	5.169044
H	7.604315	3.655912	4.487850
C	6.987534	1.617183	4.444914
H	7.975177	1.217683	4.186681
H	6.404620	1.717174	3.521844
H	6.486299	0.876514	5.078777
C	5.711446	3.522447	5.460875
H	5.753310	4.458258	6.028227
H	5.101735	2.819173	6.038720
H	5.174616	3.719928	4.527133
C	11.596056	3.146658	7.541250
H	11.945989	2.886203	6.533380
C	11.871727	4.634779	7.736061
H	11.360772	5.258570	6.996662

H	12.947378	4.829315	7.640722
H	11.556184	4.965187	8.734309
C	12.428921	2.326948	8.515658
H	12.254196	1.253276	8.395019
H	12.218931	2.588541	9.560004
H	13.493024	2.514005	8.338039
C	10.916759	3.560975	1.276254
C	12.166417	3.754376	0.658698
C	12.357317	3.267025	-0.636019
H	13.322026	3.414937	-1.118352
C	11.344606	2.593906	-1.304492
H	11.504708	2.225746	-2.314407
C	10.131490	2.367416	-0.664640
H	9.353997	1.809065	-1.179321
C	9.896766	2.828166	0.632912
C	13.306798	4.416706	1.396221
H	12.881883	4.858074	2.298922
C	14.329201	3.375138	1.848205
H	13.855993	2.591566	2.450383
H	15.115219	3.833297	2.461975
H	14.807948	2.895905	0.985844
C	13.977597	5.530375	0.602072
H	13.255735	6.278524	0.254967
H	14.502947	5.150932	-0.282785
H	14.722285	6.056389	1.214257
C	8.583950	2.538283	1.336502
H	8.810120	2.461928	2.410544
C	7.575054	3.675464	1.168818
H	7.936076	4.614029	1.600458
H	6.629455	3.429687	1.667159
H	7.356040	3.852376	0.108776
C	7.966693	1.212745	0.906472
H	8.683494	0.390570	0.990746
H	7.606202	1.242880	-0.127994
H	7.104316	0.973220	1.535794
O	12.901850	4.013778	4.699820
C	13.014792	5.929479	4.451747
H	13.909692	5.865372	3.851964
H	12.048870	5.965642	3.981289
H	13.083661	6.226792	5.493596
C	14.038033	3.489923	5.216092
C	14.204188	2.091243	5.312893
C	15.095668	4.294015	5.683055
C	15.359407	1.542112	5.851098
H	13.400563	1.453080	4.955887
C	16.250595	3.727723	6.218725
H	15.027118	5.374887	5.635968
C	16.398691	2.349321	6.312325
H	15.443853	0.459438	5.907911
H	17.042847	4.388373	6.566844
H	17.300020	1.912898	6.732059
Al	13.161788	8.561315	3.831904
N	13.135303	9.830850	5.340932
N	14.465119	9.716280	2.880163
C	13.586355	11.092595	5.367920
C	14.368290	11.630246	4.340045
H	14.700895	12.653519	4.471092
C	14.845721	10.960722	3.206364
C	13.284606	11.964157	6.551172
H	12.210399	12.166052	6.623497
H	13.809192	12.918143	6.485508
H	13.564571	11.468687	7.485850
C	15.846076	11.684584	2.351324
H	15.621572	11.578846	1.286356
H	16.848132	11.264570	2.495215
H	15.886058	12.744306	2.607372
C	12.457061	9.306795	6.493025
C	11.084573	9.558174	6.673505
C	10.439044	8.947136	7.752188
H	9.373757	9.114094	7.898275
C	11.132511	8.127999	8.630578
H	10.613854	7.653700	9.459337
C	12.491060	7.897893	8.441635
H	13.015290	7.239606	9.127463
C	13.181969	8.466898	7.369522
C	10.296370	10.437614	5.720130
H	11.010148	11.005691	5.111310
C	9.464405	9.594192	4.755676
H	10.097188	8.898782	4.190372
H	8.927253	10.226190	4.040704
H	8.720176	8.998418	5.297983
C	9.414223	11.444583	6.454496
H	9.984083	12.040585	7.175114
H	8.608995	10.949703	7.007369
H	8.941899	12.131646	5.745939
C	14.657384	8.167994	7.138099
H	14.762805	7.899294	6.070361
C	15.570651	9.371772	7.387549
H	15.397976	10.196253	6.693624
H	16.619095	9.074160	7.278849
H	15.442016	9.749491	8.408502
C	15.173742	6.990934	7.956542
H	14.563852	6.090867	7.840877
H	15.215201	7.236546	9.023731
H	16.191993	6.738514	7.645226
C	15.072983	9.119777	1.721412
C	16.363672	8.564602	1.830251
C	16.944686	8.021291	0.682362
H	17.939410	7.587579	0.742284
C	16.270068	8.022995	-0.531873
H	16.740236	7.600881	-1.415543
C	14.982783	8.538759	-0.609961
H	14.449623	8.500151	-1.555620
C	14.351341	9.083498	0.510983
C	17.078448	8.486544	3.167934
H	16.714724	9.305994	3.803038
C	16.709678	7.180522	3.874752
H	15.625531	7.105435	4.024496
H	17.186643	7.105847	4.859246
H	17.013081	6.306764	3.285739
C	18.592364	8.629828	3.058039
H	18.879892	9.525539	2.498127
H	19.048953	7.768372	2.559901
H	19.041147	8.694867	4.053522
C	12.930187	9.611984	0.430564
H	12.430142	9.316502	1.370764
C	12.880516	11.138474	0.349670
H	13.293761	11.617615	1.241171
H	11.847548	11.484363	0.241137
H	13.443035	11.498386	-0.519729
C	12.122387	9.005243	-0.710296
H	12.178915	7.912078	-0.722309
H	12.462157	9.367578	-1.686945
H	11.068999	9.284580	-0.614604

