Supporting Information

Functionalization and Hydrogenation of Carbon Chains Derived from CO

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1 GENERAL EXPERIMENTAL

All manipulations were carried out using standard Schlenk-line and glovebox techniques under an inert atmosphere of argon or dinitrogen. A MBraun Labmaster glovebox was employed, operating at <0.1 ppm O\textsubscript{2} and <0.1 ppm H\textsubscript{2}O. A Polar Bear Cub reactor located inside this MBraun Labmaster glovebox was used as the low-temperature reactor. Solvents were dried over activated alumina from a SPS (solvent purification system) based upon the Grubbs design and degassed before use. Glassware was dried for 12 h at 120 °C prior to use. C\textsubscript{6}D\textsubscript{6} was dried over 3 Å molecular sieves and freeze-pump-thaw degassed thrice before use.

NMR Spectra were recorded on Bruker 400 MHz at 25 °C unless otherwise stated and values recorded in ppm. Data were processed in MestReNova software. Where needed, chemical shifts were assigned with the assistance of 2D NMR (HSQC, HMBC, COSY) spectra. \textsuperscript{1} and \textsuperscript{2} and \textsuperscript{3b} were synthesized according to literature procedures. IR spectra were recorded on an Agilent Cary630 ATR FTIR spectrometer located inside an MBraun glovebox operating at <0.1 ppm O\textsubscript{2} and <0.1 ppm H\textsubscript{2}O. Chemicals were purchased from Sigma Aldrich, Fluorochem, Alfa Aesar, or VWR and used as received. CO was purchased from BOC Ltd and used as received. Elemental analyses were performed by Elemental Labs (https://www.elementallab.co.uk/).
2 EXPERIMENTAL METHODS

2.1 – Preparation of Compounds

Preparation of 3a

In a glovebox, 2 (15 mg, 0.012 mmol, 1 equiv) and benzophenone (2.6 mg, 0.014 mmol, 1.2 equiv) were dissolved in C$_6$D$_6$ (0.6 mL) and transferred to a J-Young NMR tube. The mixture was heated for 24 h at 100 °C. The reaction was monitored by $^1$H NMR spectroscopy and was deemed to be complete upon consumption of 2. The formation of both 3a and 4a was observed at this point in an approximate 4:1 ratio, respectively. The J-Young NMR tube was returned to the glovebox, and the headspace of the NMR tube was evacuated. CO gas (~1 atm) was introduced to the NMR tube and the reaction mixture was subsequently heated for a further 1 h at 100 °C. A $^1$H NMR spectrum was taken at this time point and showed the full conversion of 4a to 3a. The J-Young NMR tube was returned to the glovebox, the reaction mixture was diluted with toluene (~0.5 mL), decanted into a 20 mL scintillation vial, and concentrated in vacuo until approx. 0.5 mL of solution remained. The solution was then filtered into a 4 mL vial, and further concentrated until approximately 0.2 mL of solution remained. n-Pentane (~2.5 mL) was layered on top, the vial was placed in the glovebox freezer (~35 °C), and 3a was allowed to recrystallize as bright orange crystals. The supernatant was decanted, and the resultant crystals were washed with cold n-pentane (3 x 1 mL) before the crystals were dried in vacuo. Yield: 10 mg, 0.0068 mmol, 56%.

$^1$H NMR (400 MHz, C$_6$D$_6$, 298 K) δ 0.60 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (C$_3$H$_2$)$_2$CH), 0.74 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (C$_3$H$_2$)$_2$CH), 0.93 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (C$_3$H$_2$)$_2$CH), 1.02 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (C$_3$H$_2$)$_2$CH), 1.05 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (C$_3$H$_2$)$_2$CH), 1.23 (d, $^3$J$_{HH} = 6.7$ Hz, 6H, (C$_3$H$_2$)$_2$CH), 1.27 (s, 6H, ((C$_3$H)$_2$C)$_2$CH), 1.37 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (C$_3$H)$_2$CH), 1.44 (s, 6H, ((C$_3$H)$_2$C)$_2$CH), 1.57 (d, $^3$J$_{HH} = 6.7$ Hz, 6H, (C$_3$H)$_2$CH), 2.54 (hept, $^3$J$_{HH} = 6.8$ Hz, 2H, (C$_3$)$_2$C$_2$H), 3.02 (hept, $^3$J$_{HH} = 6.9$ Hz, 2H, (C$_3$)$_2$C$_2$H), 3.23 (hept, $^3$J$_{HH} = 6.8$ Hz, 2H, (C$_3$)$_2$C$_2$H), 3.58 (hept, $^3$J$_{HH} = 6.6$ Hz, 2H, (C$_3$)$_2$C$_2$H), 4.86 (s, 1H, ((C$_3$)$_2$C)$_2$H), 4.99 (s, 1H, ((C$_3$)$_2$C)$_2$H), 6.40 – 6.47
(overlapping signals, 4H, Ar-H), 6.51 – 6.59 (overlapping signals, 4H, Ar-H), 6.80 (m, 2H, Ar-H), 6.90 (m, 2H, Ar-H), 6.96 (m, 2H, Ar-H), 7.08 – 7.22 (overlapping signals, 8H, Ar-H).

$^{13}$C{^1H} NMR (101 MHz, C$_6$D$_6$, 298 K) δ 23.4 (2x (CH$_3$)$_2$CH), 24.0 (2x ((CH$_3$)$_2$C)$_2$CH), 24.1 (2x ((CH$_3$)$_2$C)$_2$CH), 24.2 (2x (CH$_3$)$_2$CH), 24.4 (2x (CH$_3$)$_2$CH), 24.6 (4x (CH$_3$)$_2$CH), 24.9 (2x (CH$_3$)$_2$CH), 27.3 (2x (CH$_3$)$_2$CH), 27.9 (2x (CH$_3$)$_2$CH), 28.4 (2x (CH$_3$)$_2$CH), 28.8 (4x (CH$_3$)$_2$CH), 29.1 (2x (CH$_3$)$_2$CH), 85.4 (C$l$), 100.2 ((CH$_3$)$_2$C)$_2$CH), 100.6 ((CH$_3$)$_2$C)$_2$CH), 124.2 (Ar-C), 124.7 (Ar-C), 125.0 (Ar-C), 125.6 (Ar-C), 127.3 (Ar-C), 127.4 (Ar-C), 139.8 (Ar-C), 140.6 (Ar-C), 142.8 (Ar-C), 143.5 (Ar-C), 144.7 (Ar-C), 146.0 (Ar-C), 148.3 (Ar-C), 152.9 (C$^{2/2}$), 155.9 (C$^{2/2}$), 172.7 ((CH$_3$)$_2$C)$_2$CH), 174.5 ((CH$_3$)$_2$C)$_2$CH), 203.2 (W(CO)$_4$), 205.1 (WCO), 315.6 (C$l$). Some Ar-C resonances are overlapping and cannot be observed.

IR (ATR), 𝜈$_{CO}$ (cm$^{-1}$): 2050, 1897, 1871.

Anal. Calc. (C$_{79}$H$_{92}$Al$_2$N$_4$O$_9$W): C, 64.14; H, 6.44; N, 3.79. Found: C, 64.63; H, 6.47; N, 3.88.
Preparation of 4a

In a glovebox, 3a (40 mg, 0.027 mmol) was dissolved in toluene (~5 mL) and transferred to a J-Young ampoule with an approximate headspace of 100 mL. The headspace of the ampoule was evacuated and the ampoule was removed from the glovebox. The reaction mixture was heated at 100 °C. After one hour, the ampoule was returned to the glovebox vacuum was applied to the headspace of the ampoule, and the ampoule was returned to heat at 100 °C. This process was repeated 5 times, for a total of 6 hours of heating, and a colour change from the characteristic yellow-orange of 3a to deep red of 4a was observed over the course of the reaction. After 6 hours, the reaction mixture was returned to the glovebox, decanted into a 20 mL scintillation vial, and the mixture was concentrated to a red oil. Pentane (ca. 2 mL) was added to the reaction mixture and the resultant solution was placed in the glovebox freezer to crystallise at –35 °C. 4a crystallised as deep red blocks from this solution. The supernatant was decanted, and the crystals were washed thrice with pentane (3 x 1mL) before the crystals were dried in vacuo. Yield: 26 mg, 0.018 mmol, 66%.

1H NMR (400 MHz, C₆D₆, 298 K) δ 0.41 (d, 3JHH = 6.6 Hz, 6H, (CH₃)₂CH), 0.68 (d, 3JHH = 6.8 Hz, 6H, (CH₃)₂CH), 0.80 (d, 3JHH = 6.8 Hz, 6H, (CH₃)₂CH), 0.95 (d, 3JHH = 6.7 Hz, 6H, (CH₃)₂CH), 1.07 (d, 3JHH = 6.7 Hz, 6H, (CH₃)₂CH), 1.15 (d, 3JHH = 6.7 Hz, 6H, (CH₃)₂CH), 1.32 (s, 6H, ((CH₃)₂C)₂CH), 1.49 (d, 3JHH = 6.6 Hz, 6H, (CH₃)₂CH), 1.66 (s, 6H, ((CH₃)₂C)₂CH), 1.78 (d, 3JHH = 6.7 Hz, 6H, (CH₃)₂CH), 2.62 (hept, 3JHH = 6.8 Hz, 2H, (CH₃)₂CH), 3.11 (hept, 3JHH = 6.7 Hz, 2H, (CH₃)₂CH), 3.24 (hept, 3JHH = 6.7 Hz, 2H, (CH₃)₂CH), 3.40 (hept, 3JHH = 6.6 Hz, 2H, (CH₃)₂CH), 5.11 (s, 1H, ((CH₃)C)₂CH), 5.33 (s, 1H, ((CH₃)C)₂CH), 6.43 (m, 4H, Ar-H), 6.60 (m, 4H, Ar-H), 6.83 (m, 2H, Ar-H), 6.99 (m, 2H, Ar-H), 7.08 (m, 4H, Ar-H), 7.16 – 7.26 (overlapping signals, 6H, Ar-H).
\(^{13}\)C\(^{1}H\) NMR (101 MHz, C\(_6\)D\(_6\), 298 K) \(\delta\) 24.0 (2x (A\(_{3}\)H\(_{2}\))CH), 24.2 (2x (A\(_{3}\)H\(_{2}\))CH), 24.2 (2x (A\(_{3}\)H\(_{2}\))CH), 24.3 (2x ((A\(_{3}\)H\(_{2}\))C\(_{2}\))CH), 24.6 (2x (A\(_{3}\)H\(_{2}\))CH), 24.6 (2x (A\(_{3}\)H\(_{2}\))CH), 24.9 (2x ((A\(_{3}\)H\(_{2}\))C\(_{2}\))CH), 24.9 (2x (A\(_{3}\)H\(_{2}\))CH), 25.1 (2x (A\(_{3}\)H\(_{2}\))CH), 27.8 (2x (A\(_{3}\)H\(_{2}\))CH), 28.2 (2x (CH\(_{3}\))\(_{2}\)A\(_{1}\)), 28.7 (2x (CH\(_{3}\))\(_{2}\)A\(_{1}\)), 29.0 (2x (CH\(_{3}\))\(_{2}\)A\(_{1}\)), 29.3 (2x (CH\(_{3}\))\(_{2}\)A\(_{1}\)), 82.3 (C\(^2\)), 100.7 ((((CH\(_{3}\))\(_{2}\)C\(_{2}\))A\(_{1}\)), 101.0 (((((CH\(_{3}\))\(_{2}\)C\(_{2}\)A\(_{1}\)), 124.0 (ArC), 124.5 (ArC), 125.4 (ArC), 126.0 (ArC), 126.1 (ArC), 127.4 (ArC), 127.6 (ArC), 128.8 (ArC), 139.9 (ArC), 140.0 (ArC), 142.8 (C\(^2/3\)), 143.2 (ArC), 143.4 (ArC), 146.1 (ArC), 146.9 (ArC), 147.5 (ArC), 161.8 (C\(^2/3\)), 174.6 (((((CH\(_{3}\))\(_{2}\)C\(_{2}\)CH), 174.6 (((((CH\(_{3}\))\(_{2}\)C\(_{2}\)CH), 215.5 (2 x W(CO)\(_{4}\)), 218.8 (W(CO)\(_{4}\)), 221.4 (W(CO)\(_{4}\)), 310.6 (C\(^s\)). Some ArC resonances are overlapping and cannot be observed.

IR (ATR), \(\nu_{CO}\) (cm\(^{-1}\)): 1988, 1874, 1862, 1825.

Anal. Calc. (C\(_{78}\)H\(_{92}\)Al\(_{2}\)N\(_{4}\)O\(_{8}\)W): C, 64.55; H, 6.39; N, 3.86. Found: C, 64.61; H, 6.33; N, 3.61.
Preparation of 5a

In a glovebox, 4a (10 mg, 0.007 mmol) was dissolved in C\textsubscript{6}D\textsubscript{6} (0.6 mL) and transferred to a j-Young NMR tube. The headspace of the NMR tube was evacuated, H\textsubscript{2} gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 2 h at 100 °C. After this time, conversion >95 % of 4a to 5a was observed. All attempts to separate 5a from reaction mixture were unsuccessful. Compound 5a was characterized by NMR spectroscopy.

5b can be also obtained in similar yield by reaction of 3a (8 mg, 0.0055 mmol) with H\textsubscript{2}, following the former procedure (see section 2.6 below).

\[ ^1\text{H NMR} \ (400 \text{ MHz, C}_6\text{D}_6, \text{298 K}) \delta 0.37 \text{ (d, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 6H, (CH}_3)_2\text{CH}), 0.96 \text{ (d, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 12H, (CH}_3)_2\text{CH}) \]

\[ 1.12 \text{ (d, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 6H, (CH}_3)_2\text{CH}), 1.13 \text{ (d, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 6H, (CH}_3)_2\text{CH}), 1.18 \text{ (d, } ^3\text{J}_{HH} = 6.7 \text{ Hz, 12H, (CH}_3)_2\text{CH}) \]

\[ 1.42 \text{ (s, 6H, ((CH}_3)_2\text{C})_2\text{CH}), 1.44 \text{ (s, 6H, ((CH}_3)_2\text{C})_2\text{CH}), 1.69 \text{ (d, } ^3\text{J}_{HH} = 6.7 \text{ Hz, 6H, (CH}_3)_2\text{CH}) \]

\[ 2.84 \text{ (hept, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 2H, (CH}_3)_2\text{C}), 2.96 \text{ (hept, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 2H, (CH}_3)_2\text{C}) \]

\[ 3.34 \text{ (hept, } ^3\text{J}_{HH} = 6.8 \text{ Hz, 2H, (CH}_3)_2\text{C}), 3.49 \text{ (hept, } ^3\text{J}_{HH} = 6.7 \text{ Hz, 2H, (CH}_3)_2\text{C}) \]

\[ 4.38 \text{ (s, 2H, CH}_2\text{), 4.84 \text{ (s, 1H, ((CH}_3)_2\text{C})_2\text{CH}), 4.86 \text{ (s, 1H, ((CH}_3)_2\text{C})_2\text{CH})} \]

\[ 6.72 – 6.84 \text{ (overlapping signals, 8H, Ar-H), 6.94 (m, 2H, Ar-H), 6.98 (m, 2H, Ar-H), 7.03 (m, 2H, Ar-H), 7.11 – 7.21 (overlapping signals, 4H, Ar-H), 7.26 (m, 4H, Ar-H)} \]

\[ ^13\text{C}[^1\text{H}] \text{ NMR} \ (101 \text{ MHz, C}_6\text{D}_6, \text{298 K}) \delta 23.2 \text{ (2x (CH}_3)_2\text{CH), 23.5 \text{ (2x (CH}_3)_2\text{CH}) \]

\[ 24.0 \text{ (2x ((CH}_3)_2\text{C})_2\text{CH), 24.1 \text{ (2x ((CH}_3)_2\text{C})_2\text{CH), 24.4 \text{ (2x (CH}_3)_2\text{CH), 24.7 \text{ (2x (CH}_3)_2\text{CH), 24.9 \text{ (2x (CH}_3)_2\text{C})_2\text{CH), 25.0 \text{ (2x (CH}_3)_2\text{C})_2\text{CH, 25.5 \text{ (2x (CH}_3)_2\text{C})_2\text{CH), 26.0 \text{ (2x (CH}_3)_2\text{C})_2\text{CH, 28.0 \text{ (2x (CH}_3)_2\text{C})_2\text{CH, 28.7 \text{ (2x (CH}_3)_2\text{C})_2\text{CH, 28.8 \text{ (2x (CH}_3)_2\text{C})_2\text{CH, 28.9 \text{ (2x (CH}_3)_2\text{C})_2\text{CH, 69.2 (CH}_2\text{), 84.5 (C1), 97.6 ((CH}_3)_2\text{C})_2\text{CH, 97.8 ((CH}_3)_2\text{C})_2\text{CH, 124.2 (Ar-C), 124.4 (Ar-C), 124.6 (Ar-C), 124.8 (Ar-C), 125.2 (Ar-C), 126.9 (Ar-C), 127.3 (Ar-C), 127.5 (Ar-C), 129.4 (Ar-C), 135.9 (C2/3), 138.8 (C2/3), 140.1 (Ar-C), 140.5 (Ar-C), 143.0 (Ar-C), 143.9 (Ar-C), 144.8 (Ar-C), 145.0 (Ar-C), 145.2 (Ar-C))}} \]

S8
(ArC150.1, ArC150.4, ArC171.1, (CH3)2C2CH, 172.2, ((CH3)2C)2CH. Some ArC resonances are overlapping and cannot be observed.

Also observed resonances corresponding to W(CO)6: δ 191.2 (JWC = 126.7 Hz), and (C6D6)W(CO)3: δ 209.3.

Attempts to obtain mass spectra data of 5a by ES and APCI (both +ve and -ve mode) were unsuccessful. Submission of CH3CN/H2O (20:80) solutions of 5a to LC-MS allowed detection of hydrolyzed species: m/z calcd for C16H17O4 [M+H]+ 273.1, found 273.4; calcd for C16H14O3 [M-H2O]+ 254.1, found 254.3.

**Preparation of **5a-**d2**

In a glovebox, 4a (10 mg, 0.007 mmol) was dissolved in C6D6 (0.6 mL) and transferred to a J-Young NMR tube. The headspace of the NMR tube was evacuated, D2 gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 2 h at 100 °C. After this time, an 1H NMR spectrum was recorded to check that reaction was completed and expected product was formed. Data for 5a-d2 are consistent with those reported for 5a but the resonance at δ = 4.38 ppm corresponding to CH2 fragment was not observed. The J-Young NMR tube was returned to the glovebox, the solvent was removed under reduced pressure and the residue dissolved in C6H6. A 2H NMR spectra was recorded.

2H NMR (61 MHz, C6H6, 298 K) δ 4.21 (bs).

Attempts to obtain mass spectra data of 5a-d2 by ES and APCI (both +ve and -ve mode) were unsuccessful. Submission of CH3CN/H2O (20:80) solutions of 5a-d2 to LC-MS allowed detection of hydrolyzed species: m/z calcd for C16H13D2O4 [M-H]- 273.1, found 273.2; calcd for C16H11D2O3 [M-H2O-H]- 255.1, found 255.1.
Preparation of 5b

In a glovebox, 3b (10 mg, 0.007 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube. The headspace of the NMR tube was evacuated, H₂ gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 12 h at 100 °C. After this time, conversion >95 % of 3b to 5b was observed. All attempts to separate 5b from reaction mixture were unsuccessful. Compound 5b was characterized by NMR spectroscopy.

¹H NMR (400 MHz, C₆D₆, 298 K) δ 0.56 (d, 3J_HH = 6.8 Hz, 6H, (CH₂)₂CH), 0.87 (d, 3J_HH = 6.8 Hz, 6H, (CH₂)₂CH), 0.89 (d, 3J_HH = 6.8 Hz, 6H, (CH₂)₂CH), 1.01 (d, 3J_HH = 6.8 Hz, 6H, (CH₂)₂CH), 1.10 (d, 3J_HH = 6.7 Hz, 6H, (CH₂)₂CH), 1.14 (d, 3J_HH = 6.7 Hz, 6H, (CH₂)₂CH), 1.44 (s, 6H, ((CH₂)₂C)₂CH), 1.52 (d, 3J_HH = 6.8 Hz, 6H, (CH₂)₂CH), 1.54 (s, 6H, ((CH₂)₂C)₂CH), 1.71 (d, 3J_HH = 6.7 Hz, 6H, (CH₂)₂CH), 3.13 (hept, 3J_HH = 6.8 Hz, 2H, (CH₃)₂CH), 3.21 (hept, 3J_HH = 6.8 Hz, 2H, (CH₃)₂CH), 3.27 (hept, 3J_HH = 6.8 Hz, 2H, (CH₃)₂CH), 3.32 (hept, 3J_HH = 6.8 Hz, 2H, (CH₃)₂CH), 4.28 (s, 2H, CH₂), 4.85 (s, 1H, ((CH₃)₂C)₂CH), 4.94 (s, 1H, ((CH₃)₂C)₂CH), 6.97-7.28 (overlapping signals, 12H, Ar-CH₃).

¹³C NMR (101 MHz, C₆D₆, 298 K) δ 22.9 (2x ((CH₂)₂C)₂CH), 23.0 (2x ((CH₂)₂C)₂CH), 24.3 (2x (CH₂)₂C)₂CH), 24.6 (2x (CH₂)₂C)₂CH), 24.7 (2x (CH₂)₂C)₂CH), 24.8 (2x (CH₂)₂C)₂CH), 24.9 (2x (CH₂)₂C)₂CH), 24.9 (2x (CH₂)₂C)₂CH), 25.1 (2x (CH₂)₂C)₂CH), 27.8 (2x (CH₂)₂C)₂CH), 28.3 (2x (CH₂)₂C)₂CH), 28.9 (4x (CH₂)₂C)₂CH), 29.6 (2x (CH₂)₂C)₂CH), 67.5 (CH₃), 96.8 ((CH₂)₂C)₂CH), 98.2 ((CH₂)₂C)₂CH), 123.8 (Ar-C), 124.4 (Ar-C), 124.6 (Ar-C), 124.9 (Ar-C), 125.4 (Ar-C), 127.3 (Ar-C), 137.8 (Ar-C), 138.5 (Ar-C), 138.7 (Ar-C), 143.8 (Ar-C), 144.4 (Ar-C), 145.0 (Ar-C), 146.0 (Ar-C), 151.8 (C²), 168.4 (C²), 171.2 ((CH₂)₂C)₂CH), 171.9 ((CH₂)₂C)₂CH). Some Ar-C resonances are overlapping and cannot be observed. The Al-C resonance could not be observed in the ¹³C NMR spectrum due to coupling to the quadrupolar ²⁷Al (I = 5/2) nucleus.
Preparation of 3c

3c was prepared following the reaction sequence shown in Scheme S1. Reaction of 2 at 25 °C gives the kinetic product S1 by C=O insertion into Al–O bond. S1 evolves to the thermodynamic product 3c after heating at 60 °C for 48 h.

**Scheme S1**: Reaction of 2 with 3-tolualdehyde.

Preparation of S1: 2 was prepared in-situ in an NMR tube from 1 (17.8 mg, 0.04 mmol), [W(CO)₆] (8 mg, 0.023 mmol) and CO gas (~1 bar) following the reported procedure. Once formation of 2 was confirmed by ¹H NMR spectroscopy, the NMR tube was returned to the glovebox, the reaction mixture was cooled to −35 °C using a low temperature reactor and the headspace of the NMR tube was evacuated to remove the remaining CO gas and 3-tolualdehyde (4.8 µL, 0.04 mmol) was added via microsyringe. After 12 h at 25 °C the reaction mixture was returned to the glovebox, diluted with ~0.5 mL of toluene and decanted into a 20 mL scintillation vial. The resultant solution was concentrated *in vacuo* and residue dissolved in THF (~0.2 mL), filtered into a 4 mL vial, and carefully layered with n-pentane (~2 mL). The vial was placed in the glovebox freezer (−35 °C) and S1 crystallised as orange blocks. The supernatant was decanted, and the resultant crystals were washed with cold n-pentane thrice (3 x 0.5mL) before being dried *in vacuo*. Yield: 15.3 mg, 0.011 mmol, 53%.
$^1$H NMR (400 MHz, THF-$_d_8$, 298 K) $\delta$ 0.49 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 0.51 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 0.61 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 0.85 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 0.86 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 0.94 (d, $^3$J$_{HH} = 6.9$ Hz, 3H, (CH$_3$)$_2$CH), 0.95 (d, $^3$J$_{HH} = 6.8$ Hz, 3H, (CH$_3$)$_2$CH), 1.07 (d, $^3$J$_{HH} = 6.9$ Hz, 3H, (CH$_3$)$_2$CH), 1.10 (d, $^3$J$_{HH} = 6.6$ Hz, 3H, (CH$_3$)$_2$CH), 1.18 (d, $^3$J$_{HH} = 6.8$ Hz, 3H, (CH$_3$)$_2$CH), 1.25 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 1.33 (d, $^3$J$_{HH} = 6.9$ Hz, 3H, (CH$_3$)$_2$CH), 1.38 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 1.43 (d, $^3$J$_{HH} = 6.8$ Hz, 3H, (CH$_3$)$_2$CH), 1.47 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 1.53 (d, $^3$J$_{HH} = 6.7$ Hz, 3H, (CH$_3$)$_2$CH), 1.65 (s, 3H, (CH$_3$)$_2$CH), 1.82 (s, 3H, (CH$_3$)$_2$CH), 1.84 (s, 3H, (CH$_3$)$_2$CH), 1.96 (s, 3H, (CH$_3$)$_2$CH), 2.09 (s, 3H, CH$_3$-C$_6$H$_4$), 2.60 - 2.80 (hept overlapping, 3H, (CH$_3$)$_2$CH), 2.87 (hept, $^3$J$_{HH} = 6.8$ Hz, 1H, (CH$_3$)$_2$CH), 3.13 (hept overlapping, 2H, (CH$_3$)$_2$CH), 3.24 (hept overlapping, 2H, (CH$_3$)$_2$CH), 5.40 (s, 1H, (CH$_3$)$_2$CH), 5.43 (s, 1H, HC$^t$), 5.75 (s, 1H, (CH$_3$)$_2$CH), 6.20 (s, 1H, Ar-H), 6.23 (m, 1H, Ar-H), 6.72 - 6.77 (m, 2H, Ar-H), 6.93 - 7.01 (overlapping signals, 2H, Ar-H), 7.03 - 7.12 (overlapping signals, 4H, Ar-H), 7.21 (m, 1H, Ar-H), 7.25 - 7.41 (overlapping signals, 5H, Ar-H).

$^{13}$C NMR (101 MHz, THF-$_d_8$, 298 K) $\delta$ 21.7 (CH$_3$-C$_6$H$_4$), 23.1 ((CH$_3$)$_2$CH), 23.6 ((CH$_3$)$_2$CH), 23.6 ((CH$_3$)$_2$CH), 24.1 (((CH$_3$)$_2$C)$_2$CH), 24.6 - 26.1 (overlapping signals, 3 x ((CH$_3$)$_2$C)$_2$CH and 8 x (CH$_3$)$_2$CH), 26.2 ((CH$_3$)$_2$CH), 26.3 ((CH$_3$)$_2$CH), 26.6 ((CH$_3$)$_2$CH), 26.6 ((CH$_3$)$_2$CH), 27.2 ((CH$_3$)$_2$CH), 28.8 ((CH$_3$)$_2$CH), 29.1 ((CH$_3$)$_2$CH), 29.2 ((CH$_3$)$_2$CH), 29.2 ((CH$_3$)$_2$CH), 29.4 ((CH$_3$)$_2$CH), 29.4 ((CH$_3$)$_2$CH), 29.4 ((CH$_3$)$_2$CH), 29.5 ((CH$_3$)$_2$CH), 100.1 (((CH$_3$)$_2$C)$_2$CH), 101.6 (((CH$_3$)$_2$C)$_2$CH), 103.5 (C$^t$), 123.9 (Ar-C), 124.7 (Ar-C), 125.3 (Ar-C), 125.4 (Ar-C), 125.5 (Ar-C), 125.7 (Ar-C), 125.8 (Ar-C), 126.2 (Ar-C), 126.7 (Ar-C), 127.1 (Ar-C), 128.1 (Ar-C), 128.2 (Ar-C), 128.6 (Ar-C), 128.7 (Ar-C), 129.3 (Ar-C), 136.4 (Ar-C), 139.1 (Ar-C), 139.9 (Ar-C), 140.8 (Ar-C), 141.1 (Ar-C), 141.8 (Ar-C), 143.3 (Ar-C), 144.2 (Ar-C), 144.5 (Ar-C), 145.2 (Ar-C), 145.4 (Ar-C), 145.6 (Ar-C), 145.7 (Ar-C), 146.6 (Ar-C), 162.1 (Ar-C), 169.7 (C$^t$), 173.0 (((CH$_3$)$_2$C)$_2$CH), 173.1 (((CH$_3$)$_2$C)$_2$CH), 174.8 (((CH$_3$)$_2$C)$_2$CH), 174.8 (((CH$_3$)$_2$C)$_2$CH), 200.5 (W(CO)$_4$), 206.6 (W(CO$^t$)), 300.4 (C$^t$). The Al-C$^t$ resonance could not be observed in the $^{13}$C NMR spectrum due to coupling to the quadrupolar $^{27}$Al (I = 5/2) nucleus.

IR (ATR), $\nu_{CO}$ (cm$^{-1}$): 2050, 1905, 1871.
Preparation of 3c: In a glovebox, S1 (8 mg, 0.0056 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube. The solution was heated for 48 h at 60 °C. The reaction was monitored by ¹H NMR spectroscopy and was deemed to be complete upon consumption of S1. Then the NMR tube was returned to the glovebox, diluted with ~0.5 mL of toluene and decanted into a 20 mL scintillation vial. The resultant solution was concentrated in vacuo and residue was extracted with pentane (3 x 0.5 mL). The resultant yellow solution was concentrated (~0.7 mL) and placed in the glovebox freezer (~35 °C) for 2 days to allow crystallization of 3c as brown blocks. The mother liquor was decanted and the crystals washed with cold n-pentane thrice (3 x 0.5 mL) before being dried in vacuo. Yield: 4.4 mg, 0.0031 mmol, 55%.

¹H NMR (400 MHz, C₆D₆, 298 K) δ 0.43 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 0.43 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 0.68 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 0.76 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 0.96 (d, 3J_HH = 6.9 Hz, 3H, (CH₃)₂CH), 0.97 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 1.07 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 1.08 (d, 3J_HH = 6.9 Hz, 3H, (CH₃)₂CH), 1.09 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 1.13 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 1.31 (s, 3H, (CH₃)₂C₂CH), 1.32 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 1.33 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 1.33 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 1.44 (s, 3H, (CH₃)₂C₂CH), 1.40 (s, 3H, (CH₃)₂C₂CH), 1.38 (s, 3H, (CH₃)₂C₂CH), 1.55 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 1.56 (d, 3J_HH = 6.7 Hz, 3H, (CH₃)₂CH), 1.65 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 2.05 (s, 3H, CH₃C₆H₄), 2.40 (hept, 3J_HH = 6.7 Hz, 1H, (CH₃)₂CH), 2.99 - 3.11 (hept overlapping, 2H, (CH₃)₂CH), 3.11 - 3.25 (hept overlapping, 3H, (CH₃)₂CH), 3.49 (hept, 3J_HH = 6.7 Hz, 1H, (CH₃)₂CH), 3.74 (hept, 3J_HH = 6.7 Hz, 1H, (CH₃)₂CH), 4.81 (s, 1H, (CH₃)C₂CH), 4.95 (s, 1H, (CH₃)C₂CH), 5.14 (s, 1H, C₄H), 6.46 (d, 3J_HH = 7.5, 1H, Ar-H), 6.71 (t, 3J_HH = 7.5 Hz, 1H, Ar-H), 6.78 - 6.86 (overlapping signals, 3H, Ar-H), 6.96 - 7.00 (m, 1H, Ar-H), 7.03 - 7.12 (overlapping signals, 6H, Ar-H), 7.17 - 7.30 (overlapping signals, 4H, Ar-H).

¹³C{¹H} NMR (101 MHz, C₆D₆, 298 K) δ 21.3 (CH₃C₆H₄), 23.5 ((CH₃)₂C₂CH), 23.8 ((CH₃)₂C₂CH), 23.9 ((CH₃)₂CH), 23.9 ((CH₃)₂CH), 24.3 (2x (CH₃)₂CH), 24.5 (2x (CH₃)₂CH), 24.6 (2x (CH₃)₂CH), 24.7 (2x (CH₃)₂CH), 25.4 (2x (CH₃)₂CH), 25.9 (2x (CH₃)₂CH), 26.0 (2x (CH₃)₂CH), 27.7 ((CH₃)₂CH), 27.8 ((CH₃)₂CH), 28.0 ((CH₃)₂CH), 28.1 ((CH₃)₂CH), 28.7 ((CH₃)₂CH), 28.8 ((CH₃)₂CH), 28.8 ((CH₃)₂CH), 28.9 ((CH₃)₂CH), 80.3 (C₄H), 99.7 ((CH₃)C₂CH), 99.8 ((CH₃)C₂CH), 124.2 (Ar-C), 124.7 (Ar-C), 124.8 (Ar-C),
124.9 (Ar C), 125.1 (Ar C), 125.4 (Ar C), 125.5 (Ar C), 136.2 (Ar C), 138.1 (Ar C), 138.6 (Ar C), 140.4 (Ar C), 140.6 (Ar C), 142.8 (Ar C), 143.4 (Ar C), 143.8 (Ar C), 143.9 (Ar C), 144.3 (Ar C), 144.4 (Ar C), 146.0 (Ar C), 146.2 (Ar C), 151.2 (C²), 154.6 (C²), 173.8 \((\text{CH}_3)_2\text{C}_2\text{CH}\), 173.3 \((\text{CH}_3)_2\text{C}_2\text{CH}\), 172.6 \((\text{CH}_3)_2\text{C}_2\text{CH}\), 172.5 \((\text{CH}_3)_2\text{C}_2\text{CH}\), 202.1 (W(CO)₄), 211.7 (W(CO)), 314.1 (C¹). Some Ar C resonances are overlapping and cannot be observed.

IR (ATR), νCO (cm⁻¹): 2052, 1927, 1901, 1867.

Anal. Calc. (C₇₄H₉₀Al₂N₄O₉W): C, 62.71; H, 6.40; N, 3.95. Found: C, 60.64; H, 6.29; N, 4.28. The low C content, but accurate H and N content likely reflect limitations of the technique (e.g. incomplete C combustion).
Preparation of 5c

In a glovebox, 3c (5 mg, 0.0036 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube containing a capillary with 1,3,5-trimethoxybenzene as external standard. The headspace of the NMR tube was evacuated, H₂ gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 48 h at 100 °C. After this time, 3c was not observed by ¹H NMR spectroscopy in the reaction mixture. NMR yield: 60 %.

Compound 5c was characterized by NMR spectroscopy.

¹H NMR (400 MHz, C₆D₆, 298 K) δ 0.57 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 0.87 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 0.93 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 0.97 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 0.99 (d, 3JHH = 6.6 Hz, 3H, (CH₃)₂CH), 1.05 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.07 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.09 (d, 3JHH = 6.9 Hz, 3H, (CH₃)₂CH), 1.10 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.13 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.16 (d, 3JHH = 6.8 Hz, 6H, (CH₃)₂CH), 1.22 (d, 3JHH = 6.9 Hz, 3H, (CH₃)₂CH), 1.34 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.42 (s, 3H, (CH₃)₂C₂CH), 1.44 (s, 3H, (CH₃)₂C₂CH), 1.45 (s, 3H, (CH₃)₂C₂CH), 1.48 (s, 3H, (CH₃)₂C₂CH), 1.50 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.51 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 2.14 (s, 3H, CH₃C₆H₄), 2.78 (hept, 3JHH = 6.8 Hz, 1H, (CH₃)₂CH), 3.01 (hept, 3JHH = 6.9 Hz, 1H, (CH₃)₂CH), 3.21 – 3.37 (hept overlapping, 4H, (CH₃)₂CH), 3.42 (hept, 3JHH = 6.9 Hz, 1H, (CH₃)₂CH), 3.53 (hept, 3JHH = 6.8 Hz, 1H, (CH₃)₂CH), 4.42 (AB spin system, Δν = 83.2 Hz, JAB = 13.8 Hz, 2H, CH₂), 4.83 (s, 1H, (CH₃)₂CH), 4.88 (s, 1H, (CH₃)₂CH), 5.01 (s, 1H, CH₃), 6.46 (m, 1H, Ar-H), 6.70 (s, 1H, Ar-H), 6.78 (m, 1H, Ar-H), 6.83 – 6.89 (overlapping signals, 2H, Ar-H), 6.94 (m, 1H, Ar-H), 7.04 – 7.09 (overlapping signals, 2H, Ar-H), 7.13 – 7.23 (overlapping signals, 6H, Ar-H), 7.32 (m, 2H, Ar-H).