Int7e.log

SCF (M06L) = -1587.99203913
E(SCF)+ZPE(0 K)= -1587.218873
H(298 K)= -1587.174760
G(298 K)= -1587.292689
Lowest Frequency = 26.0292cm-1

Al	0.783401	-0.303041	0.432368
O	-2.408839	-0.208879	1.074459
N	0.375699	1.486523	-0.455073
N	0.093229	-1.201661	-1.254234
C	-0.300675	1.723688	-1.583528
C	-0.854900	0.704587	-2.371294

H	-1.434985	1.022341	-3.230936
C	-0.621912	-0.671720	-2.252656
C	-0.450149	3.130951	-2.091717
H	-1.244502	3.196030	-2.837728
H	0.480408	3.463426	-2.566411
H	-0.652575	3.839000	-1.283609
C	-1.193520	-1.561807	-3.320961
H	-0.424595	-2.210980	-3.751411
H	-1.652013	-0.978497	-4.121122
H	-1.954424	-2.230377	-2.901977
C	1.047986	2.594303	0.161402
C	2.256120	3.063151	-0.391387
C	2.897087	4.138172	0.228941
H	3.833447	4.507641	-0.183988
C	2.367470	4.728729	1.367788
H	2.877133	5.566741	1.835297
C	1.194824	4.229789	1.922216
H	0.801349	4.678301	2.829878
C	0.518535	3.154189	1.342981
C	2.914554	2.379449	-1.575495
H	2.175221	1.728215	-2.059166
C	4.054186	1.484724	-1.084935
H	4.833015	2.080910	-0.596057
H	4.517810	0.944674	-1.918686
H	3.700084	0.746897	-0.353997
C	3.421253	3.360255	-2.629315
H	2.636066	4.044766	-2.967111
H	3.797286	2.821434	-3.505059
H	4.246487	3.972866	-2.250652
C	-0.748371	2.596871	1.961099
H	-0.692369	1.502892	1.857134
C	-2.003531	3.049375	1.215573
H	-2.089392	4.142699	1.219478
H	-2.898359	2.642976	1.702672
H	-2.008648	2.712084	0.175060
C	-0.889192	2.900484	3.446389
H	-0.004249	2.589109	4.010293
H	-1.752692	2.366804	3.855064
H	-1.050179	3.968782	3.632214
C	0.445206	-2.589886	-1.335783
C	-0.462637	-3.589421	-0.939736
C	-0.060206	-4.924227	-1.027615
H	-0.750628	-5.706796	-0.720208
C	1.203697	-5.265192	-1.488006
H	1.497876	-6.309048	-1.553778
C	2.100469	-4.265513	-1.845604
H	3.096933	-4.538468	-2.181745
C	1.749403	-2.916334	-1.767444
C	-1.820563	-3.247441	-0.361904
H	-2.030475	-2.198227	-0.596224
C	-1.785849	-3.363866	1.161382
H	-1.573018	-4.394601	1.467691
H	-2.743476	-3.067648	1.604219
H	-1.007569	-2.720714	1.587333
C	-2.946960	-4.095589	-0.945818
H	-2.970349	-4.054795	-2.040323
H	-3.918661	-3.754129	-0.574170
H	-2.850401	-5.149186	-0.662354
C	2.740632	-1.829876	-2.144623
H	2.554334	-0.976493	-1.473219
C	2.523408	-1.325698	-3.571922
H	2.635474	-2.142008	-4.295223
H	3.258738	-0.552940	-3.825251
H	1.529737	-0.888435	-3.707460
C	4.191889	-2.244653	-1.940560
H	4.361630	-2.638276	-0.934054
H	4.854220	-1.385244	-2.082281
H	4.505203	-3.009395	-2.659953
C	-2.799055	-0.178959	2.386591
C	-1.808690	-0.489881	3.324673
H	-0.808733	-0.726574	2.963216
C	-2.110782	-0.468757	4.677831
H	-1.332683	-0.707150	5.397634
C	-3.395960	-0.141712	5.114645
H	-3.628426	-0.125761	6.174962
C	-4.374860	0.162575	4.176598
H	-5.380082	0.418006	4.500885
C	-4.089664	0.144821	2.810368
H	-4.868631	0.385081	2.094948
C	-3.417937	0.004846	0.105746
H	-3.871549	0.999662	0.206857
H	-4.206982	-0.756806	0.177966
H	-2.925065	-0.060540	-0.866324

TS6e.log

SCF (M06L) = -1587.93973612
E(SCF)+ZPE(0 K)= -1587.169574
H(298 K)= -1587.125736
G(298 K)= -1587.242703
Lowest Frequency = -327.7030cm-1

Al	11.886360	10.474886	11.885283
O	10.151759	10.099999	12.643592
N	11.741016	12.183840	10.903437
N	11.601471	9.395824	10.226035
C	11.338350	12.314664	9.628470
C	10.950220	11.239497	8.824857
H	10.594906	11.494219	7.832083
C	11.142700	9.868206	9.068177
C	11.368256	13.668357	8.974994
H	10.740332	13.682251	8.082366
H	12.390588	13.914210	8.665026
H	11.052734	14.465240	9.652923
C	10.842734	8.949223	7.917224
H	11.340252	7.982502	8.014682
H	11.143022	9.410119	6.973418
H	9.765210	8.764379	7.853208
C	12.373099	13.322420	11.512743
C	13.707284	13.629714	11.182693
C	14.293515	14.753652	11.770282
H	15.325871	14.999047	11.528951
C	13.588234	15.548995	12.662079
H	14.058667	16.422546	13.104718
C	12.284981	15.209971	13.006912
H	11.747840	15.819653	13.728013
C	11.658223	14.092439	12.452114
C	14.544359	12.740401	10.282263
H	13.882085	12.011837	9.795851
C	15.548289	11.953275	11.126317
H	16.243781	12.629545	11.636307
H	16.139625	11.275209	10.500057
H	15.041135	11.356402	11.894243
C	15.266263	13.516544	9.183601
H	14.578079	14.114843	8.577595
H	15.793770	12.830703	8.512813
H	16.014031	14.201317	9.598303
C	10.249885	13.700313	12.851914
H	10.243071	12.603697	12.901004
C	9.205916	14.102719	11.809256
H	9.233237	15.182841	11.623551
H	8.198456	13.852832	12.159756
H	9.357405	13.589099	10.856235
C	9.843958	14.225570	14.223929
H	10.601310	14.016698	14.985962
H	8.906829	13.760000	14.545558
H	9.675020	15.308242	14.210857
C	11.864693	7.998433	10.407635
C	10.817805	7.067231	10.566425

C	11.152161	5.734358	10.828351
H	10.351013	5.008436	10.953750
C	12.471917	5.326596	10.941081
H	12.707727	4.287285	11.151818
C	13.493517	6.256301	10.784443
H	14.526397	5.933070	10.873725
C	13.216961	7.596777	10.516176
C	9.348429	7.433624	10.479328
H	9.272611	8.507729	10.267816
C	8.631507	7.165855	11.802600
H	8.627371	6.094203	12.032138
H	7.586873	7.491954	11.749666
H	9.114798	7.680754	12.636159
C	8.644748	6.660252	9.361433
H	9.150579	6.755870	8.396805
H	7.612137	7.003852	9.240806
H	8.603310	5.591217	9.598069
C	14.338061	8.595729	10.299791
H	14.031528	9.536082	10.788837
C	14.531385	8.901957	8.814035
H	14.809741	7.996438	8.262596
H	15.330968	9.638488	8.671235
H	13.623925	9.307545	8.356513
C	15.656131	8.179958	10.937022
H	15.533816	7.936929	11.996700
H	16.385203	8.992110	10.861137
H	16.096436	7.309469	10.437827
C	11.094562	9.756188	13.914454
C	11.114565	8.370982	14.226013
H	11.200698	7.642579	13.422436
C	11.126037	7.948619	15.546293
H	11.190902	6.881811	15.751349
C	11.055103	8.858300	16.604624
H	11.060449	8.516125	17.634390
C	10.969524	10.218769	16.302522
H	10.911745	10.951092	17.105635
C	10.958799	10.669673	14.991071
H	10.921505	11.737795	14.792127
C	8.788322	10.430488	12.889801
H	8.704646	11.295928	13.558541
H	8.274263	9.579788	13.348271
H	8.331965	10.665292	11.923169

4a.log

SCF (M06L) = -1588.09068542
E(SCF)+ZPE(0 K)= -1587.318123
H(298 K)= -1587.273777
G(298 K)= -1587.391745
Lowest Frequency = 25.1569cm-1

Al	10.949113	10.510925	11.815908
O	9.234717	10.483860	12.089313
N	11.506236	12.108537	10.903026
N	11.303515	9.359902	10.302952
C	11.297473	12.241793	9.580648
C	11.061152	11.157025	8.728786
H	10.882257	11.394390	7.686365
C	11.168770	9.790474	9.047433
C	11.341314	13.612221	8.973347
H	10.665892	14.287860	9.509209
H	11.060721	13.588893	7.919947
H	12.337284	14.057123	9.056463
C	11.145541	8.803214	7.919534
H	11.939207	8.058401	8.029116
H	11.250319	9.298456	6.953587
H	10.200993	8.247590	7.918881
C	12.075359	13.217744	11.615172
C	13.466131	13.441248	11.526219
C	14.012867	14.503132	12.249956
H	15.084067	14.686420	12.188269
C	13.221833	15.312521	13.055554
H	13.668709	16.128988	13.615988
C	11.858908	15.065713	13.146497
H	11.237702	15.690120	13.785255
C	11.260357	14.026900	12.429170
C	14.393295	12.546606	10.722823
H	13.794019	11.753526	10.258075
C	15.417768	11.876202	11.638497
H	16.056609	12.620027	12.128042
H	16.073266	11.211277	11.064982
H	14.934058	11.285802	12.423431
C	15.111529	13.308566	9.609685
H	14.416052	13.782796	8.910475
H	15.752103	12.633577	9.032390
H	15.752081	14.097363	10.020280
C	9.775451	13.773085	12.574207
H	9.488022	13.033260	11.819844
C	8.941812	15.028637	12.331646
H	9.130408	15.794035	13.092643
H	7.873924	14.790564	12.371151
H	9.151079	15.478142	11.355610
C	9.467118	13.174361	13.946720
H	10.056581	12.272518	14.139949
H	8.411364	12.896140	14.021631
H	9.688542	13.896356	14.741916
C	11.558758	7.973652	10.573785
C	10.502622	7.044004	10.602759
C	10.798847	5.721236	10.946724
H	9.990764	4.993261	10.980292
C	12.092181	5.328983	11.256283
H	12.301247	4.296131	11.521006
C	13.118736	6.266076	11.243553
H	14.125197	5.957466	11.510308
C	12.877091	7.600861	10.916094
C	9.059081	7.423962	10.336862
H	9.034191	8.459645	9.975331
C	8.246011	7.370330	11.631223
H	8.293919	6.370471	12.077925
H	7.191786	7.593913	11.434655
H	8.613135	8.098008	12.360737
C	8.419915	6.532628	9.272324
H	9.005260	6.500938	8.347206
H	7.414868	6.888408	9.025058
H	8.318692	5.500297	9.624669
C	14.002417	8.619200	10.929523
H	13.573819	9.576436	11.259832
C	14.571262	8.837819	9.526560
H	14.961806	7.901687	9.110652
H	15.395301	9.560437	9.549825
H	13.817149	9.224827	8.833256
C	15.107853	8.265669	11.917007
H	14.702554	8.086765	12.918362
H	15.828287	9.085326	11.987407
H	15.668107	7.376248	11.607495
C	11.983631	9.996492	13.405942
C	11.846131	8.687133	13.908003
H	11.152910	7.992639	13.429975
C	12.579947	8.228676	15.000267
H	12.450529	7.207460	15.351670
C	13.479241	9.079102	15.639382
H	14.056967	8.726567	16.490377
C	13.627321	10.386219	15.183487
H	14.318910	11.061765	15.681956
C	12.887022	10.831427	14.088857
H	13.022906	11.864121	13.765241
C	8.226407	10.773078	11.177483
H	8.567924	10.798399	10.125502
H	7.760395	11.752852	11.383406