¹³C NMR (101 MHz, C₆D₆, 298 K) δ 22.2 (CH₃C₆H₄), 23.3 ((CH₃)₂C₂CH), 23.5 ((CH₃)₂C₂CH), 23.5 ((CH₃)₂C₂CH), 23.6 ((CH₃)₂C₂CH), 24.4 ((CH₃)₂CH), 24.5 ((CH₃)₂CH), 24.5 ((CH₃)₂CH), 24.5 ((CH₃)₂CH), 24.6 ((CH₃)₂CH), 24.7 ((CH₃)₂CH), 24.7
([CH₃]₂CH), 24.7 ([CH₃]₂CH), 24.8 ([CH₃]₂CH), 24.8 ([CH₃]₂CH), 24.8 ([CH₃]₂CH), 24.9 ([CH₃]₂CH), 25.0 ([CH₃]₂CH), 25.3 ([CH₃]₂CH), 25.4 ([CH₃]₂CH), 25.6 ([CH₃]₂CH), 28.1 ([CH₃]₂CH₂), 28.2 ([CH₃]₂CH₂), 28.3 ([CH₃]₂CH₂), 28.6 ([CH₃]₂CH₂), 28.7 ([CH₃]₂CH₂), 28.7 ([CH₃]₂CH₂), 28.8 ([CH₃]₂CH₂), 29.0 ([CH₃]₂CH₂), 68.6 (CH₂), 79.8 (C⁴H), 97.6 ([CH₃]₂CH₂), 97.9 ([CH₃]₂CH₂), 123.6 (ArC), 123.7 (ArC), 123.9 (ArC), 124.2 (ArC), 124.4 (ArC), 124.5 (ArC), 124.7 (ArC), 124.8 (ArC), 124.9 (ArC), 125.4 (ArC), 125.9 (ArC), 126.1 (ArC), 127.4 (ArC), 129.1 (ArC), 129.7 (ArC), 135.7 (C⁴), 136.0 (C³), 136.8 (ArC), 139.4 (ArC), 139.6 (ArC), 139.7 (ArC), 140.3 (ArC), 141.3 (ArC), 142.8 (ArC), 144.0 (ArC), 144.2 (ArC), 144.3 (ArC), 144.5 (ArC), 144.7 (ArC), 144.8 (ArC), 145.2 (ArC), 148.0 (ArC), 171.3 ([CH₃]₂CH₂), 171.4 ([CH₃]₂CH₂), 171.5 ([CH₃]₂CH₂), 171.6 ([CH₃]₂CH₂).
Preparation of 3d

2 was prepared in-situ in an NMR tube from 1 (8.9 mg, 0.02 mmol), [W(CO)₆] (4 mg, 0.011 mmol) and CO gas (~1 bar) following the reported procedure. Once formation of 2 was confirmed by ¹H NMR spectroscopy, the NMR tube was returned to the glovebox, the reaction mixture was cooled to ~35 °C using a low temperature reactor and the headspace of the NMR tube was evacuated to remove the remaining CO gas and 2-butanone (1.8 μL, 0.02 mmol) was added via microsyringe. After 24 h at 25 °C reaction mixture was returned to the glovebox, diluted with ~0.5 mL of toluene and decanted into a 20 mL scintillation vial. The resultant solution was concentrated in vacuo to ~0.2 mL, filtered into a 4 mL vial, and carefully layered with n-pentane (~2 mL). The vial was placed in the glovebox freezer (~35 °C) and 3d crystallised as yellow blocks. The supernatant was decanted, and the resultant crystals were washed with cold n-pentane thrice (3 x 0.5mL) before being dried briefly in vacuo (~2 min). Yield: 7.0 mg, 0.0051 mmol, 51%.

¹H NMR (400 MHz, CDCl₃, 298 K) δ -0.03 (t, 3JHH = 7.3 Hz, 3H, CH₂CH₂), 0.49 (s, 3H, CH₂C₆H₅), 0.68 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 0.77 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 0.81 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 0.90 (m, 2H, CH₂CH₃), 1.03 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.06 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.13 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.16 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.19 (d, 3JHH = 6.9 Hz, 6H, (CH₃)₂CH), 1.25 (overlapping signals, 3H, (CH₃)₂CH), 1.27 (d, 3JHH = 6.6 Hz, 3H, (CH₃)₂CH), 1.34 (overlapping signals, 3H, (CH₃)₂CH), 1.35 (s, 3H, ((CH₃)₂C)₂CH), 1.35 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.38 (s, 3H, ((CH₃)₂C)₂CH), 1.41 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.48 (s, 3H, ((CH₃)₂C)₂CH), 1.50 (s, 3H, ((CH₃)₂C)₂CH), 1.64 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.77 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 2.86 (hept, 3JHH = 6.8 Hz, 1H, (CH₃)₂CH), 3.01 - 3.20 (hept overlapping, 5H, (CH₃)₂CH), 3.62 (hept, 3JHH = 6.6 Hz, 1H, (CH₃)₂CH), 3.73 (hept, 3JHH = 6.7 Hz, 1H, (CH₃)₂CH), 4.77 (s, 1H, ((CH₃)C)₂CH), 4.98 (s, 1H, ((CH₃)C)₂CH), 6.88 (m, 1H, Ar-H), 6.99 (m, 4H, Ar-H), 7.07 (m, 2H, Ar-H), 7.10 - 7.20 (overlapping signals, 5H, Ar-H).
$^{13}$C{$^1$H} NMR (101 MHz, CD$_6$, 298 K) $\delta$ 7.5 (CH$_2$CH$_3$), 23.1 ((CH$_3$)$_2$CH), 23.3 ((CH$_3$)$_2$CH), 23.4 ((CH$_3$)$_2$CH), 23.6 (((CH$_3$)$_2$C)$_2$CH), 23.8 (((CH$_3$)$_2$C)$_2$CH), 24.1 ((CH$_3$)$_2$CH), 24.1 ((CH$_3$)$_2$CH), 24.2 ((CH$_3$)$_2$CH), 24.4 ((CH$_3$)$_2$CH), 24.5 (CH$_3$)$_2$CH), 24.6 (((CH$_3$)$_2$C)$_2$CH), 24.6 (((CH$_3$)$_2$C)$_2$CH), 24.7 (CH$_3$)$_2$CH), 24.9 (CH$_3$)$_2$CH), 25.0 (CH$_3$)$_2$CH), 25.3 (CH$_3$)$_2$CH), 25.3 (CH$_3$)$_2$CH), 26.8 (CH$_3$)$_2$CH), 27.7 (CH$_3$)$_2$CH), 27.9 ((CH$_3$)$_2$CH), 28.3 ((CH$_3$)$_2$CH), 28.4 ((CH$_3$)$_2$CH), 28.7 ((CH$_3$)$_2$CH), 28.7 ((CH$_3$)$_2$CH), 28.7 (CH$_3$C'), 28.9 ((CH$_3$)$_2$CH), 29.0 ((CH$_3$)$_2$CH), 29.1 ((CH$_3$)$_2$CH), 29.5 ((CH$_3$)$_2$CH), 35.4 (CH$_2$CH$_3$), 78.4 (C'), 99.8 (((CH$_3$)$_2$C)$_2$CH), 99.9 (((CH$_3$)$_2$C)$_2$CH), 123.6 (Ar C), 123.9 (Ar C), 124.0 (Ar C), 124.1 (Ar C), 124.6 (Ar C), 124.8 (Ar C), 125.4 (Ar C), 125.9 (Ar C), 127.2 (Ar C), 127.5 (Ar C), 139.0 (Ar C), 139.3 (Ar C), 140.3 (Ar C), 140.4 (Ar C), 142.1 (Ar C), 142.6 (Ar C), 143.8 (Ar C), 144.9 (Ar C), 144.8 (Ar C), 145.4 (Ar C), 146.3 (Ar C), 146.4 (Ar C), 154.9 (C'), 157.2 (C'), 172.1 (((CH$_3$)$_2$C)$_2$CH), 172.3 (((CH$_3$)$_2$C)$_2$CH), 173.8 (((CH$_3$)$_2$C)$_2$CH), 174.3 (((CH$_3$)$_2$C)$_2$CH), 203.6 (W(CO)$_4$), 205.2 (W(CO)), 311.3 (C'). Some ArC resonances are overlapping and cannot be observed.

IR (ATR), $\nu_{\text{CO}}$ (cm$^{-1}$): 2043, 1923, 1893, 1871.

Anal. Calc. (C$_{71}$H$_{92}$Al$_{2}$N$_{4}$O$_{9}$W): C, 61.65; H, 6.70; N, 4.05. Found: C, 61.79; H, 6.65; N, 4.49.
In a glovebox, 3d (5 mg, 0.0036 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube containing a capillary with 1,3,5-trimethoxybenzene as external standard. The headspace of the NMR tube was evacuated, H₂ gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 4 h at 100 °C. After this time, 3d was not observed by ¹H NMR spectroscopy in the reaction mixture. NMR yield: 87%. Compound 5d was characterized by NMR spectroscopy.

¹H NMR (400 MHz, C₆D₆, 298 K) δ -0.37 (t, 3JHH = 7.2 Hz, 3H, CH₂CH₃), 0.56 (s, 3H, CH₃C¹), 0.76 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 0.81 (m, 1H, CH₂CH₃), 0.98 (d, 3JHH = 6.8 Hz, 3H, (CH₃)₂CH), 1.03 (d, 3JHH = 6.8 Hz, 6H, (CH₃)₂CH), 1.14 (d, 3JHH = 6.8 Hz, 6H, (CH₃)₂CH), 1.17 (d, 3JHH = 6.8 Hz, 6H, (CH₃)₂CH), 1.21 (d, 3JHH = 6.9 Hz, 3H, (CH₃)₂CH), 1.30 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.46 (d, 3JHH = 6.7 Hz, 6H, (CH₃)₂CH), 1.52 (d, 3JHH = 6.7 Hz, 3H, (CH₃)₂CH), 1.64 (s, 6H, ((CH₃)₂C)₂CH), 1.59 (d, 3JHH = 6.6 Hz, 3H, (CH₃)₂CH), 2.98 (hept, 3JHH = 6.9 Hz, 2H, (CH₃)₂CH), 3.08 (hept, 3JHH = 6.7 Hz, 2H, (CH₃)₂CH), 3.24 – 3.58 (hept overlapping, 4H, (CH₃)₂CH), 4.67 (s, 2H, CH₂), 4.90 (s, 1H, ((CH₃)₂C)₂CH), 4.93 (s, 1H, ((CH₃)₂C)₂CH), 6.94 (m, 1H, Ar-H), 7.02 (m, 2H, Ar-H), 7.10 – 7.20 (overlapping signals, 9H, Ar-H).

¹³C NMR (101 MHz, C₆D₆, 298 K) δ 6.9 (CH₂CH₃), 22.7 ((CH₃)₂CH), 23.4 ((CH₃)₂CH), 23.4 ((CH₃)₂CH), 23.5 (((CH₃)₂C)₂CH), 23.5 (((CH₃)₂C)₂CH), 23.8 (((CH₃)₂C)₂CH), 23.9 (((CH₃)₂C)₂CH), 24.0 (((CH₃)₂C)₂CH), 24.1 (((CH₃)₂C)₂CH), 24.4 (((CH₃)₂C)₂CH), 24.5 (((CH₃)₂C)₂CH), 24.5 (((CH₃)₂C)₂CH), 24.7 ((CH₃)₂CH), 24.8 ((CH₃)₂CH), 24.8 ((CH₃)₂CH), 24.9 ((CH₃)₂CH), 25.3 ((CH₃)₂CH), 25.5 ((CH₃)₂CH), 26.2 ((CH₃)₂CH), 26.7 ((CH₃)₂CH), 27.9 ((CH₃)₂CH), 28.0 ((CH₃)₂CH), 28.2 ((CH₃)₂CH), 28.5 ((CH₃)₂CH), 28.7 ((CH₃)₂CH), 28.8 ((CH₃)₂CH), 28.8 ((CH₃)₂CH), 30.3 (CH₃C¹), 35.1 (CH₂CH₃), 69.1 (CH₂), 78.4 (C¹), 97.3 (((CH₃)₂C)₂CH), 97.8 (((CH₃)₂C)₂CH), 123.6 (Ar-C), 123.7 (Ar-C), 124.0 (Ar-C), 124.1 (Ar-C), 124.2 (Ar-C), 124.5 (Ar-C), 124.8 (Ar-C), 125.5 (Ar-C), 125.9 (Ar-C), 135.3 (C²), 138.3 (C²), 19.
140.0 (Ar $\mathbf{C}$), 140.5 (Ar $\mathbf{C}$), 140.6 (Ar $\mathbf{C}$), 141.1 (Ar $\mathbf{C}$), 142.8 (Ar $\mathbf{C}$), 143.3 (Ar $\mathbf{C}$), 143.4 (Ar $\mathbf{C}$), 144.1 (Ar $\mathbf{C}$), 144.2 (Ar $\mathbf{C}$), 144.5 (Ar $\mathbf{C}$), 144.9 (Ar $\mathbf{C}$), 145.4 (Ar $\mathbf{C}$), 171.0 ({$(\text{CH}_3)_2\mathbf{C}$}2CH), 171.3 ({$(\text{CH}_3)_2\mathbf{C}$}2CH), 171.7 ({$(\text{CH}_3)_2\mathbf{C}$}2CH), 172.2 ({$(\text{CH}_3)_2\mathbf{C}$}2CH). Some Ar $\mathbf{C}$ resonances are overlapping and cannot be observed.
Preparation of 3e

2 was prepared in-situ in an NMR tube from 1 (8.9 mg, 0.02 mmol), [W(CO)₆] (4 mg, 0.011 mmol) and CO gas (~1 bar) following the reported procedure. Once formation of 2 was confirmed by ¹H NMR spectroscopy, the NMR tube was returned to the glovebox, reaction mixture was cooled to ~35 °C using a low temperature reactor and the headspace of the NMR tube was evacuated to remove the remaining CO gas. 2,6-Dimethylphenyl isocyanide (1.3 mg, 0.01 mmol) was dissolved in 0.3 mL of C₆D₆ and added to the reaction mixture. After 24 h at 60 °C reaction mixture was returned to the glovebox, diluted with ~0.5 mL of toluene and decanted into a 20 mL scintillation vial. The resultant solution was concentrated in vacuo and the residue dissolved in ~0.2 mL of THF. A dark purple solid precipitated after addition of n-pentane (~0.5 mL) to the solution. The supernatant was decanted, and the solid washed with n-pentane thrice (3 x 0.5mL) before being dried in vacuo. Yield: 8.5 mg, 0.006 mmol, 60%.

¹H NMR (400 MHz, THF-d₈, 298 K) δ 0.14 (d, ³JHH = 6.7 Hz, 6H, (CH₃)₂CH), 0.60 (s, 6H, Xyl-CH₃), 0.74 (d, ³JHH = 6.7 Hz, 6H, (CH₃)₂CH), 0.87 (d, ³JHH = 6.7 Hz, 6H, (CH₃)₂CH), 0.92 (d, ³JHH = 6.8 Hz, 6H, (CH₃)₂CH), 1.00 (d, ³JHH = 6.6 Hz, 6H, (CH₃)₂CH), 1.18 (d, ³JHH = 6.7 Hz, 6H, (CH₃)₂CH), 1.26 (d, ³JHH = 6.7 Hz, 6H, (CH₃)₂CH), 1.54 (d, ³JHH = 6.9 Hz, 6H, (CH₃)₂CH), 1.64 (s, 6H, ((CH₃)₂C)₂CH), 1.84 (s, 6H, ((CH₃)₂C)₂CH), 2.37 (hept, ³JHH = 6.9 Hz, 2H, (CH₃)₂C), 2.98 (hept, ³JHH = 6.8 Hz, 2H, (CH₃)₂C), 3.25 (hept, ³JHH = 6.7 Hz, 2H, (CH₃)₂C), 3.33 (hept, ³JHH = 6.9 Hz, 2H, (CH₃)₂C), 5.48 (s, 1H, ((CH₃)C)₂CH), 5.66 (s, 1H, ((CH₃)C)₂CH), 6.41 (m, 3H, Ar-H), 6.96 (m, 2H, Ar-H), 7.02 – 7.10 (overlapping signals, 4H, Ar-H), 7.15 (m, 3H, Ar-H), 7.24 (m, 3H, Ar-H).
$^{13}$C NMR (101 MHz, THF, 298 K) δ 17.1 (Xyl-CH$_3$), 24.2 (2x (CH$_3$)$_2$CH), 24.5 (2x ((CH$_3$)$_2$C)$_2$CH) 24.5 (2x ((CH$_3$)$_2$C)$_2$CH), 26.3 (2x (CH$_3$)$_2$CH), 26.4 (2x (CH$_3$)$_2$CH), 28.1 (2x (CH$_3$)$_2$CH), 28.6 (2x (CH$_3$)$_2$CH), 29.3 (2x (CH$_3$)$_2$CH), 29.4 (2x (CH$_3$)$_2$CH), 30.0 (2x (CH$_3$)$_2$CH), 100.5 ([(CH$_3$)$_2$C]$_2$CH), 102.2 ([(CH$_3$)$_2$C]$_2$CH), 121.9 (ArC), 124.0 (ArC), 124.9 (ArC), 125.3 (ArC), 125.5 (ArC), 125.8 (ArC), 128.2 (ArC), 128.6 (ArC), 129.0 (ArC), 139.3 (ArC), 140.8 (ArC), 144.2 (ArC), 145.0 (ArC), 145.0 (ArC), 145.8 (C$^{2/3}$), 146.5 (ArC), 156.5 (ArC), 161.2 (C$^{2/3}$), 173.8 ([(CH$_3$)$_2$C]$_2$CH), 175.0 ([(CH$_3$)$_2$C]$_2$CH), 202.5 (W(CO)$_4$), 206.5 (W(CO)$_4$), 329.2 (C$^i$). Some ArC resonances are overlapping and cannot be observed. The Al–C$^4$ resonance could not be observed in the $^{13}$C NMR spectrum due to coupling to the quadrupolar $^{27}$Al (I = 5/2) nucleus.

IR (ATR), ν$_{CO}$ (cm$^{-1}$): 2051, 1907, 1879.

Anal. Calc. (C$_{75}$H$_{91}$Al$_2$N$_5$O$_8$W): C, 63.07; H, 6.42; N, 4.90. Found: C, 51.79; H, 4.95; N, 4.50.$^1$

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$^1$ Accurate CHN analysis could not be obtained likely due to the air-sensitive nature of the compound.
Preparation of S2

In a glovebox, 3f (24 mg, 0.019 mmol) and 2,6-dimethylphenyl isocyanide (7 mg, 0.053 mmol) were dissolved in C₆D₆ (0.600 mL) and transferred to a J-Young NMR tube. The mixture was heated at 100°C for 6 h. At 2 hr intervals, the headspace of the NMR tube was removed under vacuum and refreshed with dinitrogen. The J-Young NMR tube was returned to the glovebox, diluted with toluene (~0.5 mL), decanted into a 20 mL scintillation vial, and concentrated in vacuo until approx 0.3 mL of solution remains. The solution was then filtered into 10 mL of n-pentane. S2 directly crystallises from this mixture as dark purple-black needles. The vial was placed in the freezer at –35°C for 18 h. The supernatant was decanted, and the resultant crystals were washed with cold n-pentane thrice (3x 1mL) before the crystals were dried briefly in vacuo (~2 minutes).

Yield: 14 mg, 0.0091 mmol, 48%.

¹H NMR (400 MHz, C₆D₆, 298 K) δ 0.46 (d, ³J_HH = 6.7 Hz, 6H, (CH₃)₂CH), 0.87 (d overlapping, ³J_HH= 6.7 Hz, 12H, 2x CH(₃)₂CH), 0.92 (d, ³J_HH = 6.8 Hz, 6H, (CH₃)₂CH), 0.95 (d, ³J_HH = 6.8 Hz, 6H, (CH₃)₂CH), 1.03 (s, 6H, 2x Xyl-CH₃), 1.37 (s, 6H, {(CH₃)₂C}₂CH), 1.40 (d, ³J_HH = 6.8 Hz, 6H, (CH₃)₂CH), 1.44 (d, ³J_HH = 6.5 Hz, 6H, (CH₃)₂CH), 1.49 (s, 6H, {(CH₃)₂C}₂CH), 1.78 (d, ³J_HH = 6.8 Hz, 6H, (CH₃)₂CH), 2.51 (hept, ³J_HH = 6.7 Hz, 2H, 2x (CH₃)₂CH), 2.53 (s, 6H, 2x Xyl-CH₃), 3.06 (hept, ³J_HH = 6.8 Hz, 2H, 2x (CH₃)₂CH), 3.18 (hept, ³J_HH = 6.6 Hz, 2H, 2x (CH₃)₂CH), 4.95 (s, 1H, {(CH₃)₃C}₂CH), 5.21 (s, 1H, {(CH₃)C}₂CH), 6.67 – 7.23 (m, overlapping signals, 24H, Ar-H).

¹³C NMR (101 MHz, C₆D₆, 298 K) δ 17.0 (2x Xyl-CH₃), 19.1 (2x Xyl-CH₃), 23.9 ({{CH₃}₂C}₂CH), 24.0 ({{CH₃}₂C}₂CH), 24.1 ({{CH₃}₂C}₂CH), 24.8 (2x (CH₃)₂CH), 25.3 ({{CH₃}₂C}₂CH), 25.3 ({{CH₃}₂C}₂CH), 25.5 ({{CH₃}₂C}₂CH), 26.0 ({{CH₃}₂C}₂CH), 27.7 ({{CH₃}₂C}₂CH), 28.5 (2x (CH₃)₂CH), 28.7 (4x (CH₃)₂CH), 29.4 (2x (CH₃)₂CH), 99.3 ({{CH₃}₂C}₂CH), 102.0...
((CH$_3)_2C)_2CH, 121.5 (ArC), 123.7 (ArC), 124.2 (2x ArC), 124.7 (2x ArC), 125.1 (2x ArC), 125.1 (2x ArC), 126.8 (ArC), 127.6 (ArC), 129.9 (ArC), 135.0 (ArC), 138.7 (ArC), 140.6 (ArC), 143.6 (ArC), 144.4 (ArC), 144.4 (ArC), 146.5 (ArC), 156.5 ($C^{2/3}$), 160.9 ($C^{2/3}$), 173.1 ((CH$_3)_2C)_2CH), 173.3 ((CH$_3)_2C)_2CH), 205.8 (W(CO)$_2$), 211.4 (W(CO)$_2$), 319.4 ($C^I$).

Some ArC resonances are overlapping and cannot be observed. The Al–C resonance could not be observed due to quadrupolar broadening to the $^27$Al ($I = 5/2$) nucleus.

IR (ATR), $\nu$CO (cm$^{-1}$): 1976, 1911, 1889, 1859.

Anal. Calc. (C$_{83}$H$_{100}$Al$_2$N$_6$O$_7$: C, 65.09; H, 6.58; N, 5.49. Found: C, 65.22; H, 6.73; N, 5.44.
Preparation of **S3**

In a glovebox, 3e (5 mg, 0.0035 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube containing a capillary with 1,3,5-trimethoxybenzene as external standard. The headspace of the NMR tube was evacuated, H₂ gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 16 h at 100 °C. After this time, reaction mixture contained 3e, S3 and 5e in 7, 60 and 20 % NMR yield, respectively. Compound S3 was characterized by NMR spectroscopy from the mixture.

**1H NMR** (400 MHz, C₆D₆, 298 K) δ 0.71 (d, 3J_HH = 6.8 Hz, 3H, (CH₃)₂CH), 0.88 (d, 3J_HH = 6.7 Hz, 6H, (CH₃)₂CH), 0.96 (d, 3J_HH = 6.6 Hz, 6H, (CH₃)₂CH), 1.12 (d, 3J_HH = 6.6 Hz, 6H, (CH₃)₂CH), 1.21 (d, 3J_HH = 6.7 Hz, 6H, (CH₃)₂CH), 1.39 (s, 6H, ((CH₃)₂C)₂CH), 1.51 (s, 6H, ((CH₃)₂C)₂CH), 1.53 (d, 3J_HH = 6.7 Hz, 6H, (CH₃)₂CH), 1.56 (d, 3J_HH = 6.7 Hz, 6H, (CH₃)₂CH), 1.61 (d, 3J_HH = 6.7 Hz, 6H, (CH₃)₂CH), 1.86 (s, 6H, Xyl-CH₃), 2.04 (m, 3H, (CH₃)₂CH), 2.54 (hept, 3J_HH = 6.6 Hz, 2H, (CH₃)₂CH), 3.19 (hept, 3J_HH = 6.7 Hz, 2H, (CH₃)₂CH), 3.58 (hept, 3J_HH = 6.7 Hz, 2H, (CH₃)₂CH), 3.63 (hept, 3J_HH = 6.8 Hz, 2H, (CH₃)₂CH), 4.86 (s, 2H, CH₂), 4.90 (s, 1H, ((CH₃)C)₂CH), 4.99 (s, 1H, ((CH₃)C)₂CH), 6.44-7.34 (overlapping signals, 15H, Ar-H).

**13C NMR** (101 MHz, C₆D₆, 298 K) δ 68.7 (CH₂), 97.2 ((CH₃)₂C)₂CH), 98.6 ((CH₃)₂C)₂CH), 146.3 (C³), 156.2 (C²), 171.2 ((CH₃)₂C)₂CH), 171.8 ((CH₃)₂C)₂CH). Resonances corresponding to Xyl-CH₃, (CH₃)₂CH, ((CH₃)C)₂CH, (CH₃)₂CH and Ar-C are overlapping and cannot be assigned. The Al-C⁴ resonance could not be observed in the 13C NMR spectrum due to coupling to the quadrupolar 27Al (I = 5/2) nucleus.

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S25
Preparation of 5e

In a glovebox, 3e (5 mg, 0.0035 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube containing a capillary with 1,3,5-trimethoxybenzene as external standard. The headspace of the NMR tube was evacuated, H₂ gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 4 days at 100 °C. After this time, no signals corresponding to 3e or S2 were observed by NMR spectroscopy from the mixture. NMR yield: 85%. Compound 5e was characterized by NMR spectroscopy.

¹H NMR (400 MHz, C₆D₆, 298 K) δ 0.62 (d, ¹³JHH = 6.6 Hz, 3H, (CH₃)₂CH)), 1.02 (d, ¹³JHH = 6.9 Hz, 6H, (CH₃)₂CH)), 1.04 (d, ¹³JHH = 6.8 Hz, 6H, (CH₃)₂CH)), 1.07 (d, ¹³JHH = 6.8 Hz, 6H, (CH₃)₂CH)), 1.11 (d, ¹³JHH = 6.7 Hz, 6H, (CH₃)₂CH)), 1.20 (d, ¹³JHH = 6.9 Hz, 6H, (CH₃)₂CH)), 1.30 (d, ¹³JHH = 6.8 Hz, 6H, (CH₃)₂CH)), 1.36 (d, ¹³JHH = 6.7 Hz, 6H, (CH₃)₂CH)), 1.47 (s, 6H, {(CH₃)₂C}₂CH), 1.48 (s, 6H, {(CH₃)₂C}₂CH), 1.86 (s, 6H, Xyl-CH₂), 2.09 (m, 3H, (CH₃)₂CH), 3.06 (hept, ¹³JHH = 6.8 Hz, 2H, (CH₃)₂CH), 3.08 (hept, ¹³JHH = 6.8 Hz, 2H, (CH₃)₂CH), 3.31 (hept, ¹³JHH = 6.9 Hz, 2H, (CH₃)₂CH), 3.68 (hept, ¹³JHH = 6.8 Hz, 2H, (CH₃)₂CH)), 4.90 (s, 1H, {(CH₃)C}₂CH), 4.94 (s, 1H, {(CH₃)C}₂CH), 5.61 (s, 1H, NH), 6.47 (s, 1H, C-H), 6.50 (m, 2H, Ar-H), 6.68 (m, 1H, Ar-H), 6.79 (m, 1H, Ar-H), 6.98 (m, 2H, Ar-H), 7.12 – 7.22 (overlapping signals, 9H, Ar-H).

¹³C NMR (101 MHz, C₆D₆, 298 K) δ 18.3 (Xyl-CH₃), 19.8 (2x (CH₃)₂CH), 23.3 (2x {(CH₃)₂C}₂CH), 23.6 (2x{(CH₃)C}₂CH), 24.1 (2x (CH₃)₂CH), 24.4 (2x (CH₃)₂CH), 24.7 (2x (CH₃)₂CH), 24.9 (2x (CH₃)₂CH), 25.2 (2x (CH₃)₂CH), 25.3 (2x (CH₃)₂CH), 25.7 (2x (CH₃)₂CH), 28.3 (2x (CH₃)₂CH), 28.6 (2x (CH₃)₂CH), 28.6 (2x (CH₃)₂CH), 28.7 (2x (CH₃)₂CH), 98.6 (2{(CH₃)C}₂CH), 99.1 (2{(CH₃)C}₂CH), 119.3 (Ar-C), 124.2 (Ar-C), 124.3 (Ar-C), 124.4 (Ar-C), 125.1 (Ar-C), 127.1 (Ar-C), 127.4 (Ar-C), 128.6 (C′H), 129.2 (Ar-C), 135.3 (Ar-C), 138.6 (C′), 139.5 (Ar-C), 140.4 (Ar-C), 143.2 (Ar-C), 144.7 (Ar-C), 145.1 (Ar-C), 145.5 (Ar-C), 146.3 (Ar-C), 151.2 (C′), 171.0 (2{(CH₃)C}₂CH), 171.8 (2{(CH₃)C}₂CH). Some Ar-C resonances are overlapping and cannot be observed. The Al–C resonance could not be
observed in the $^{13}$C NMR spectrum due to coupling to the quadrupolar $^{27}$Al (I = 5/2) nucleus.

NH group was confirmed by $^{15}$N-$^1$H HSQC experiment. $^{15}$N NMR (41 MHz, 298 K) δ 79.5.
Preparation of 5f

In a glovebox, 2 (10 mg, 0.008 mmol) was dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube. The headspace of the NMR tube was evacuated, H₂ gas (~1 bar) was introduced into the NMR tube and the reaction mixture was heated for 72 h at 100 °C. After this time, conversion >95% of 2 to 5f was observed. All attempts to separate 5f from reaction mixture were unsuccessful. Compound 5f was characterized by NMR spectroscopy.

¹H NMR (400 MHz, C₆D₆, 298 K) δ 1.00 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆Ha)₂CH), 1.07 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆Hb)₂CH), 1.08 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆Hc)₂CH), 1.11 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆Hd)₂CH), 1.13 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆He)₂CH), 1.15 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆Hf)₂CH), 1.30 (d, ³Jₘₘₘ = 6.8 Hz, 6H, (C₆Hg)₂CH), 1.36 (d, ³Jₘₘₘ = 6.7 Hz, 6H, (C₆Hh)₂CH), 1.48 (s, 6H, ((C₆H)₂C)₂CH), 1.50 (s, 6H, ((C₆H)₂C)₂CH), 2.98 (hept, ³Jₘₘₘ = 6.8 Hz, 2H, (CH₃)₂CH), 2.98 (hept, ³Jₘₘₘ = 6.8 Hz, 2H, (CH₃)₂CH), 3.32 (hept, ³Jₘₘₘ = 6.8 Hz, 2H, (CH₃)₂CH), 3.67 (hept, ³Jₘₘₘ = 6.8 Hz, 2H, (CH₃)₂CH), 4.69 (s, 2H, CH₂), 4.90 (s, 1H, ((CH₃)C)₂CH), 4.94 (s, 1H, ((CH₃)C)₂CH), 6.93 (m, 2H, Ar-H), 7.05 (m, 2H, Ar-H), 7.09 (m, 2H, Ar-H), 7.11 (m, 2H, Ar-H), 7.16 (m, 1H, Ar-H), 7.19 (m, 1H, Ar-H), 7.21 (m, 1H, Ar-H), 7.23 (m, 1H, Ar-H).

¹³C NMR (101 MHz, C₆D₆, 298 K) δ 23.3 (2x ((CH₃)₂C)₂CH), 23.4 (2x ((CH₃)₂C)₂CH), 24.6 (4x (CH₃)₂C), 24.7 (4x (CH₃)₂C), 24.9 (2x (CH₃)₂C), 25.0 (2x (CH₃)₂C), 25.2 (2x (CH₃)₂C), 25.6 (2x (CH₃)₂C), 28.2 (4x (CH₃)₂C), 28.6 (2x (CH₃)₂C), 29.1 (2x (CH₃)₂C), 67.5 (CH₃), 97.7 (((CH₃)₂C)₂CH), 97.9 (((CH₃)₂C)₂CH), 124.1 (Ar-C), 124.1 (Ar-C), 124.8 (Ar-C), 124.9 (Ar-C), 126.9 (Ar-C), 127.4 (Ar-C), 139.3 (Ar-C), 140.2 (Ar-C), 143.2 (Ar-C), 143.4 (Ar-C), 144.9 (Ar-C), 145.1 (Ar-C), 155.9 (C²), 171.0 (((CH₃)₂C)₂CH), 171.1 (((CH₃)₂C)₂CH). Some Ar-C resonances are overlapping and cannot be observed. The Al–C₃ resonance could not be observed in the ¹³C NMR spectrum due to coupling to the quadrupolar ²⁷Al (I = 5/2) nucleus.
Preparation of $^{13}$C$_3$-5f

$[^{13}\text{C}]$ labelled $^{13}$C$_3$-3f was prepared according to literature procedure. In a glovebox, $^{13}$C$_3$-3f (18 mg) was dissolved in C$_6$D$_6$ (0.6 mL) and transferred to an NMR tube with a capillary of pyridine in C$_6$D$_6$ as an internal standard. The headspace of the NMR tube was evacuated in vacuo, and the NMR tube was removed from the glovebox. An atmosphere of H$_2$ (~ 1 atm) was introduced to the NMR tube. The NMR tube was heated at 100°C for 6 days. The reaction was monitored using $^1$H NMR spectroscopy and deemed completed upon the total consumption of $^{13}$C$_3$-3f and formation of $^{13}$C$_3$-5f. Yield 39% (relative to internal pyridine standard).

$^1$H NMR (400 MHz, C$_6$D$_6$, 298 K) $\delta$ 1.00 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.07 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.08 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.10 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.13 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.15 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.30 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, (CH$_3$)$_2$CH), 1.48 (s, 6H, (CH$_3$)$_2$C)$_2$CH), 1.50 (s, 6H, ((CH$_3$)$_2$C)$_2$CH), 2.98 (hept, $^3$J$_{HH} = 6.8$ Hz, 2H, (CH$_3$)$_2$CH), 3.22 (hept, $^3$J$_{HH} = 6.8$ Hz, 2H, (CH$_3$)$_2$CH), 3.67 (hept, $^3$J$_{HH} = 6.8$ Hz, 2H, (CH$_3$)$_2$CH), 4.70 (ddd, $^1$J$_{HC} = 140.7$ Hz, $^2$J$_{HC} = 6.6$ Hz, $^3$J$_{HC} 3.2$ Hz, 2H, (CH$_3$)$_2$C), 4.90 (s, 1H, ((CH$_3$)$_2$C)$_2$CH), 6.93 (m, 2H, Ar-$^H$), 7.05 (m, 2H, Ar-$^H$), 7.09 (m, 2H, Ar-$^H$), 7.11 (m, 2H, Ar-$^H$), 7.16 (m, 1H, Ar-$^H$), 7.19 (m, 1H, Ar-$^H$), 7.21 (m, 1H, Ar-$^H$), 7.23 (m, 1H, Ar-$^H$).

$^{13}$C NMR (101 MHz, C$_6$D$_6$, 298 K) $\delta$ 23.3 (2x ((CH$_3$)$_2$C)$_2$CH), 23.4 (2x ((CH$_3$)$_2$C)$_2$CH), 24.6 (4x (CH$_3$)$_2$CH), 24.7 (4x (CH$_3$)$_2$CH), 24.9 (2x (CH$_3$)$_2$CH), 25.0 (2x (CH$_3$)$_2$CH), 25.2 (2x (CH$_3$)$_2$CH), 25.6 (2x (CH$_3$)$_2$CH), 26.2 (4x (CH$_3$)$_2$CH), 28.6 (2x (CH$_3$)$_2$CH), 29.1 (2x (CH$_3$)$_2$CH), 67.48 (d, $^1$J$_{CC} = 48.6$ Hz, $^{13}$CH$_2$), 97.7 (((CH$_3$)$_2$C)$_2$CH), 97.9 (((CH$_3$)$_2$C)$_2$CH), 124.1 (Ar-$^C$), 124.1 (Ar-$^C$), 124.8 (Ar-$^C$), 124.9 (Ar-$^C$), 126.9 (Ar-$^C$), 127.4 (Ar-$^C$), 139.3 (Ar-$^C$), 140.2 (Ar-$^C$), 143.2 (Ar-$^C$), 143.4 (Ar-$^C$), 144.9 (Ar-$^C$), 145.1 (Ar-$^C$), 146.9 (d, $^1$J$_{CC} = 51.6$ Hz, $^{13}$C$_2$), 155.9 (dd, $^1$J$_{CC} = 53.1$, 48.7 Hz, $^{13}$C$_2$), 171.0 (((CH$_3$)$_2$C)$_2$CH), 171.1 (((CH$_3$)$_2$C)$_2$CH).
A proton coupled $^{13}$C spectrum was also recorded (Figure S2) and key $^{13}$C-labelled resonances were identified:

$^{13}$C NMR (101 MHz, C$_6$D$_6$, 298 K) δ 67.48 (td, $^1J_{CH} = 140.5$, $^1J_{CC} = 48.7$ Hz, $^{13}$C$^1$H$_2$), 146.9 (d, $^1J_{CC} = 52.4$ Hz, $^{13}$C$^3$), 155.9 (ddt, $^1J_{CC} = 53.1$, 48.6 Hz, $^2J_{CH} = 6.6$ Hz, $^{13}$C$^2$).

**Figure S1:** $^{13}$C{H} spectrum of 5f-$^{13}$C with key $^{13}$C resonances of the carbon chain expanded. [W($^{13}$CO)$_6$] and [W(C$_6$D$_6$)($^{13}$CO)$_3$] are also observed in the spectrum.

**Figure S2:** $^{13}$C proton-coupled spectrum of 5f-$^{13}$C with key $^{13}$C resonances of the carbon chain expanded. [W($^{13}$CO)$_6$] and [W(C$_6$D$_6$)($^{13}$CO)$_3$] are also observed in the spectrum.
2.2 – Reversible conversion of 3a to 4a

In a glovebox, 2 (15 mg, 0.012 mmol) and benzophenone (2.6 mg, 0.014 mmol) were dissolved in C₆D₆ (0.6 mL) and transferred to a J-Young NMR tube containing a capillary with ferrocene dissolved in C₆D₆ as external standard. The mixture was heated for 24 h at 100 °C. The reaction mixture was monitored by ¹H NMR spectroscopy and was deemed to be complete upon consumption of 2. After this time, a ¹H NMR spectrum was recorded to determine the initial ratio between 3a and 4a (4:1). 81 % NMR yield.

**Conversion to 3a:** The reaction mixture was frozen by placing it into a liquid-nitrogen bath (~196 °C), the headspace of the NMR tube was evacuated, and CO gas (~1 bar) was introduced into the NMR tube at 25 °C, the mixture was heated for 12h at 100 °C and a second ¹H NMR spectrum was recorded showing only resonances corresponding to 3a.

**Conversion back to a mixture of 3a/4a:** The reaction mixture was frozen again at ~196 °C, and CO removed under reduced pressure. The NMR tube was heated under static vacuum for 12h at 100 °C and a ¹H NMR spectrum was recorded showing the presence of 3a and 4a in a ratio ca. 1:1. This mixture was converted to 3a again by introducing CO gas (~1 bar) at 25 °C into the NMR tube and heating for 12h at 100 °C. A Final ¹H NMR spectrum was recorder and signals corresponding to 4a were not detected in the reaction mixture.