H	7.422342	10.022970	11.235414

Int7f.log

SCF (M06L) = -1587.98187408
E(SCF)+ZPE(0 K)= -1587.209546
H(298 K)= -1587.164872
G(298 K)= -1587.286487
Lowest Frequency = 15.5955cm-1

Al	-1.111110	0.047332	-0.082353
N	-0.331436	1.608748	-1.153524
N	-0.556242	-1.150310	-1.624901
C	-0.015669	1.639644	-2.454401
C	-0.109627	0.519364	-3.290550
H	0.107331	0.682470	-4.340388
C	-0.287731	-0.811229	-2.889966
C	0.520420	2.902294	-3.070675
H	0.014003	3.793561	-2.690355
H	0.433177	2.873249	-4.158430
H	1.582394	3.022926	-2.826890
C	-0.115297	-1.880199	-3.931437
H	0.639067	-2.610059	-3.619683
H	0.180700	-1.456447	-4.892265
H	-1.043062	-2.444528	-4.073314
C	-0.000899	2.754958	-0.361062
C	1.340998	2.979081	0.010659
C	1.641850	4.114816	0.766051
H	2.674183	4.298946	1.057826
C	0.647072	4.999866	1.160464
H	0.899613	5.883261	1.740777
C	-0.677586	4.738395	0.829086
H	-1.456176	5.419331	1.162292
C	-1.029577	3.615244	0.076023
C	2.437939	1.981051	-0.310661
H	2.063851	1.284537	-1.071494
C	2.759989	1.158076	0.937624
H	3.189912	1.794685	1.721226
H	3.489839	0.370887	0.717093
H	1.862491	0.683466	1.353404
C	3.703889	2.632118	-0.860585
H	3.500298	3.261614	-1.732999
H	4.428683	1.868130	-1.159623
H	4.193370	3.263420	-0.110896
C	-2.474964	3.339551	-0.287199
H	-2.598075	2.244753	-0.285533
C	-2.803934	3.833448	-1.695741
H	-2.625830	4.911896	-1.782611
H	-3.855937	3.649113	-1.936636
H	-2.198750	3.330234	-2.455363
C	-3.465493	3.897596	0.725848
H	-3.216247	3.586567	1.745164
H	-4.474953	3.540655	0.502566
H	-3.502847	4.992709	0.705668
C	-0.529271	-2.534808	-1.256193
C	-1.639836	-3.364825	-1.497013
C	-1.579428	-4.694567	-1.071693
H	-2.433113	-5.345859	-1.247219
C	-0.460480	-5.189934	-0.418383
H	-0.431235	-6.226977	-0.095315
C	0.616463	-4.349796	-0.159171
H	1.478069	-4.737566	0.376516
C	0.604920	-3.012453	-0.560231
C	-2.913407	-2.839699	-2.130469
H	-2.695183	-1.861443	-2.576149
C	-3.980568	-2.622385	-1.056964
H	-4.235959	-3.569487	-0.568045
H	-4.898055	-2.210482	-1.490511
H	-3.628091	-1.933810	-0.280793
C	-3.441036	-3.750018	-3.236676
H	-2.682856	-3.954893	-4.000101
H	-4.304014	-3.294495	-3.732076
H	-3.771653	-4.716180	-2.840589
C	1.774034	-2.092741	-0.250011
H	1.341116	-1.130645	0.073565
C	2.636885	-1.808626	-1.481689
H	3.039049	-2.741224	-1.895011
H	3.489610	-1.173934	-1.212100
H	2.086988	-1.295262	-2.274617
C	2.653875	-2.592355	0.887724
H	2.073204	-2.840034	1.779554
H	3.377570	-1.821655	1.171168
H	3.229045	-3.478259	0.593765
C	0.528167	2.256669	3.613935
H	-0.126100	3.018172	3.185994
H	0.592766	2.387035	4.702862
H	1.530160	2.379133	3.181227
O	-0.046209	1.013379	3.274927
C	0.579282	-0.113085	3.713493
C	1.806844	-0.125118	4.381166
C	-0.087708	-1.317090	3.450315
C	2.348677	-1.342425	4.795426
H	2.336695	0.800346	4.582714
C	0.464980	-2.516969	3.873265
H	-1.032342	-1.275919	2.916631
C	1.685462	-2.539764	4.552581
H	3.301412	-1.344405	5.318755
H	-0.060794	-3.445194	3.662481
H	2.113845	-3.481351	4.882916