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²The ratio of the formation of 3a to 4a under these reaction conditions is dependent on the concentration of the solution. The conversion of 3a to 4a involves the release of one CO molecule. The released CO molecule equilibrates between the headspace of the NMR tube (ca. 2mL) and solution. Hence, a more dilute sample will result in a larger relative proportion of 4a in solution, whereas a more concentrated solution would result in a smaller relative proportion of 4a in solution.
### Conditions

| Time  | Description                                      | Ratio 3a:4a |
|-------|--------------------------------------------------|-------------|
| t = 0 | Initial reaction mixture                         | 4:1         |
| t = 1 | 100 °C for 12h under CO                          | 99:1        |
| t = 2 | 100 °C for 12h under vacuum                       | 1:1         |
| t = 3 | 100 °C for 12h under CO                          | 99:1        |

**Table S1:** Ratio between 3a and 4a calculated by integration of $^1$H NMR signals against an external standard of ferrocene.

**Figure S3:** $^1$H NMR experiments showing the reversible interconversion of 3 and 4. Descriptions of conditions at each time detailed in Table S1.
Figure S4: Detail of $^1$H NMR experiments showing the reversible interconversion of $3a$ and $4a$. Descriptions of conditions at each time detailed in Table S1.
2.3 – Direct reaction of 2, H₂ and benzophenone

2 was prepared in-situ in an NMR tube from 1 (8.9 mg, 0.02 mmol), [W(CO)₆] (4 mg, 0.011 mmol) and CO gas (~1 bar) following the reported procedure. Once formation of 2 was confirmed by ¹H NMR spectroscopy, the NMR tube was returned to the glovebox, the reaction mixture was cooled to −35 °C using a low temperature reactor and the headspace of the NMR tube was evacuated to remove the remaining CO gas. A capillary containing a solution of 1,3,5-trimethoxybenzene in C₆D₆ as external standard and a solution of Ph₂CO (1.82 mg, 0.01 mmol) in C₆D₆ (0.3 mL) were added to the NMR tube and the mixture cooled to −35 °C. The headspace of the NMR tube was evacuated, the NMR tube was removed from the glovebox and H₂ gas (~1 bar) was introduced into the headspace of the NMR. The resultant mixture was heated at 100 °C and conversion to 5a was complete after 24 h, as monitored by ¹H NMR spectroscopy. NMR yield: 42%.
2.4 – Direct reaction of \([\text{W(CO}_6])\), \(\mathbf{1}\) and syngas \((1:1 \text{ H}_2: \text{ CO})\)

In a glovebox, an NMR tube was charged with a suspension of \(\mathbf{1}\) (8.9 mg, 0.02 mmol) in \(\text{C}_6\text{D}_6\) (0.3 mL) was cooled to \(-35^\circ\text{C}\) using a low temperature reactor. \([\text{W(CO}_6])\) (4 mg, 0.011 mmol) was added slowly as a slurry in \(\text{C}_6\text{D}_6\) (0.3 mL) via Pasteur pipette. Care was taken to ensure that the reaction mixture remains frozen and a capillary containing a solution of 1,3,5-trimethoxybenzene in \(\text{C}_6\text{D}_6\) as external standard was introduced. The headspace of the NMR tube was evacuated, and the NMR tube was removed from the glovebox quickly and placed into a liquid-nitrogen bath \((-196^\circ\text{C})\). The tube was removed from the liquid nitrogen bath, and syngas (1:1 mixture of \(\text{H}_2/\text{CO}\), \(\sim\)1 bar) was introduced at room temperature into the headspace of the NMR tube while the mixture was still frozen. Upon addition of syngas, the mixture was allowed to thaw, and during this process the tube was shaken vigorously to ensure incorporation of gas into solution. A \(^1\text{H}\) NMR spectrum was taken at this point to show formation of \(\mathbf{2}\). Reaction mixture was heated at 100 \(^\circ\text{C}\) and monitored by \(^1\text{H}\) NMR spectroscopy until conversion to \(\mathbf{5b}\) was completed after 10 days. NMR yield: 50\%.\(^3\)

During the progress of the reaction only signals corresponding to \(\mathbf{2}, \mathbf{3b}\) and \(\mathbf{5b}\) were observed. \(\mathbf{5f}\) was not detected at any time.

\(^3\) Calculated against 1,3,5-trimethoxybenzene external standard in relation to initial concentration of \(\mathbf{2}\).
2.5 – Kinetic experiments

In a glovebox, 4a (8 mg, 0.0055 mmol) and ferrocene (0.2 mg, 0.0011 mmol) as internal
standard were placed in a vial and dissolved in 1.2 mL of C₆D₆. Then, a portion 0.55 mL
was transferred to a J-Young NMR tube. The headspace of the NMR tube was evacuated
and H₂ (or D₂) gas (~1 bar) was introduced. The tube was transferred to an NMR
spectrometer preheated at 80 °C and allowed to warm to 100 °C. The reaction mixture
was monitored as a function of time over 8000 sec (133 min) with data points acquired
every 68 sec. The concentration of 5a was constant after 6000 sec (100 min) in both
cases.

A plot of Ln[4a] (determined from initial concentration and integration against internal
standard) vs time for both reactions using H₂ or D₂ gave a linear fit with high R-factor
(Figure S5) indicating the reaction is first order in [4a]. Standard errors were calculated
by use of the regression analysis calculation in Microsoft Excel software. The rate
constant for the H₂ reaction was found to be $k_{obs}(H_2) = 6.28 \times 10^{-4} (\pm 6 \times 10^{-6}) \text{ s}^{-1}$ and
$k_{obs}(D_2) = 6.16 \times 10^{-4} (\pm 6 \times 10^{-6}) \text{ s}^{-1}$ for D₂. This gave a $k_{obs}(H_2) / k_{obs}(D_2)$ of 1.02 (±0.01)
for the reaction.
**Figure S5:** Ln[4a] versus time plot for reaction of 4a with H₂ (a) and D₂ (b).
2.6 – Monitoring of reaction of 3a with H₂

In a glovebox, 3a (8 mg, 0.0055 mmol) and ferrocene (0.4 mg, 0.0021 mmol) as internal standard were placed in a vial and dissolved in 1.2 mL of C₆D₆. Then, a portion 0.45 mL was transferred to a J-Young NMR tube. The headspace of the NMR tube was evacuated and H₂ (or D₂) gas (~1 bar) was introduced. The tube was transferred to an NMR spectrometer preheated at 100 °C. The reaction mixture was monitored as a function of time over 8400 sec (140 min) with data points acquired every 68 sec. First spectrum was taken after 300 sec (5 min) and signals corresponding to 4a and 5a were detected. Complex 3a was consumed after 5000 sec (83 min) and concentration of 5a was constant after 8000 sec (133 min).

Figure S6: Plot of variation of concentration with time of compounds 3a, 4a and 5a for hydrogenation of 3a.
3 X-RAY DATA

The X-ray structure of 3a

*Figure S7*: The X-ray structure of 3a. All hydrogen atoms are omitted for clarity.

3a was found to crystallise in the P-1 space group with an included toluene and pentane molecule in the asymmetric unit.

The isopropyl group C33>C35 was found to be disordered over two sites in a ca. 58:42 ratio for the major and minor components respectively. The thermal parameters of both orientations were restrained to be similar, and only the non-hydrogen atoms of the major component were refined anisotropically (those in the minor component were refined isotropically).

The included toluene molecule (C81>C87) was found to be disordered. No convincing model of a second orientation of a toluene molecule could be found and the residual electron density most resembled a pentane molecule. As a result, the toluene molecule was modelled as the major component of the disordered fragment with ca. 74% occupancy, while the pentane molecule (C91>C95) was modelled as the minor component of the disordered fragment with ca. 26% occupancy. The geometries of both major and minor components were optimized, their thermal parameters restrained to be similar and only the non-hydrogen atoms of the major component were refined anisotropically (those in the minor component were refined isotropically).
**Crystal Data for C₈₅.H₁₀₁.Al₂N₄O₉W, M=1566.31**, triclinic, space group P-1 (no. 2), \(a = 13.1875(3)\ \text{Å},\ b = 16.3826(5)\ \text{Å},\ c = 18.6982(5)\ \text{Å},\ \alpha = 99.300(2)^\circ,\ \beta = 99.5985(19)^\circ,\ \gamma = 92.952(2)^\circ,\ V = 3917.95(17)\ \text{Å}^3,\ Z = 2,\ \rho_{\text{calc}} \text{g/cm}^3 = 1.328,\ \mu(\text{MoK} \alpha) = 1.556\ \text{mm}^{-1},\ T = 173.05(10),\ \text{yellow needles, } F^2\ \text{refinement},^{5,6} R_1(\text{obs}) = 0.0429,\ wR_2(\text{all}) = 0.1025,\ 15462\ \text{independent observed reflections } (R_{\text{int}} = 0.0286),\ 12739\ \text{independent measured reflections } ([|F_o| > 4\sigma(|F_o|),\ 2\theta_{\text{full}} = 56.498],\ 981\ \text{parameters. CCDC 2130349.}
The X-ray structure of 4a

4a was found to crystallise in the P2₁/n space group with two included hexane molecules with respective occupancies of 0.25 and 0.5 for a total of 0.75 molecules in the asymmetric unit, for a total of 3 within the unit cell.

A significant amount of electron density (ca 4 e⁻) was observed approximately 1 Å from W1. This unresolved electron density was assigned to be a minor component of co-crystallised material. Accordingly, the tungsten centre was split over these two sites resulting in a ca 96:4 occupancy for the major and minor components respectively. The major component corresponds to the structure of 4a, while the minor component appears to be trace amounts of 3a, based on inspection of the W1’–C1–C2 angle and W1’–O2 distance. No other electron density associated with 3a was observed in the Fourier difference map. This is not unexpected for two reasons: i) it is apparent from the geometry of the C1–W1 and C1–W1’ orientations that it is likely that the ligands at the tungsten centres (both CO and the C1 to C4 carbon chain) overlap to a significant degree ii) the comparatively small percentage of the minor component (4%) preclude observation of the C and O carbonyl atoms bound to the W1’ centre.

The isopropyl group C32>C34 was found to be disordered over two sites in a ca. 54:46 ratio for the major and minor components respectively. The thermal parameters of both
orientation were restrained to be similar, and only the non-hydrogen atoms of the major component were refined anisotropically (those in the minor component were refined isotropically).

The arene ring C38>C43 was found to be disordered over two sites in a ca. 62:38 for the major and minor components respectively. The geometries of both were optimised using AFIX 66, the thermal parameters were restrained to be similar, and only the non-hydrogen atoms of the major component were refined anisotropically (those in the minor component were refined isotropically).

The isopropyl group C44>C46 was found to be disordered over two sites in a ca. 58:42 ratio for the major and minor components respectively. Their geometries were optimized, the thermal parameters were restrained to be similar, and only the non-hydrogen atoms of the major component were refined anisotropically (those in the minor component were refined isotropically).

The hexane molecule C79>C85 was found to be a 0.5 occupancy molecule by inspection of the thermal ellipsoids.

The hexane molecule C86>C92 was found to be disordered about a special position. The molecule was modelled in the Part -1. The occupancy of the molecule was set at 0.25 by inspection of the thermal ellipsoids.

Crystal Data for C_{83.25}H_{104}Al_{2}N_{4}O_{8}W, M =1526.51, monoclinic, space group P2_1/n (no. 14), a = 13.5044(3) Å, b = 42.6353(10) Å, c = 14.7867(5) Å, β = 103.943(3)°, V = 8262.8(4) Å³, Z = 4, \( \rho_{\text{calc}} \) = 1.227, \( \mu(\text{CuK}\alpha) \) = 3.215 mm\(^{-1}\), \( T = 173.00(10) \), red needles, \( F^2 \) refinement, \( R_1(\text{obs}) = 0.0513, wR_2(\text{all}) = 0.1423, 15844 \) independent observed reflections \( (R_{\text{int}} = 0.0440) \), 12208 independent measured reflections \( [|F_o| > 4\sigma(|F_o|), 2\theta_{\text{full}} = 147.192] \), 989 parameters. CCDC 2130349.
The X-ray structure of S1

Figure S9: The X-ray structure of S1. All hydrogen atoms are omitted for clarity.

Difference electron density maps for the structure of S1 suggested the presence of a second orientation of the whole molecule (of ca. 13% occupancy) overlaying the main occupancy orientation in a manner corresponding to a ca. 180° rotation about an axis passing through the middle of the complex (along the b axis direction, approximately coincident with the C66–C62 bond). Unsurprisingly, the only atom of this second orientation that could be reliably located was the minor occupancy tungsten atom, W1', which was refined anisotropically. The C64-bound m-tolyl group and the O80-based included tetrahydrofuran solvent molecule were both found to be disordered. For the former, two orientations were identified of ca. 67 and 33% occupancy, whilst for the latter three orientations were identified of ca. 52, 30 and 18% occupancy. The geometries of each set of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically).

Crystal data for S1: C_{74}H_{90}Al_{2}N_{4}O_{9}W·C_{4}H_{8}O, M = 1489.41, monoclinic, P2_{1}/c (no. 14), a = 14.9640(6), b = 21.4758(5), c = 24.2362(8) Å, \( \beta = 107.909(4)^\circ \), \( V = 7411.2(4) \text{ Å}^3 \), Z =
$D_c = 1.335 \text{ g cm}^{-3}$, $\mu(\text{Cu-K}\alpha) = 3.592 \text{ mm}^{-1}$, $T = 173 \text{ K}$, orange tablets, Agilent Xcalibur PX Ultra A diffractometer; 14495 independent measured reflections ($R_{int} = 0.0404$), $F^2$ refinement,$^5$ $^6$ $R_1(\text{obs}) = 0.0647$, $wR_2(\text{all}) = 0.1700$, 11508 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$], completeness to $\theta_{\text{full}}(67.7^\circ) = 99.8\%$, 935 parameters. CCDC 2129492.
The X-ray structure of 3c

The W1-based W(CO)$_5$ unit in the structure of 5c was found to be disordered. Two orientations were identified of ca. 70 and 30% occupancy, their geometries were optimised, and the thermal parameters of adjacent atoms were restrained to be similar. All of the atoms of the major occupancy orientation, and the tungsten centre of the minor occupancy orientation, were refined anisotropically (the oxygen and carbon atoms of the minor occupancy orientation were refined isotropically).

The included solvent was found to be highly disordered, and the best approach to handling this diffuse electron density was found to be the SQUEEZE routine of PLATON. This suggested a total of 231 electrons per unit cell, equivalent to 28.9 electrons per asymmetric unit. Before the use of SQUEEZE the solvent most resembled pentane (C$_5$H$_{12}$, 42 electrons), and 0.75 pentane molecules corresponds to 31.5 electrons, so this was used as the solvent present. As a result, the atom list for the asymmetric unit is low by 0.75(C$_5$H$_{12}$) = C$_3$.75H$_9$ (and that for the unit cell low by C$_{30}$H$_{72}$) compared to what is actually presumed to be present.
Crystal data for 3c: C74H90Al2N4O9W·0.75(C5H12), M = 1471.41, monoclinic, I2/a (no. 15), a = 30.6403(15), b = 21.7168(5), c = 23.4001(12) Å, β = 98.775(6)°, V = 15388.4(12) Å³, Z = 8, Dc = 1.270 g cm⁻³, μ(Cu-Kα) = 3.443 mm⁻¹, T = 173 K, orange plates, Agilent Xcalibur PX Ultra A diffractometer; 14796 independent measured reflections (Rint = 0.0484), F² refinement,⁵,⁶ R₁(obs) = 0.0503, wR2(all) = 0.1461, 8502 independent observed absorption-corrected reflections [|Fo| > 4σ(|Fo|), completeness to θ full(67.7°) = 98.9%], 882 parameters. CCDC 2129490.
The crystal of 3d that was studied was found to be a two component twin in a ca. 56:44 ratio, with the two lattices related by the approximate twin law [1.00 0.00 0.00 0.00 –1.00 0.00 –0.09 0.00 –1.00]. The C65-based C(Et)(Me) unit was found to be disordered. Two orientations were identified of ca. 56 and 44% occupancy, their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically). The included solvent was found to be highly disordered, and the best approach to handling this diffuse electron density was found to be the SQUEEZE routine of PLATON. This suggested a total of 159 electrons per unit cell, equivalent to 39.8 electrons per asymmetric unit. Before the use of SQUEEZE the solvent most resembled pentane (C\textsubscript{5}H\textsubscript{12}, 42 electrons), and one pentane molecule corresponds to 42 electrons, so this was used as the solvent present. As a result, the atom list for the asymmetric unit is low by C\textsubscript{5}H\textsubscript{12} (and that for the unit cell low by C\textsubscript{20}H\textsubscript{48}) compared to what is actually presumed to be present.

Figure S11: The X-ray structure of 3d. All hydrogen atoms are omitted for clarity.
Crystal data for S11: C_{70}H_{90}Al_{2}N_{4}O_{9}W·C_{5}H_{12}, M = 1441.41, monoclinic, P2_1/n (no. 14), a = 20.4694(5), b = 17.5544(4), c = 20.6800(4) Å, β = 92.606(2)°, V = 7423.2(3) Å³, Z = 4, D_c = 1.290 g cm⁻³, μ(Cu-Kα) = 3.555 mm⁻¹, T = 173 K, yellow blocks, Agilent Xcalibur PX Ultra A diffractometer; 20698 independent measured reflections (R_{int} = 0.0772), F² refinement, R₁(obs) = 0.0593, wR₂(all) = 0.1749, 15250 independent observed absorption-corrected reflections [||F_o|| > 4σ(|F_o|), completeness to θ_{full}(67.7°) = 98.3%], 813 parameters. CCDC 2129491.
**The X-ray structure of S2**

*Figure S12*: The X-ray structure of S2. All hydrogen atoms are omitted for clarity.

S2 was found to crystallise in the P-1 space group with one included pentane molecule and half of a toluene molecule for a total of two pentane molecules and one toluene molecule within the unit cell.

The included toluene molecule (C84>C90) was found to be disordered across two positions. Inspections of the thermal parameters of the ellipsoids suggest that the molecule has a total of one half occupancy across the two orientations. Their geometries were optimized, the thermal parameters were restrained to be similar, and only the non-hydrogen atoms of the major component were refined isotropically.

The included solvent was found to be highly disordered, and the best approach to handling this diffuse electron density was found to be the SQUEEZE routine of PLATON. This suggested a total of 144 electrons per unit cell, equivalent to 72 electrons per asymmetric unit. Before the use of SQUEEZE the solvent most resembled two pentane molecules (C5H12, 84 electrons), and two pentane molecule corresponds to 84 electrons, so this was used as the solvent present. As a result, the atom list for the asymmetric unit is low by C10H24 (and that for the unit cell low by C20H48) compared to what is actually presumed to be present.
Crystal Data for C_{86.5}H_{104}Al_{2}N_{6}O_{7}W, M = 1577.56, triclinic, space group P-1 (no. 2), a = 13.3538(2) Å, b = 13.8568(4) Å, c = 26.7693(6) Å, α = 75.930(2)°, β = 77.1228(16)°, γ = 83.7504(18)°, V = 4676.11(19) Å³, Z = 2, ρ_{calc}/cm³ = 1.120, μ(Mo Kα) = 1.303 mm⁻¹, T = 172.95(10), violet blocks, F² refinement, R₁(obs) = 0.0435, wR₂(all) = 0.1110, 18515 independent observed reflections (R_{int} = 0.0261), 15316 independent measured reflections [||Fₒ|| > 4σ(|Fₒ|), 2θ_{full} = 56.594], 987 parameters. CCDC 2130351.
4 DENSITY FUNCTIONAL THEORY CALCULATIONS

4.1 – Computational methods

DFT calculations were performed using Gaussian 09 (Revision D.01) using an ultrafine integration grid (int=ultrafine). Geometry optimisations and frequency calculations were performed using the ωB97X functional with SDDAll (W, Al) and 6-31G** (C, H, N, O) basis set. Frequency analyses for all stationary points were performed using the enhanced criteria to confirm the nature of the structures as either minima (no imaginary frequency) or transition states (only one imaginary frequency). The electronic energies of the optimised geometries were calculated using the ωB97XD functional with def2tzvp (W, Al) and 6-311+G** (C, H, N, O) basis sets with solvent corrections (PCM, benzene, ϵ = 2.2706). The Gibbs free energy correction from the frequency calculation was added to this electronic energy to generate Gibbs free energy values for the calculated stationary points.

Intrinsic reaction coordinate (IRC) calculations were used to connect transition states and minima located on the potential energy surface allowing a full energy profile (calculated at 298.15 K, 1 atm) of the reaction to be constructed. Natural Bond Orbital analysis was carried out using NBO 6.0 with the ωB97x functional.

Functional testing was performed with the B3LYP, and B3PW91 in addition to the M06L and ωB97X functionals with SDDAll (W, Al) and 6-31G** (C, H, N, O) basis set. The electronic energies of the optimised geometries were calculated using the corresponding functional with the same basis set with solvent corrections (PCM, benzene, ϵ = 2.2706) and an empirical dispersion correction (Grimme, D3: B3LYP, B3PW91, M06L; Grimme D2: ωB97X).
4.2 – Calculated stationary points

4.2.1 – Transformation of 3a to 4a (Interchange mechanism).

Calculated stationary points for transformation of 3a to 4a.

*Figure S13*: Calculated pathway for transformation of 3a to 4a. All energies in kcal mol$^{-1}$. 

[Diagram showing the calculated pathway for transformation of 3a to 4a with energy levels and structures of 3a, TS-3a_4a, and 4a.]
|      | 3a   | TS-3a_4a | 4a   |
|------|------|----------|------|
| **WBI** |      |          |      |
| W-C1 | 0.51 | 0.56     | 0.61 |
| W-C5 | 0.78 | 0.14     | -    |
| W-O2 | 0.003| 0.05     | 0.17 |
| **NPA** |      |          |      |
| W    | -0.86| -0.51    | -0.43|
| C1   | 0.31 | 0.28     | 0.26 |
| O2   | -1.00| -1.00    | -0.96|
| **Bond distance (Å)** |      |          |      |
| W-C1 | 2.270| 2.197    | 2.167|
| W-C5 | 2.067| 2.876    | -    |
| W-O2 | 3.463| 2.903    | 2.423|

Table S2: Selected calculated NBO data of **3a**, **TS-3a_4a**, and **4a**.
4.2.2 - Calculated mechanism for hydrogenation of 4a.
Figure S14: Calculated pathway for hydrogenation of 4a. All energies in kcal mol$^{-1}$. 
Table S3: Selected calculated NBO data of calculated mechanisms for hydrogenation of 4a.

To find the most plausible mechanism, a range of different pathways were investigated. All alternative pathways found for hydrogenation of 4a are shown below.
Alternative calculated mechanism (a) for hydrogenation of 4a: CO dissociation prior to oxidative addition.
Figure S15: Calculated alternative pathway ($\alpha$) for hydrogenation of 4a. All energies in kcal mol$^{-1}$. 

TS-5a  \hspace{1.5cm} Int-6a  \hspace{1.5cm} TS-6a  

Int-7a
Gibbs Energies

Alternative calculated mechanism (b) for hydrogenation of 4a: concerted CO dissociation migration.
Figure S16: Calculated alternative pathway (b) for hydrogenation of 4a. All energies in kcal mol\(^{-1}\).
Alternative calculated mechanism (C) for hydrogenation of 4a, without CO dissociation.
Figure S17: Calculated alternative pathway (c) for hydrogenation of 4a. All energies in kcal mol$^{-1}$. 
Figure S18: Comparison of key steps of alternative calculated mechanisms (a), (b) and (c) for hydrogenation of 4a with most plausible mechanism. All energies in kcal mol⁻¹.
4.2.3 – Rotation barriers for Int-1

Figure S19: Calculated mechanism for isomerization of Int-1. All energies in kcal mol\(^{-1}\).
4.3 - Functional testing on key stationary points

To investigate the hydrogenation reaction of 4a, functional testing was performed on key stationary points within the calculated pathways. A simplified version of 4a (4a') was used for these calculations.

![Image of chemical structure]

|        | TS-2 | TS-6 | TS-9 | TS-2a | TS-3b | Int-7c | TS-7c |
|--------|------|------|------|-------|-------|--------|-------|
| ωB97xD | 20.0 | 31.1 | 35.7 | 42.5  | 42.0  | 1.7    | 33.2  |
| M06l   | 21.9 | 37.0 | 40.5 | 40.5  | 48.2  | 0.1    | 26.8  |
| b3pw91 | 21.1 | 36.8 | 38.7 | 46.9  | 49.4  | -0.1   | 29.5  |
| b3lyp  | 21.8 | 38.8 | 41.3 | 46.3  | 49.7  | 1.0    | -     |

**Table S4**: All Gibbs free energies provided in kcal mol⁻¹. Gibbs free energies relative to 4a'. TS-7c with b3lyp functional could not be found.
5 NMR SPECTRA
### 6 COMPUTATIONAL COORDINATES

```
01_3.log

SCF (wB97x) = -4032.58831321
E(SCF)+ZPE(0 K)= -4031.018350
H(298 K)= -4030.919353
G(298 K)= -4031.150263

Lowest Frequency = 16.5812 cm⁻¹

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| O       | -1.556713  | 9.158067   | 8.336676   |
| C       | 0.959097   | 12.379280  | 16.703011  |
| H       | 1.782203   | 12.802040  | 16.132301  |
| C       | -1.972912  | 7.194946   | 16.383895  |
| C       | -0.833237  | 10.492665  | 13.048799  |
| C       | 0.549892   | 13.519368  | 8.782457   |
| H       | -0.193985  | 14.148869  | 9.280781   |
| C       | 0.398325   | 11.164660  | 16.298400  |
| C       | -1.446745  | 15.185060  | 15.088301  |
| C       | 2.070464   | 6.932152   | 12.713412  |
| C       | 1.019166   | 16.520312  | 10.070254  |
| H       | 1.991819   | 16.083527  | 9.844201   |
| H       | 1.150432   | 17.563117  | 10.369195  |
| H       | 0.414165   | 16.513037  | 9.157610   |
| C       | -3.333982  | 7.550253   | 16.384923  |
| C       | 2.390260   | 10.515954  | 14.811820  |
| C       | -2.605109  | 14.595318  | 15.614304  |
| C       | 1.757404   | 13.360322  | 9.699511   |
| C       | 0.101986   | 11.097048  | 13.866921  |
| C       | -2.905253  | 14.811165  | 16.961577  |
| H       | -3.797137  | 14.354986  | 17.383989  |
| C       | 2.863981   | 12.645350  | 9.232623   |
| H       | 2.821374   | 12.191209  | 8.245386   |
| C       | 0.235392   | 5.446731   | 12.978611  |
| C       | 1.836926   | 13.923259  | 10.986275  |
| C       | -2.492079  | 17.125012  | 13.415898  |
| H       | -3.428280  | 16.586241  | 13.595009  |
| H       | -2.668795  | 17.909895  | 12.679543  |
| H       | -2.205119  | 17.583500  | 14.365010  |
```

C 0.286576  15.775079  11.156900  C  4.299881  10.354170  13.326771
C  4.641934  10.378592  15.775079  H  4.686670  10.299790  12.312500
H  5.305457  10.345999  16.564992  C  3.623642  7.654787  11.025350
C  3.266879  10.469020  15.899210  H  3.816279  8.076100  10.041194
H  2.868077  10.491215  16.909998  C  -4.202893  7.513341  15.136981
C  -0.587478  15.956031  15.899324  H  -3.664048  6.983071  14.347531
H  0.221394   7.697111  10.973426  C  0.707273  16.574816  15.381413
C  -0.877697  4.936391  13.651864  H  0.880569  16.205727  14.365193
H  -1.180380  3.931265  13.387194  C  4.080542  13.104049  11.253795
C  0.941875  4.511641  12.029617  H  4.986066  13.000554  11.843215
H  1.067128  4.981227  11.051280  C  4.159658  13.965348  14.057484
H  0.378791  3.585310  11.912293  H  3.973314  12.904258  14.241536
H  1.944430  4.272140  12.395601  H  4.112943  14.493385  15.015647
C  2.946410  5.939839  14.926354  H  5.182680  14.078000  13.680407
H  1.871739  5.838841  15.110953  C  0.271224  6.866718  17.589366
C  -1.205177  7.243251  17.566838  H  0.696236  7.153650  16.624509
C  0.870695  10.415066  15.034474  C  -1.530718  5.510371  14.751894
C  2.926105  10.461422  13.525386  C  -4.722570  11.075704  12.043906
H  2.269107  10.502763  12.660670  C  -3.532764  13.725266  14.784314
C  -0.130539  12.178686  8.508053  H  -3.208006  13.766198  13.737698
H  0.546033  11.485118  7.996482  C  0.939261  14.191908  7.457970
H  -1.010804  12.321933  7.872649  H  1.480003  15.131408  7.608767
H  -0.458465  11.714686  9.441290  H  0.042630  14.401926  6.865590
C  3.004658  13.823185  11.770647  H  1.580844  13.536439  6.858968
C  0.484748  13.038865  17.831095  C  -0.829392  16.440320  11.708093
H  0.936726  13.979836  18.134501  H  -1.143663  17.343649  11.198597
C  2.300491  7.490807  11.445246  C  -0.947448  16.168393  17.229308
C  -1.445920  16.157008  12.921894  H  -0.309679  16.780669  17.863281
C  3.144037  6.559864  13.548699  C  -0.661919  10.643562  17.037509
C  -1.143060  11.304892  18.165569  H  -1.112574  9.706658  16.732078
H  -1.967826  10.868108  18.724119  C  -3.909152  7.971350  17.586518
H    1.572515  18.518506  14.939224  C    -4.822679  9.018715  11.427789
H    0.431855  18.538937  16.293952  N    1.059412  14.562446  11.492453
C    1.185815   7.909965   10.498182  N   -1.143756   6.926363  15.302180
C    1.246957   7.145570    9.167575  C    -2.428903   7.391095  11.776038
H    2.155132   7.397736   8.608075  N   -0.850312  15.210368  13.539313
H    0.387289   7.413634    8.545675  N    0.894965   7.023788  13.307268
H    1.239950   6.059719   9.307835  C    -2.465845   9.597258   9.758380
C    1.245728   9.417054  10.226364  O    -5.800031   8.396408  11.352789
H    1.802751  16.489028  17.273533  O    -4.531236  12.385322   9.907334
H    2.832555  16.575064  15.844395  C   -4.033759  11.560309  10.572124
H    2.009537  15.056607  16.252166  O   -2.590586   6.431424  11.184370
H    2.250574   9.733748   9.921868  O   -4.262150  11.680823  14.198172
H    0.959584   9.996922  11.109219  C   -1.398448  11.327086  12.231854
H    0.558133   9.675982   9.421139  O   -2.155936   9.371095   8.666692
                                           C   -1.760677  7.219767  16.580505
02_TS3_4.log  C   -0.639315  10.695290  13.296094  C   -1.922615  15.061644  14.507944
SCF (wB97x) =  -4032.5474530  C    2.185360  7.468472  12.832243
E(SCF)+ZPE(0 K)=  -4030.976674  C    2.015033  16.529205  10.348944
H(298 K)=  -4030.878673  H    2.942101  15.979782  10.181174
G(298 K)=  -4031.108696  H    2.245879  17.562681  10.611136
Lowest Frequency = -138.1393cm-1  H    1.464507  16.531122   9.403309
                                           C   -3.098282  7.661013  16.622637
                                           C   -3.255544  14.982931  14.049115
                                           C    1.067078  13.616268   9.219151
                                           C    0.284638  11.316158  14.099729
                                           C   -4.262459  14.987716  15.018652
W   -3.156274  10.168494  11.603204  H   -5.300368  14.933632  14.711952
Al   -0.041476  13.695456  12.750103  C    1.755776  12.940504   8.208556
Al   -0.132574   8.234071  14.365771  H    1.273520  12.792995   7.245318
O   -1.114901  9.424642  13.527938  C    0.518429   5.763793  13.091513
O   -1.126302  12.570885  11.914719  O    0.280190   5.763793  13.091513
O    0.990846   9.246946  15.218046  O    0.280190   5.763793  13.091513
O    0.655984  12.582964  13.928417

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 4.937981   | 15.108312  | 11.598219  |
| H    | 3.446645   | 15.533948  | 12.449742  |
| H    | 4.757740   | 14.757637  | 13.330947  |
| C    | -0.090451  | 10.903866  | 16.547583  |
| C    | -1.396751  | 11.365069  | 16.383631  |
| C    | 0.330276   | 10.540053  | 17.831845  |
| C    | -2.267516  | 11.450659  | 17.470888  |
| H    | -1.763264  | 11.660481  | 15.405009  |
| C    | 1.346436   | 10.178121  | 17.971653  |
| C    | -1.840677  | 11.079318  | 18.739034  |
| C    | -3.277549  | 11.820436  | 17.309532  |
| C    | -0.186200  | 10.340605  | 19.906395  |
| C    | -2.518402  | 11.137967  | 19.586667  |
| C    | 2.280606   | 11.192889  | 15.625584  |
| C    | 3.376670   | 10.512007  | 15.097736  |
| C    | 2.509564   | 12.341532  | 16.381386  |
| C    | 4.673774   | 10.942751  | 15.361335  |
| C    | 3.208984   | 9.625920   | 14.495260  |
| C    | 3.803855   | 12.788987  | 16.627879  |
| C    | 1.666487   | 12.875370  | 16.803904  |
| C    | 4.895079   | 12.082490  | 16.128850  |
| C    | 5.512907   | 10.382741  | 14.953337  |
| C    | 3.958908   | 13.682440  | 17.228510  |
| C    | 5.908129   | 12.417038  | 16.338567  |

G(298 K) = -3917.838153

Lowest Frequency = 17.4664 cm

H(298 K)= -3917.613759


03_4.log

SCF (wB97x) = -3919.27240046

E(SCF)+ZPE(0 K)= -3917.709899

H(298 K)= -3917.613759

H 3.104422
H 7.665334
H 8.407030
H 9.272682
H 10.186706
| Atom | X       | Y            | Z     |
|------|---------|--------------|-------|
| H    | 12.86553| 10.488980    | 9.209906 |
| H    | 13.852087 | 9.014993    | 9.360170 |
| C    | 9.697850 | -1.086120    | 5.098132 |
| C    | 13.428026 | 4.116604    | 3.202411 |
| C    | 11.329095 | 9.743189    |    9.36 |
| H    | 11.243380 | 10.735835    | 7.777225 |
| C    | 12.014771 | 3.645758    | 3.585467 |
| C    | 13.654072 | 0.630013    | 6.089287 |
| C    | 10.525012 | -1.389176   | 6.808355 |
| H    | 12.808421 | 3.213673    | 8.268388 |
| C    | 11.045091 | 3.799587    | 2.3924846 |
| C    | 12.124429 | 8.833294     | 8.067629 |
| C    | 14.224476 | -0.363151    | 3.793194 |
| H    | 13.190444 | -0.92950     | 3.560146 |
| C    | 8.477775 | -1.952209    | 4.912691 |
| H    | 7.604803 | -1.383528    | 5.253294 |
| C    | 8.549241 | -2.857170    | 5.517077 |
| H    | 8.315431 | -2.223844    | 3.868606 |
| C    | 10.759658 | 9.552221    | 6.097884 |
| C    | 14.600490 | 0.352136    | 5.081117 |
| C    | 8.067099 | 0.572201     | 2.722595 |
| C    | 9.990004 | 2.799825     | 0.458252 |
| H    | 9.835540 | 1.927928     | -0.172579 |
| C    | 7.694070 | 6.373845     | 4.265913 |
| H    | 7.384971 | 6.176312     | 3.232094 |
| H    | 6.866839 | 6.099297     | 4.927021 |

S89
|   | C   | H   | H   | H   | H   | C   | H   |
|---|-----|-----|-----|-----|-----|-----|-----|
| C | 10.136124 | 10.752278 | 5.433168 | C | 15.795885 | 4.061234 | 3.709810 |
| H | 10.702081 | 11.039961 | 4.542205 | H | 16.599105 | 3.780080 | 4.386869 |
| H | 10.105691 | 11.598340 | 6.120330 | C | 10.394929 | 5.292955 | 10.370023 |
| H | 9.119829 | 10.521490 | 5.101481 | H | 10.292469 | 4.875962 | 9.367084 |
| C | 13.526578 | 5.659648 | 10.709822 | H | 9.384797 | 5.484973 | 10.747177 |
| H | 13.175460 | 5.320609 | 11.681034 | H | 10.857124 | 4.538373 | 11.018565 |
| C | 16.317207 | 1.395797 | 6.444092 | C | 15.926131 | 0.731531 | 5.289427 |
| H | 17.355317 | 1.688173 | 6.582418 | H | 16.666449 | 0.520360 | 4.524175 |
| C | 11.137892 | -1.692423 | 2.122315 | C | 13.506000 | 1.308925 | 9.748158 |
| H | 11.608654 | -1.344804 | 3.046410 | H | 14.362545 | 1.911085 | 10.072716 |
| C | 9.534532 | 5.090692 | 1.022967 | H | 13.800696 | 0.255228 | 9.807342 |
| H | 9.026768 | 6.029124 | 0.821889 | H | 12.691436 | 1.478672 | 10.458159 |
| C | 8.070380 | 7.848267 | 4.452819 | C | 15.046522 | 4.986500 | 1.623346 |
| H | 8.398466 | 7.977415 | 5.490451 | H | 15.257744 | 5.445965 | 0.660771 |
| C | 14.839806 | 5.420336 | 10.338596 | C | 14.297437 | -1.884099 | 3.985257 |
| H | 15.513842 | 4.906857 | 11.019463 | H | 15.303344 | -2.182280 | 4.303072 |
| C | 9.229869 | 8.217436 | 3.539663 | H | 14.071907 | -2.410242 | 3.051026 |
| C | 11.217922 | 6.586503 | 10.358874 | H | 13.586028 | -2.232756 | 4.742389 |
| H | 10.725075 | 7.276002 | 9.664989 | C | 15.371850 | 1.688168 | 7.412615 |
| C | 9.324611 | 3.991902 | 0.194860 | H | 15.666837 | 2.225227 | 8.311186 |
| H | 8.646592 | 4.067106 | -0.651434 | C | 7.398435 | 2.926027 | 3.234089 |
| C | 13.523257 | 10.382173 | 3.265195 | H | 8.414580 | 3.313220 | 3.115334 |
| H | 13.627751 | 10.461354 | 2.177581 | H | 6.859321 | 3.575533 | 3.927502 |
| H | 14.508238 | 10.570181 | 3.706039 | H | 6.900845 | 2.995410 | 2.259780 |
| H | 12.849094 | 11.180510 | 3.594340 | C | 15.070352 | 0.083753 | 2.597259 |
| C | 5.992338 | 1.014284 | 4.099011 | H | 15.085258 | 1.175601 | 2.514460 |
| H | 5.321494 | 1.087699 | 3.235242 | H | 14.653177 | -0.324327 | 1.672078 |
| H | 5.577218 | 1.642014 | 4.894051 | H | 16.103709 | -0.274556 | 2.667189 |
| H | 5.978225 | -0.023552 | 4.447417 | C | 12.115359 | -1.431817 | 0.970551 |
| C | 13.015967 | 8.995883 | 3.681054 | H | 11.724500 | -1.800340 | 0.016401 |
| H | 12.994302 | 8.976911 | 4.776179 | H | 13.064378 | -1.947865 | 1.149383 |
| Element | X     | Y     | Z     | Element | X     | Y     | Z     | Element | X     | Y     | Z     |
|---------|-------|-------|-------|---------|-------|-------|-------|---------|-------|-------|-------|
| H       | 12.32 | -0.36 | 0.85  | C       | 14.96 | 6.92  | 6.82  | H       | 14.16 | 6.74  | 6.09  |
| C       | 13.98 | 7.89  | 3.22  | C       | 13.98 | 7.89  | 3.22  | H       | 13.66 | 6.92  | 3.58  |
| H       | 13.66 | 6.92  | 3.58  | H       | 14.99 | 8.09  | 3.60  | O       | 9.78  | 4.31  | 6.71  |
| H       | 14.99 | 8.09  | 3.60  | N       | 10.04 | -0.25 | 4.11  | O       | 5.72  | 4.13  | 6.01  |
| C       | 6.78  | 1.97  | 8.61  | N       | 10.8  | 8.21  | 5.43  | C       | 9.41  | 2.49  | 9.29  |