TS6f.log

SCF (M06L) = -1587.93633168
E(SCF)+ZPE(0 K)= -1587.167104
H(298 K)= -1587.123239
G(298 K)= -1587.238899
Lowest Frequency = -552.6195cm-1

Al	10.160483	10.695782	11.676343
N	11.185271	12.208022	10.744209
N	10.999028	9.399662	10.380446
C	11.438048	12.185401	9.434846
C	11.261564	11.041435	8.637782
H	11.399714	11.175987	7.570719
C	11.168117	9.719501	9.090097
C	11.998019	13.393581	8.736857
H	11.750488	14.329613	9.241602
H	11.638468	13.434752	7.705695
H	13.090486	13.326119	8.689394
C	11.291379	8.629060	8.064513
H	12.090613	7.926650	8.321450
H	11.488604	9.038233	7.072799
H	10.370939	8.036686	8.020320
C	11.602075	13.343566	11.505406
C	12.957919	13.490763	11.861078
C	13.318968	14.570917	12.672000
H	14.362032	14.686008	12.961699
C	12.378749	15.492376	13.108723
H	12.679912	16.326429	13.736669
C	11.047335	15.345171	12.735336
H	10.314316	16.070616	13.077068
C	10.632966	14.278310	11.936158
C	14.039957	12.531412	11.402129
H	13.589113	11.796282	10.723355
C	14.633613	11.761436	12.579100
H	15.064654	12.446111	13.319547
H	15.437158	11.096951	12.241434
H	13.874755	11.154211	13.077847

C	15.154629	13.259341	10.648764
H	14.772122	13.887739	9.838809
H	15.861011	12.541982	10.217959
H	15.724261	13.911790	11.320137
C	9.175776	14.118067	11.542640
H	8.951271	13.036284	11.573408
C	8.916825	14.580362	10.108754
H	9.206939	15.629588	9.977709
H	7.853302	14.494448	9.863964
H	9.469091	13.982277	9.379827
C	8.209340	14.808965	12.497461
H	8.403850	14.548207	13.543446
H	7.180710	14.518489	12.266326
H	8.260807	15.900752	12.414072
C	11.114035	8.019351	10.744234
C	10.004864	7.155679	10.659068
C	10.168597	5.825205	11.060467
H	9.315831	5.150815	11.008555
C	11.391273	5.354746	11.515163
H	11.501305	4.314971	11.811552
C	12.472393	6.224583	11.608544
H	13.418517	5.858786	11.997527
C	12.353932	7.567323	11.248841
C	8.637908	7.616754	10.191412
H	8.734355	8.639164	9.803100
C	7.660963	7.663905	11.366167
H	7.541938	6.670533	11.815096
H	6.673209	8.007078	11.041073
H	8.013448	8.352277	12.142838
C	8.079222	6.733591	9.076395
H	8.767147	6.647119	8.228843
H	7.133740	7.138091	8.702051
H	7.877376	5.717619	9.433461
C	13.512568	8.529274	11.442517
H	13.073530	9.493565	11.736653
C	14.294781	8.774340	10.150496
H	14.687873	7.834304	9.744994
H	15.149285	9.435050	10.340361
H	13.682699	9.248589	9.377740
C	14.460366	8.089290	12.553484
H	13.921144	7.832537	13.471180
H	15.163839	8.892933	12.791513
H	15.057896	7.219572	12.255899
C	10.272492	11.858981	14.168236
H	9.773934	12.608659	13.568781
H	9.615037	11.165963	14.680237
H	11.129387	12.223255	14.725756
O	11.398620	10.659641	13.235918
C	11.730455	9.674262	14.117262
C	12.658589	9.958263	15.130837
C	11.115668	8.414279	14.082707
C	12.997329	8.983992	16.061519
H	13.114175	10.944529	15.164198
C	11.468023	7.445348	15.016876
H	10.386232	8.193097	13.307619
C	12.411967	7.719184	16.004600
H	13.729428	9.211445	16.831746
H	10.999695	6.466044	14.962828
H	12.688493	6.955032	16.724887

TS7g.log

SCF (M06L) = -1587.35522959
E(SCF)+ZPE(0 K)= -1586.601235
H(298 K)= -1586.557556
G(298 K)= -1586.672974
Lowest Frequency = -466.6388cm-1