SCF (wB97x) = -3920.42475443
E(SCF)+ZPE(0 K) = -3918.848881
H(298 K) = -3918.751104
G(298 K) = -3918.978608

Lowest Frequency = -216.1987 cm⁻¹
|   |   |   |   |
|---|---|---|---|
|   |   |   |   |
| H | 16.412227 | 5.426731 | 8.591331 |
| C | 14.493180 | 3.712765 | 3.991193 |
| H | 14.303961 | 3.221250 | 4.943497 |
| C | 9.297876 | -1.079082 | 0.558734 |
| H | 9.740743 | -1.652352 | -0.252686 |
| C | 7.481429 | 1.260033 | 3.704094 |
| H | 8.094355 | -1.652352 | -0.252686 |
| C | 13.243463 | 6.641403 | 8.543285 |
| C | 10.095664 | 10.576578 | 5.439729 |
| H | 10.623090 | 10.865644 | 4.526076 |
| C | 10.081893 | 11.425669 | 6.123683 |
| H | 9.069736 | 10.33238 | 5.150012 |
| C | 13.739942 | 5.597186 | 10.650898 |
| H | 13.437596 | 5.300899 | 11.651812 |
| C | 16.270907 | 1.384348 | 6.589887 |
| H | 17.290984 | 1.705026 | 6.786786 |
| C | 11.307346 | -1.706012 | 1.926328 |
| H | 11.728871 | -1.444520 | 2.901716 |
| C | 9.489810 | 4.965140 | 1.048868 |
| H | 8.960914 | 5.897089 | 0.874211 |
| C | 8.055225 | 7.704710 | 4.440620 |
| H | 8.385629 | 7.807143 | 5.485035 |
| C | 15.016958 | 5.295007 | 10.207031 |
| H | 15.711709 | 4.770806 | 10.858339 |
| C | 9.218303 | 8.073192 | 3.532841 |
| C | 11.456164 | 6.609550 | 10.416937 |
| H | 10.959534 | 7.330413 | 9.759497 |
| C | 9.302828 | 3.885246 | 0.190961 |
| H | 8.621598 | 3.968421 | -0.652031 |
| C | 13.483464 | 10.255237 | 3.307126 |
| H | 13.567367 | 10.382168 | 2.222183 |
SCF (wB97x) = -3920.43862282
E(SCF)+ZPE(0 K)= -3918.861300
H(298 K)= -3918.763625
G(298 K)= -3918.992330
Lowest Frequency = 13.8683 cm⁻¹
C   2.722520 -3.127023 -1.942035  C   -0.630970  5.281709  3.991623
C  -1.012589  5.414265 -0.341693  H   -0.018102  5.873250  4.668480
C   3.694573 -4.163850  0.062199  C   -0.197684 -0.099821  3.657174
C  -0.693047  0.545398  4.787471  H   -0.677286 -1.006667  3.306598
H  -1.555273  0.127047  5.301429  C   -3.389414 -2.779408  4.204076
C   4.763233 -0.334689 -0.097699  H   -4.436749 -2.488099  4.213578
H   5.124301 -0.368936 -1.122082  C   5.131092 -3.350892 -1.708192
C   4.164390 -2.470280 -3.396225  C   3.876201  5.376901 -0.313824
C  -3.674156 -3.253089  1.751912  H   4.824883  5.500498 -0.848589
H  -3.130311 -3.791438  0.971012  H   3.960150  5.898580  0.645576
C   1.056399  5.803049  2.200973  H   3.094404  5.874475 -0.896797
H   1.255289  5.489419  1.170702  C   0.973386 -5.392536  4.472289
C   4.605575  2.510877 -1.964090  H   0.527300 -5.685132  5.430285
H   5.503478  2.421216 -1.360982  H   2.039511 -5.647406  4.505167
C   4.595583  3.274662  0.864892  H   0.513148 -5.998585  3.684237
H   4.429543  2.202842  1.002619  C   1.596354 -3.066254  5.226000
H   4.510950  3.763666  1.841080  H   1.419999 -1.995231  5.083184
H   5.625372  3.425191  0.520900  H   2.665316 -3.256931  5.089107
C   0.790183 -3.890638  4.218738  H   1.352602 -3.325495  6.262760
H   1.206486 -3.662164  3.235082  C  -1.929122 -6.155512  2.157661
C  -0.976816 -5.258796  1.404600  H  -1.796804 -6.059374  3.237823
H  -2.651311  1.417652 -3.593367  H  -1.780849 -7.196687  1.869341
C  -3.120218  2.923257  1.369369  H   -2.963389 -5.878985  1.932561
H  -2.760612  3.009734  0.337471  C  -1.316042 -3.099889  5.368858
C   1.471836  3.565504 -5.785631  H  -0.745644 -3.051609  6.291472
H   1.966770  4.525631 -5.611175  C  -1.789636  4.682553  4.467296
H   0.573103  3.745420 -6.384629  H  -2.081019  4.806711  5.507151
H   2.150471  2.951974 -6.388436  C   3.577553  3.885446 -0.099284
C  -0.374483  5.727964 -1.537872  H   2.598319  3.803015  0.387657
H  -0.687832  6.638302 -2.035211  C   4.967249 -3.938190 -0.465147
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| H  | 5.841943 | -4.232689 | 0.109605 | H  | 4.161251 | -6.815624 | 0.741589 |
| C  | -4.580078 | 3.391413 | 1.381974 | H  | 4.191147 | -6.600782 | 2.500579 |
| H  | -5.035193 | 3.259301 | 2.370056 | H  | 5.472349 | -5.908865 | 1.503783 |
| H  | -5.161072 | 2.801741 | 0.666087 | C  | 0.943116 | 7.333151 | 2.202160 |
| H  | -4.673002 | 4.449832 | 1.113394 | H  | 0.150198 | 7.684417 | 1.534315 |
| C  | 5.657355  | -0.379138 | 0.967095 | H  | 1.883819 | 7.784840 | 1.868094 |
| H  | 6.726964  | -0.443712 | 0.783388 | H  | 0.727546 | 7.712046 | 3.207648 |
| C  | -0.085750 | 1.706717 | 5.249667 | C  | 1.516942 | -2.658689 | -2.754381 |
| H  | -0.467412 | 2.215118 | 6.131537 | C  | 0.797344 | -3.809060 | -3.474700 |
| C  | 4.574858  | 1.938695  | -3.229992 | H  | 1.489875 | -4.360648 | -4.122497 |
| H  | 5.446762  | 1.412102  | -3.609859 | H  | -0.005074 | -3.409744 | -4.105325 |
| C  | -3.026993 | 1.449047 | 1.770937 | H  | 0.334755 | -4.511637 | -2.777855 |
| H  | -2.001552 | 1.070771 | 1.694999 | C  | 1.888922 | -1.585702 | -3.779362 |
| H  | -3.669169 | 0.848349 | 1.125036 | H  | 2.118477 | 5.638930 | 4.106242 |
| H  | -3.349982 | 1.302627 | 2.809147 | H  | 3.171728 | 5.833542 | 2.704578 |
| C  | 2.249023  | 5.358181 | 3.055220 | H  | 2.381741 | 4.272965 | 3.009382 |
| C  | 4.000976  | -3.822184 | 2.525064 | H  | 2.523068 | -1.989602 | -4.577620 |
| H  | 5.027992  | -3.475463 | 2.360885 | H  | 2.409495 | -0.734119 | -3.324849 |
| H  | 3.958018  | -4.299118 | 3.511786 | H  | 0.984784 | -1.208438 | -4.261410 |
| H  | 3.349488  | -2.943102 | 2.528525 | H  | -1.522983 | -1.107216 | -4.071589 |
| C  | -3.922917 | -1.839827 | 1.224877 | C  | -1.152873 | 0.474024 | -1.268378 |
| H  | -4.412722 | -1.220477 | 1.985393 | H  | -0.983881 | -0.899350 | -3.485634 |
| H  | -4.571058 | -1.864926 | 0.342871 | H  | 0.982033 | -1.358364 | 0.938393 |
| C  | -5.006628 | -3.977262 | 1.983979 | 06_TS2.log SCF (wB97x) = -3920.42594079 |
| H  | -4.871117 | -4.962503 | 2.443970 | SCF (wB97x) = -3920.42594079 |
| H  | -5.525742 | -4.113505 | 1.029940 | E(SCF)+ZPE(0 K)= -3918.851583 |
| H  | -5.671235 | -3.399565 | 2.635719 | H(298 K)= -3918.754417 |
| C  | -2.655314 | -2.732055 | 5.378573 | G(298 K)= -3918.981261 |
| H  | -3.124784 | -2.408443 | 6.304224 | Lowest Frequency = -676.2239 cm-1 |
| C  | 4.395912  | -6.108088 | 1.544035 |   |   |   |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| W    | -2.630041 | -0.439863 | -2.708578 |
| Al   | 0.097100 | 2.861611 | -0.454304 |
| Al   | 0.230665 | -2.753226 | 0.799462 |
| O    | -0.629960 | -1.578302 | -0.164051 |
| O    | -1.034649 | 1.777946 | -1.279732 |
| O    | 1.137599 | -1.708908 | 1.849988 |
| O    | 0.923978 | 1.653482 | 0.497533 |
| C    | -4.123290 | -1.113587 | -3.925967 |
| N    | 1.138730 | 3.859077 | -1.703161 |
| C    | -0.825139 | -4.003899 | 1.785579 |
| C    | -4.111788 | 0.305000 | -1.470139 |
| N    | -0.699429 | 4.322896 | 0.416209 |
| N    | 1.239640 | -4.051141 | -0.174556 |
| C    | -2.485153 | -2.324011 | -1.884696 |
| O    | -4.952709 | -1.504094 | -4.629942 |
| O    | -4.952718 | 0.754403 | -0.819595 |
| O    | -2.479672 | 2.369262 | -4.234525 |
| O    | -2.425512 | -3.417409 | -1.515870 |
| C    | 1.469207 | 1.600004 | 3.413466 |
| H    | 2.297922 | 2.031864 | 2.857747 |
| C    | -1.488277 | -3.577762 | 2.998638 |
| C    | -0.365008 | -0.241220 | -0.231483 |
| C    | 1.126780 | 2.837851 | -4.521024 |
| H    | 0.319161 | 3.384944 | -4.023078 |
| C    | 0.910335 | 0.392780 | 2.984650 |
| C    | -1.034566 | 4.399297 | 1.822917 |
| C    | 2.552123 | -3.738676 | -0.697592 |
| C    | 1.456167 | 5.840098 | -3.157657 |
| H    | 2.444455 | 5.433728 | -3.371714 |
| H    | 1.552487 | 6.882064 | -2.843294 |
| H    | 0.866996 | 5.827060 | -4.080370 |
| Atom | X      | Y      | Z      | Atom | X      | Y      | Z      |
|------|--------|--------|--------|------|--------|--------|--------|
| C    | 1.379551 | -0.334600 | 1.706813 | C    | -0.983417 | -5.275938 | 1.401325 |
| C    | 3.388459 | -0.249386 | 0.144884 | C    | -2.537048 | 1.358516  | -3.677266 |
| H    | 2.701954 | -0.236155 | -0.700512 | H    | -3.095112 | 2.916281  | 1.457460  |
| C    | 0.564883 | 1.467734  | -4.900694 | H    | -2.749569 | 2.975427  | 0.418848  |
| H    | 1.319836 | 0.858729  | -5.410805 | C    | 1.521078  | 3.600881  | -5.795242 |
| H    | -0.290243 | 1.581567  | -5.573877 | H    | 2.000160  | 4.561230  | -5.583270 |
| H    | 0.224495 | 0.921985  | -4.017973 | C    | 3.480678  | 3.182765  | -1.453875 |
| C    | 0.982402 | 2.244179  | 4.545759  | C    | -0.405931 | 5.699709  | -1.543405 |
| H    | 1.433525 | 3.178822  | 4.869359  | H    | -0.731909 | 6.602416  | -2.046539 |
| C    | 2.672766 | -3.105582 | 1.950540  | C    | -0.583743 | 5.344216  | 3.992005  |
| C    | -1.023886 | 5.398720  | -0.334568 | H    | 0.033816  | 5.954512  | 4.647860  |
| C    | 3.820761 | -4.123896 | 0.048294  | C    | -0.163435 | -0.133198 | 3.701293  |
| C    | -0.657146 | 0.513179  | 4.832130  | H    | -0.617118 | -1.061790 | 3.375257  |
| H    | -1.492547 | 0.072920  | 5.371660  | C    | -3.444189 | -2.792121 | 4.155963  |
| C    | 4.758280 | -0.318984 | -0.092458 | H    | -4.491097 | -2.498807 | 4.148162  |
| H    | 5.117887 | -0.361939 | -1.116887 | C    | 3.506635  | 3.297529  | -1.740398 |
| C    | 3.960207 | -2.908421 | -2.454351 | H    | 6.077207  | -3.130629 | -2.155700 |
| H    | 4.089057 | -2.433988 | -3.421646 | C    | 3.855174  | 5.385210  | -0.338298 |
| C    | -3.687480 | -3.276070 | 1.698883  | H    | 4.806154  | 5.499144  | -0.870988 |
| H    | -3.122244 | -3.805293 | 0.926109  | H    | 3.937404  | 5.918299  | 0.614843  |
| C    | 1.082522 | 5.831862  | 2.175382  | H    | 3.077605  | 5.878361  | -0.930833 |
| H    | 1.277354 | 5.490855  | 1.153259  | C    | 0.920905  | -5.416622 | 4.451169  |
| C    | 4.598955 | 2.520685  | -1.956245 | H    | 0.458677  | -5.737492 | 5.392354  |
| H    | 5.491865 | 2.440626  | -1.344622 | H    | 1.987942  | -5.665332 | 4.497641  |
| C    | 4.561626 | 3.292613  | 0.867303  | H    | 0.480937  | -6.004090 | 3.638341  |
| H    | 4.391901 | 2.222475  | 1.013010  | C    | 1.524989  | -3.114843 | 5.279844  |
| H    | 4.472848 | 3.790280  | 1.838583  | H    | 1.352909  | -2.039491 | 5.168329  |
| H    | 5.593857 | 3.437298  | 0.528607  | H    | 2.595784  | -3.302692 | 5.152132  |
| C    | 0.735287 | -3.908942 | 4.236075  | H    | 1.265795  | -3.406087 | 6.304451  |
| H    | 1.168600 | -3.652011 | 3.266422  | C    | -1.942799 | -6.175995 | 2.141511  |
H  -1.836776  -6.070735  3.223601  H  -4.476026  -1.259452  1.911610
H  -1.777334  -7.217777  1.864561  H  -4.569548  -1.909354  0.263836
H  -2.974196  -5.912229  1.889429  H  -3.010128  -1.368935  0.906432
C  -1.390765  -3.116559  5.357548  C  -5.013462  -4.018790  1.909966
H  -0.836615  -3.068408  6.290087  H  -4.871837  -5.003047  2.369737
C  -1.731613  4.749706  4.495781  H  -5.518420  -4.159743  0.948964
H  -2.011192  4.892657  5.536176  H  -5.693502  -3.451145  2.554689
C   3.551209  3.896878  -0.109019  C  -2.729496  -2.745395  5.342747
H   2.569174  3.822482  0.373469  H  -3.214252  -2.419922  6.259835
C   4.944596  -3.883088  -0.493237  C   4.432274  -6.048373  1.531303
H   5.829647  -4.164107  0.072344  H   4.217508  -6.760270  0.727013
C  -4.552739  3.392119  1.480784  H   4.238249  -6.547696  2.486669
H  -4.994504  3.281525  2.477433  H   5.503324  -5.821488  1.494004
H  -5.148578  2.795042  0.783835  C   0.964400  7.361000  2.135109
H  -4.643219  4.445822  1.194016  H   0.170009  7.691283  1.458369
C   5.654567  -0.336469  0.971517  H   1.903374  7.806206  1.787775
H   6.724697  -0.388249  0.786727  H   0.748628  7.766616  3.130086
C  -0.083273  1.703811  5.260734  C   1.450352  -2.653031  -2.746369
H  -0.464292  2.214187  6.141760  C   0.712115  -3.809391  -3.437573
C   4.585833  1.946818  -3.221293  H   1.387515  -4.365496  -4.099914
H   5.465515  1.426857  -3.592174  H  -0.104797  -3.406427  -4.046199
C  -2.998596  1.453506  1.900747  H   0.265073  -4.507147  -2.725896
H  -1.976322  1.069466  1.814611  C   1.791501  -1.594428  -3.795409
H  -3.655841  0.831966  1.290206  H   2.152796  5.726305  4.080461
H  -3.299098  1.338879  2.949291  H   3.200463  5.877698  2.670238
C   2.278955  5.413601  3.038092  H   2.412602  4.327390  3.025358
C   3.974408  -3.775064  2.515626  H   2.407799  -2.007877  -4.603341
H   4.992705  -3.401354  2.355999  H   2.320129  -0.734286  -3.366132
H   3.939720  -4.255258  3.501495  H   0.866683  -1.232182  -4.248907
H   3.299703  -2.913704  2.518558  H  -1.963363  -1.151754  -4.172406
C  -3.949723  -1.867178  1.165834  C  -1.190798  0.478160  -1.213220
### 07_Int2.log

**SCF (wB97x) =** -3920.42725268

**E(SCF)+ZPE (0 K) =** -3918.851732

**H(298 K) =** -3918.754359

**G(298 K) =** -3918.981534

**Lowest Frequency =** 15.5464 cm⁻¹

| Atom | x    | y    | z    |
|------|------|------|------|
| H    | -0.987138 | -0.719304 | -3.237180 |
| C    | 9.024347  | 1.644422  | 0.502138  |
| O    | -0.636672  | -1.585939  | -0.141005  |
| O    | 1.145028  | -1.716367  | 1.857910  |
| O    | 0.924347  | 1.644422  | 0.502138  |
| W    | -2.606099  | -0.455622  | -2.711494  |
| Al   | 0.094743  | 2.852065  | -0.448272  |
| Al   | 0.238114  | -2.762373  | 0.808637  |
| O    | -1.049046 | 1.766886  | -1.259893  |
| O    | 1.145028  | -1.716367  | 1.857910  |
| O    | 0.924347  | 1.644422  | 0.502138  |
| C    | -0.182628  | 3.590815  | 2.993921  |
| C    | 0.914342  | 0.384516  | 2.995210  |
| C    | -2.850183  | 5.817503  | -4.080390  |
| C    | 1.134215  | 2.836709  | -4.541228  |
| C    | 0.317745  | 3.371448  | -4.043806  |
| C    | 0.914342  | 0.384516  | 2.995210  |
| C    | -2.850183  | 5.817503  | -4.080390  |
| W    | -2.606099  | -0.455622  | -2.711494  |
| Al   | 0.094743  | 2.852065  | -0.448272  |
| Al   | 0.238114  | -2.762373  | 0.808637  |
| O    | -1.049046 | 1.766886  | -1.259893  |
| O    | 1.145028  | -1.716367  | 1.857910  |
| O    | 0.924347  | 1.644422  | 0.502138  |
| C    | -0.182628  | 3.590815  | 2.993921  |
| C    | 0.914342  | 0.384516  | 2.995210  |
| C    | -2.850183  | 5.817503  | -4.080390  |
| C    | 1.134215  | 2.836709  | -4.541228  |
| C    | 0.317745  | 3.371448  | -4.043806  |
| C    | 0.914342  | 0.384516  | 2.995210  |
| C    | -2.850183  | 5.817503  | -4.080390  |
| C    | 1.134215  | 2.836709  | -4.541228  |
| C    | 0.317745  | 3.371448  | -4.043806  |
| C    | 0.914342  | 0.384516  | 2.995210  |
| C    | -2.850183  | 5.817503  | -4.080390  |
H  0.751651  -2.203344  -2.030032  C  1.101314  5.827810  2.166891
C  -0.269872  -5.861911  0.336922  H  1.293756  5.473505  1.148953
H  -0.515467  -6.888420  0.095303  C  4.592448  2.510896  -1.958551
C  1.638433  -6.283799  -1.165256  H  5.483763  2.431451  -1.344621
H  2.091406  -5.804112  -2.032975  C  4.554755  3.287807  0.861653
H  0.999805  -7.105104  -1.495379  H  4.386203  2.217980  1.010399
H  2.449435  -6.707259  -0.562956  H  4.466663  3.788002  1.831611
C  3.590200  -4.776341  1.434557  H  5.586474  3.432593  0.521552
H  2.547792  -5.067070  1.608313  C  0.723007  -3.928250  4.243733
C  -0.752151  -3.545190  4.194240  H  1.163334  -3.661936  3.279604
C  1.383248  -0.341316  1.716509  C  -0.978086  -5.286198  1.395807
C  3.389549  -0.254871  0.152006  C  -2.519314  1.318125  -3.719140
H  2.702158  -0.246773  -0.692775  C  -3.090260  2.918141  1.496740
C  0.585243  1.470603  -4.954074  H  -2.754347  2.969499  0.454503
H  1.351239  0.873940  -5.462430  C  1.540508  3.621533  -5.798992
H  -0.257866  1.593584  -5.640653  H  2.017346  4.578626  -5.568839
H  0.230221  0.905243  -4.090207  H  0.659730  3.815654  -6.419901
C  3.472224  3.171500  -1.458800  H  2.246617  3.042506  -6.404431
C  0.978194  2.241911  4.549404  C  -0.417143  5.683252  -1.540319
H  1.422151  3.182012  4.867013  H  -0.746971  6.584365  -2.043824
C  2.685415  -3.104976  -1.939722  C  -0.554668  5.356648  3.995931
C  -1.026850  5.386292  -0.326626  H  0.067222  5.971310  4.643049
C  3.691235  -4.124146  0.060166  C  -0.149850  -0.149450  3.719962
C  -0.643000  0.496158  4.851557  H  -0.596190  -1.083513  3.399613
H  -1.470932  0.049718  5.397556  C  -3.453947  -2.802864  4.139372
C  4.759241  -0.321230  -0.086713  H  -4.499904  -2.506318  4.125135
H  5.117652  -0.366737  -1.111406  C  5.098646  -3.297691  -1.727156
C  3.973383  -2.907994  -2.442218  H  6.090038  -3.131091  -2.141365
H  4.102363  -2.432910  -3.409257  C  3.846293  5.376194  -0.349708
C  -3.680320  -3.275930  1.678245  H  4.795392  5.488017  -0.886141
H  -3.108069  -3.798788  0.906051  H  3.932333  5.912140  0.601429
| X   | Y   | Z   |
|-----|-----|-----|
| 3.066976 | 5.868082 | -0.940985 |
| 0.907363  | -5.437965  | 4.445331  |
| 0.438384  | -5.768003  | 5.379986  |
| 1.974165  | -5.686562  | 4.497292  |
| 0.473931  | -6.017748  | 3.623629  |
| 1.506196  | -3.145331  | 5.300744  |
| 1.336415  | -2.068623  | 5.199204  |
| 2.577614  | -3.333183  | 5.178171  |
| 1.239802  | -3.446774  | 6.320568  |
| -1.943917 | -6.186793  | 2.126715  |
| -1.844758 | -6.085583  | 3.209858  |
| -1.779362 | -7.227961  | 1.847159  |
| -2.973023 | -5.919797  | 1.868736  |
| -1.409725 | -3.136265  | 5.354662  |
| -0.862092 | -3.091763  | 6.291237  |
| -1.699442 | 4.765133   | 4.511966  |
| -1.972005 | 4.917672   | 5.553102  |
| 3.542841  | 3.888449   | -0.115392 |
| 2.561579  | 3.814959   | 0.368712  |
| 4.955656  | -3.883000  | -0.479853 |
| 5.840168  | -4.163806  | 0.086689  |
| -4.544731 | 3.403334   | 1.532258  |
| -4.978729 | 3.294992   | 2.532539  |
| -5.150090 | 2.811549   | 0.839453  |
| -4.630451 | 4.457953   | 1.247447  |
| 5.656832  | -0.332830  | 0.976270  |
| 6.726852  | -0.382461  | 0.790287  |
| -0.078348 | 1.693999   | 5.272326  |
| -0.459151 | 2.203956   | 6.153691  |
| 4.583577  | 1.938653   | -3.224204 |
| 5.464477  | 1.419459   | -3.593233 |

S103
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| H       | 0.286254 | -4.509916| -2.730870|
| C       | 1.801487 | -1.583208| -3.776824|
| H       | 2.176394 | 5.750117 | 4.070762 |
| H       | 3.220745 | 5.876941 | 2.656158 |
| H       | 2.430640 | 4.334144 | 3.037487 |
| H       | 2.418403 | -1.98866 | -4.588384|
| H       | 2.328579 | -0.724884| -3.341576|
| H       | 0.872846 | -1.221496| -4.222881|
| H       | -2.237117| -1.165822| -4.281670|
| C       | -1.197815| 0.468535 | -1.189785|
| H       | -0.906053| -0.610502| -3.089562|

08_TS3.log

SCF (wB97x) = -3920.42621948
E(SCF)+ZPE(0 K)= -3918.851855
H(298 K)= -3918.754855
G(298 K)= -3918.981719
Lowest Frequency = -412.5183 cm⁻¹

W  -3.027619 10.295764 10.638424
    10.638424
Al  -0.354780 13.576224 12.868813
    12.868813
Al  -0.218190 7.969574 14.143455
    14.143455
O    -1.094594 9.144432 13.190277
    13.190277
O    -1.491919 12.498205 12.048753
    12.048753
O    0.674409 9.017098 15.200524
    15.200524
O    0.471690 12.379089 13.830747
    13.830747
C    -4.565016 9.482145 9.524172
    9.524172
N    0.685722 14.572917 11.612936
    11.612936
N    -1.272687 6.713078 15.119095
    15.119095

C    -4.511619 11.095227 11.814476
N    -1.153169 15.043751 13.731562
N    0.785704 6.679101 13.153409
C    -2.828829 8.402501 11.445440
O    -5.383250 8.989621 8.880327
O    -5.339569 11.602779 12.425168
O    -2.974835 13.066696 9.042515
O    -2.772277 7.301987 11.789851
C    0.983877 12.328839 16.761610
H    1.816490 12.760523 16.211786
H    -1.935187 7.138183 16.332044
C    -0.823939 10.478694 13.120221
C    0.691860 13.581985 8.777654
H    -0.114083 14.134789 9.272117
C    0.430145 11.120454 16.329845
C    -1.490427 15.124913 15.137462
C    2.088614 7.002897 12.612839
C    1.016649 16.558865 10.167698
C    2.003284 16.148034 9.954657
C    1.118777 17.597633 10.490852
C    0.431131 16.557346 9.242670
C    -3.329275 7.501957 16.299999
C    2.423913 10.524023 14.810439
C    -2.651897 14.514598 15.633525
C    1.856337 13.427214 9.750249
C    0.125358 11.081904 13.908685
C    -2.976102 14.701073 16.979564
H    -3.870369 14.228137 17.377992
C    2.998951 12.753064 9.308010
H    3.003086 12.321921 8.309807
C    0.378499 5.413023 13.005013

S104
| Element | X       | Y       | Z       | Element | X       | Y       | Z       |
|---------|---------|---------|---------|---------|---------|---------|---------|
| C       | 1.874108| 13.962692| 11.052135| C       | 2.184834| 7.643759| 11.361972|
| C       | -2.538316| 17.069226| 13.469593| C       | -1.474147| 16.119177| 12.979230|
| H       | -3.472898| 16.518783| 13.619195| C       | 3.231054| 6.621651| 13.339425|
| H       | -2.707875| 17.865874| 12.744307| C       | -1.153513| 11.242652| 18.163389|
| H       | -2.275181| 17.512195| 14.432771| H       | -1.993145| 10.802703| 18.696607|
| C       | 0.278304| 15.776695| 11.223577| C       | 4.304503| 10.397113| 13.286559|
| C       | 4.695421| 10.443648| 15.657122| H       | 4.672114| 10.346677| 12.265346|
| H       | 5.377266| 10.431356| 16.503980| C       | 3.462546| 7.858502| 10.840982|
| C       | 3.322722| 10.502129| 15.879725| H       | 3.571134| 8.341545| 9.875265|
| H       | 2.944010| 10.518085| 16.892188| C       | -4.128583| 7.459782| 15.028116|
| C       | -0.655888| 15.893042| 15.976446| H       | -3.562098| 6.933676| 14.253684|
| H       | 0.233034| 8.502731| 11.304942| C       | 0.634934| 16.544269| 15.490105|
| C       | -0.723057| 4.865685| 13.672569| H       | 0.832395| 16.193134| 14.472007|
| H       | -0.965381| 3.837507| 13.434969| C       | 4.134305| 13.204109| 11.374618|
| C       | 1.174380| 4.450340| 12.155320| H       | 5.022665| 13.114418| 11.991447|
| H       | 1.621541| 4.930953| 11.285121| C       | 4.104968| 14.000779| 14.190363|
| H       | 0.535478| 3.627844| 11.828639| H       | 3.934626| 12.932076| 14.343603|
| H       | 1.989461| 4.027961| 12.752999| H       | 4.017754| 14.504955| 15.158419|
| C       | 3.155921| 5.959095| 14.710436| H       | 5.136710| 14.142888| 13.848877|
| H       | 2.121027| 5.646840| 14.891802| C       | 0.287153| 6.796981| 17.568424|
| C       | -1.187036| 7.183523| 17.526848| H       | 0.715766| 7.025739| 16.589729|
| C       | 0.911143| 10.393883| 15.056796| C       | -1.427685| 5.441057| 14.733981|
| C       | 2.932910| 10.470482| 13.512261| C       | -2.999325| 12.072796| 9.629749|
| H       | 2.252993| 10.480048| 12.661654| C       | -3.562977| 13.659036| 14.770775|
| C       | 0.111821| 12.229908| 8.361639| H       | -3.215244| 13.714276| 13.732678|
| H       | 0.863238| 11.615265| 7.852876| C       | 1.120569| 14.358997| 7.522554|
| H       | -0.728770| 12.373249| 7.675566| H       | 1.614634| 15.306278| 7.756944|
| H       | -0.255392| 11.671809| 9.224777| H       | 0.247647| 14.571196| 6.896383|
| C       | 3.021310| 13.880374| 11.869649| H       | 1.818810| 13.766720| 6.920845|
| C       | 0.487026| 12.974517| 17.88713| C       | -0.853544| 16.418204| 11.771424|
| H       | 0.934452| 13.910392| 18.213998| H       | -1.174877| 17.322729| 11.268494|

S105
H  3.833363  3.995736  13.996398  W  -2.544035  -0.427044  -2.719357
H  3.853970  4.194160  15.758028  Al  0.100981  2.853003  -0.492125
H  5.100081  4.956073  14.768849  Al  0.263724  -2.744250  0.790970
C  0.524112  18.073497  15.435232  O  -0.585570  -1.581388  -0.207161
H  -0.264387  18.401070  14.750304  O  -0.986175  1.795264  -1.375334
H  1.467316  18.511325  15.089902  O  1.106244  -1.689619  1.876453
H  0.303788  18.489015  16.425150  O  0.923622  1.676596  0.495168
C  0.945949  8.081609  10.585034  C  -4.162782  -1.285074  -3.661603
C  0.232209  6.919482  9.878274  N  1.171895  3.867578  -1.719515
H  0.916230  6.395986  9.198420  N  -0.795685  -4.003960  1.756808
H  -0.601321  7.313380  9.286378  C  -3.944775  0.448354  -1.532338
H  -0.186863  6.194606  10.580105  N  -0.690721  4.329973  0.370676
C  1.245547  9.170370  9.554771  N  1.269031  -4.034924  -0.202680
H  1.698380  16.454047  17.399959  C  -2.343801  -2.313260  -1.886958
H  2.751376  16.581891  15.991434  O  -5.027156  -1.812974  -4.206330
H  1.952208  15.041101  16.362146  O  -4.760476  0.995203  -0.924319
H  1.860334  8.790660  8.729070  O  -2.617712  2.309171  -4.381093
H  1.760361  10.032979  9.996194  O  -2.312807  -3.412918  -1.540897
H  0.302880  9.517838  9.126377  C  1.402124  1.628733  3.425798
H  -2.468198  9.638336  9.085516  C  2.234714  2.061120  2.876710
C  -1.651251  11.195678  12.121984  C  -1.454305  -3.580015  2.972385
H  -1.271360  10.418704  10.593196  C  -0.328302  -0.242429  -0.252048
          C  1.166456  2.878886  -4.548422

09_Int3.log

SCF (wB97x)  =  -3920.43031309
E(SCF)+ZPE(0 K)=  -3918.852999
H(298 K)=  -3918.755817
G(298 K)=  -3918.983359
Lowest Frequency = 13.6270 cm⁻¹

      H  0.375793  3.454704  -4.056340
      C  0.854148  0.417189  2.995631
      C  -1.024374  4.419530  1.776429
      C  2.562232  -3.700326  -0.760089
      C  1.523315  5.852403  -3.161859
      H  2.503984  5.429116  -3.378329
      H  1.641757  6.885735  -2.826499
      H  0.939033  5.872166  -4.087521

S107
| C  | -2.809741 | -3.208078 | 2.943293 | C  | 1.346224 | -0.310969 | 1.728841 |
| C  | 2.863904  | -0.187214 | 1.504311 | C  | 3.391129 | -0.249209 | 0.213749 |
| C  | -2.185871 | 3.816559  | 2.280228 | H  | 2.721796 | -0.238923 | -0.644999|
| C  | 2.329527  | 2.706578  | -3.577158| C  | 0.552505 | 1.537115  | -4.947405|
| C  | 0.581425  | 0.368992  | 0.564154 | H  | 1.286201 | 0.895729  | -5.448581|
| C  | -2.509286 | 4.017784  | 3.624459 | C  | 2.863904 | -0.187214 | 1.504311 |
| H  | -3.404120 | 3.550397  | 4.028130 | C  | 3.987151 | 3.148023  | -1.458456|
| C  | 3.458827  | 1.576907  | -5.013335| C  | 0.899122 | 2.276989  | 4.548542 |
| C  | 0.867479  | -5.303250 | -0.347273| H  | 1.341645 | 3.216133  | 4.871217 |
| C  | 2.353847  | 3.245904  | -2.277010| C  | 2.634821 | -3.054538 | -2.009824|
| C  | -2.066093 | 6.362168  | 0.104647 | C  | -1.000746| 5.409608  | -0.379830|
| H  | -3.001260 | 5.812955  | 0.255072 | C  | 3.718723 | -4.073386 | -0.051839|
| H  | -2.233593 | 7.156100  | -0.624268| C  | -0.736790| 0.540937  | 4.822805 |
| H  | -1.804466 | 6.809610  | 1.066243 | H  | -1.577092| 0.100389  | 5.354615 |
| C  | 0.771437  | 5.070242  | -2.114532| C  | 4.765423 | -0.329326 | 0.006939 |
| C  | 5.124290  | -0.268809 | 2.381964 | H  | 5.146567 | -0.385788 | -1.009035|
| H  | 5.794502  | -0.276941 | 3.238154 | C  | 3.902258 | -2.815616 | -2.544918|
| C  | 3.748765  | -0.205333 | 2.585524 | H  | 3.991331 | -2.324975 | -3.509019|
| H  | 3.357148  | -0.180660 | 3.598893 | C  | -3.645421| -3.241491 | 1.671166 |
| C  | -0.186519 | 5.191848  | 2.608722 | H  | -3.081593| -3.770917 | 0.897152 |
| H  | 0.655888  | -2.270045 | -2.040753| C  | 1.109913 | 5.828266  | 2.117863 |
| C  | -0.233027 | -5.853873 | 0.319589 | H  | 1.309247 | 5.459620  | 1.106446 |
| H  | -0.469137 | -6.884258 | 0.084992 | C  | 4.600896 | 2.451576  | -1.949873|
| C  | 1.669158  | -6.265545 | -1.192354| H  | 5.486897 | 2.349678  | -1.331457|
| H  | 2.118126  | -5.786610 | -2.062541| C  | 4.583116 | 3.269933  | 0.862345 |
| H  | 1.034399  | -7.091443 | -1.518550| H  | 4.400726 | 2.204811  | 1.025012 |
| H  | 2.483483  | -6.683453 | -0.590234| H  | 4.502194 | 3.782919  | 1.826337 |
| C  | 3.667704  | -4.747471 | 1.314349 | H  | 5.616145 | 3.397707  | 0.518683 |
| H  | 2.643266  | -5.092160 | 1.496027 | C  | 0.764909 | -3.944203 | 4.211946 |
| C  | -0.705376 | -3.544740 | 4.166362 | H  | 1.183275 | -3.790257 | 3.214248 |