Al	10.229172	10.687461	11.603094
N	11.013135	12.263860	10.727330
N	11.178558	9.437990	10.436273
C	11.357743	12.219337	9.385559
C	11.420468	11.075883	8.643116
H	11.584206	11.204869	7.576266
C	11.385942	9.691703	9.078576
C	11.630658	13.528799	8.688123
H	12.519215	14.030839	9.088030
H	10.809963	14.243670	8.817987
H	11.788991	13.370141	7.618483
C	11.612734	8.716728	8.142072
H	11.675041	7.664523	8.392431
H	11.824779	9.003687	7.117572
C	11.498958	13.369318	11.456206
C	12.885161	13.466147	11.724379
C	13.372200	14.602236	12.376180
H	14.441771	14.685479	12.570102
C	12.514263	15.610166	12.798981
H	12.906693	16.490931	13.302671
C	11.142769	15.469939	12.602632
H	10.472080	16.241927	12.973845
C	10.612534	14.359147	11.943605
C	13.831436	12.331043	11.373051
H	13.220778	11.489322	11.023641
C	14.592037	11.857050	12.609203
H	15.237366	12.642864	13.022171
H	15.232951	11.002820	12.359774
H	13.895668	11.535345	13.389199
C	14.808824	12.697011	10.257519
H	14.293269	12.906094	9.316229
H	15.505193	11.871413	10.071504
H	15.404518	13.580457	10.523707
C	9.112914	14.172721	11.801314
H	8.920171	13.094589	11.942673
C	8.595361	14.507398	10.404014
H	8.868481	15.529531	10.112006
H	7.502355	14.430405	10.370841
H	8.997781	13.813484	9.663111
C	8.313734	14.927644	12.856949
H	8.693339	14.737644	13.867102
H	7.263306	14.620456	12.826947
H	8.335491	16.012818	12.693400
C	11.242442	8.064803	10.793050
C	10.136087	7.208922	10.594501
C	10.231667	5.870091	10.989128
H	9.371869	5.215443	10.844737
C	11.396420	5.364800	11.548642
H	11.456518	4.319240	11.844411
C	12.484094	6.210358	11.739705
H	13.387302	5.820183	12.203344
C	12.426611	7.558329	11.382519
C	8.842413	7.690694	9.968647
H	8.971515	8.747354	9.708523
C	7.684551	7.591995	10.959707
H	7.512690	6.553269	11.270839
H	6.754287	7.963442	10.513849
H	7.887079	8.189465	11.855894
C	8.524796	6.930031	8.682841
H	9.339641	7.039442	7.961045
H	7.606591	7.313210	8.222391
H	8.372761	5.859795	8.874913
C	13.599110	8.479332	11.658568
H	13.169487	9.448624	11.943698
C	14.443335	8.715463	10.405831
H	14.884846	7.772900	10.056049
H	15.268356	9.407139	10.622815
H	13.846663	9.128341	9.587553
C	14.478472	8.003215	12.809544
H	13.888503	7.752154	13.697719
H	15.190220	8.787623	13.091282

H	15.069045	7.119875	12.532861
C	10.681881	12.174156	14.258782
H	9.772285	12.463175	13.748153
H	10.559817	11.643018	15.195001
H	11.540119	12.826082	14.158422
O	11.416755	10.672512	13.291511
C	11.667663	9.668993	14.161005
C	12.548469	9.891125	15.237737
C	11.012414	8.426321	14.082598
C	12.792110	8.895461	16.174813
H	13.041071	10.857312	15.315660
C	11.271917	7.435261	15.022646
H	10.321605	8.240294	13.265477
C	12.164964	7.653438	16.070873
H	13.488644	9.088459	16.988302
H	10.767743	6.476639	14.922859
H	12.370461	6.869000	16.794497

Int7h.log

SCF (M06L) = -1587.98914118
E(SCF)+ZPE(0 K)= -1587.216023
H(298 K)= -1587.171699
G(298 K)= -1587.291154
Lowest Frequency = 18.1543cm-1