S108
10_TS4.log

SCF (wB97x) = -3920.41101624

E(SCF)+ZPE(0 K) = -3918.833187

H(298 K) = -3918.736730

G(298 K) = -3918.961495

Lowest Frequency = -37.4264 cm⁻¹
|   |   |   |   |
|---|---|---|---|
| C | 1.034403 | 5.718536 | 2.222350 |
| H | 1.260781 | 5.424763 | 1.191989 |
| C | 4.619156 | 2.357419 | -1.921340 |
| H | 5.507215 | 2.228916 | -1.310556 |
| C | 4.646250 | 3.183227 | 0.893393 |
| H | 4.466934 | 2.116592 | 1.046998 |
| H | 4.570913 | 3.685875 | 1.863741 |
| C | 0.861477 | -3.906898 | 4.256212 |
| H | 1.230143 | -3.874526 | 3.227761 |
| C | -0.958916 | -5.251021 | 1.482025 |
| C | -3.446758 | 1.477494 | -2.321406 |
| C | -3.199859 | 3.034453 | 1.126947 |
| H | -2.789144 | 3.163902 | 0.120482 |
| C | 1.622909 | 3.546429 | -5.789703 |
| H | 2.205816 | 4.457124 | -5.618991 |
| H | 0.754821 | 3.803970 | -6.405828 |
| H | 2.246723 | 2.861439 | -6.374422 |
| C | -0.242333 | 5.763639 | -1.566962 |
| H | -0.508435 | 6.693586 | -2.055733 |
| C | -0.723887 | 5.173753 | 3.943289 |
| H | -0.118057 | 5.719103 | 4.664054 |
| C | -0.322934 | -0.032535 | 3.625510 |
| H | -0.828783 | -0.905491 | 3.226551 |
| C | -3.295466 | -2.716884 | 4.308919 |
| H | -4.336142 | -2.403752 | 4.339621 |
| C | 4.962969 | -3.226913 | -1.961171 |
| H | 5.926041 | -3.029902 | -2.425614 |
| C | 3.940838 | 5.285799 | -0.278346 |
| H | 4.891243 | 5.407134 | -0.810997 |
| H | 4.028652 | 5.797583 | 0.686501 |
C   -3.196974  1.535576  1.435379   H   0.224458 -4.598734  -2.810152
H   -2.182903  1.120643  1.415804   C   1.488982 -1.511479  -3.736829
H   -3.797413  0.993633  0.697200   H   2.047224  5.505182  4.150385
H   -3.613275  1.339759  2.431652   H   3.134525  5.712993  2.775514
C    2.198637  5.242130  3.097280   H   2.318899  4.157088  3.032209
C    4.041036 -3.813039  2.344226   H   2.082898 -1.820682  -4.605890
H    5.037714 -3.393794  2.164540   H   1.988703 -0.656208  -3.266387
H    4.050993 -4.310256  3.322170   H   0.521391 -1.169725  -4.115847
H    3.333633 -2.978572  2.381904   H  -2.578992  0.605717  -3.926196
C   -3.831197 -1.730673  1.345040   C  -1.120660  0.445898  -1.299359
H   -4.304639 -1.110595  2.115048   H  -0.797260  0.081239  -2.353268
H   -4.481073 -1.719783  0.461934
H   -2.877766 -1.266212  1.073520   11_Int4.log
C   -4.977330 -3.843618  2.090485
H   -4.866105 -4.843792  2.523807   SCF (wB97x) =  -3920.41607082
H   -5.517692 -3.939630  1.143246   E(SCF)+ZPE(0 K) =  -3918.838555
H   -5.611112 -3.260668  2.767418   H(298 K) =  -3918.741140
H   -2.538593 -2.690094  5.470614   G(298 K) =  -3918.969300
H   -2.984590 -2.361349  6.405892   Lowest Frequency = 13.8025 cm^-1
C    4.580158 -6.040085  1.292896
H    4.376133 -6.740381  0.475377   W  -2.704692 -0.306880  -2.666657
H    4.441573 -6.572491  2.239703   Al  0.028502  2.876996  -0.495828
H    5.636852 -5.758514  1.231000   Al  0.264580 -2.720905  0.742433
C    0.939387  7.249796  2.254615   O   -0.470179  1.598669  -0.382732
H    0.171336  7.626264  1.571680   O  -1.148109  1.838236  -1.266746
H    1.895310  7.696839  1.959619   O  1.070125  1.661000  1.840046
H    0.697817  7.608126  3.261909   O  0.898730  1.696594  0.444558
C    1.266426 -2.662200 -2.755790   C  -1.862962  1.660904  -3.954253
C    0.594197 -3.829727 -3.493435   N  1.105240  3.857025  -1.752396
H    1.288670 -4.298378 -4.201348   N  -0.795152  3.916288  1.808609
H   -0.266249 -3.462717 -4.065641   C  -4.656362  0.774281  -3.014487
N  -0.715878  4.390732  0.350104  C  -2.029029  6.462629  0.091605
N  1.221743  -4.063326  -0.216915  H  -2.992350  5.951714  0.195775
C  -2.814341  -1.984316  -1.523722  H  -2.141181  7.287267  -0.613357
O  -1.417909  -2.371536  -4.742297  H  -1.776198  6.863901  1.075342
O  -5.770613  -1.020026  -3.179298  C  0.743394  5.072340  -2.148659
O  -4.189642  2.443188  -1.830459  C  5.113518  -0.394675  2.337931
O  -2.949614  -3.043926  -1.077921  H  5.776871  -0.444575  3.190872
C  1.463496  1.613141  3.402396  C  3.739915  -0.286490  2.534044
H  2.338152  2.006048  2.889869  H  3.342159  -0.269605  3.545358
C  -1.348466  -3.498229  3.084567  C  -0.222247  5.165757  2.622446
C  -0.300899  -0.243887  -0.349361  H  0.647204  -3.117723  -2.447857
C  1.047931  2.852300  -4.572130  C  -0.415120  -5.760812  0.297240
H  0.286283  3.462519  -4.076387  H  -0.748477  -6.758200  0.040305
C  0.855557  0.451024  2.923939  C  1.355756  -6.233931  -1.368376
C  -1.075789  4.461493  1.749343  H  1.427537  -5.779150  -2.35934
C  2.551524  -3.819425  -0.738557  H  0.789117  -7.162488  -1.442481
C  1.510028  5.821514  -3.210399  H  2.376661  -6.465596  -1.052078
H  2.478205  5.370093  -3.426395  C  3.514604  -4.832279  1.428981
H  1.657675  6.855631  -2.89706  H  2.448416  -4.933038  1.657915
H  0.922209  5.844702  -4.133809  C  -0.513480  -3.492559  4.221191
C  -2.697399  -3.109792  3.179260  C  1.342119  -0.293583  1.663670
C  2.863070  -0.212924  1.447580  C  3.398079  -0.267850  0.160523
C  -2.276582  3.895351  2.203253  H  2.738292  -0.206861  -0.701639
C  2.216909  2.655299  -3.611924  C  0.378290  1.529650  -4.947580
C  0.582237  0.378076  0.490610  H  1.076901  0.862193  -5.465551
C  -2.608799  4.037285  3.551764  H  -0.478426  1.704732  -5.606815
H  -3.531162  3.594712  3.920082  H  0.005258  1.014761  -4.061519
C  3.328394  1.934958  -4.059425  C  3.418987  3.090724  -1.509233
H  3.307090  1.494272  -5.053624  C  0.970140  2.259776  4.531395
C  0.698050  -5.282035  -0.401441  H  1.463473  3.157330  4.896246
C  2.266514  3.203292  -2.315850  C  2.738231  -3.252958  -2.011699
C   -4.657513  3.647360  1.362060
H   -5.108313  3.407652  2.331680
H   -5.264665  3.170723  0.585998
H   -4.722827  4.732607  1.225084
C    5.634992 -0.457493  1.048173
H    6.706843 -0.553981  0.893595
C   -0.153439  1.769017  5.189644
H    0.538564  2.280019  6.068603
C    4.454332  1.780193 -3.266890
H    5.306174  1.213019 -3.633897
C    3.141258  1.642809  1.537176
H    2.121990  1.256146  1.427077
H    3.785550  1.099333  0.837822
H    3.469323  1.411989  2.558231
C    2.270835  5.336340  3.015374
H    4.200168 -3.751758  2.299952
H    1.727941 -4.729376  1.126991
H    3.855550  1.099333  0.837822
H    3.469323  1.411989  2.558231
C    2.270835  5.336340  3.015374
C    4.140353 -3.940139  2.505065
H    4.072611 -4.422848  3.486707
H    3.633805 -2.971261  2.551769
H    3.785550 -1.576584  1.550450
H    4.195417 -0.978893  2.373684
H    4.467857 -1.485958  0.696218
H    -2.826416 -1.139301  1.257900
C    -4.989810 -3.681622  2.226586
H    -4.902691 -4.699917  2.621761
C    -5.554076 -3.727541  1.289553
H    -5.588083 -3.102601  2.938708
H    -2.398238 -2.746675  5.558039
C    -2.806476 -2.458941  6.523573
H    3.680682 -6.899702  0.715037
H    3.518571 -6.899702  0.715037

SCF (wB97x) =  -3920.40701687
E(SCF)+ZPE(0 K)= -3918.828892
H(298 K)= -3918.732057
G(298 K)= -3918.957865
Lowest Frequency = -131.3931 cm^-1

W   -3.040508  10.548415
     10.536381
| Atomic Symbol | Atomic Coordinates |
|---------------|--------------------|
| C             | 2.919222 10.442963 13.592426 |
| H             | 2.246518 10.460785 12.737676 |
| C             | -0.174617 12.277274 8.318346 |
| H             | 0.503489 11.633080 12.737676 |
| C             | -1.070287 12.453092 7.712668 |
| H             | -0.477827 11.73691 9.215606 |
| C             | 2.932895 13.783266 11.708844 |
| H             | 0.489187 13.058167 17.867263 |
| C             | 2.370816 7.602070 11.550349 |
| C             | -1.515741 16.076464 12.971670 |
| C             | 3.287018 6.562956 13.579496 |
| C             | -1.077342 11.285114 18.279223 |
| H             | 1.871995 10.835050 18.870847 |
| C             | 4.293082 10.355682 13.387445 |
| C             | 4.676850 10.296672 12.372248 |
| C             | 3.676639 7.774791 11.087841 |
| C             | 3.844035 8.248903 10.125088 |
| C             | -4.10682 7.574653 14.796867 |
| C             | -3.525168 7.059043 14.053085 |
| C             | 0.776781 16.527309 15.288553 |
| H             | 0.920175 16.087223 14.296856 |
| C             | 3.998512 13.060873 11.175253 |
| H             | 4.903203 12.935931 11.761633 |
| C             | 4.130321 13.928418 13.976716 |
| C             | 3.934081 12.874244 14.184525 |
| H             | 4.112181 14.473404 14.926080 |
| C             | 5.145914 14.022119 13.574568 |
| C             | 0.068990 6.775333 17.630978 |
| C             | 0.574703 7.043394 16.699340 |
| C             | -1.482950 5.460473 14.684959 |
| Element | X  | Y  | Z   |
|---------|----|----|-----|
| W       | -2.799129 | 0.811671 | -2.381167 |
| Al      | 0.070359  | 2.738958  | -0.511636 |
| Al      | 0.124121  | -2.829146 | 2.738958 |
| O       | -0.723236 | -1.701820 | -0.216856 |
| O       | -1.162822 | 1.719525  | -1.292638 |
| O       | 0.958228  | -1.766899 | 1.935128 |
| O       | 0.931578  | 1.525876  | 0.371717 |
| C       | -4.549843 | 0.506568  | -3.398124 |
| N       | 1.170326  | 3.638595  | -1.820359 |
| N       | -0.864153 | -4.122706 | 1.868971 |
| C       | -2.443155 | -1.127038 | -2.894768 |
| N       | -0.692282 | 4.265243  | 0.281322 |
| N       | 1.170347  | -4.139873 | -0.104802 |
| C       | -2.105307 | 1.682254  | -4.102844 |
| O       | -5.547400 | 1.682254  | -4.102844 |
| O       | -2.225378 | -2.217126 | -3.199621 |
| O       | -4.861797 | 0.355339  | -0.007244 |
| O       | -1.916885 | 2.271842  | -5.076934 |
| C       | 1.059915  | 1.684044  | 3.305807 |
| H       | 1.783217  | 2.175836  | 2.660238 |
| C       | -1.506481 | -3.722726 | 3.102071 |
| C       | -0.338757 | -0.386861 | -0.287029 |
|     | 2.68418 | -5.991011 | 0.466773 | H  | 1.327162 | 5.459193 | 0.912017 |
|-----|---------|-----------|----------|----|---------|----------|----------|
|     | -0.466777 | -7.036271 | 0.265332 | C  | 4.622991 | 2.252579 | -1.764345|
|     | 1.664866  | -6.392716 | -1.004116| H  | 5.461188 | 2.189972 | -1.078279|
|     | 2.156112  | -5.929050 | -1.858959| C  | 4.401641 | 3.211948 | 0.990547 |
|     | 1.049165  | -7.227118 | -1.345991| H  | 4.160422 | 2.169197 | 1.211715 |
|     | 2.446841  | -6.799133 | -0.353182| H  | 4.275748 | 3.795939 | 1.907708 |
|     | 3.619075  | -4.713679 | 1.412483 | H  | 5.461146 | 3.274072 | 0.717486 |
|     | 2.607549  | -5.080494 | 1.622503 | C  | 0.753315 | -3.984632| 4.291516 |
|     | -0.738110 | -3.663265 | 4.282411 | H  | 1.155216 | -3.686071| 3.320277 |
|     | 1.209328  | -0.387015 | 1.794660 | C  | -0.975908| -5.411995| 1.522002 |
|     | 3.355401  | -0.387987 | 0.420518 | C  | -3.982881| 0.452899 | -0.748502|
|     | 2.744060  | -0.462285 | -0.477101| H  | -3.036123| 2.908256 | 1.573242 |
|     | 0.914629  | 1.206774  | -5.159711| H  | -2.707578| 2.804785 | 0.532115 |
|     | 1.739638  | 0.567027  | -5.490262| H  | 1.988261 | 3.342175 | -5.856435|
|     | 0.238153  | 1.350394  | -6.006656| H  | 2.467261 | 4.280720 | -5.566557|
|     | 0.365758  | 0.672701  | -4.382383| H  | 1.186874 | 3.568801 | -6.57725 |
|     | 3.486227  | 2.965393  | -1.391259| H  | 2.738485 | 2.743586 | -6.385023|
|     | 0.528913  | 2.362432  | 4.397050 | C  | -0.406017| 5.458162 | -1.802816|
|     | 0.826250  | 3.390757  | 4.588333 | H  | -0.742710| 6.309652 | -2.382913|
|     | 2.476858  | -3.175881 | -1.950914| C  | -0.589682| 5.761104 | 3.690282 |
|     | -1.031042 | 5.256868  | -0.576663| H  | 0.016744 | 6.469437 | 4.249973 |
|     | 3.624499  | -4.070869 | 0.030558 | C  | -0.241309| -0.247889| 3.875817 |
|     | -0.766679 | 0.425940  | 4.977184 | H  | -0.549677| -1.264125| 3.667520 |
|     | -1.480718 | -0.085281 | 5.619481 | H  | -3.470322| -3.024340 | 4.299262 |
|     | 4.742412  | -0.425352 | 0.310437 | H  | -4.526808| -2.769792| 4.315144 |
|     | 5.193412  | -0.533579 | -0.672447| C  | 4.899752 | -3.167067| -1.820963|
|     | 3.724585  | -2.878628 | -2.502931| H  | 5.861130 | -2.930771| -2.270690|
|     | 3.779745  | -2.415542 | -3.483577| C  | 3.887946 | 5.223448 | -0.438839|
|     | -3.721555 | -3.514927 | 1.835272 | H  | 4.874061 | 5.244112 | -0.916632|
|     | -3.179926 | -4.124034 | 1.105127 | H  | 3.939962 | 5.838317 | 0.465089 |
|     | 1.101025  | 5.968890  | 1.853555 | H  | 3.174573 | 5.694255 | -1.123840|
SCF (wB97x) = -3920.40740769
E(SCF)+ZPE(0 K)= -3918.828994
H(298 K)= -3918.731882
G(298 K)= -3918.959846
Lowest Frequency = -101.9528 cm⁻¹

14_TS6.log

123
|   | C           | H           | C          | H          |
|---|-------------|-------------|------------|------------|
| 1 | -0.333144   | -5.013434   | -0.198745  | 3.317090   |
| 2 | -0.679978   | -5.176184   | -1.194314  | 2.745148   |
| 3 | -3.389771   | -4.727871   | -2.886955  | 4.432822   |
| 4 | -4.432234   | -5.617347   | -2.578325  | -0.339699  |
| 5 | 4.909609    | 6.702839    | -3.079635  | 0.365973   |
| 6 | 5.853539    | -0.479348   | -2.809590  | 1.771751   |
| 7 | 3.847237    | -0.930688   | 5.142331   | 2.317994   |
| 8 | 4.821508    | 4.543921    | 5.759315   | -0.305874  |
| 9 | 3.912629    | 5.398968    | 0.403955   | -0.327092  |
|10 | 3.111563    | -2.935420   | 5.603888   | 1.555667   |
|11 | 0.958783    | -1.908199   | -5.502049  | 1.199261   |
|12 | 0.540606    | -3.609550   | -5.661622  | 0.866376   |
|13 | 2.023254    | -3.154689   | -5.761719  | 1.509912   |
|14 | 0.468365    | 2.253071    | -6.200787  | 5.528123   |
|15 | 1.609628    | 4.034413    | -3.101440  | -3.695737  |
|16 | 1.456846    | 4.988734    | -2.060581  | -3.187974  |
|17 | 2.673795    | 4.092374    | -3.334744  | -4.191623  |
|18 | 1.361467    | 3.253664    | -3.199926  | -2.930155  |
|19 | -1.875832   | -3.849281   | -6.289440  | -1.917369  |
|20 | -1.712678   | -4.356321   | -6.215340  | -1.291159  |
|21 | -1.756845   | -4.474501   | -7.328278  | -1.946447  |
|22 | -2.910313   | -2.895379   | -5.985992  | -1.447220  |
|23 | -1.334658   | -4.983529   | -3.255212  | -4.038383  |
|24 | -0.775022   | -4.870999   | -3.229048  | -5.032278  |
|25 | -1.793549   | -5.490039   | 5.109141   | -4.152439  |
|26 | -2.092631   | -5.648140   | 5.364992   | -3.458242  |
|27 | 3.480624    | -2.668857   | 3.692972   | -0.143730  |
|28 | 2.481854    | -3.145953   | 3.695527   | -0.306381  |
|29 | 4.901433    | 4.756338    | -3.694809  | -0.650532  |
|30 | 5.843326    | 4.613088    | -3.894383  | -0.145765  |
|31 | -4.590646   | 4.657714    | 3.398470   | -6.414786  |

S125
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | 5.786966 | -5.508866 | 1.334713 |
| C    | 1.025599  | 7.399964  | 1.725700  |
| H    | 0.263082  | 7.670620  | 0.988136  |
| H    | 1.987765  | 7.779885  | 1.364251  |
| H    | 0.789106  | 7.920489  | 2.660738  |
| C    | 1.180128  | -2.896325 | -2.711882 |
| C    | 0.691542  | -4.141836 | -3.465782 |
| H    | 1.465411  | -4.516253 | -4.147414 |
| H    | -0.192650 | -3.892148 | -4.061916 |
| H    | 0.405098  | -4.952008 | -2.790604 |
| C    | 1.273507  | -1.724942 | -3.687119 |
| H    | 2.117561  | 5.977176  | 3.872626  |
| H    | 3.203775  | 5.900431  | 2.485592  |
| H    | 2.338058  | 4.444153  | 3.014185  |
| H    | 1.714835  | -0.837545 | -3.218917 |
| H    | 0.268069  | -1.467847 | -4.035600 |
| H    | -3.904652 | 1.948692  | -2.408570 |
| C    | -0.740121 | 0.347619  | 1.469942  |
| H    | 0.018339  | 0.412277  | -2.263595 |

15_Int6.log

SCF (wB97x) = -3807.12573523
E(SCF)+ZPE(0 K) = -3805.554191
H(298 K) = -3805.459324
G(298 K) = -3805.682702
Lowest Frequency = 14.4480 cm⁻¹

W   -2.727916 0.564764 -2.222279
Al  0.086041 2.619361 -0.566979

H  0.274660 -2.957732 0.793824
O  -0.543375 -1.852752 -0.298444
C  -1.055585 1.557245 -1.440484
H  1.022091 -1.876153 1.923150
H  0.949553 1.440287 0.365106
C  -4.561929 0.399558 -1.490633
N  1.105479 3.580858 -1.876452
N  -0.806460 -4.221224 1.727893
C  -3.089387 -1.346945 -2.741196
N  -0.748111 4.115355 0.210100
C  1.325564 -4.263530 -0.150316
C  -3.223355 0.873838 -4.096684
O  -5.603838 0.334209 -0.984084
H  -3.289479 -2.442809 -3.046067
O  -3.432985 1.096367 -5.217367
C  1.230051 1.493470 3.396442
H  2.086501 1.912027 2.874037
C  -1.540445 -3.757255 2.882730
O  -0.201794 -0.528566 -0.345942
C  1.014356 2.508663 -4.678439
H  0.263252 3.142123 -4.195612
C  0.713586 0.262553 2.982919
C  -1.108838 4.248114 1.605247
C  2.597671 -3.892211 -0.731117
C  1.454939 5.506071 -3.393614
H  2.421984 5.054254 -3.614466
H  1.603930 6.544263 -3.086005
H  0.855579 5.518245 -4.309578
C  -2.881451 -3.359240 2.739917
C  2.809956 -0.376933 1.639885
C  -2.289992 3.672450 2.097001

S126
C 2.171095 2.293022 -3.703408  C 0.301826 1.215975 -5.087913
C 0.604008 0.114593 0.528810  H 0.989900 0.515530 -5.574709
C -2.637900 3.912010 3.427867  H -0.504022 1.441034 -5.794783
H -3.546470 3.467184 3.826129  H -0.145246 0.708683 -4.231021
C 3.254659 1.510557 -4.114771  C 3.403356 2.793525 -1.627899
H 3.214266 1.020251 -5.085052  C 0.670938 2.174922 4.472244
C 0.970067 -5.548432 -0.256325  H 1.092828 3.127279 4.783701
C 2.251632 2.902226 -2.435637  C 2.626585 -3.267995 -1.993404
C -2.127945 6.131671 -0.132213  C -1.058118 5.166732 -0.580970
H -3.061855 5.585822 0.037872  C 3.777469 -4.204047 -0.030292
H -2.297885 6.896918 -0.890477  C -0.964458 0.435429 4.725496
H -1.867300 6.615771 0.811934  H -1.826112 0.006388 5.232209
C 0.707691 4.768813 -2.311276  C 4.799947 -0.559969 0.264560
C 5.017991 -0.369385 2.648840  H 5.240706 -0.659928 -0.723858
H 5.636475 -0.319035 3.541778  C 3.875602 -2.960963 -2.538523
C 3.631497 -0.324189 2.769014  H 3.930546 -2.478861 -3.510055
H 3.183260 -0.251031 3.756137  C -3.625053 -3.452717 1.414170
C -0.278178 5.033694 2.429501  H -3.010187 -4.030137 0.716146
H 0.578974 -2.672779 -2.054226  C 1.028790 5.647368 1.937117
C -0.132668 -6.111189 0.398551  H 1.221426 5.275210 0.925415
H -0.324646 -7.158620 0.202050  C 4.455217 2.006330 -2.091197
C 1.824577 -6.514658 -1.044619  H 5.345053 1.890666 -1.480553
H 2.276817 -6.056124 -1.924054  C 4.532518 3.017862 0.669699
H 1.228118 -7.376282 -1.350018  H 4.307332 1.978791 0.919591
H 2.639665 -6.877602 -0.408360  H 4.497508 3.607211 1.592115
C 3.762556 -4.874295 1.339220  H 5.560953 3.072677 0.293899
H 2.779768 -5.334819 1.488979  C 0.563596 -4.153839 4.310142
C -0.880877 -3.702441 4.125981  H 1.015316 -4.262419 3.319005
C 1.277712 -0.494542 1.768832  C -0.907640 -5.511545 1.395296
C 3.414751 -0.497439 0.387274  C -3.182988 2.799945 1.232537
H 2.795942 -0.540441 -0.507065  H -2.857062 2.901028 0.191022
S128
C  -1.587413  15.092120  14.969055  H  1.770783  4.822869  11.402694
C   2.117854   6.979429   12.589900  H  0.696303  3.516051  11.959687
C   1.139485  16.350065  10.050504  H  2.126232  3.961395  12.899271
H   2.115570  15.900915   9.867628  C  3.347342   5.995638  14.624606
H  1.273375  17.359236  10.361266  H  2.352898   5.584594  14.832213
H   0.575892  16.357996   9.112031  C  -1.027407   7.053647  17.605751
C  -3.149905   7.426918  16.431471
C   2.386533  10.489221   15.094521
C   2.117854  14.269186  16.431471
C   1.139485  16.350065  10.050504
H   2.115570  15.900915   9.867628
H   1.273375  17.359236  10.361266
H   0.575892  16.357996   9.112031
C  -2.796303  14.520623  15.394681  H  2.427451  10.286666  12.950225
C   1.875548  13.144318   9.754341  C   0.073237   12.082819   8.273097
C   0.205361  10.964328  13.929041
C  -3.149905   7.426918  16.431471
C   2.386533  10.489221   15.094521
C   1.139485  16.350065  10.050504
H   2.115570  15.900915   9.867628
H   1.273375  17.359236  10.361266
H   0.575892  16.357996   9.112031
C   0.353872  15.611834  13.095358  H   0.509004  13.958001  18.206758
C   1.900405  13.746972  11.027489  C   2.112760   7.611285  11.330072
C  -2.520752  17.002118  13.212428  C  -1.448459  16.026960  12.791950
C   0.353872  15.611834  13.095358
C   1.900405  13.746972  11.027489  C   2.112760   7.611285  11.330072
C   3.347342   5.995638  14.624606
H   2.352898   5.584594  14.832213
H   0.575892  16.357996   9.112031
C  -1.027407   7.053647  17.605751
C   0.781765  11.386431  7.810759
C  -3.149905   7.426918  16.431471
C   2.386533  10.489221   15.094521
C   1.139485  16.350065  10.050504
H   2.115570  15.900915   9.867628
H   1.273375  17.359236  10.361266
H   0.575892  16.357996   9.112031
H  -2.352428  10.772856  18.564652
C  -4.410878  10.286011  13.772877
C   4.568417  10.513927  16.158746  H   4.876363  10.168229  12.797607
C   5.164012  10.577827  17.066215  C   3.346810   7.941793  10.764925
C   3.179062  10.559774  16.243138  H   3.376681   8.433409  9.797451
C   2.706092  10.646810  17.217455  C  -3.986320   7.477617  15.162163
C  -0.787403  15.854186  15.843455  H  -3.452169   6.938543  14.372651
C   0.067472   8.219980  11.307434  C   0.535387  16.480883  15.413182
C  -0.596233   4.766718  13.778751  H   0.766860  16.128788  14.402333
C  -0.811345   3.726372  13.568964  C   4.093304  12.861027  11.454975
C   1.315876   4.357090  12.276684  H   4.959375  12.748552  12.099197
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | 4.072995     | 13.872467    | 14.210701    |
| H       | 3.854348     | 12.828436    | 14.444659    |
| H       | 3.998208     | 14.453723    | 14.444659    |
| C       | 0.448389     | 6.676544     | 17.624436    |
| C       | 0.470237     | 4.943374     | 17.644826    |
| H       | 0.820591     | 6.717766     | 16.597177    |
| H       | -1.308162    | 5.351049     | 14.82965    |
| C       | -3.671118    | 13.701411    | 14.461013    |
| H       | -3.294145    | 13.836771    | 13.440689    |
| H       | 1.324571     | 14.093968    | 7.490655     |
| H       | 1.996792     | 13.434054    | 6.931229     |
| C       | 0.783182     | 16.286603    | 11.598834    |
| H       | 1.071761     | 17.184463    | 11.064866    |
| C       | -0.873901    | 10.553995    | 17.027139    |
| H       | -1.262878    | 9.596605     | 16.700682    |
| C       | -3.723915    | 7.812722     | 17.644826    |
| H       | -4.766199    | 8.121195     | 17.665726    |
| C       | 4.540299     | 7.651855     | 11.413505    |
| H       | 5.488326     | 7.915821     | 10.950788    |
| C       | 3.434672     | 15.904066    | 12.883594    |
| H       | 4.406454     | 15.976284    | 12.381751    |
| H       | 3.492629     | 16.480725    | 13.813722    |
| H       | 2.688740     | 16.382759    | 12.241910    |
| C       | 0.650890     | 5.244377     | 18.134492    |
| H       | 0.269076     | 5.132730     | 19.156184    |
| H       | 1.716928     | 4.989100     | 18.143210    |
| H       | 0.137998     | 4.511687     | 17.501239    |
| C       | 1.280309     | 7.674734     | 18.434976    |
| H       | 1.110118     | 8.693318     | 18.074282    |
| H       | 2.346035     | 7.447386     | 18.330166    |
| H       | 1.041383     | 7.635846     | 19.503738    |
| C       | -2.249493    | 4.454435     | 15.596210    |
| H       | -2.030371    | 4.479259     | 16.666982    |
| H       | -2.176516    | 3.426422     | 15.239982    |
| C       | -3.282306    | 4.795466     | 15.476136    |
| H       | -1.080462    | 7.431593     | 19.719245    |
| C       | 4.520835     | 7.027354     | 12.650757    |
| C       | 5.458054     | 6.813225     | 13.158275    |
| H       | -5.134336    | 14.158403    | 14.470090    |
| C       | -5.617665    | 13.946128    | 15.430135    |
| H       | -5.696648    | 13.630447    | 13.692906    |
| C       | -5.226997    | 15.233638    | 14.281168    |
| H       | 5.191720     | 10.375113    | 14.921747    |
| C       | 6.276293     | 10.335173    | 14.854723    |
| H       | -0.991498    | 12.446829    | 18.517621    |
| C       | -1.464612    | 12.972321    | 19.343630    |
| H       | 4.062596     | 12.202748    | 10.230946    |
| H       | 4.900737     | 11.580263    | 9.927832     |
| H       | -3.568666    | 12.212228    | 14.799304    |
| C       | -2.536141    | 11.845555    | 14.729356    |
| H       | -4.187793    | 11.623356    | 14.113857    |
| H       | -3.911505    | 12.018278    | 15.822327    |
| H       | 1.687413     | 16.043708    | 16.324836    |

S131
C      3.657758  7.014869  15.726048  H      1.553826  8.701296  8.679086
H      4.621484  7.504705  15.546002  H      1.432957  9.909844  9.972571
H      3.706723  6.515170  16.701466  H     -0.030418  9.293126  9.175873
H      2.892080  7.795610  15.771921  H     -3.173649 12.188387  9.444658
C     -4.134937  8.928962  14.699251  C     -1.017553 11.033201 11.786128
H     -4.586159  9.540036  15.490024  H     -0.179592 11.087139 11.079014
H     -4.775169  8.983775  13.813988
H     -3.160086  9.357183  14.442254  17_Int7.log
C     -5.360714  6.819391  15.329296
H     -5.286000  5.799742  15.724093  SCF (wB97x) = -3807.12157481
H     -5.871973  6.775635  14.362540  E(SCF)+ZPE(0 K)= -3805.549824
H     -6.001896  7.390499  16.009604  H(298 K)= -3805.454893
C     -2.989560  7.801390  18.821518  G(298 K)= -3805.679146
H     -3.455940  8.092631  19.759348
C     -4.341186  4.828435  14.672919
H     -4.184618  4.118564  13.853132  Lowest Frequency = 9.6642 cm^{-1}
H     -4.235748  4.286350  15.618546
H     -5.377528  5.178177  14.614000  W     -2.706295  0.584289  -2.332136
H     -4.508288  18.011834  15.358368  Al    0.057403  2.600777  -0.546923
H     -0.310301  18.353134  14.649393  Al    0.311997  -2.979453  0.769089
C     -0.030418  9.293126  9.175873
H     -1.553826  8.701296  8.679086
C     -1.017553 11.033201 11.786128
C     -2.989560  7.801390  18.821518
C     -4.341186  4.828435  14.672919
C     -4.184618  4.118564  13.853132
C     -4.235748  4.286350  15.618546
C     -5.377528  5.178177  14.614000
| Atoms | X    | Y    | Z    | Atoms | X    | Y    | Z    | Atoms | X    | Y    | Z    | Atoms | X    | Y    | Z    |
|-------|------|------|------|-------|------|------|------|-------|------|------|------|-------|------|------|------|
| C     | -3.874595 | 12.421171 | 9.635983 | H     | 2.810752  | 11.924280 | 8.326836 |
| N     | 0.626011  | 14.411340 | 11.547925 | C     | 0.642105  | 5.311519  | 13.095031 |
| N     | -1.151640 | 6.609185  | 15.084323 | C     | 1.789526  | 13.759246 | 10.988553 |
| C     | -4.824965 | 11.621434 | 11.779668 | C     | -2.578368 | 16.966480 | 13.349456 |
| N     | -1.189197 | 14.952989 | 13.675701 | H     | -3.509613 | 16.424613 | 13.544807 |
| N     | 0.992715  | 6.594931  | 13.220591 | H     | -2.763541 | 17.727087 | 12.590088 |
| C     | -3.765804 | 9.450689  | 10.832075 | O     | -4.287203 | 13.099254 | 8.792300  |
| O     | -1.151640 | 6.609185  | 15.084323 | C     | -4.824965 | 11.621434 | 11.779668 |
| N     | 0.626011  | 14.411340 | 11.547925 | O     | -1.189197 | 14.952989 | 13.675701 |
| N     | -1.151640 | 6.609185  | 15.084323 | H     | -2.578368 | 16.966480 | 13.349456 |
| O     | -4.287203 | 13.099254 | 8.792300  | C     | -1.151640 | 6.609185  | 15.084323 |
| C     | 0.785663  | 12.322584 | 16.815843 | C     | 0.785663  | 12.322584 | 16.815843 |
| H     | -0.190442 | 13.969485 | 9.209259  | O     | -1.151640 | 6.609185  | 15.084323 |
| C     | 0.534434  | 10.312276 | 13.031639 | H     | 0.221855  | 8.158781  | 11.325081 |
| C     | 0.585102  | 13.366373 | 8.725168  | C     | 0.585102  | 13.366373 | 8.725168  |
| H     | -0.190442 | 13.969485 | 9.209259  | C     | 0.534434  | 10.312276 | 13.031639 |
| C     | 0.306480  | 11.079623 | 16.393047 | C     | 0.306480  | 11.079623 | 16.393047 |
| C     | -1.536052 | 15.088178 | 15.074144 | H     | 1.980294  | 4.823790  | 11.446072 |
| C     | 2.262553  | 6.985307  | 12.648044 | H     | 0.922266  | 3.496150  | 11.985336 |
| C     | 0.950492  | 16.352032 | 10.042470 | H     | 2.314366  | 3.986233  | 12.959782 |
| H     | 1.925517  | 15.918321 | 9.821126  | C     | 3.436831  | 6.006864  | 14.714389 |
| H     | 1.080731  | 17.392019 | 10.352072 | H     | 2.454459  | 5.545590  | 14.865754 |
| H     | 0.351046  | 16.354965 | 9.126490  | C     | -1.203629 | 7.049320  | 17.497555 |
| C     | -3.214312 | 7.449191  | 16.143691 | C     | 0.900862  | 10.346996 | 15.179036 |
| C     | 2.433126  | 10.489428 | 15.074735 | C     | 3.057870  | 10.377297 | 13.830959 |
| C     | -2.720395 | 14.524394 | 15.571846 | H     | 2.452664  | 10.321359 | 12.928068 |
| C     | 1.732856  | 13.162104 | 9.713341  | C     | -0.083099 | 12.063802 | 8.273253  |
| C     | 0.240456  | 10.955941 | 13.932954 | H     | 0.634101  | 11.394131 | 7.785262  |
| C     | -3.054597 | 14.759133 | 16.907044 | H     | -0.876467 | 12.285527 | 7.551003  |
| H     | -3.963904 | 14.321483 | 17.311040 | H     | -0.538042 | 11.521636 | 9.103875  |
| C     | 2.834356  | 12.404671 | 9.302514  | C     | 2.940833  | 13.668901 | 11.799956 |
| C  | 0.201219 | 12.982320 | 17.891492 | H  | -1.236003 | 17.147331 | 11.134728 |
| H  | 0.594174 | 13.944419 | 18.210430 | C  | -1.089946 | 16.102564 | 17.210297 |
| C  | 2.285767 | 7.620308  | 11.391142 | H  | -0.465705 | 16.720772 | 17.852163 |
| C  | -1.518699| 15.997599 | 12.884212 | C  | -0.794737 | 10.535072 | 17.052749 |
| C  | 3.444583 | 6.687336  | 13.350385 | H  | -1.187852 | 9.578853  | 16.727485 |
| C  | -1.386771| 11.196694 | 18.125624 | C  | -3.871374 | 7.883048  | 17.297239 |
| H  | -2.238911| 10.740749 | 18.624858 | H  | -4.904312 | 8.215495  | 17.227192 |
| C  | 4.44519  | 10.339608 | 13.728095 | C  | 4.708828  | 7.666941  | 11.530741 |
| H  | 4.902210 | 10.246093 | 12.746156 | H  | 5.667416  | 7.932613  | 11.091387 |
| C  | 3.531053 | 7.954547  | 10.853739 | C  | 3.363106  | 15.932955 | 12.783936 |
| H  | 3.580079 | 8.446383  | 9.886618  | H  | 4.313023  | 16.013013 | 12.242958 |
| C  | -3.962226| 7.446701  | 14.817310 | H  | 3.452652  | 16.514398 | 13.708406 |
| H  | -3.350862| 6.922238  | 14.075502 | H  | 2.586916  | 16.401092 | 12.170880 |
| C  | 0.610205 | 16.476241 | 15.392349 | C  | 0.339272  | 5.216887  | 18.282020 |
| H  | 0.801548 | 16.090321 | 14.385711 | H  | -0.108394 | 5.209951  | 19.282729 |
| C  | 4.009635 | 12.903782 | 11.338185 | H  | 1.386572  | 4.909711  | 18.379906 |
| H  | 4.897541 | 12.800648 | 11.953713 | H  | -0.175698 | 4.460916  | 17.679032 |
| C  | 4.073080 | 13.913494 | 14.093877 | C  | 1.076259  | 7.626463  | 18.443581 |
| H  | 3.872897 | 12.869000 | 14.342167 | H  | 1.023193  | 8.613213  | 17.975937 |
| H  | 4.028198 | 14.499407 | 15.017832 | H  | 2.125605  | 7.313808  | 18.468779 |
| H  | 5.098496 | 13.993269 | 13.714295 | H  | 0.734081  | 7.710237  | 19.481219 |
| C  | 0.248620 | 6.611682  | 17.649225 | C  | -2.247624 | 4.430923  | 15.424600 |
| H  | 0.692335 | 6.550893  | 16.650550 | H  | -2.134620 | 4.488205  | 16.510104 |
| C  | -1.255492| 5.325744  | 14.724103 | H  | -2.125054 | 3.395574  | 15.105147 |
| C  | -3.637563| 13.677908 | 14.706346 | H  | -3.268845 | 4.749666  | 15.194424 |
| H  | -3.330077| 13.800561 | 13.660687 | C  | -1.913265 | 7.465997  | 18.624255 |
| C  | 1.082625 | 14.116906 | 7.477616  | H  | -1.418146 | 7.475102  | 19.591877 |
| H  | 1.636219 | 15.026877 | 7.723147  | C  | -2.260466 | 15.555527 | 17.717694 |
| H  | 0.237651 | 14.389540 | 6.836246  | H  | -2.549795 | 15.745375 | 18.748202 |
| H  | 1.749954 | 13.478333 | 6.888275  | C  | 3.050775  | 14.462124 | 13.098896 |
| C  | -0.911496| 16.256993 | 11.660696 | H  | 2.079391  | 14.422530 | 13.604539 |
|   | X          | Y          | Z          |   | X          | Y          | Z          |
|---|------------|------------|------------|---|------------|------------|------------|
| C | 4.661660   | 7.044485   | 12.769209  | C | 4.481924   | 4.889697   | 14.818850  |
| H | 5.587790   | 6.834660   | 13.297950  | H | 4.408427   | 4.178030   | 13.988799  |
| C | -5.105290  | 14.110432  | 14.805433  | H | 4.346467   | 4.337853   | 15.754815  |
| H | -5.517560  | 13.911890  | 15.800903  | H | 5.501894   | 5.288905   | 14.824446  |
| H | -5.708195  | 13.552317  | 14.082558  | C | 0.526628   | 18.004631  | 15.289244  |
| H | -5.228570  | 15.180434  | 14.602912  | H | -0.257220  | 18.323413  | 14.594580  |
| C | 5.237475   | 10.424656  | 14.869497  | H | 1.476913   | 18.414906  | 14.929709  |
| H | 6.321719   | 10.404869  | 14.789867  | H | 0.314461   | 18.455347  | 16.265479  |
| C | -0.887902  | 12.421641  | 18.553044  | C | 1.006410   | 7.896274   | 10.608328  |
| H | -1.345241  | 12.942185  | 19.390972  | C | 0.527201   | 6.661264   | 9.831155   |
| C | 3.951214   | 12.255929  | 10.109758  | H | 1.315681   | 6.285414   | 9.167204   |
| H | 4.789402   | 11.650456  | 9.774154   | H | -0.338267  | 6.923809   | 9.213477   |
| C | -3.483883  | 12.196466  | 15.061416  | H | 0.216098   | 5.847940   | 10.491825  |
| H | -2.458954  | 11.840169  | 14.904752  | C | 1.138880   | 9.074201   | 9.642647   |
| H | -4.156610  | 11.592521  | 14.446083  | H | 1.677517   | 16.431412  | 17.301745  |
| H | -3.731663  | 12.016988  | 16.114752  | H | 2.727707   | 16.481935  | 15.884474  |
| C | 1.793217   | 16.064226  | 16.275861  | H | 1.895733   | 14.975241  | 16.316013  |
| C | 3.630435   | 7.037309   | 15.832414  | H | 1.763247   | 8.828179   | 8.773950   |
| H | 4.575259   | 7.578089   | 15.704990  | H | 1.568290   | 9.958708   | 10.127201  |
| H | 3.651492   | 6.537616   | 16.808918  | H | 0.146550   | 9.338753   | 9.264659   |
| H | 2.822899   | 7.776233   | 15.836490  | H | -2.940279  | 10.584052  | 9.459174   |
| C | -4.158430  | 8.877584   | 14.311377  | C | -1.002630  | 11.035063  | 11.805325  |
| H | -4.714983  | 9.472476   | 15.044779  | H | -0.186660  | 11.139305  | 11.078591  |
| H | -4.725317  | 8.876245   | 13.374115  |   |            |            |            |
| H | -3.192948  | 9.359743   | 14.126385  |   |            |            |            |
| C | -5.312315  | 6.724683   | 14.912190  |   |            |            |            |
| H | -5.216837  | 5.717386   | 15.332599  | SCF (wB97x)= -3807.12288674 |
| H | -5.760226  | 6.638753   | 13.917098  | E(SCF)+ZPE(0 K)= -3805.551694 |
| H | -6.018453  | 7.277374   | 15.541610  | H(298 K)= -3805.456588 |
| C | -3.233671  | 7.885454   | 18.529476  | G(298 K)= -3805.680960 |
| H | -3.765929  | 8.214553   | 19.418491  | Lowest Frequency = 12.1798cm⁻¹ |
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 1.282686 | -0.527795| 1.729663 |
| C       | 3.410977 | -0.463673| 0.335713 |
| H       | 2.786695 | -0.501275| -0.555070|
| C       | 0.298955 | 1.264065 | -5.061046|
| H       | 0.994115 | 0.574383 | -5.552863|
| H       | -0.516952| 1.472114 | -5.761656|
| C       | 3.382123 | 2.858672 | -1.610099|
| C       | 0.638580 | 2.094790 | 4.472046 |
| H       | 1.044170 | 3.050677 | 4.794893 |
| C       | 2.699806 | -3.225008| -2.048522|
| C       | -1.144310| 5.117312 | -0.549271|
| C       | 3.857348 | -4.171939| -0.095327|
| C       | -0.962618| 0.321766 | 4.708433 |
| H       | -1.813445| -0.130591| 5.213201 |
| C       | 4.796281 | -0.501572| 0.204490 |
| H       | 5.233061 | -0.577250| -0.787820|
| C       | 3.946013 | -2.894383| -2.586096|
| H       | 3.997149 | -2.398366| -3.550788|
| C       | -3.546998| -3.582704| 1.374658 |
| H       | -2.926844| -4.146518| 0.670248 |
| C       | 0.939265 | 5.603999 | 1.970994 |
| H       | 1.141359 | 5.238818 | 0.958576 |
| C       | 4.449753 | 2.101407 | -2.086911|
| H       | 5.342201 | 1.994099 | -1.478571|
| C       | 4.503562 | 3.065503 | 0.692395 |
| H       | 4.297761 | 2.018118 | 0.923789 |
| H       | 4.456056 | 3.637977 | 1.624815 |
| H       | 5.531284 | 3.146227 | 0.319359 |
| C       | 0.670377 | -4.226750| 4.240702 |
| H       | 1.118747 | -4.313445| 3.245936 |