Al	0.874124	0.296208	-1.303794
N	1.798403	-0.692464	0.223290
N	-0.377119	1.096782	0.075455
C	1.429108	-0.779562	1.508855
C	0.248761	-0.207246	1.997341
H	-0.005832	-0.433199	3.026736
C	-0.581582	0.712961	1.342240
C	2.312076	-1.480472	2.503018
H	2.769239	-2.382502	2.087939
H	1.756572	-1.738902	3.406345
H	3.139349	-0.824561	2.799017
C	-1.711508	1.307606	2.132778
H	-2.675454	1.006449	1.707391
H	-1.686086	2.401614	2.104893
H	-1.683025	0.978190	3.172797
C	3.082239	-1.211143	-0.150448
C	3.151437	-2.423280	-0.868691
C	4.408707	-2.901459	-1.242902
H	4.479875	-3.837553	-1.790099
C	5.567887	-2.199970	-0.935265
H	6.536563	-2.589253	-1.235999
C	5.480522	-0.991421	-0.258654
H	6.386125	-0.427945	-0.043534
C	4.246452	-0.473148	0.140474
C	1.897113	-3.210892	-1.191621
H	1.089257	-2.479222	-1.348284
C	2.006460	-4.030066	-2.471253
H	2.343173	-3.419058	-3.313550
H	1.032065	-4.455321	-2.730465
H	2.701116	-4.870395	-2.363661
C	1.498434	-4.103714	-0.015853
H	1.276099	-3.522298	0.884816
H	2.308159	-4.800518	0.229768
H	0.609607	-4.698090	-0.253835
C	4.189349	0.894612	0.793148
H	3.183422	1.042143	1.207253
C	5.188187	1.051950	1.936892
H	5.086417	0.259942	2.686070
H	5.045982	2.013107	2.441304
H	6.222447	1.027655	1.577033
C	4.411801	1.978070	-0.262551
H	3.668253	1.915037	-1.066992
H	5.401076	1.875037	-0.722485
H	4.351347	2.977764	0.181892
C	-1.066859	2.259706	-0.412768
C	-0.349445	3.477993	-0.436522
C	-0.991756	4.615695	-0.929086
H	-0.459584	5.562307	-0.948216
C	-2.293411	4.557142	-1.409824
H	-2.773196	5.452794	-1.794682
C	-2.970731	3.347148	-1.410560
H	-3.981878	3.298903	-1.807162
C	-2.379194	2.181792	-0.915605
C	1.079513	3.563026	0.071722
H	1.576264	2.613521	-0.187173
C	1.881820	4.678704	-0.586126
H	1.831109	4.624788	-1.677731
H	2.933645	4.612877	-0.293650
H	1.530367	5.670077	-0.280183
C	1.137874	3.692343	1.594555
H	0.687112	2.832921	2.099205
H	0.611589	4.594445	1.927798
H	2.176718	3.766763	1.937024
C	-3.139054	0.872901	-0.984227
H	-2.656415	0.167779	-0.297545
C	-4.597515	1.013369	-0.555632
H	-4.688573	1.455440	0.442628
H	-5.089073	0.036083	-0.536027
H	-5.163148	1.645993	-1.248181
C	-3.044908	0.278409	-2.389964
H	-2.001223	0.118162	-2.688635
H	-3.497633	0.949688	-3.128714
H	-3.572264	-0.681732	-2.439469
C	-4.260745	-2.642207	-0.375727
C	-5.648611	-2.732971	-0.485196
C	-6.476742	-2.296362	0.542666
C	-5.904781	-1.766307	1.700697
C	-4.527047	-1.668837	1.826123
C	-3.699249	-2.103365	0.784678
H	-3.631191	-2.983420	-1.190462
H	-6.079183	-3.149701	-1.391748
H	-7.555507	-2.368642	0.446674
H	-6.539084	-1.422649	2.513190
H	-4.063406	-1.258160	2.718456
O	-2.361444	-1.949815	0.990912
C	-1.502570	-2.325382	-0.067400
H	-1.704648	-1.744346	-0.980776
H	-0.490160	-2.113557	0.279301
H	-1.589621	-3.394604	-0.303316

TS6h.log

SCF (M06L) = -1587.92660666
E(SCF)+ZPE(0 K)= -1587.157025
H(298 K)= -1587.113047
G(298 K)= -1587.231240
Lowest Frequency = -576.9033cm-1

Al	0.400133	-0.091577	-0.943019
N	1.763723	-0.735462	0.351723
N	-0.298922	1.250763	0.334081
C	1.630443	-0.594125	1.681290
C	0.629479	0.181800	2.279929
H	0.598287	0.158457	3.362969
C	-0.188993	1.140031	1.663388
C	2.614660	-1.251559	2.605737
H	2.883357	-2.255924	2.268056
H	2.215276	-1.305323	3.619579
H	3.547046	-0.677902	2.643437
C	-0.927264	2.091523	2.557168
H	-2.008297	1.951293	2.463251
H	-0.728036	3.130092	2.274684

H	-0.650606	1.948882	3.602083
C	2.974051	-1.363005	-0.115275
C	2.935622	-2.694472	-0.583359
C	4.135165	-3.293221	-0.971836
H	4.124673	-4.319087	-1.327926
C	5.338817	-2.599958	-0.922588
H	6.260885	-3.086378	-1.228130
C	5.351742	-1.277970	-0.504938
H	6.287356	-0.722404	-0.499950
C	4.179434	-0.635651	-0.096779
C	1.619743	-3.438640	-0.685326
H	0.908117	-2.713245	-1.098867
C	1.656054	-4.615841	-1.651225
H	2.058585	-4.334695	-2.628824
H	0.645087	-5.006385	-1.800266
H	2.261577	-5.442459	-1.262813
C	1.072640	-3.895553	0.667955
H	0.922881	-3.065898	1.363564
H	1.756062	-4.611824	1.139196
H	0.100488	-4.382728	0.544338
C	4.240888	0.834264	0.271994
H	3.274015	1.131180	0.698592
C	5.323126	1.147005	1.303263
H	5.225810	0.538553	2.207835
H	5.276594	2.199145	1.602046
H	6.325921	0.970151	0.899784
C	4.466003	1.666816	-0.990766
H	3.670514	1.510057	-1.727808
H	5.413953	1.396554	-1.469356
H	4.507828	2.735757	-0.753668
C	-0.977450	2.401973	-0.203523
C	-0.181869	3.463519	-0.691753
C	-0.822538	4.601884	-1.183835
H	-0.226960	5.430285	-1.555528
C	-2.208451	4.692988	-1.212090
H	-2.688504	5.588431	-1.596690
C	-2.972816	3.626960	-0.766204
H	-4.058095	3.683616	-0.815922
C	-2.383549	2.463636	-0.261117
C	1.334851	3.397178	-0.657918
H	1.627385	2.350394	-0.845598
C	1.991313	4.247925	-1.738749
H	1.574173	4.040231	-2.728414
H	3.066110	4.051826	-1.777100
H	1.871877	5.318651	-1.541768
C	1.882862	3.772331	0.720421
H	1.544637	3.084643	1.501618
H	1.564956	4.783504	0.999765
H	2.978985	3.756859	0.720299
C	-3.293037	1.312216	0.123820
H	-2.690118	0.520679	0.591307
C	-4.382327	1.714429	1.117796
H	-3.980361	2.162253	2.032364
H	-4.971207	0.835218	1.397159
H	-5.071617	2.443049	0.677318
C	-3.954396	0.739379	-1.133070
H	-3.218450	0.443536	-1.888975
H	-4.599364	1.494050	-1.597652
H	-4.573425	-0.129889	-0.890005
C	-4.294528	-2.890695	-1.042427
C	-5.642956	-2.707702	-1.314801
C	-6.508904	-2.217718	-0.334328
C	-6.000363	-1.910910	0.928487
C	-4.648264	-2.072595	1.206171
C	-3.758742	-2.584833	0.231664
H	-3.621136	-3.271069	-1.807615
H	-6.028239	-2.949698	-2.303003
H	-7.563566	-2.077402	-0.552311
H	-6.664458	-1.528409	1.701435
H	-4.240315	-1.826936	2.183987
O	-2.489520	-2.767286	0.529735
C	-1.308326	-1.654358	-0.598457
H	-2.108101	-0.973593	-0.842491
H	-0.786456	-1.575859	0.352243
H	-1.087028	-2.460861	-1.277796