### SCF (wB97x) = -3807.10643037

### E(SCF)+ZPE(0 K)= -3805.535542

### H(298 K)= -3805.441188

### G(298 K)= -3805.662782

**Lowest Frequency = -784.5541 cm⁻¹**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| W    | -3.342363 | 11.527312 | 11.376098 |
| Al   | -0.325078  | 13.473484 | 12.812351 |
| O    | -0.952506  | 8.993456  | 13.104683 |
| O    | -1.372440  | 12.386472 | 11.864163 |
| O    | 0.661971   | 8.957955  | 15.276232 |
| O    | 0.487122   | 12.305706 | 13.805639 |
| C    | -3.264622  | 11.166452 | 9.484196  |
| N    | 0.742923   | 14.493261 | 11.597302 |
| N    | -1.135789  | 6.605384  | 15.140902 |
| C    | -4.548247  | 13.109839 | 10.963481 |
| N    | -1.217221  | 14.941092 | 13.589274 |
| N    | 0.921187   | 6.594560  | 13.174649 |
| C    | -4.952731  | 10.380578 | 11.453956 |
| O    | -3.184906  | 10.939593 | 8.338245  |
| O    | -5.228617  | 14.009443 | 10.696603 |
| O    | -5.879991  | 9.680880  | 11.523148 |
| C    | 0.808759   | 12.272459 | 16.845109 |
| H    | 1.686816   | 12.701581 | 16.369483 |
| C    | -1.791756  | 7.024712  | 16.359990 |
| C    | -0.654793  | 10.325459 | 13.073928 |

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.730071 | 13.470359 | 8.796648 |
| H    | -0.011968 | 14.128695 | 9.257857 |
| C    | 0.295043 | 11.065495 | 16.366514 |
| C    | -1.633045 | 15.023238 | 14.973203 |
| C    | 2.184744 | 6.977771  | 12.582025 |
| C    | 1.134363 | 16.447021 | 10.127864 |
| H    | 2.114032 | 16.008679 | 9.937575  |
| H    | 1.258786 | 17.482829 | 10.453791 |
| H    | 0.570946 | 16.463662 | 9.189227  |
| C    | -3.147235 | 7.395267  | 16.331588 |
| C    | 2.410063 | 10.490948 | 15.005221 |
| C    | -2.847206 | 14.450258 | 15.384934 |
| C    | 1.877528 | 13.262046 | 9.781625  |
| C    | 0.176482 | 10.972604 | 13.922571 |
| C    | -3.243249 | 14.613206 | 16.712112 |
| H    | -4.177071 | 14.170839 | 17.048577 |
| C    | 2.982467 | 12.505378 | 9.379723  |
| H    | 2.971793 | 12.033481 | 8.399675  |
| C    | 0.559097 | 5.312966  | 13.058739 |
| C    | 1.916439 | 13.840835 | 11.063971 |
| C    | -2.588571 | 16.966680 | 13.256346 |
| H    | -3.535267 | 16.420047 | 13.328698 |
| H    | -2.705509 | 17.775908 | 12.534707 |
| H    | -2.391330 | 17.392877 | 14.242642 |
| C    | 0.352256 | 15.686231 | 11.168851 |
| C    | 4.622540 | 10.474478 | 16.003934 |
| H    | 5.245330 | 10.502967 | 16.894773 |
| C    | 3.236835 | 10.516913 | 16.131879 |
| H    | 2.793496 | 10.561582 | 17.122852 |
| C    | -0.828607 | 15.755435 | 15.867049 |
| H    | 0.134156 | 8.167857  | 11.294694 |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| H | 0.216938 | 5.162990 | 19.161595 | H | -3.983027 | 11.606716 | 13.758194 |
| H | 1.684271 | 4.998690 | 18.180482 | H | -3.744328 | 11.782048 | 15.490121 |
| H | 0.117180 | 4.513867 | 17.515596 | C | 1.644027 | 15.979112 | 16.360876 |
| C | 1.250202 | 7.688201 | 18.419510 | C | 3.673536 | 6.995057 | 15.734860 |
| H | 1.090196 | 8.702311 | 18.042149 | H | 4.639764 | 7.487036 | 15.574770 |
| H | 2.316899 | 7.455265 | 18.337662 | H | 3.703527 | 6.493430 | 16.710115 |
| H | 0.991730 | 7.664975 | 19.484146 | H | 2.905890 | 7.774686 | 15.765999 |
| C | -2.199842 | 4.419253 | 15.534782 | C | -4.153764 | 8.838418 | 14.553132 |
| H | -2.009816 | 4.463290 | 16.610348 | H | -4.661186 | 9.445641 | 15.312968 |
| H | -2.099015 | 3.388078 | 15.195008 | H | -4.760879 | 8.853377 | 13.643082 |
| H | -3.235129 | 4.738984 | 15.382113 | H | -3.187038 | 9.298025 | 14.323719 |
| C | -1.695013 | 7.447006 | 18.724518 | C | -5.323947 | 7.817631 | 15.723367 |
| H | -1.139938 | 7.473749 | 19.658269 | H | -5.226142 | 5.697228 | 15.623325 |
| C | -2.475888 | 15.352933 | 17.600826 | H | -5.823383 | 6.635629 | 14.240222 |
| H | -2.808812 | 15.487618 | 18.626758 | H | -5.987908 | 7.271548 | 15.875823 |
| C | 3.117705 | 14.488734 | 13.223653 | C | -3.033018 | 7.816731 | 18.716798 |
| H | 2.133642 | 14.421668 | 13.703060 | H | -3.518925 | 8.123774 | 19.639849 |
| C | 4.586796 | 7.018118 | 12.668554 | C | 4.387729 | 4.816832 | 14.683964 |
| H | 5.518260 | 6.797032 | 13.183460 | H | 4.248871 | 4.110175 | 13.858240 |
| C | -5.208581 | 13.942480 | 14.557498 | H | 4.269222 | 4.269587 | 15.624987 |
| H | -5.602248 | 13.544976 | 15.499447 | H | 5.422985 | 5.172349 | 14.644515 |
| H | -5.754535 | 13.455839 | 13.742387 | C | 0.378185 | 17.933336 | 15.404900 |
| H | -5.430996 | 15.014324 | 14.523691 | H | -0.383333 | 18.267523 | 14.693069 |
| C | 5.207929 | 10.380429 | 14.744150 | H | 1.334002 | 18.374834 | 15.101652 |
| H | 6.289779 | 10.340347 | 14.642964 | H | 0.118548 | 18.338334 | 16.389683 |
| C | -0.911633 | 12.381488 | 18.535526 | C | 0.909076 | 7.912905 | 10.564192 |
| H | -1.373745 | 12.891126 | 19.377440 | C | 0.417703 | 6.688152 | 9.778296 |
| C | 4.088072 | 12.351683 | 10.202257 | H | 1.198844 | 6.317727 | 9.103026 |
| H | 4.933382 | 11.753480 | 9.871240 | H | -0.452700 | 6.959173 | 9.171685 |
| C | -3.416838 | 12.174324 | 14.520179 | H | 0.112376 | 5.868600 | 10.433940 |
| H | -2.350731 | 11.939491 | 14.437273 | C | 1.039215 | 9.100712 | 9.609927 |
21_Int9.log

SCF (wB97x) = -3807.15629040
E(SCF)+ZPE(0 K) = -3805.578986
H(298 K) = -3805.484189
G(298 K) = -3805.709313
Lowest Frequency = 12.2468 cm⁻¹
S148

22_Int1a.log

SCF (wB97x) = -3920.43645857
E(SCF)+ZPE(0 K)= -3918.858565
H(298 K)= -3918.760955
G(298 K)= -3918.987935

Lowest Frequency = 16.6896 cm⁻¹
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| C | 0.602295 | 0.446232 | 0.488790 | H | 1.005894 | 0.891140 | -5.380228 |
| C | -2.416954 | 4.101763 | 3.574948 | H | -0.546639 | 1.736907 | -5.438010 |
| H | -3.304830 | 3.633463 | 3.992498 | H | 0.063376 | 1.116352 | -3.894995 |
| C | 3.378540 | 2.045575 | -4.154254 | C | 3.522420 | 3.197792 | -1.603025 |
| H | 3.333560 | 1.597363 | -5.144087 | C | 0.995695 | 2.372582 | 4.465279 |
| C | 0.816739 | -5.221494 | -0.328716 | H | 1.448842 | 3.311812 | 4.772462 |
| C | 2.354688 | 3.304916 | -2.385050 | C | 2.800127 | -3.062470 | -1.860051 |
| C | -2.004955 | 6.456052 | 0.053524 | H | -0.952099 | 5.497874 | -0.445932 |
| H | -2.937541 | 5.910582 | 0.230650 | C | 3.684833 | -4.108356 | 0.175770 |
| H | -2.186195 | 7.244695 | -0.677827 | C | -0.629750 | 0.635855 | 4.796588 |
| H | -1.720722 | 6.910752 | 1.005214 | H | -1.452028 | 0.195066 | 5.355699 |
| C | 0.800113 | 5.150105 | -2.197790 | C | 4.773714 | -0.291989 | -0.099744 |
| C | 5.153084 | -0.243265 | 2.272383 | H | 5.145745 | -0.353729 | -1.118908 |
| H | 5.830477 | -0.263909 | 3.122628 | C | 4.111213 | -2.923853 | -2.319772 |
| C | 3.780576 | -0.160539 | 2.488347 | H | 4.290942 | -2.461877 | -3.285929 |
| H | 3.397233 | -0.132715 | 3.504882 | C | -3.727502 | 3.172699 | 1.693058 |
| C | -0.107660 | 5.275948 | 2.525919 | H | -3.167922 | 3.693031 | 0.911245 |
| H | 0.826033 | -2.261100 | -2.043044 | C | 1.184560 | 5.907943 | 2.016608 |
| C | -0.319502 | -5.737805 | 0.304845 | H | 1.363803 | 5.549171 | 0.997610 |
| H | -0.583993 | -6.757671 | 0.054723 | C | 4.598210 | 2.485157 | -2.129736 |
| C | 1.612306 | -6.208600 | 1.150669 | H | 5.504278 | 2.375005 | 1.542318 |
| H | 2.138821 | -5.738337 | -1.980938 | C | 4.669127 | 3.309036 | 0.689051 |
| H | 0.951073 | -6.988605 | -1.533139 | H | 4.476015 | 2.247301 | 0.861122 |
| H | 2.363645 | -6.687606 | -0.513763 | H | 4.621800 | 3.827030 | 1.652735 |
| C | 3.513100 | -4.732066 | 1.555113 | H | 5.694050 | 3.420072 | 0.316677 |
| H | 2.449441 | -4.942569 | 1.714556 | C | 0.708311 | -3.791254 | 4.217975 |
| C | -0.767431 | -3.411939 | 4.172510 | H | 1.148960 | -3.508118 | 3.258841 |
| C | 1.370900 | -0.237597 | 1.653795 | C | -1.021923 | -5.157816 | 1.366803 |
| C | 3.402637 | -0.196009 | 0.119917 | C | -4.186373 | 0.388152 | -1.365607 |
| H | 2.725015 | -0.180405 | -0.731770 | C | -3.028129 | 3.020664 | 1.391083 |
| C | 0.357261 | 1.586893 | -4.836738 | H | -2.689690 | 3.055193 | 0.348435 |
H -4.901206 -4.903847 2.374210
H -5.555118 -4.067980 0.952136
H -5.730392 -3.355765 2.556397
C -2.756266 -2.637198 5.328417
H -3.239391 -2.313198 6.246881
C 4.271192 -6.057508 1.701065
H 4.017334 -6.769436 0.908539
H 4.030944 -6.522898 2.663227
H 5.355786 -5.905646 1.673368
C 1.095544 7.438359 1.955725
H 0.303411 7.774800 1.279338
H 2.040669 7.860398 1.596366
H 0.894362 7.861869 2.946272
C 1.636608 -2.572953 -2.713224
C 1.082115 -3.686647 -3.613976
H 1.881560 -4.126677 -4.223216
H 0.324216 -3.281906 -4.291061
C 0.610963 -4.484903 -3.033603
C 2.014312 -1.358702 -3.564886
H 2.274912 5.810962 3.911048
H 3.308261 5.919070 2.485906
H 2.495255 4.390518 2.876054
H 2.705369 -1.624756 -4.374196
H 2.480734 -0.563211 -2.971693
H 1.118061 -0.954268 -4.035091
H -2.376482 1.587392 -3.160796
H -2.958955 1.396616 -3.667312

E(SCF)+ZPE(0 K)= -3918.804960
H(298 K)= -3918.706203
G(298 K)= -3918.939043

Lowest Frequency = -51.1712 cm⁻¹

23_TS1a.log
SCF (wB97x) = -3920.37906419
24_Int2a.log

SCF (wB97x) = -3807.09878597
E(SCF)+ZPE(0 K)= -3805.530035
H(298 K)= -3805.434833
G(298 K)= -3805.657867
Lowest Frequency = 14.8746 cm⁻¹
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -0.262481  | -0.203215      | C    | 5.317247     | -3.380512     | -1.240339 |
| H    | -0.288243  | -1.228307      | H    | 6.356426     | -3.202706     | -1.505935 |
| C    | -3.154159  | -2.169234      | C    | 3.892064     | 5.364782      | -0.774622 |
| H    | -2.803712  | -3.166065      | H    | 4.815645     | 5.460035      | -1.357023 |
| C    | -3.055707  | 1.092379       | H    | 4.014603     | 5.943635      | 0.147783  |
| H    | -3.585021  | 0.399026       | H    | 3.082693     | 5.824432      | -1.351141 |
| C    | 5.861160   | 1.959903       | C    | 0.514800     | -5.387161     | 4.274191  |
| H    | 5.524096   | 0.925833       | H    | -0.090266    | -5.820837     | 5.079498  |
| C    | 2.411482   | -2.297354      | H    | 1.564468     | -5.632991     | 4.474633  |
| H    | 2.392012   | -1.762262      | H    | 0.238878     | -5.877118     | 3.335512  |
| C    | 3.35827   | 0.485435       | C    | 0.943522     | -3.218878     | 5.462109  |
| H    | 2.279836   | 0.712202       | H    | 0.790060     | -2.135088     | 5.468794  |
| C    | 3.896022   | 1.425729       | H    | 2.022030     | -3.405735     | 5.476652  |
| H    | 3.443519   | 0.068788       | H    | 0.529812     | -3.637549     | 6.387321  |
| C    | -3.864362  | 4.215706       | C    | -2.159882    | -6.075629     | 1.828929  |
| H    | -3.481671  | 3.362181       | H    | -2.101374    | -6.016628     | 2.918512  |
| C    | -5.222064  | 1.178134       | H    | -2.053340    | -7.116060     | 1.520532  |
| C    | 3.081322   | 1.447890       | H    | -3.156689    | -5.730135     | 1.540945  |
| H    | 3.090835   | 0.400941       | C    | -1.919878    | -3.037005     | 5.051658  |
| C    | 3.056264   | -5.927629      | H    | -1.501270    | -3.003509     | 6.052820  |
| H    | 4.034749   | -5.879009      | C    | -1.479597    | 4.925827      | 4.398796  |
| H    | 3.168931   | -6.460624      | H    | -1.717064    | 5.100561      | 5.444993  |
| H    | 2.401859   | -6.531239      | C    | 3.612456     | 3.888200      | -0.457918 |
| C    | -0.366349  | 5.660493       | H    | 2.660716     | 3.835538      | 0.084938  |
| H    | 6.550122   | -2.259276      | C    | 4.993214     | -3.837202     | 0.029729  |
| C    | 5.471276   | 3.842784       | H    | 5.785088     | -4.018265     | 0.753165  |
| H    | 6.071779   | 4.463642       | C    | -4.442547    | 3.626963      | 1.490457  |
| C    | -0.157307  | 3.612126       | H    | -4.864542    | 3.570570      | 2.500011  |
| H    | -1.100464  | 3.300080       | H    | -5.089325    | 3.040536      | 0.828817  |
| C    | -2.643652  | 3.575840       | H    | -4.492239    | 4.672657      | 1.168418  |
| H    | -2.311751  | 3.423412       | C    | 5.699669     | -0.279048     | 0.859348  |
| Atom | X  | Y  | Z  | Atom | X  | Y  | Z  |
|------|----|----|----|------|----|----|----|
| C    | -0.051862 | 1.704588 | 5.143536 | C    | 1.900820 | -3.136816 | -2.905893 |
| H    | -0.440595 | 2.220137 | 6.018198 | C    | 2.226694 | -3.826961 | -4.236348 |
| C    | 4.429102 | 1.735449 | -3.506636 | H    | 3.080720 | -3.356211 | -4.736685 |
| H    | 5.284373 | 1.200148 | -3.911624 | H    | 1.366714 | -3.751360 | -4.909032 |
| C    | -2.971387 | 1.630298 | 1.936980 | H    | 2.466947 | -4.888121 | -4.105955 |
| H    | -1.973360 | 1.191099 | 1.829742 | C    | 1.672086 | -1.642390 | -3.134926 |
| H    | -3.677536 | 1.020945 | 1.366451 | H    | 2.442806 | 5.680330 | 3.807597 |
| H    | -3.244230 | 1.562105 | 2.996611 | H    | 3.426145 | 5.782892 | 2.345683 |
| C    | 2.499670 | 5.368687 | 2.758657 | H    | 2.571609 | 4.276617 | 2.734293 |
| C    | 3.809991 | -3.711019 | 2.896056 | H    | 2.598534 | -1.133981 | -3.433893 |
| H    | 4.880256 | -3.482361 | 2.834202 | H    | 1.285822 | -1.153835 | -2.233867 |
| H    | 3.623436 | -4.174651 | 3.872782 | H    | 0.928034 | -1.504647 | -3.922035 |
| H    | 3.257290 | -2.769508 | 2.841187 | H    | -3.856136 | 1.031179 | -0.959633 |
| C    | -3.743001 | -1.610782 | 0.597213 | H    | -4.493301 | 0.823507 | -1.422508 |
| H    | -4.436681 | -1.025989 | 1.211328 | H    | -4.160280 | -1.625579 | -0.429784 | 25_TS2a.log |
| H    | -2.759550 | -1.136485 | 0.623702 | C    | -5.033046 | -3.719072 | 1.038010 | SCF (wB97x) = | -3807.08533154 |
| H    | -5.021214 | -4.740374 | 1.432904 | E(SCF)+ZPE(0 K)= | -3805.520150 |
| H    | -5.386847 | -3.758939 | 0.002535 | H(298 K)= | -3805.425099 |
| H    | -5.772773 | -3.153488 | 1.615206 | G(298 K)= | -3805.648286 |
| C    | -3.233505 | -2.629194 | 4.851954 | Lowest Frequency = -605.4264 cm^-1 |
| H    | -3.832370 | -2.294225 | 5.694985 | C    | 4.012302 | -6.039418 | 1.941363 | W  | -3.120938 | -0.227646 | -1.999638 |
| H    | 3.688996 | -6.736224 | 1.160418 | Al  | 0.177172 | 2.949814 | -0.511099 |
| H    | 3.736657 | -6.470002 | 2.910616 | Al  | 0.355705 | -2.658139 | 0.707993 |
| H    | 5.105746 | -5.979153 | 1.902277 | O  | -0.498018 | -1.496953 | -0.280642 |
| C    | 1.248517 | 7.394638 | 1.943228 | O  | -1.035639 | 1.892672 | -1.231530 |
| H    | 0.435222 | 7.776153 | 1.317869 | O  | 1.260380 | -1.624086 | 1.765386 |
| H    | 2.188260 | 7.794068 | 1.546114 | O  | 1.013659 | 1.748153 | 0.445534 |
| Atomic Symbol | x-coordinate  | y-coordinate  | z-coordinate  |
|----------------|---------------|---------------|---------------|
| C              | -4.609149     | -1.276809     | -2.893865     |
| N              | 1.175560      | 3.851192      | -1.848811     |
| N              | -0.821284     | -3.870573     | 1.601702      |
| C              | -1.859516     | -1.646792     | -2.822425     |
| N              | -0.514453     | 4.476919      | 0.339504      |
| N              | 1.395723      | -4.005187     | -0.155313     |
| C              | -2.963916     | 0.931548      | -3.547597     |
| O              | -5.466077     | -1.861079     | -3.41894      |
| O              | -1.200549     | -2.445716     | -3.335298     |
| C              | -1.253005     | 0.610801      | -1.073213     |
| O              | -2.899810     | 1.681034      | -4.442776     |
| C              | 1.577983      | 1.693976      | 3.417840      |
| H              | -2.899810     | 1.681034      | -4.442776     |
| O              | -2.899810     | 1.681034      | -4.442776     |
| C              | -0.795386     | 4.256932      | 3.658988      |
| H              | 2.775280      | -3.743712     | 0.506497      |
| C              | 1.418488      | 5.693006      | -3.484140     |
| C              | 2.402185      | 5.277934      | -3.704557     |
| H              | 1.506484      | 6.767849      | -3.311497     |
| C              | 0.780057      | 5.548824      | -4.362203     |
| C              | -2.941240     | -2.989828     | 2.496091      |
| C              | 3.016287      | -0.105745     | 1.370479      |
| C              | -1.953534     | 4.033698      | 2.305760      |
| C              | 2.160741      | 2.507857      | -3.675345     |
| C              | 0.698326      | 0.448454      | 0.503905      |
| C              | -2.219800     | 4.256932      | 3.658988      |
| H              | -3.112668     | 3.820405      | 4.100143      |

S158
C  3.527954  3.184613 -1.742539  C  -0.288686  5.753869 -1.696890
C  1.084309  2.342500  4.451740  H  -0.616094  6.643152 -2.222095
H  1.513404  3.294106  4.755409  C  -0.227709  5.571756  3.883932
C  3.107420 -3.295366 -1.795088  H  0.437558  6.169780  4.503346
C  -0.834940  5.534960 -0.434816  C  -0.008914 -0.074271  3.649337
C  3.765975 -3.995375  0.462532  H  -0.441529 -1.017339  3.336877
C  -0.509123  0.574378  4.776169  C  -3.691869 -2.564379  3.594477
H  -1.331078  0.122052  5.327081  H  -4.714189 -2.226893  3.442302
C  4.885894 -0.163046 -0.170110  C  5.443825 -3.305420 -1.145063
H  5.246136 -0.179585 -1.195228  H  6.487581 -3.130076 -1.393527
C  4.454831 -3.079117  2.090592  C  3.963105  5.457724 -0.775061
H  4.730432 -2.730759  3.083473  H  4.880299  5.556342 -1.366954
C  -3.562455 -2.933459  1.106987  H  4.092068  6.038593  0.145240
H  -2.898731 -3.443844  0.402068  H  3.145492  5.912355 -1.343706
C  1.386263  5.955269  1.995944  C  0.587573 -5.321798  4.286037
H  1.504438  5.623502  0.959126  H  -0.023955 -5.757222  5.085460
C  4.606189  2.497334 -2.295986  H  1.634975 -5.573116  4.491483
H  5.556724  2.482548 -1.771934  H  0.314845 -5.805777  3.343186
C  4.776589  3.435933  0.480856  C  1.017778 -3.160527  5.487175
H  4.615435  2.379782  0.712879  H  0.865750 -2.076562  5.498942
H  4.766523  3.998845  1.419592  H  2.095822 -3.349055  5.506189
H  5.779446  3.547567  0.052932  H  0.599241 -3.583372  6.408211
C  0.410261 -3.798104  4.234637  C  -2.084268 -5.978433  1.819088
H  0.984599 -3.412414  3.385375  H  -2.027709 -5.932373  2.909447
C  -1.014239 -5.126017  1.181729  H  -1.985980 -7.016094  1.498892
C  -2.916547  3.181334  1.497391  H  -3.077086 -5.619972  1.533515
H  -2.591246  3.167406  0.451376  C  -1.842292 -2.978042  5.070790
C  1.096953  3.115330 -5.885501  H  -1.426671 -2.956885  6.073457
H  1.579593  4.096892 -5.847091  C  -1.378882  5.031830  4.441568
H  0.139090  3.220594 -6.404805  H  -1.614392  5.209233  5.487839
H  1.731510  2.463097 -6.495972  C  3.693772  3.980602 -0.452283
H  2.748382  3.925808  0.101430  H  -3.756351  -2.241884  5.717372
C  5.097070  -3.759285  0.119727  C  4.079097  -5.959858  2.012688
H  5.876203  -3.759285  0.119727  H  3.761842  -6.654759  1.227578
C  -4.346705  3.733632  1.518620  H  3.789394  -6.389522  2.978188
H  -4.779198  3.692348  2.524883  H  5.173226  -5.905244  1.987062
H  -4.982157  3.137878  0.855269  C  1.356725  7.488991  1.987887
H  -4.389980  4.775289  1.181950  H  0.540089  7.878405  1.371797
C  5.782762  -0.189819  0.892793  H  2.295350  7.885384  1.584976
H  6.853441  -0.225154  0.707086  H  1.232472  7.888203  3.000852
C  0.036559  1.786665  5.181931  C  2.058851  -3.055786  -2.869156
H  -0.352151  2.301457  6.056996  C  2.406461  -3.754411  -4.189926
C  4.480774  1.815278  -3.500689  H  3.273962  -3.292003  -4.674243
H  5.332666  1.280415  -3.913380  H  1.562507  -3.676489  -4.882578
C  -2.894311  1.737281  2.005474  H  2.636593  -4.816424  -4.049824
H  -1.892758  1.297931  1.933228  C  1.846305  -1.560280  -3.108550
H  -3.578759  1.130608  1.408844  H  2.551271  5.756290  3.835484
H  -3.199135  1.681259  3.057513  H  3.527319  5.862732  2.368532
C  2.600770  5.451086  2.784259  H  2.666398  4.358710  2.752924
C  3.877864  -3.630651  2.965450  H  2.785329  -1.057902  -3.375436
H  4.949396  -3.405506  2.914612  H  1.432869  -1.068258  -2.221451
H  3.680525  -4.094854  3.939545  H  1.133553  -1.416203  -3.923319
H  3.328793  -2.687160  2.906521  H  -3.696992  1.062787  -0.939499
C  -3.658723  -1.475074  0.655891  H  -4.687728  0.527121  -1.815119
H  -4.328224  -0.902260  1.305504
H  -4.117159  -1.447047  -0.352829
H  -2.675039  -1.002005  0.667173
C  -4.941696  -3.595357  1.035234  SCF (wB97x) = -3807.0866073
H  -4.929489  -4.629807  1.406331  E(SCF)+ZPE(0 K)= -3805.521044
H  -5.293794  -3.616139  -0.001535  H(298 K)= -3805.425397
H  -5.683679  -3.048224  1.623029  G(298 K)= -3805.651192
C  -3.155077  -2.567214  4.872334  Lowest Frequency = 9.8690 cm⁻¹

26_Int3a.log

SCF (wB97x) = -3807.0866073
E(SCF)+ZPE(0 K) = -3805.521044
H(298 K) = -3805.425397
G(298 K) = -3805.651192

Lowest Frequency = 9.8690 cm⁻¹
W  -3.177443  -0.342618  -2.068942  
Al  0.086668   2.867319  -0.566479  
Al  0.257470  -2.742049   0.678514  
O  -0.601430  -1.582910  -0.311606  
O  -1.114735   1.800930  -1.303798  
C  -4.516189  -1.760442  -2.571791  
N  -0.902987  -3.967801   1.574597  
C   1.878397  -1.653968  -2.981396  
N   0.595769   4.404931   0.273330  
C   1.325863  -0.228189  -0.304898  
H   2.369674   5.173361  -3.737316  
H   1.508927   6.679407  -3.330358  

H   0.760148   5.494798  -4.403949  
C  -3.012440  -3.132021   2.534298  
C   2.894081  -0.177944   1.414458  
C  -2.052330   4.005551   2.235539  
C   2.078965   2.416592  -3.725480  
C   0.593072   0.366733   0.478119  
C  -2.320481   4.246058   3.585411  
C   3.180986   1.717552  -4.226369  
C   3.088329   1.195729  -5.176019  
C   0.836063  -5.300586  -0.449418  
C   2.228573   3.074839  -2.491661  
C  -1.876270   6.498826   0.009624  
C  -2.827411   6.013388   0.235999  
C   2.037494   7.276117  -0.737225  
C  -1.526449   6.960858   0.936800  
C   0.717446   4.954744  -2.342298  
C   5.144076  -0.252111   2.316764  
C   5.804448  -0.265192   3.180387  
C   3.766024  -0.196379   2.505312  
C   3.361978  -0.181172   3.514082  
C   0.028715   5.278626   2.475606  
H   0.989723  -3.420044  -2.546708  
H  -0.347869  -5.798772  0.103402  
H   0.636552  -6.798347  -0.195118  
C   1.630607  -6.242559  -1.318011  
C   1.767186  -5.816548  -2.315622  
H   1.122788  -7.202972  -1.409797  
C   2.629186  -6.405485  -0.902630  
C   3.379365  -4.682981   1.760383  
H   2.293978  -4.792642   1.855265
| Atoms | X   | Y   | Z   |
|-------|-----|-----|-----|
| C     | -1.084913 | -3.557466 | 3.995592 |
| H     | 0.929202  | -3.553635 | 3.327751 |
| C     | 1.378507  | -0.325980 | 1.625374 |
| C     | -1.101906 | -5.213299 | 1.128215 |
| C     | 3.435696  | -0.216911 | 0.129239 |
| C     | -3.027510 | 3.170336  | 1.425374 |
| C     | 2.781188  | -0.195804 | -0.739244 |
| C     | -2.696382 | 3.143180  | 0.381421 |
| C     | 0.163876  | 1.073610  | -4.695377 |
| C     | 1.052176  | 3.056042  | -5.943304 |
| H     | 0.836316  | 0.391246  | -5.226922 |
| H     | 1.563657  | 4.022610  | -5.898222 |
| C     | -0.770027 | 1.142920  | -5.259850 |
| H     | 0.103245  | 3.191116  | -6.472230 |
| C     | -0.069818 | 0.637947  | -3.719310 |
| C     | 1.671943  | 2.385909  | -6.549329 |
| C     | 3.445594  | 3.058549  | -1.779482 |
| C     | -0.337230 | 5.682915  | -1.757739 |
| C     | 0.832670  | 2.253581  | 4.431264 |
| H     | -0.646559 | 6.578528  | -2.283131 |
| C     | 1.232624  | 3.215476  | 4.741822 |
| H     | -0.296247 | 5.512422  | 3.811343 |
| C     | 3.008272  | -3.345095 | -1.842597 |
| C     | 0.380197  | 6.098563  | 4.429991 |
| C     | -0.897338 | 5.467975  | -0.500804 |
| C     | -0.182994 | -0.192740 | 3.613096 |
| C     | 3.684389  | -4.092995 | 0.389200 |
| C     | -0.583310 | -1.149024 | 3.297572 |
| C     | -0.721883 | 0.445621  | 4.727878 |
| C     | -3.752685 | -2.761648 | 3.659195 |
| C     | -1.541543 | -0.027169 | 5.264559 |
| C     | -4.782387 | -2.435511 | 3.535108 |
| C     | 4.812338  | -0.285627 | -0.062115 |
| C     | 5.353196  | -3.395229 | -1.224523 |
| C     | 5.205822  | -0.327623 | -1.074180 |
| C     | 6.396465  | -3.232096 | -1.483313 |
| C     | 4.355446  | -3.131486 | -2.150163 |
| C     | 3.882312  | 5.330565  | -0.808243 |
| C     | 4.623140  | -2.763831 | -3.138353 |
| C     | 4.794497  | 5.430818  | -1.407545 |
| C     | -3.644690 | -3.003805 | 1.156334 |
| C     | 4.020085  | 5.907198  | 0.113467 |
| C     | -2.997221 | -3.492431 | 0.421233 |
| C     | 3.060276  | 5.788985  | -1.366916 |
| C     | 1.336877  | 5.838932  | 1.926546 |
| C     | 0.569866  | -5.461405 | 4.247894 |
| C     | 1.457601  | 5.480341  | 0.899001 |
| H     | -0.016085 | -5.896487 | 5.066344 |
| C     | 4.514396  | 2.353745  | -2.329602 |
| H     | 1.624344  | -5.704947 | 4.424527 |
| H     | 5.461267  | 2.319422  | -1.799948 |
| H     | 0.272253  | -5.951777 | 3.315518 |
| C     | 4.704454  | 3.311491  | 0.440920 |
| C     | 1.002560  | -3.282801 | 5.425732 |
| H     | 4.548300  | 2.255638  | 0.675901 |
| H     | 0.833355  | -2.201076 | 5.428101 |
| H     | 4.695618  | 3.875822  | 1.378878 |
| H     | 2.083292  | -3.454955 | 5.426240 |
| H     | 5.705023  | 3.426910  | 0.008401 |
| H     | 0.608263  | -3.700640 | 6.359496 |
| C     | 0.378221  | -3.940016 | 4.191628 |
| C     | -2.165604 | -6.079046 | 1.757933 |
| Element | X | Y | Z | X | Y | Z |
|---------|---|---|---|---|---|---|
| C       | 0.951268 | 2.904291 | -4.643423 |
| H       | 0.229036 | 3.565384 | -4.154534 |
| C       | 0.750318 | 0.525675 | 2.880699 |
| W       | -3.000644 | 0.016318 | -2.500690 |
| Al      | 0.048613 | 2.995790 | -0.656748 |
| Al      | 0.051084 | -2.604164 | 0.700234 |
| O       | -0.796648 | -1.431578 | -0.285588 |
| O       | -1.016812 | 1.899224 | -1.563199 |
| O       | 0.990478 | -1.567398 | 1.727395 |
| C       | -4.996512 | 0.160668 | -2.864952 |
| N       | 1.103192 | 3.990948 | -1.881127 |
| N       | -1.057891 | -3.844456 | 1.639850 |
| C       | -3.452919 | -1.880953 | -2.308300 |
| N       | -0.750442 | 4.463282 | 0.204727 |
| N       | 1.108808 | -3.911943 | -0.211984 |
| C       | -1.873894 | -0.833489 | -3.951125 |
| O       | -6.132025 | 0.285908 | -3.029363 |
| O       | -3.694383 | -3.009614 | -2.147493 |
| C       | -1.241189 | 0.618673 | -1.350272 |
| O       | -1.278493 | -1.338262 | -4.810437 |
| C       | 1.272311 | 1.754233 | 3.294559 |
| H       | 2.083334 | 2.205910 | 2.728735 |
| C       | -1.777779 | -3.434400 | 2.827740 |
| C       | -0.465325 | -0.105318 | -0.359286 |