Int8h.log

SCF (M06L) = -1588.04206729
E(SCF)+ZPE(0 K)= -1587.271291
H(298 K)= -1587.227233
G(298 K)= -1587.343353
Lowest Frequency = 22.9631cm-1

Al	-0.150589	-0.712202	-0.374756
N	1.531934	-0.253428	0.513724
N	-1.159734	0.733154	0.400339
C	1.390349	0.031678	1.819004
C	0.167638	0.442753	2.385088
H	0.162692	0.546897	3.465347
C	-0.980055	0.906000	1.718869
C	2.556321	-0.064009	2.759738
H	3.359675	-0.686306	2.360879
H	2.220552	-0.477191	3.714374
H	2.974891	0.923553	2.975500
C	-2.048029	1.573488	2.532953
H	-2.939034	0.933361	2.551330
H	-2.362476	2.524418	2.095322
H	-1.722368	1.746636	3.559375
C	2.849176	-0.270748	-0.057779
C	3.325276	-1.443975	-0.687488
C	4.619067	-1.452313	-1.209631
H	4.985568	-2.358296	-1.683720
C	5.441489	-0.337462	-1.126728
H	6.450211	-0.366714	-1.528878
C	4.951215	0.820818	-0.545728
H	5.574093	1.712421	-0.515941
C	3.658587	0.887738	-0.017864
C	2.491150	-2.700068	-0.749365
H	1.434981	-2.425033	-0.844957
C	2.763290	-3.577163	-1.963432
H	2.750933	-2.993853	-2.889336
H	1.979647	-4.334694	-2.033391
H	3.729932	-4.089451	-1.897665
C	2.634502	-3.506626	0.540465
H	2.416850	-2.902245	1.429683
H	3.658820	-3.882308	0.646205
H	1.953074	-4.363562	0.533252
C	3.171850	2.247431	0.448343
H	2.181889	2.144863	0.910564
C	4.106527	2.909465	1.461116
H	4.343345	2.259985	2.308614
H	3.658819	3.828365	1.853450
H	5.058481	3.189187	0.997134
C	3.022932	3.158111	-0.770757
H	2.333290	2.736466	-1.508977
H	3.989853	3.297910	-1.266476
H	2.656073	4.147993	-0.478862
C	-2.167873	1.512285	-0.267920
C	-1.854580	2.839727	-0.638755
C	-2.869373	3.634708	-1.175442
H	-2.651361	4.663963	-1.445075
C	-4.145052	3.131298	-1.395580
H	-4.920301	3.768693	-1.811459
C	-4.405268	1.799802	-1.118153
H	-5.387054	1.383771	-1.334525
C	-3.431098	0.966837	-0.558972
C	-0.446912	3.397370	-0.517314
H	0.242886	2.542433	-0.585317

C	-0.127439	4.355094	-1.663974
H	-0.356539	3.910963	-2.637129
H	0.929672	4.629096	-1.656650
H	-0.693230	5.288882	-1.582210
C	-0.189585	4.087380	0.824266
H	-0.230425	3.392140	1.667768
H	-0.926021	4.879914	1.002577
H	0.803369	4.551781	0.834907
C	-3.779295	-0.487844	-0.333565
H	-2.923132	-0.986317	0.134733
C	-4.970057	-0.646132	0.609049
H	-4.785393	-0.182045	1.583645
H	-5.186444	-1.705561	0.778877
H	-5.873061	-0.187208	0.190735
C	-4.057310	-1.181111	-1.668377
H	-3.180108	-1.163485	-2.323111
H	-4.881279	-0.694217	-2.202413
H	-4.330313	-2.227754	-1.506922
C	-2.520331	-3.931320	-0.236440
C	-3.272268	-3.681194	0.872146
C	-2.783608	-2.886336	1.956560
C	-1.538495	-2.344489	1.873165
C	-0.710144	-2.483754	0.686136
C	-1.150826	-3.449913	-0.357090
H	-2.878683	-4.584140	-1.028129
H	-4.266564	-4.120625	0.953418
H	-3.395813	-2.750171	2.843523
H	-1.131868	-1.793509	2.718392
H	0.341452	-2.642927	0.954310
O	-0.409654	-3.815568	-1.284739
C	-0.092013	-0.692435	-2.322689
H	-0.848435	-0.028314	-2.756925
H	-0.234851	-1.690906	-2.746731
H	0.884652	-0.332320	-2.670932