**27_TS3a.log**

**SCF (wB97x) = -3807.09097171**

**E(SCF)+ZPE(0 K)= -3805.524482**

**H(298 K)= -3805.429845**

**G(298 K)= -3805.652176**

**Lowest Frequency = -10.8288 cm⁻¹**
|   | C       | H       | C       | H       | C       | H       |
|---|---------|---------|---------|---------|---------|---------|
|   | -0.484634 | -5.679266 | 0.178862 | 1.260916 | 5.550120 | 0.956461 |
| H | -0.741372 | -6.697182 | -0.087147 | 4.509910 | 2.547067 | -2.198485 |
| C | 1.508966  | -6.153586 | -1.187569 | 5.415394 | 2.443383 | -1.608920 |
| H | 2.114642  | -5.684822 | -1.962213 | 4.581115 | 3.366337 | 0.612232  |
| H | 0.857310  | -6.904999 | -1.638335 | 4.425657 | 2.295548 | 0.762393  |
| H | 2.189122  | -6.669874 | -0.501188 | 4.515671 | 3.861427 | 1.586885  |
| C | 3.310399  | -4.638261 | 1.589037  | 5.601046 | 3.522025 | 0.241715  |
| H | 2.241674  | -4.845558 | 1.715218  | 0.388125 | -3.773993 | 4.163920  |
| C | -1.087225 | -3.401142 | 4.058728  | 0.879937 | -3.429350 | 3.249660  |
| C | 1.241647  | -0.193568 | 1.608596  | -1.220025 | -5.107073 | 1.221804  |
| C | 3.284131  | -0.148126 | 0.094966  | -3.142873 | 3.033358 | 1.258752  |
| H | 2.613616  | -0.153777 | -0.762562 | -2.723513 | 2.964295 | 0.248334  |
| C | 0.251676  | 1.557774  | -4.829786 | 1.304922 | 3.500891 | -6.013615 |
| H | 0.896984  | 0.846719  | -5.356756 | 1.874819 | 4.432661 | -5.934658 |
| H | -0.665019 | 1.679429  | -5.416721 | 0.392470 | 3.701252 | -6.584486 |
| H | -0.025446 | 1.123968  | -3.866511 | 1.908572 | 2.800860 | -6.601217 |
| C | 3.428020  | 3.254217  | -1.676669 | -0.375417 | 5.880061 | -1.715345 |
| C | 0.774888  | 2.389864  | 4.426521  | -0.665780 | 6.804552 | -2.199028 |
| H | 1.196347  | 3.342356  | 4.737514  | -0.641180 | 5.498971 | 3.771600  |
| C | 2.700924  | -3.020898 | -1.872252 | -0.021684 | 6.109231 | 4.425369  |
| C | -1.025036 | 5.566715  | -0.522800 | -0.294976 | -0.033436 | 3.612917  |
| C | 3.525557  | -4.025833 | 0.210716  | -0.716117 | -0.981536 | 3.300877  |
| C | -0.801011 | 0.604817  | 4.743082  | -3.797313 | -2.708599 | 3.912752  |
| H | -1.615777 | 0.139563  | 5.293306  | -4.847469 | -2.432226 | 3.862496  |
| C | 4.657134  | -0.232274 | -0.113693 | 5.083142 | -3.301750 | -1.496799 |
| H | 5.037132  | -0.302967 | -1.129220 | 6.106196 | -3.187068 | -1.846496 |
| C | 4.024742  | -2.889506 | -2.295410 | 3.816124 | 5.460693 | -0.540370 |
| H | 4.233761  | -2.447335 | -3.264910 | 4.710086 | 5.597074 | -1.159827 |
| C | -3.921575 | -3.103147 | 1.435988  | 3.996017 | 5.957198 | 0.419166  |
| H | -3.322891 | -3.595390 | 0.662780  | 2.983131 | 5.977548 | -1.026798 |
| C | 1.056279  | 5.923516  | 1.965162  | 0.576743 | -5.293501 | 4.267383  |
H  2.108302  5.859361  3.883799  O  -4.624467 -3.196121 -1.657973
H  3.168816  5.942826  2.477178  O  -1.294558 -3.080762 -4.160235
H  2.349498  4.421249  2.877502  C  -1.175824  0.674767 -1.420949
H  2.688481 -1.623778 -4.396429  O  -3.116223  0.551902 -4.775753
H  2.368760 -0.527614 -3.040170  C  1.214497  1.776144  3.381345
H  1.066897 -0.988209 -4.155580  H  2.076581  2.194622  2.868759
H  3.680575  0.746937 -0.991246  C  -1.783000 -3.369361  2.864566
H  2.368760 -0.527614 -3.040170  C  -0.392825  0.006343 -0.374635
H  1.066897 -0.988209 -4.155580  C  0.909777  2.802864 -4.615355

28_Int4a.log

SCF (wB97x) = -3807.10497111
E(SCF)+ZPE(0 K)= -3805.537283
H(298 K)= -3805.442107
G(298 K)= -3805.665410
Lowest Frequency = 15.3774 cm⁻¹
| X  | Y  | Z   |  X  | Y  | Z   |
|----|----|-----|----|----|-----|
| -1.724144 | 7.095580 | 0.828671 | H  | -1.855528 | 0.276059 | 5.188263 |
| 0.764216  | 5.179329 | -2.335313 | C  | 4.667205  | -0.254466 | 0.081179 |
| 4.931117  | -0.244095 | 2.469441 | C  | 5.087172  | -0.309216 | -0.919650 |
| 5.565696  | -0.289592 | 3.351094 | C  | 4.093317  | -2.939451 | -2.264643 |
| 3.551403  | -0.132695 | 2.619844 | H  | 4.349269  | -2.543626 | -3.244851 |
| 3.119270  | -0.104500 | 3.616737 | C  | -0.401287 | -2.863406 | 1.655809 |
| -0.249185 | 5.370568 | 2.407371 | H  | -3.432292 | -3.174123 | 0.780838 |
| 0.726517  | -3.107310 | -2.602427 | C  | 1.083926  | 5.949470  | 1.943002 |
| -0.660067 | -5.518871 | 0.050301 | H  | 1.265371  | 5.611858  | 0.917188 |
| -0.989250 | -6.500148 | -0.266525 | C  | 4.459650  | 2.403606  | -2.162924 |
| 1.199799  | -5.963896 | -1.521044 | H  | 5.367910  | 2.301259  | -1.577234 |
| 1.147474  | -5.537443 | -2.527734 | C  | 4.565332  | 3.345549  | 0.617541 |
| 0.719639  | -6.942603 | -1.532861 | H  | 4.361456  | 2.294018  | 0.833752 |
| 2.257806  | -6.084487 | -1.276711 | H  | 4.531644  | 3.901454  | 1.560346 |
| 3.152640  | -4.621281 | 1.593311 | H  | 5.588501  | 3.429640  | 0.233039 |
| 2.071981  | -4.598167 | 1.762150 | C  | 0.454837  | -3.773029 | 4.072275 |
| -1.024324 | -3.411912 | 4.055170 | H  | 0.889670  | -3.437567 | 3.128028 |
| 1.186803  | -0.132916 | 1.661839 | C  | -1.339512 | -4.970576 | 1.150029 |
| 3.289723  | -0.129357 | 0.233892 | C  | -3.281371 | 3.365736  | 1.114072 |
| 2.661118  | -0.078693 | -0.652593 | H  | -2.894692 | 3.396316  | 0.089152 |
| 0.183840  | 1.475950  | -4.848191 | C  | 1.302017  | 3.424060  | -5.964399 |
| 0.829363  | 0.764277  | -5.376098 | H  | 1.867790  | 4.354042  | -5.849756 |
| -0.711403 | 1.634779  | -5.457649 | H  | 0.405243  | 3.636167  | -6.555817 |
| -0.135596 | 1.022474  | -3.906511 | H  | 1.921222  | 2.733470  | -6.547473 |
| 3.404015  | 3.164828  | -1.664526 | C  | -0.326149 | 5.904697  | -1.810315 |
| 0.677618  | 2.425731  | 4.487204  | H  | -0.583820 | 6.819732  | -2.330521 |
| 1.121402  | 3.356648  | 4.831446  | C  | -0.640856 | 5.558266  | 3.732145 |
| 2.746626  | -3.110839 | -1.935726 | H  | 0.006808  | 6.115572  | 4.405797 |
| -0.986337 | 5.655563  | -0.611882 | C  | -0.449691 | 0.058995  | 3.583090 |
| 3.439371  | -3.981614 | 0.242584  | H  | -0.892514 | -0.867587 | 3.235966 |
| -0.991811 | 0.709284  | 4.689107  | C  | -3.736611 | -2.743970 | 4.132104 |
H  2.037260  7.870163  1.590476  O  0.910618  1.774731  0.408050
H  0.874071  7.887525  2.925896  C  -3.660369 -2.519379 -1.819819
C  1.698563 -2.779878 -2.980538  N  1.225721  3.862109 -1.897667
C  1.958456 -3.508627 -4.306331  N  -1.012423 -3.842966  1.607344
H  2.838513 -3.101737 -4.817433  C  -1.529977 -2.415435 -3.406152
H  1.096951 -3.386170 -4.163365  N  -0.640013  4.447227  0.144158
H  2.131232 -4.580680 -4.163365  N  1.160242 -3.953995 -0.284917
C  1.617409 -1.273193 -3.227667  C  -2.725626 -0.153545 -3.818671
H  2.137673  5.753810  3.850281  O  -4.491981 -3.305126 -1.643196
H  3.196730  5.841708  2.441369  O  -1.181828 -3.222709 -4.165904
H  2.301495  4.348196  2.783856  C  -1.050862  0.557581 -1.431349
H  2.586908 -0.872188 -3.548456  O  -2.980839  0.403473 -4.807136
H  1.305563 -0.729601 -2.329646  C  1.343723  1.661227  3.377460
H  0.884479 -1.062091 -4.009989  H  2.206085  2.078128  2.864035
H  -3.014569 -0.030389 -0.655890  C  -1.657397 -3.479121  2.860836
H  -4.027246 -0.361504 -2.379959  C  -0.274359 -0.107683 -0.375575
       C  1.032518  2.693589 -4.621450
       H  0.315241  3.359701 -4.132197
       C  0.788762  0.464923  2.918315
SCF (wB97x) = -3807.10495920  C  -1.002096  4.549762  1.541482
E(SCF)+ZPE(0 K)= -3805.537544  C  2.542605 -3.733425 -0.673725
H(298 K)= -3805.443132  C  1.652088  5.750900 -3.440187
G(298 K)= -3805.664150  H  2.614813  5.278433 -3.635294
Lowest Frequency = -54.0836cm^-1
       H  1.808668  6.800496 -3.179869
       H  1.060141  5.724347 -4.361053
W  -2.286599 -1.028446 -2.109292  C  -3.018952 -3.122573  2.888383
Al  0.123060  2.925307 -0.657358  C  2.836019 -0.183014  1.495145
Al  0.134523 -2.644276  0.647611  C  -2.211932  4.015319  2.007852
O  -0.646109 -1.455768 -0.431409  C  2.248656  2.539424 -3.713833
O  -0.952620  1.858086 -1.584827  C  0.605935  0.463140  0.486131
O  0.986524 -1.610726  1.733530  C  -2.544268  4.201887  3.351807
| X      | Y      | Z      | X      | Y      | Z      |
|--------|--------|--------|--------|--------|--------|
| H      | 2.045682 | 2.626817 | -6.552795 | C      | 3.660234 | 3.821741 | -0.356957 |
| C      | -0.209495 | 5.789855 | -1.814452 | H      | 2.691043 | 3.786366 | 0.155011  |
| H      | -0.467835 | 6.704998 | -2.334153 | C      | 4.887846 | -3.919241 | -0.146073 |
| C      | -0.523544 | 5.438426 | 3.726801  | H      | 5.679209 | -4.202600 | 0.543542  |
| H      | 0.124032  | 5.995747 | 4.400512  | C      | -4.568438 | 3.860893 | 1.090668  |
| C      | -0.324355 | -0.051965 | 3.580011  | H      | -5.047874 | 3.790330 | 2.073473  |
| H      | -0.770134 | -0.977028 | 3.232596  | H      | -5.201614 | 3.327951 | 0.374345  |
| C      | -3.608582 | -2.836129 | 4.122833  | H      | -4.551302 | 4.919055 | 0.807312  |
| H      | -4.659927 | -2.560097 | 4.150951  | C      | 5.615889 | -0.426520 | 1.183827  |
| C      | 5.219908  | -3.397355 | -1.387273 | H      | 6.692063 | -0.522388 | 1.063291  |
| H      | 6.262862  | -3.267281 | -1.665127 | C      | -0.297372 | 1.783498 | 5.143772  |
| C      | 3.994286  | 5.293884 | -0.641065 | H      | -0.715786 | 2.297539 | 6.005557  |
| H      | 4.936217  | 5.369615 | -1.196432 | C      | 4.486126 | 1.653790 | -3.397606 |
| H      | 4.110514  | 5.851086 | 0.295305  | H      | 5.318792 | 1.059150 | -3.765269 |
| H      | 3.216426  | 5.791018 | -1.228574 | C      | -3.228798 | 1.777244 | 1.534180  |
| C      | 0.759996  | -5.405690 | 4.183344  | H      | -2.238619 | 1.306486 | 1.507634  |
| H      | 0.272251  | -5.787318 | 5.088118  | H      | -3.882612 | 1.218432 | 0.859385  |
| H      | 1.823196  | -5.666211 | 4.239911  | H      | -3.612692 | 1.678708 | 2.557095  |
| H      | 0.335583  | -5.932803 | 3.321180  | C      | 2.360926 | 5.326779 | 2.799781  |
| C      | 1.350096  | -3.158098 | 5.175634  | C      | 3.939654 | -3.966412 | 2.725952  |
| H      | 1.149513  | -2.081923 | 5.147017  | H      | 5.026546 | -3.917543 | 2.598274  |
| H      | 2.424622  | -3.306456 | 5.037587  | H      | 3.746426 | -4.463130 | 3.683220  |
| H      | 1.098802  | -3.533274 | 6.174247  | H      | 3.562002 | -2.940612 | 2.777587  |
| C      | -2.204683 | -5.993879 | 1.835017  | C      | -4.216128 | -1.493032 | 1.449327  |
| H      | -2.075549 | -5.968631 | 2.919640  | H      | -4.800218 | -1.114132 | 2.296874  |
| H      | -2.085937 | -7.018766 | 1.482798  | H      | -4.795087 | -1.338749 | 0.533736  |
| H      | -3.226740 | -5.670977 | 1.621886  | H      | -3.304670 | -0.897766 | 1.364581  |
| C      | -1.539588 | -3.229255 | 5.257090  | C      | -5.180081 | -3.790920 | 1.703422  |
| H      | -0.971193 | -3.258633 | 6.181148  | H      | -5.013896 | -4.841916 | 1.960919  |
| C      | -1.719924 | 4.919457 | 4.203721  | H      | -5.676538 | -3.759356 | 0.728933  |
| H      | -2.005266 | 5.070409 | 5.241697  | H      | -5.873061 | -3.380623 | 2.446495  |
C -2.885960 -2.896064 5.301076  
H -3.365222 -2.678034 6.252006  
C 3.698887 -6.210911 1.593693  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  
H 3.192115 -6.785034 1.242766  

Lowest Frequency = 10.5650 cm⁻¹

30_Int5a.log

SCF (wB97x) = -3807.12256177

E(SCF)+ZPE(0 K)= -3805.551733

H(298 K)= -3805.456924

G(298 K)= -3805.680272

S173
| X       | Y       | Z       | X       | Y       | Z       |
|---------|---------|---------|---------|---------|---------|
| C -4.400994 | -1.416520 | 0.923180 | H -3.751946 | -1.219381 | -2.273954 |
| H -5.031370 | -0.863059 | 1.629078 | 31_TS5a.log |
| H -4.957632 | -1.531673 | -0.013309 |
| H -3.516529 | -0.809464 | 0.716420 |
| C -5.259663 | -3.615762 | 1.768460 |
| H -5.027047 | -4.571767 | 2.246706 |
| H -5.786024 | -3.820946 | 0.830256 |
| H -5.953219 | -3.079892 | 2.426004 |
| C -3.015806 | -1.860092 | 5.038470 |
| H -3.487030 | -1.397832 | 5.902087 |
| C 3.049724 | -6.449619 | 1.716073 |
| H 2.406173 | -6.843380 | 0.923004 |
| H 2.735886 | -6.911159 | 2.659232 |
| H 4.076846 | -6.770613 | 1.507125 |
| C 1.100260 | 7.003512 | 2.717078 |
| H 0.292187 | 7.655162 | 2.367528 |
| H 2.049489 | 7.436052 | 2.382035 |
| H 1.095227 | 7.027738 | 3.812396 |
| C 2.015125 | -2.740570 | -2.74507 |
| C 2.351852 | -3.416107 | -4.080902 |
| C 3.311985 | -3.062678 | -4.473253 |
| H 1.580138 | -3.187175 | -4.820322 |
| H 2.419555 | -4.505056 | -3.979760 |
| C 2.025980 | -1.216584 | -2.898387 |
| H 2.056692 | 4.590935 | 3.790989 |
| H 3.066791 | 5.127235 | 2.436764 |
| H 2.033768 | 3.681064 | 2.277548 |
| H 3.037673 | -0.843745 | -3.102418 |
| H 1.663599 | -0.717433 | -1.993750 |
| H 1.382103 | -0.917324 | -3.730590 |
| H -2.350371 | 0.433116 | -0.861388 |

SCF (wB97x) = -3807.11819660
E(SCF)+ZPE(0 K)= -3805.547622
H(298 K)= -3805.452996
G(298 K)= -3805.676342
Lowest Frequency = -84.3405 cm⁻¹
|  |   |   |   |  |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| C | 1.448268 | 0.904874 | 5.357941 | C | -2.652996 | -1.508515 | 5.085382 |
| H | 0.991783 | 0.458156 | 6.239005 | H | -3.571894 | -0.945908 | 5.230780 |
| C | 4.439268 | -0.201110 | -1.111324 | C | 4.577381 | -3.590310 | -1.917964 |
| H | 4.491210 | -0.136847 | -2.195118 | H | 5.545656 | -3.553206 | -2.410322 |
| C | 3.436518 | -3.182266 | -2.589822 | C | 4.080716 | 5.391716 | -0.189620 |
| H | 3.514930 | -0.136847 | -2.195118 | H | 4.870652 | 5.720719 | -0.875785 |
| C | -3.321539 | -1.707479 | 2.676364 | H | 4.405813 | 5.631165 | 0.828573 |
| H | -2.986800 | -2.249900 | 1.784203 | H | 3.184051 | 5.982921 | -0.385560 |
| C | -1.521975 | 3.988560 | 2.837679 | C | 0.961608 | -5.135668 | 4.520820 |
| H | -0.641872 | 4.397192 | 2.329372 | H | 0.522663 | -5.487984 | 5.461795 |
| C | 4.590954 | 2.843911 | -2.515034 | H | 1.951273 | -5.597012 | 4.419914 |
| H | 5.581329 | 2.722421 | -2.087433 | H | 0.344345 | -5.503753 | 3.695815 |
| C | 5.039040 | 3.157896 | 0.329588 | C | 2.135371 | -3.174462 | 5.554442 |
| H | 4.975571 | 2.072799 | 0.227652 | H | 2.225159 | -2.084604 | 5.605674 |
| H | 5.074631 | 3.396643 | 1.398181 | H | 3.113434 | -3.578177 | 5.276642 |
| H | 5.990301 | 3.492499 | -0.102003 | H | 1.904070 | -3.554416 | 6.556212 |
| C | 1.088284 | -3.606138 | 4.523004 | C | -2.355477 | -5.126639 | 2.888312 |
| H | 1.470854 | -3.291837 | 3.544838 | H | -2.027167 | -5.133212 | 3.930738 |
| C | -1.331231 | -4.467106 | 2.000928 | H | -2.545296 | -6.149917 | 2.563450 |
| C | -3.300572 | 4.218439 | -1.990280 | H | -3.295464 | -4.568355 | 2.849771 |
| H | -2.283508 | 4.589163 | -2.157736 | C | -0.612226 | -2.407945 | 5.967749 |
| C | 0.780616 | 4.050284 | -5.615768 | H | 0.060633 | -2.541037 | 6.808898 |
| H | 1.264673 | 5.020677 | -5.460967 | C | -4.872973 | 3.069701 | 1.283005 |
| H | -0.216615 | 4.228346 | -6.031448 | H | -5.831939 | 2.678358 | 1.612998 |
| H | 1.361112 | 3.511871 | -6.373354 | C | 3.848963 | 3.876916 | -0.314355 |
| C | 0.180139 | 6.272808 | -0.970274 | H | 2.954000 | 3.617180 | 0.265448 |
| H | 0.227477 | 7.348461 | -1.087267 | C | 4.475944 | -4.047558 | -0.612439 |
| C | -3.854758 | 3.286213 | 2.199903 | H | 5.370695 | -4.374214 | -0.087567 |
| H | -4.022308 | 3.065814 | 3.252056 | C | -4.275905 | 5.338157 | -2.382557 |
| C | 1.331206 | 0.259343 | 4.128632 | H | -5.315869 | 5.007755 | -2.282423 |
| H | 0.790705 | -0.676985 | 4.057967 | H | -4.120098 | 5.626983 | -3.427413 |
SCF (wB97x) = -3807.11491573
E(SCF)+ZPE(0 K)= -3805.544175
H(298 K)= -3805.449491
G(298 K)= -3805.672724

Lowest Frequency = -818.5346cm⁻¹

33_TS6a.log
O  1.609850 -1.468480  1.927213  C  -4.454442  3.160884  -0.029116
O  1.067836  1.945687  0.710396  H  -5.254474  2.988230  -0.745216
C  -3.943653 -1.208303  -0.966702  C  3.240851  2.287157  -4.316181
N  1.443961  4.011976  -1.541292  H  3.044434  1.906258  -5.315873
N  -0.601551 -3.483927  2.359674  C  0.346378  -5.095332  0.016521
C  -2.316826 -3.282767  -1.597772  C  2.484130  3.361203  -2.306801
N  -0.916144  4.310571  0.009892  C  -1.672130  6.616651  0.359335
N  1.056660 -3.960170  0.075419  H  -2.646373  6.511187  -0.125968
C  -2.341352 -1.117537  -3.270038  H  -1.310601  7.634047  0.205762
O  -5.068818 -1.143742  -0.658192  H  -1.830309  6.447541  1.428195
O  -2.538800 -4.399598  -1.815661  C  1.318625  5.338922  -1.653239
C  -1.221292  0.746983  -0.589151  C  5.674456  -0.755915  0.991973
O  -2.435383 -0.998144  -4.424426  H  6.562963  -0.95146  1.571458
C  2.796120  1.816984  3.108925  C  4.473999  -0.503111  1.644631
H  3.255837  2.246208  2.224157  H  4.426955  -0.551317  2.729738
C  -0.961910  -2.926652  3.647635  C  -2.413601  3.598407  1.837217
C  -0.164312  0.017764  0.223782  H  0.272271  -3.282726  -2.175350
C  0.826628  3.001560  -4.248213  C  -0.724180  -5.382396  0.872544
H  0.160985  3.530757  -3.556631  H  -1.251598  -6.308157  0.682287
C  2.102425  0.609386  3.003711  C  0.708978  -6.143587  -1.002002
C  -2.218221  3.886153  0.476126  H  0.508792  -5.761246  -2.008031
C  2.321303  -3.897816  -0.632155  H  0.120827  -7.048897  -0.852051
C  2.169312  6.095499  -2.645206  H  1.772864  -6.390161  -0.954372
H  3.184038  5.704875  -2.719770  C  3.441504  -4.858911  1.478233
H  2.205092  7.155284  -2.387522  H  2.404729  -4.837477  1.830624
H  1.708771  6.002706  -3.635267  C  -0.077860  -3.116238  4.732381
C  -2.160792  -2.208786  3.796088  C  1.967562  -0.125118  1.659060
C  3.315632  -0.196730  0.922504  C  3.395045  -0.128827  -0.466323
C  -3.246239  3.699445  -0.473137  H  2.514488  0.134135  -1.046556
C  2.199802  2.881804  -3.596327  C  0.205311  1.624130  -4.507636
C  0.893155  0.596448  0.821218  H  0.832668  1.025988  -5.179846
H  -0.779096  1.732678  -4.976692  H  -0.113367  3.963395  -5.952207
H  0.067417  1.087113  -3.566048  H  1.478494  3.288364  -6.313211
C  3.764967  3.234782  -1.724836  C  0.384041  6.097817  -0.936136
C  2.912914  2.463519  4.334952  H  0.437793  7.172102  -1.062533
H  3.463837  3.398927  4.398369  C  -3.648451  3.078426  2.231287
C  2.386636  -3.462279  -1.967396  H  -3.814780  2.844814  3.280679
C  -0.694384  5.610244  -0.188958  C  1.516311  0.074804  4.148688
C  3.480016  -4.301580  0.060476  H  0.963823  -0.854526  4.074264
C  1.634054  0.717722  5.379148  C  -2.489548  -1.731664  5.068280
H  1.165710  0.276518  6.256666  H  -3.414009  -1.174952  5.201192
C  4.595344  -0.391890  -1.124906  C  4.789437  -3.798772  -1.915702
H  4.629233  -0.338051  -2.209911  H  5.753313  -3.754990  -2.416153
C  3.637289  -3.421329  -2.586936  C  4.283798  5.206859  -0.170877
H  3.703578  -3.085583  -3.619344  H  5.068818  5.533373  -0.863756
C  -3.084947  -1.873440  2.633343  H  4.617740  5.446378  0.844374
H  -2.716843  -2.379609  1.733572  H  3.386901  5.800020  -0.360178
C  -1.336174  3.833876  2.885177  C  1.160495  -5.332138  4.555879
H  -0.459315  4.255385  2.381608  H  0.715847  -5.685730  5.493692
C  4.771961  2.662121  -2.499991  H  2.154804  -5.785599  4.465062
H  5.768539  2.549869  -2.084521  H  0.553699  -5.707135  3.726247
C  5.241176  2.970200  0.341392  C  2.308010  -3.358014  5.595178
H  5.174887  1.885580  0.236319  H  2.388021  -2.267283  5.643727
H  5.285031  3.205933  1.410327  H  3.292192  -3.754634  5.328154
H  6.189783  3.304268  -0.096200  H  2.070097  -3.736536  6.595914
C  1.274746  -3.801653  4.555043  C  -2.146198  -5.322584  2.901871
H  1.665397  -3.488625  3.579616  H  -1.811977  -5.347388  3.942327
C  -1.113727  -4.672811  2.017026  H  -2.356373  -6.338312  2.566308
C  -3.117329  4.098601  -1.941437  H  -3.075178  -4.746281  2.876852
H  -2.119442  4.523582  -2.097587  C  -0.459791  -2.627959  5.981844
C  0.893569  3.812852  -5.549361  H  0.197864  -2.765279  6.834469
H  1.353067  4.796268  -5.402629  C  -4.656395  2.842804  1.308052

S184
|   | SCF (wB97x) | E(SCF)+ZPE(0 K) | H(298 K) |
|---|-------------|-----------------|----------|
| H | -5.604110   | 2.418332        | 1.628670 |
| C | 4.047827    | 3.692535        | -0.292429|
| H | 3.157706    | 3.435919        | 0.296538 |
| C | 4.705390    | -4.235903       | -0.601943|
| H | 5.609047    | -4.539871       | -0.078571|
| C | -4.146277   | 5.182008        | -2.299397|
| H | -5.167588   | 4.790853        | -2.234767|
| H | -3.989848   | 5.528430        | -3.326397|
| H | -4.085398   | 6.051961        | -1.636630|
| C | 5.737354    | -0.709152       | -0.399796|
| H | 6.673166    | -0.916206       | -0.913262|
| C | 2.337772    | 1.913195        | 5.479070 |
| H | 2.437570    | 2.415136        | 6.438257 |
| C | 4.516984    | 2.194276        | -3.784861|
| H | 5.318318    | 1.745262        | 4.366624 |
| C | -3.257370   | 2.905898        | -2.895898|
| H | -2.442939   | 2.194228        | -2.738891|
| C | -3.219705   | 3.252578        | -3.935486|
| H | -4.213289   | 2.388183        | -2.754740|
| C | -0.898959   | 2.521967        | 3.541396 |
| C | 4.272413    | -4.009491       | 2.444270 |
| H | 5.316614    | -3.938619       | 2.119322 |
| H | 4.265447    | -4.459340       | 3.443962 |
| H | 3.871132    | -2.993757       | 2.512514 |
| C | -3.047579   | -0.363396       | 2.369003 |
| H | -3.433705   | 0.189802        | 3.233652 |
| H | -3.669244   | -0.103708       | 1.505891 |
| H | -2.027278   | -0.011260       | 2.183949 |
| C | -4.534617   | -2.320452       | 2.861027 |
| H | -4.615761   | -3.388171       | 3.090190 |
| H | -5.124879   | -2.119638       | 1.960993 |

34_Int7a.log

SCF (wB97x) = -3807.16079222
E(SCF)+ZPE(0 K) = -3805.584590
H(298 K) = -3805.489473
$G(298 \text{ K}) = -3805.714945$

Lowest Frequency = 10.9045 cm$^{-1}$

W  -2.548716  -1.643002  -1.143121
Al  0.166326   3.117680  -0.717862
Al  0.250274  -2.372623   0.999552
O  -0.724780  -1.197602   0.032143
O  -0.706753   1.961047  -1.683261
O    1.378100  -1.322684   1.752440
O   0.934345    2.063353  -0.469795
C   4.372459  -0.994748  -1.206930
N   1.359429   4.259541  -1.634547
N  -0.799763  -3.338750   2.234002
C  -3.307629  -3.323634  -0.590336
N  -1.074678   4.446455  -0.175161
N   0.811536  -3.805407  -0.088724
C  -2.822234  -2.219133  -2.967007
O  -5.457771  -0.555621  -1.189672
O  -3.804168  -4.324664  -0.229970
C  -1.248887   0.863438  -1.029793
O  -2.915087  -2.578384  -4.078428
C   2.545216   1.963167   2.940358
H   3.026532   2.381622   2.062881
C  -1.096745  -2.769694   3.533465
C  -0.323124   0.144209  -0.066975
C   0.900466   3.346414  -4.407098
H   0.194383   3.848457  -3.735933
C   1.839620   0.763050   2.826969
C  -2.366576   3.956006   0.257994
C   2.028183  -3.702429  -0.868729
C   2.075407   6.394651  -2.640306

H    3.104180   6.035473  -2.666088
H    2.064130   7.447341  -2.353230
H    1.675485   6.316598  -3.657588
C   -2.258407  -2.004726   3.729140
C    3.096313  -0.041561   0.770887
C   -3.333062   3.653367  -0.726614
C    2.240955   3.225850  -3.691664
C    0.695274    0.729669   0.593882
C   -4.545436   3.105825  -0.304667
H   -5.301270   2.847982  -1.041630
C    3.324856   2.671552  -0.437857
H    3.185999   2.329614  -5.401852
C    0.133475  -4.964736  -0.104997
C    2.449863   3.655859  -2.370426
C   -1.896242   6.724822   0.23925
H    2.922460   6.415383   0.026516
H   -1.734961   7.731774  -0.152766
H   -1.783832   6.748258   1.323796
C    1.194721   5.586249  -1.718565
C    5.462314  -0.562043   0.893940
C    6.338418   0.796435   1.493897
C    4.240220  -0.340857  1.517899
H    4.165846  -0.408400   2.600412
C   -2.615592   3.742842   1.623377
H   -0.129883  -3.062706  -2.253480
C   -0.895203  -5.270411   0.788384
H   -1.416654  -6.203795   0.619562
C    0.498263  -6.015156  -1.120278
C    0.308023   5.638011  -2.129554
H   -0.089453  -6.920415   0.968213
H    1.561982  -6.262064  -1.064822
|  | x       | y       | z       |  | x       | y       | z       |
|---|---------|---------|---------|---|---------|---------|---------|
| H | -2.193692 | 1.127916 | -0.513886 | C | -1.513102 | -3.577665 | 2.952474 |
| H | -1.504480 | 0.134499 | -1.849092 | C | -0.332149 | -0.191589 | -0.210671 |
|   |          |         |         | C | 1.028093  | 2.951755  | -4.527650 |
| 35_TS3b.log |         |         |         | H | 0.298382  | 3.584036  | -4.012988 |
|   |          |         |         | C | 0.878163  | 0.402042  | 3.018410  |
| SCF (wB97x) = | -3920.3843637 |         |         | C | -1.020549 | 4.410296  | 1.797833  |
| E(SCF)+ZPE(0 K)= | -3918.811062 |         |         | C | 2.592873  | -3.680683 | -0.669704 |
| H(298 K)= | -3918.713210 |         |         | C | 1.507306  | 5.899825  | -3.148711 |
| G(298 K)= | -3918.942783 |         |         | H | 2.480612  | 5.467866  | -3.380736 |
| Lowest Frequency = | -137.5456cm^-1 |         |         | H | 1.638849  | 6.932493  | -2.816428 |
|   |          |         |         | H | 0.910156  | 5.922602  | -4.066168 |
| W | -2.538352 | -0.672833 | -2.430873 | C | -2.870914 | -3.214679 | 2.929145  |
| Al | 0.115820  | 2.893129 | -0.482948 | C | 2.893399  | -0.174861 | 1.514963  |
| Al | 0.223798  | -2.701599 | 0.779600  | C | -2.202011 | 3.827921  | 2.278888  |
| O | -0.670572 | -1.519577 | -0.161988 | C | 2.232061  | 2.753349  | -3.612766 |
| O | -0.974797 | 1.797080  | -1.362966 | C | 0.608742  | 0.402442  | 0.592696  |
| O | 1.127812  | -1.675054 | 1.842581  | C | -2.516175 | 3.987694  | 3.630660  |
| O | 0.933524  | 1.701367  | 0.508905  | H | -3.425774 | 3.535847  | 4.018816  |
| C | -4.257209 | -1.773584 | -2.364297 | C | 3.338556  | 2.049871  | -4.096778 |
| N | 1.155362  | 3.910591  | -1.713582 | H | 3.296134  | 1.620699  | -5.095102 |
| N | -0.845889 | -3.966032 | 1.727513  | C | 0.830307  | -5.236797 | -0.392663 |
| C | -3.738368 | 0.742255  | -1.676739 | C | 2.311543  | 3.277310  | -2.309350 |
| N | -0.687147 | 4.352811  | 0.389699  | C | -2.039369 | 6.405796  | 0.174376  |
| N | 1.253480  | -3.981749 | -0.204377 | H | -2.987435 | 5.869202  | 0.285092  |
| C | -2.004299 | -3.479172 | -1.866395 | H | -2.180161 | 7.233042  | -0.522258 |
| O | -5.200891 | -2.439949 | -2.323836 | H | -1.784770 | 6.805826  | 1.158352  |
| O | -4.423112 | 1.623095  | -1.349067 | C | 0.764139  | 5.123951  | -2.090570 |
| O | -3.068429 | 0.980604  | -5.013444 | C | 5.155193  | -0.292444 | 2.380683  |
| O | -2.120307 | -4.523495 | -2.303600 | H | 5.829309  | -0.320179 | 3.233270  |
| C | 1.432013  | 1.597112  | 3.482943  | C | 3.781402  | -0.215189 | 2.592263  |
| H | 2.275797  | 2.033481  | 2.954541  | H | 3.394141  | -0.200829 | 3.607531  |
C  -0.160528  5.132946  2.650999
H   0.805355  -2.198288 -2.028841
C   -0.298618  -5.779729  0.235642
H   -0.554346  -6.795878 -0.037524
C    1.628132  -6.197924 -1.242073
H    2.155835  -5.702975 -2.057028
H    0.967667  -6.966616 -1.648203
H    2.377983  -6.695244 -0.617508
C    3.533548  -4.775268  1.465637
H    2.475061  -5.011497  1.624108
C    0.772968  -3.575519  4.153654
C    1.377361  -0.296949  1.739731
C    3.413449  -0.226140  0.221072
H    2.740738  -0.201268  0.634544
C    0.316343  1.636009  -4.843370
H    0.977242  0.951089  -5.387322
H    -0.565558  1.818941  -5.465359
H    -0.022132  1.136852  -3.932162
C    3.478142  3.158146  -1.525943
C    0.922731  2.212040  4.616632
C    1.370948  3.147238  4.967565
C    2.774635  -3.017985  -1.898008
C    -0.986878  5.453054  -0.335123
C    3.687168  -4.111754  0.102387
C    -0.732613  0.493316  4.828757
H   -1.582127  0.046819  5.340465
C    4.785310  -0.317795  0.006332
C    5.161369  -0.366539  -1.011959
C    4.080473  -2.853939  -2.364098
C    4.247099  -2.361234  -3.317200
C    -3.693800  -3.155034  1.650118

H    -3.118836  -3.620636  0.841837
C    1.141022  5.766660  2.169192
C    1.328406  5.425593  1.145694
C    4.553916  2.451933  -2.061055
H    5.459474  2.332674  -1.474535
C    4.640531  3.258404  0.761271
H    4.465680  2.192577  0.925131
H    4.593088  3.766350  1.730313
H    5.660242  3.389580  0.380973
C    0.705542  -3.944554  4.192531
C    1.142788  -3.654791  3.233791
C    -1.007392  -5.227096  1.306624
C    -2.895722  0.368421  -4.00832
C    -3.143586  3.039205  1.386903
H    -2.804229  3.132643  0.349192
C    1.433932  3.655379  -5.831200
C    1.989728  4.581566  -5.653216
H    0.543046  3.895258  -6.420878
H    2.066232  3.005923  -6.446368
C    -0.354951  5.774776  -1.531312
C    -0.659921  6.695884  -2.013876
C    -0.535322  5.292837  3.984230
C     0.102745  5.867173  4.652525
C    -0.216123  -0.133115  3.697342
C    -0.666498  -1.053814  3.344315
C    -3.479587  -2.854142  4.134033
C    -4.526660  -2.561499  4.132054
C     5.171786  -3.298008  -1.629867
C     6.179568  -3.158590  -2.013230
C     3.900206  5.355185  -0.403532
C     4.833752  5.472932  -0.965529

S190
| Atoms | X   | Y   | Z   | Atoms | X    | Y   | Z   |
|-------|-----|-----|-----|-------|-----|-----|-----|
| C     | -0.95792 | 5.860030 | -0.961796 | C     | 1.597698 | -2.509802 | 1.789429 |
| C     | 1.710537 | 3.695545 | 1.441781 | H     | 5.398537 | -5.916182 | 1.549998 |
| C     | 4.481510 | 1.887071 | -3.329212 | C     | 1.740975 | 7.302897 | 2.133015 |
| C     | -0.432696 | 4.639770 | 1.232190 | H     | 0.267402 | 7.645770 | 1.455220 |
| C     | 5.662867 | -0.349524 | 1.085682 | H     | 2.001955 | 7.725766 | 1.789429 |
| H     | 6.734968 | -0.418717 | 0.919323 | H     | 0.842842 | 7.704315 | 3.128920 |
| C     | -0.161560 | 1.671609 | 5.295304 | C     | 1.597698 | -2.509802 | -2.720700 |
| H     | -0.560193 | 2.165290 | 6.178052 | C     | 1.005824 | -3.596034 | -3.629212 |
| C     | 4.481510 | 1.887071 | -3.329212 | H     | 1.764025 | -3.973236 | -4.326669 |
| H     | 5.327374 | 1.330183 | -3.724474 | H     | 1.597698 | 7.302897 | 2.133015 |
| C     | 3.105792 | 5.860030 | -0.961796 | C     | -3.103760 | 1.554447 | 1.755788 |
| C     | 0.902468 | -5.456235 | 4.365463 | H     | -2.095475 | 1.136217 | 1.654428 |
| H     | 0.433402 | -5.807992 | 5.292068 | H     | -3.778414 | 0.992563 | 1.105780 |
| H     | 1.970741 | -5.698708 | 4.415890 | H     | -3.415792 | 1.397682 | 2.795767 |
| H     | 0.474950 | -6.023052 | 3.531274 | C     | 2.331429 | 5.322775 | 3.026866 |
| C     | 1.478178 | -3.171399 | 5.264924 | C     | 3.961321 | -3.805123 | 2.573103 |
| H     | 1.291220 | -2.095685 | 5.183773 | H     | 4.997699 | -3.478965 | 2.427024 |
| H     | 2.552177 | -3.339921 | 5.139960 | H     | 3.895522 | -4.292808 | 3.553320 |
| H     | 1.216239 | -3.496076 | 6.278591 | H     | 3.328511 | -2.912359 | 2.578816 |
| C     | -1.980980 | -6.138053 | 2.013258 | C     | -3.925552 | -1.694298 | 1.260921 |
| H     | -1.836458 | -6.107888 | 3.096033 | H     | -4.426815 | -1.153248 | 2.072102 |
| H     | -1.865183 | -7.164720 | 1.664754 | H     | -4.553887 | -1.624633 | 0.367122 |
| H     | -3.008587 | -5.818606 | 1.817401 | H     | -2.975275 | -1.197583 | 1.045277 |
| C     | -1.433047 | -3.223995 | 5.331214 | C     | -5.032733 | -3.894405 | 1.765621 |
| H     | -0.884473 | -3.215534 | 6.268116 | H     | -4.914816 | -4.923760 | 2.121435 |
| C     | -1.704191 | 4.727040 | 4.475620 | H     | -5.524648 | -3.924282 | 0.788000 |
| H     | -1.977681 | 4.858957 | 5.519391 | H     | -5.712878 | -3.384701 | 2.456723 |
| C     | 3.599440 | 3.865335 | -0.179653 | C     | -2.775230 | -2.866284 | 5.327288 |
| H     | 2.633895 | 3.787892 | 0.334913 | H     | -3.268860 | -2.592415 | 6.256284 |
| C     | 4.972924 | -3.900992 | -0.398267 | C     | 4.317168 | -6.089631 | 1.572709 |
| H     | 5.831249 | -4.220790 | 0.187646 | H     | 4.077209 | -6.782848 | 0.759476 |
| C     | -4.582542 | 3.565445 | 1.441781 | H     | 4.086447 | -6.587249 | 2.520873 |
| H     | -5.033629 | 3.399206 | 2.426668 | H     | 5.398537 | -5.916182 | 1.549998 |
| H     | -5.190975 | 3.042606 | 0.698234 | C     | 1.053446 | 7.298098 | 2.133015 |
| H     | -4.633696 | 4.639770 | 1.232190 | H     | 0.267402 | 7.645770 | 1.455220 |
| C     | 5.662867 | -0.349524 | 1.085682 | H     | 2.001955 | 7.725766 | 1.789429 |
| H     | 6.734968 | -0.418717 | 0.919323 | H     | 0.842842 | 7.704315 | 3.128920 |
| C     | -0.161560 | 1.671609 | 5.295304 | C     | 1.597698 | -2.509802 | -2.720700 |
| H     | -0.560193 | 2.165290 | 6.178052 | C     | 1.005824 | -3.596034 | -3.629212 |
| C     | 4.481510 | 1.887071 | -3.329212 | H     | 1.764025 | -3.973236 | -4.326669 |
|    | X       | Y       | Z       |    | X       | Y       | Z       |
|----|---------|---------|---------|----|---------|---------|---------|
| H  | 0.178953| -3.176503| -4.212943| C  | -3.745299| 0.131206| -1.895460|
| H  | 0.610712| -4.444773| -3.063986| N  | -0.704340| 4.536190| 0.328666|
| C  | 1.954782| -1.288595| -3.568126| N  | 1.162963| -3.858103| -0.310115|
| H  | 2.220635| 5.643040  | 4.068785 | O  | -4.124905| -3.387566| -1.388177|
| H  | 3.260893| 5.763475  | 2.649729 | O  | -4.692757| 0.795852| -1.810503|
| H  | 2.440073| 4.233966  | 3.017186| O  | -2.715932| -0.588082| -5.115835|
| H  | 2.632639| -1.544372| -4.392013| C  | 1.372702| 1.698498| 3.527901|
| H  | 2.425273| -0.493949| -2.976913| H  | 2.228870| 2.125500| 3.012606|
| H  | 1.039913| -0.887198| -4.007557| C  | -1.496395| -3.434804| 2.948518|
| H  | -2.637519| -1.873839| -3.744986| C  | -0.260164| -0.009064| -0.257047|
| C  | -1.132948| 0.507625  | -1.210074| C  | 0.983279| 3.068695| -4.523600|
| H  | -0.891795| -0.698690| -3.083505| H  | 0.307468| 3.767651| -4.023229|
| H  | 0.807131 | 0.516503  | 3.045816 |
|    |         |         |         | 36_int3b.log |          |         |         |
| C  | -1.090351| 4.574986 | 1.720014 |
| C  | 2.501590 | -3.598727| -0.807244 |
| SCF (wB97x) = | -3807.12471457 | C  | 1.619866| 5.991945| -3.161804|
| E(SCF)+ZPE(0 K)= | -3805.554668 | H  | 2.572486| 5.510269| -3.382755|
| H(298 K)= | -3805.459840 | H  | 1.802447| 7.017044| -2.829788|
| G(298 K)= | -3805.683054 | H  | 1.035151| 6.045293| -4.086080|
| Lowest Frequency = 15.2223 cm^-1 | | C  | -2.841797| -3.034903| 3.030396|
|    |         |         |         | 2.838839 | -0.109252| 1.587693 |
| W  | -2.133753| -1.015678| -2.063008| C  | -2.303192| 4.006949| 2.135440|
| Al | 0.053937 | 3.023729 | -0.513619| C  | 2.167676| 2.794946| -3.599703|
| Al | 0.180028 | -2.568940| 0.702993 | C  | 0.605775| 0.557593| 0.605266|
| O  | -0.628697| -1.362738| -0.348585| C  | -2.656589| 4.113711| 3.482213|
| O  | -1.051791| 2.008075 | -1.420428| H  | -3.588758| 3.669448| 3.823106|
| O  | 0.994300 | -1.534871| 1.813445 | C  | 3.229524| 2.016746| -4.068828|
| O  | 0.900098 | 1.884060 | 0.529114 | H  | 3.165715| 1.577136| -5.061849|
| C  | -3.404344| -2.515488| -1.635457| C  | 0.660965| -5.078839| -0.530681|
| N  | 1.158433 | 4.031724 | -1.718162| C  | 2.277521| 3.335512| -2.304645|
| N  | -0.917842| -3.792400| 1.665880 | C  | -1.966912| 6.642211| 0.105162|
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -2.939732 | 6.145111  | 0.183671  |
| H       | -2.054146 | 7.484423  | -0.582439 |
| H       | -1.723816 | 7.017431  | 1.101614  |
| C       | 0.827622  | 5.256618  | -2.108169 |
| C       | 5.074875  | -0.288318 | 2.509588  |
| H       | 5.727418  | -0.319329 | 3.378690  |
| C       | 3.699505  | -0.159481 | 2.686749  |
| H       | 3.291088  | -0.106626 | 3.692192  |
| C       | 0.242063  | 5.242962  | 2.626494  |
| C       | 5.074875  | -0.288318 | 2.509588  |
| H       | 5.727418  | -0.319329 | 3.378690  |
| C       | 3.699505  | -0.159481 | 2.686749  |
| H       | 3.291088  | -0.106626 | 3.692192  |
| C       | 0.242063  | 5.242962  | 2.626494  |
| H       | 0.615571  | -2.489028 | -2.282614 |
| C       | -0.492488 | -5.573635 | 0.094183  |
| H       | -0.805227 | -6.565681 | -0.206845 |
| C       | 1.396049  | -6.065781 | -1.405347 |
| H       | 1.988668  | -5.586976 | -2.183364 |
| H       | 0.684695  | -6.758057 | -1.859950 |
| H       | 2.081167  | -6.651796 | -0.782770 |
| C       | 3.465145  | -4.711017 | 1.309290  |
| H       | 2.401217  | -4.882497 | 1.508699  |
| C       | -0.687638 | -3.505046 | 4.102113  |
| C       | 1.311968  | -0.163092 | 1.763413  |
| C       | 3.388923  | -0.207416 | 0.308441  |
| H       | 2.737647  | -0.165567 | -0.561919 |
| C       | 0.156981  | 1.816085  | -4.822605 |
| H       | 0.763142  | 1.044743  | -5.310369 |
| H       | -0.674431 | 2.061274  | -5.491801 |
| H       | -0.267625 | 1.404534  | -3.904250 |
| C       | 3.433052  | 3.159434  | -1.515278 |
| C       | 0.857703  | 2.321944  | 4.659251  |
| H       | 1.314672  | 3.239386  | 5.021911  |
| C       | 2.679854  | -2.970179 | -2.053776 |
| C       | -0.941028 | 5.652161  | -0.389412 |
C  -0.303460  -0.008294  3.706250  H  -5.134237  3.602838  2.180634
H  -0.761700  -0.919363  3.339015  H  -5.260492  3.317919  0.440596
C  -3.369025  -2.720524  4.285165  H  -4.705595  4.890379  1.046735
H  -4.406475  -2.403804  4.358134  C  5.611077  -0.392814  1.229288
C  5.078316  -3.243940  -1.801761  H  6.683915  -0.501919  1.091202
H  6.083709  -3.113628  -2.194274  C  -0.243219  1.783495  5.319204
C  3.931298  5.354068  -0.404105  H  -0.646803  2.276177  6.200370
H  4.871517  5.442636  -0.960721  H  4.058076  5.870592  0.554038
C  3.155968  5.883409  -0.965490  C  0.955719  -5.418624  4.192716
H  0.544678  -5.769327  5.146748  H  -3.820002  1.252258  0.710368
H  2.018261  -5.688744  4.163988  H  -3.556745  1.549820  2.443681
H  0.453099  -5.964572  3.386109  C  2.253030  5.347988  3.040810
C  1.624643  -3.147029  5.079968  C  4.005215  -3.793816  2.411591
H  1.444473  -2.069028  5.012424  H  5.051387  -3.527392  2.222782
H  2.687984  -3.326494  4.898229  H  3.957816  -4.297922  3.383860
H  1.413376  -3.472785  6.104727  H  3.432060  -2.863120  2.468193
C  -2.126836  -5.929070  1.916739  C  -3.921480  -1.399623  1.497380
H  -1.926432  -5.954859  2.990980  H  -4.381228  -0.881584  2.347245
H  -2.075473  -6.942473  1.517993  H  -4.568737  -1.259716  0.624953
H  -3.146515  -5.555663  1.787074  H  -2.961903  -0.917347  1.286830
C  -1.267814  -3.198593  5.333633  C  -5.094671  -3.572529  1.966165
H  -0.663876  -3.249492  6.233888  H  -5.001721  -4.612756  2.296871
C  -1.849198  4.789586  4.384254  H  -5.619728  -3.565794  1.005924
H  -2.148957  4.877288  5.425481  H  -5.727060  -3.051745  2.693760
C  3.582521  3.875581  -0.175663  C  -2.597108  -2.810979  5.431758
H  2.615987  3.828581  0.339560  H  -3.026019  -2.573638  6.401966
C  4.884384  -3.840784  -0.565581  C  4.166216  -6.074940  1.353881
H  5.745319  -4.167781  0.012636  H  3.836293  -6.735083  0.544827
C  -4.606020  3.808288  1.213976  H  3.956758  -6.574770  2.305923
|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| H | 5.253472 | -5.969610 | 1.270832 | Al | 0.286360 | -2.449422 | 0.716561 |
| C | 1.031429 | 7.405210 | 2.267755 | O | -0.431380 | -1.348223 | -0.490909 |
| H | 0.258360 | 7.817160 | 1.611600 | O | -1.283481 | 1.945107 | -1.545486 |
| H | 1.992267 | 7.831186 | 1.958146 | O | 1.207002 | -1.354604 | 1.654772 |
| H | 0.824703 | 7.749878 | 3.287455 | O | 0.725918 | 2.039894 | 0.375921 |
| C | 1.510276 | -2.513970 | -2.910296 | C | -4.040367 | -0.990549 | -1.477786 |
| C | 1.222951 | -3.486861 | -4.060954 | N | 0.837402 | 4.252428 | -1.693216 |
| H | 2.086389 | -3.568053 | -4.732454 | N | -0.902339 | -3.355417 | 1.876916 |
| H | 0.365406 | -3.129135 | -4.640550 | C | -2.966741 | -0.856717 | -3.695573 |
| H | 0.976035 | -4.490132 | -3.701634 | N | -1.338080 | 4.453014 | 0.106785 |
| C | 1.716317 | -1.105925 | -3.468794 | N | 0.990680 | -3.958218 | -0.183459 |
| H | 2.137108 | 5.601328 | 4.100837 | O | -5.160434 | -0.859605 | -1.198725 |
| H | 3.195079 | 5.793050 | 2.700554 | O | -3.421838 | -0.601817 | -4.732131 |
| H | 2.338018 | 4.260769 | 2.958485 | O | -1.770618 | -4.159729 | -3.252818 |
| H | 2.562696 | -1.057151 | -4.163981 | C | 2.766267 | 1.223911 | 3.316712 |
| H | 1.893010 | -0.366207 | -2.678833 | H | 3.680831 | 1.295851 | 2.735469 |
| H | 0.822911 | -0.802804 | -4.021350 | C | -1.285209 | -2.776981 | 3.150696 |
| H | -1.654642 | -2.548623 | -2.871901 | C | -0.240487 | 0.039570 | -0.396147 |
| C | -1.042843 | 0.650841 | -1.33481 | C | 0.964978 | 3.192156 | -4.437500 |
| H | -0.594555 | 0.181967 | -2.350142 | H | 0.128818 | 3.718263 | -3.965564 |
| C |   |   |   | C | 1.624746 | 0.660863 | 2.751227 |

37_Int4b.log

SCF (wB97x) = -3807.12427409

E(SCF)+ZPE(0 K)= -3805.553869

H(298 K)= -3805.458925

G(298 K)= -3805.682933

Lowest Frequency = 10.5486 cm⁻¹

W -2.148387 -1.266250 -1.935629

Al -0.269313 3.072330 -0.671370
C  0.620645  0.678530  0.418480  H  1.364676  1.132156  -5.013242
C  -4.011341  3.156971  2.353776  H  -0.351468  1.588888  -5.104846
H  -5.012075  2.734501  2.294247  H  0.406228  1.301766  -3.531771
C  3.452106  3.012702  -4.049903  C  3.249062  3.907472  -1.397553
H  3.540212  2.651752  -5.071602  C  2.758793  1.670377  4.639405
C  0.203867  -5.033908  -0.347479  H  3.665371  2.090781  5.067978
C  2.108760  3.809404  -2.222679  C  2.622883  -3.421068  -1.977861
C  -2.390992  6.666500  0.231481  C  -1.428991  5.687071  -0.388157
H  -3.408608  6.269681  0.228421  C  3.359204  -4.559075  0.061537
H  -2.376223  7.615551  -0.305153  C  0.448084  1.037569  4.838677
H  -2.121837  6.848104  1.276592  H  -0.465516  0.951093  5.422253
C  0.477635  5.509241  -1.992286  C  4.606275  0.249685  -1.037687
C  5.174757  -1.210698  0.783878  H  4.853660  0.733338  -1.978532
H  5.875534  -1.883078  1.273521  C  3.943648  -3.439316  -2.431479
C  3.930899  -0.978753  1.351504  H  4.173691  -3.006040  -3.402067
H  3.650794  -1.467661  2.281661  C  -3.390699  -1.743780  2.095763
C  -1.470167  4.318204  2.545144  H  -3.039134  -2.295762  1.217417
H  0.590521  -2.954888  -2.371262  C  -0.165922  5.095858  2.686613
C  -0.961952  -5.256990  0.397054  H  0.104014  5.490039  1.700379
H  -1.515246  -6.155813  0.153942  C  4.485728  3.586983  -1.956796
C  0.545984  -6.066839  -1.391152  H  5.382104  3.658583  -1.348218
H  1.621027  -6.165152  -1.546172  C  4.279705  3.796230  0.933236
H  0.093797  -5.745651  -2.337610  H  4.424199  2.722724  0.776381
H  0.124111  -7.038675  -1.129725  H  4.035510  3.955108  1.989199
C  3.087986  -5.208942  1.411902  H  5.230265  4.306754  0.736389
H  2.100169  -4.883390  1.752229  C  0.945477  -3.592717  4.123751
C  -0.410453  -2.915101  4.246937  H  1.255305  -3.522385  3.078020
C  1.605374  -0.026842  1.374713  C  -1.407589  -4.539470  1.521388
C  3.358444  0.492114  -0.457192  C  -1.894095  -3.105774  -2.791255
H  2.664651  1.168877  -0.948230  C  -4.161983  3.600316  -0.130699
C  0.572086  1.715306  -4.529178  H  -3.535914  4.081689  -0.889340

S196
H -4.987120 -3.164449 2.611971 SCF (wB97x) = -3807.11986928
H -5.428816 -1.944301 1.401514 E(SCF)+ZPE(0 K)= -3805.550274
H -5.314780 -1.500877 3.107843 H(298 K)= -3805.456023
C -2.031438 -1.768052 5.639243 G(298 K)= -3805.676912
H -2.329839 -1.389818 6.613754 Lowest Frequency = -32.7788cm-1
C 3.049689 -6.738563 1.294271
H 2.274555 -7.073235 0.597424 W -2.016952 -1.208970 -1.965722
H 2.842996 -7.192969 2.269786 Al -0.084294 3.057458 -0.579580
H 4.011016 -7.125529 0.936831 Al 0.414386 -2.489228 0.750941
C -0.342731 6.297643 3.624790 O -0.345111 -1.371255 -0.420749
H -1.173174 6.943531 3.318511 O -1.098441 1.955485 -1.481624
H 0.570659 6.902076 3.638768 O 1.357156 -1.407681 1.686401
H -0.539220 5.973376 4.652596 O 0.890057 1.996027 0.449332
C 1.546786 -2.863282 -2.891943 C -3.603996 -0.367145 -2.786040
C 1.450997 -3.668453 -4.194347 N 1.025913 4.240694 -1.585614
H 2.355901 -3.546733 -4.800695 N -0.728010 -3.422400 1.946830
H 0.599030 -3.325276 -4.790911 C -1.817984 -1.830343 -3.842930
H 1.320383 -4.738299 -4.003430 N -1.137449 4.425224 0.232171
C 1.761796 -1.379727 -3.197246 N 1.127492 -3.996628 -0.141889
H 0.803956 3.821678 4.160630 O -4.546420 0.144683 -3.223999
H 1.920355 4.798159 3.196172 O -1.707059 -2.143001 -4.957194
H 1.139463 3.363088 2.489458 O -2.811514 -4.283516 -1.611184
H 2.728825 -1.205241 -3.684224 C 2.893876 1.111649 3.419521
H 1.735002 -0.774606 -2.285234 H 3.827362 1.161488 2.867087
H 0.977474 -1.022690 -3.873190 C -1.125489 -2.814120 3.202036
H -2.871749 -2.606295 -1.087022 C -0.126568 0.015047 -0.319561
C -1.188091 0.582478 -1.410094 C 1.124932 3.167924 -4.326736
H -0.757911 0.122648 -2.428054 H 0.286350 3.672622 -3.835946
C 1.749991 0.600173 2.810417
38_TS4b.log C -1.866042 4.074151 1.429672
C 2.464126 -3.990639 -0.703526
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| C    | 1.497118     | 6.321670     | -2.825705    |
| H    | 2.551472     | 6.318104     | -2.537382    |
| H    | 1.139072     | 7.351150     | -2.855835    |
| H    | 1.440529     | 5.901626     | -3.833846    |
| C    | -2.364774    | -2.162590    | 3.309695     |
| C    | 3.135026     | -0.154303    | 0.774951     |
| C    | -3.157823    | 3.526268     | 1.333592     |
| H    | 1.139972     | 7.351150     | -2.537382    |
| H    | 1.139072     | 7.351150     | -2.855835    |
| H    | 1.440529     | 5.901626     | -3.833846    |
| C    | -2.364774    | -2.162590    | 3.309695     |
| C    | 3.135026     | -0.154303    | 0.774951     |
| C    | -3.157823    | 3.526268     | 1.333592     |
| H    | 1.139972     | 7.351150     | -2.537382    |
| H    | 1.139072     | 7.351150     | -2.855835    |
| H    | 1.440529     | 5.901626     | -3.833846    |
| Atom | x          | y          | z          |
|------|------------|------------|------------|
| H    | 5.323818   | -5.032105  | 2.241265   |
| H    | 4.068571   | -5.029152  | 3.476771   |
| H    | 4.370350   | -3.564426  | 2.520088   |
| C    | -3.288860  | -0.457585  | 1.749294   |
| H    | -3.624801  | 0.159770   | 2.590867   |
| H    | -3.954718  | -0.280559  | 0.901972   |
| H    | -2.288831  | -0.110693  | 1.461819   |
| C    | -4.770497  | -3.451527  | 2.732580   |
| H    | -5.314526  | -2.336106  | 1.466827   |
| H    | -5.219454  | -1.794088  | 3.145386   |
| C    | -1.901935  | -1.745809  | 5.653863   |
| H    | -2.210328  | -1.342239  | 6.615059   |
| C    | 3.254309   | -6.660967  | 1.402270   |
| H    | 2.454555   | -7.033193  | 0.754612   |
| H    | 3.092581   | -7.076160  | 2.403443   |
| H    | 4.204890   | -7.053111  | 1.022288   |
| C    | -0.109132  | 6.241748   | 3.759288   |
| H    | -0.951256  | 6.882317   | 3.474528   |
| H    | 0.797574   | 6.856223   | 3.768509   |
| H    | -0.286929  | 5.900922   | 4.785138   |
| C    | 1.603397   | -2.958511  | -2.894662  |
| C    | 1.504905   | -3.770998  | -4.193324  |
| H    | 2.392652   | -3.626260  | -4.819759  |
| H    | 0.631275   | -3.452072  | -4.715952  |
| H    | 1.413795   | -4.844591  | -3.997625  |
| C    | 1.804039   | -1.474889  | -3.213815  |
| H    | 1.076002   | 3.778019   | 4.246832   |
| H    | 2.165094   | 4.772655   | 3.269439   |
| H    | 1.383362   | 3.335213   | 2.566653   |
| H    | 2.772643   | -1.299004  | -3.697148  |

SCF (wB97x) = -3807.12739478
E(SCF)+ZPE(0 K)= -3805.556455
H(298 K)= -3805.462006
G(298 K)= -3805.682981
Lowest Frequency = 15.3537cm⁻¹
H  3.251769  2.202437  2.129293  H  4.219886 -0.608734  2.459945
C  -1.168246 -2.755543  3.092506  C  -2.448527  4.153535  2.587600
C  -0.119706  0.089285 -0.283665  H  0.516193 -3.402963 -2.565243
C   0.094298  2.906509 -3.951142  C  -0.844671 -5.180686  0.312197
H  -0.545588  2.763149 -3.074904  H  -1.397848 -6.075146  0.054128
C   1.929783  0.645781  2.794848  C   0.822614 -6.115926 -1.265497
C  -2.530455  4.156329  1.185120  H  1.887952 -6.325686 -1.145138
C   2.461907 -3.876056 -0.825326  H   0.661799 -5.827831 -2.309078
C   1.531163  6.270227 -2.554971  H   0.250639 -7.023084 -1.068026
H   2.592778  6.167327 -2.324159  C   3.446630 -4.448731  1.475809
H   1.269747  7.329119 -2.553761  H   2.663221 -3.793818  1.875494
H   1.392194  5.872521 -3.562795  C  -0.519951 -3.297111  4.220964
C  -2.100563 -1.711281  3.230656  C   1.786746 -0.029417  1.420921
C   3.138676 -0.076055  0.677534  C   3.240594  0.104598 -0.699999
C  -3.731745  3.841658  0.517883  H   2.373360  0.424860 -1.271628
C   1.537926  3.020289 -3.459022  C  -0.121032  1.686154 -4.855640
C   0.725316  0.699148  0.570043  H   0.304661  1.834763 -5.855275
C  -4.842005  3.504392  1.293769  H  -1.194198  1.507697 -4.982162
H  -5.778463  3.260499  0.798246  H   0.322383  0.780939 -4.427940
C   2.586918  2.561601 -4.261496  C   3.186603  3.555086 -1.701995
H   2.367780  2.145445 -5.240502  C   2.922906  2.310388  4.248695
C   0.377295 -4.999182 -0.355686  H   3.573674  3.172598  4.375453
C   1.866976  3.568606 -2.204091  C   2.612385 -3.569707 -2.189525
C  -2.082511  6.841702  0.733539  C  -1.204208  5.803681  0.080590
H  -3.140060  6.581183  0.656439  C   3.585682 -4.137721 -0.010812
H  -1.918676  7.823197  0.287674  C   1.451537  0.649100  5.170269
H  -1.847894  6.898964  1.801886  H   0.936776  0.199925  6.016656
C   0.676005  5.515405 -1.562481  C   4.449746 -0.112451 -1.362678
C   5.495173 -0.652351  0.731719  H   4.496924  0.028942 -2.439534
H   6.375507 -0.940836  1.301898  C   3.900786 -3.562042 -2.730397
C   4.284997 -0.459761  1.384924  H   4.029574 -3.326535 -3.784059
C  -2.764420 -1.028957  2.047747  H  4.314886  5.936921 -0.702272
H   -2.291425 -1.398233  1.133933  H  3.973186  5.647057  1.006234
C   -1.174471  4.516107  3.347373  H  2.643444  5.977346 -0.094242
H   -0.463681  4.937796  2.615004  C  0.261376 -5.618570  4.896149
C    4.192777  3.09706 -2.554631  H  0.169673 -5.426299  5.970879
H    5.221209  3.08142 -2.208621  H  1.058068 -6.358138  4.759306
C    4.815892  3.312848  0.243189  H -0.677182 -6.070681  4.558883
H    4.845702  2.233517  0.070195  C  1.911354 -3.731265  4.616547
H    4.917043  3.488789  1.319639  H  2.187320 -2.849465  4.027234
H    5.694733  3.764495 -0.232542  H  2.718089 -4.469314  4.546117
C    0.589753 -4.335401  4.123779  H  1.836102 -3.424040  5.665574
H    0.721544 -4.608676  3.071334  C -2.531779 -5.001659  2.128845
C   -1.357589 -4.428238  1.381188  H -2.202350 -5.424324  3.083507
C   -3.113034 -2.636929 -1.081530  H -3.009953 -5.787512  1.543443
C   -3.887343  3.898151 -0.997521  H -3.264258 -4.223579  2.354039
H   -2.896447  4.023497 -1.441984  C -0.864458 -2.815318  5.484355
C   -0.398268  4.167686 -4.675436  H -0.372664 -3.228346  6.362206
H   -0.509703  5.018991 -3.997867  C -4.775390  3.478650  2.679813
H   -1.380926  3.980247 -5.121085  H -5.652897  3.211652  3.263087
H    0.287344  4.452003 -5.483340  C  3.514981  3.953011 -0.258359
C   -0.250355  6.271039 -0.831369  H  2.696370  3.556475  0.356442
H   -0.245408  7.338440 -1.011620  C  4.847419 -4.124796 -0.603647
C   -3.586592  3.802147  3.316481  H  5.725141 -4.324559  0.002046
H   -3.537437  3.786536  4.402709  C -4.751920  5.094805 -1.418639
C    1.275942  0.102686  3.900596  H -5.755627  5.027947 -0.983166
H    0.643274 -0.768801  3.768501  H -4.861727  5.116696 -2.508128
C   -2.409877 -1.262856  4.517066  H -4.316172  6.050850 -1.108771
H   -3.132077 -0.458464  4.632436  C  5.580747 -0.487775 -0.650889
C    5.009594 -3.845459 -1.953644  H  6.524151 -0.653413 -1.165060
H    6.003674 -3.838084 -2.393093  C  2.287311  1.745510  5.352514
C    3.605413  5.467232 -0.009610  H  2.439871  2.162008  6.345263
C  3.902779  2.631210  -3.829949  H  2.271852  -3.850774  -5.037269
H  4.706185  2.286846  -4.476553  H  0.509257  -3.941603  -4.930457
C  -4.464209  2.595375  -1.557986  C  1.516744  -5.169034  -4.140774
H  -3.859096  1.741511  -1.243643  H  -1.229752  2.747727  4.606135
H  -5.499765  2.437211  -1.234141  H  0.356519  3.532999  4.523135
C  -0.529896  3.267018  3.940323  C  -4.465459  2.622712  -2.652884
H  -3.859096  1.741511  -1.243643  H  -1.229752  2.747727  4.606135
H  -4.464209  2.595375  -1.557986  C  1.487496  -1.746837  -3.499952
H  -4.465459  2.622712  -2.652884  H  -1.229752  2.747727  4.606135
C  4.720752  -4.146324  2.269475  H  5.518213  -4.864798  2.047075
H  4.516795  -4.214293  3.341811  H  5.091134  -3.139320  2.056747
H  5.499765  -2.559654  0.490223  H  -3.859096  1.741511  -1.243643
C  5.518213  -4.864798  2.047075  H  1.394723  -1.107131  -2.617396
H  4.516795  -4.214293  3.341811  H  0.666003  -1.512888  -4.187199
H  5.091134  -3.139320  2.056747  H  -3.540065  -0.606232  -1.116010
C  -2.559654  0.490223  2.092434  C  -1.154152  0.676883  -1.174898
H  -3.162898  0.955952  2.879930  H  -0.760420  0.370636  -2.270624
H  -2.860183  0.936630  1.137946  H  -1.511032  0.745760  2.275414
C  -4.259232  -1.357991  1.960196
H  -4.441315  -2.432119  1.853877  SCF (wB97x) =  -3807.11624730
H  -4.698882  -0.858471  1.089543  E(SCF)+ZPE(0 K) =  -3805.546171
H  -4.788084  -1.008223  2.854648  H(298 K) =  -3805.451992
C  -1.810666  -1.812234  5.639463  G(298 K) =  -3805.673573
H  -2.068849  -1.451148  6.631613  Lowest Frequency =  -760.0027 cm^-1
C  3.024142  -5.905917  1.712589
H  2.040058  -6.130176  1.290198  W  -1.963720  -1.149892  -1.907339
H  2.977464  -6.120993  2.786797  Al  -0.262266  3.113590  -0.268200
H  3.752504  -6.592731  1.265434  Al  0.517728  -2.406342  0.731752
C  -1.421160  5.576199  4.415799  O  -0.083027  -1.297450  -0.524369
H  -1.934260  6.459505  4.019138  O  -1.316561  1.975516  -1.099200
H  -0.468863  5.899891  4.848339  O  1.472530  -1.362448  1.706725
H  -2.032368  5.180484  5.234210  O  0.760365  2.056247  0.713261
C  1.450349  -3.230127  -3.110256  C  -3.401515  -0.442420  -3.035503
C  1.437128  -4.101988  -4.373527  N  0.827221  4.181661  -1.397232

40_TS5b.log
| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| C    | -1.228983 | 5.779164 | 0.080405 |
| C    | 3.644893  | -4.158413 | 0.082027 |
| C    | 1.501383  | 0.682109  | 5.204688 |
| H    | 0.988099  | 0.238241  | 6.054530 |
| C    | 4.531644  | -1.003900 | -1.299163 |
| H    | 4.592265  | 0.049754  | -2.374140 |
| C    | 4.014841  | -3.575978 | -2.627355 |
| H    | 4.163874  | -3.340021 | -3.678254 |
| C    | -2.657737 | -0.949136 | 2.152365 |
| H    | -2.229713 | -1.330591 | 1.221247 |
| C    | -1.092705 | 4.610663  | 3.355790 |
| H    | -0.412200 | 5.023104  | 2.602127 |
| C    | 4.212083  | 3.111936  | -2.506502 |
| H    | 5.237985  | 3.103639  | -2.153203 |
| C    | 4.826214  | 3.361776  | 0.286470 |
| H    | 4.876476  | 2.281498  | 0.122296 |
| C    | 4.923835  | 3.548807  | 1.361288 |
| H    | 5.696361  | 3.825952  | -0.192876 |
| C    | 0.581267  | -4.436569 | 4.107373 |
| H    | 0.758475  | -4.620425 | 3.042741 |
| C    | -1.353753 | -4.377259 | 1.357788 |
| C    | -3.181748 | -2.427494 | -1.021596 |
| C    | -3.907376 | 3.771103  | -0.874551 |
| H    | -2.927626 | 3.844580  | -1.353386 |
| C    | -0.357472 | 4.133075  | -4.693168 |
| H    | -0.486655 | 4.993655  | -4.030677 |
| H    | -1.330146 | 3.932698  | -5.154413 |
| H    | 0.341546  | 4.409539  | -5.492120 |
| C    | -0.292027 | 6.246221  | -0.848843 |
| H    | -0.308772 | 7.310091  | -1.048066 |
| C    | -3.476022 | 3.811558  | 3.430136 |

**S206**
41_Int6c.log

SCF (wB97x) = -3920.44183652
E(SCF)+ZPE(0 K)= -3918.858996
H(298 K)= -3918.762952
G(298 K)= -3918.986663

Lowest Frequency = 12.9693 cm^{-1}
Al  0.249653  2.531917 -0.790796  C  2.409834 -0.082033  2.271724
Al  0.380580 -3.020532  0.673997  C -1.607784  4.358267  1.950693
O  -0.527070 -1.913454 -0.356449  C  1.415757  1.845690 -4.404257
O  -1.053534  1.517892 -1.462127  C  0.552219  0.076425  0.512442
O   1.050613 -1.936273  1.844605  C -1.787434  4.789393  3.265271
O   0.925869  1.397590  0.349819  H -2.782658  4.773315  3.699660
C  -5.015017  0.214443 -1.310372  C  2.282514  1.279043 -5.340995
N   1.178373  3.187562 -2.349998  H  1.885093  0.912799 -6.283222
N  -0.583030 -4.547262  1.349772  C  1.710421 -5.369719 -0.375106
C  -3.039777 -1.174075 -2.487014  C  1.982336  2.347734 -3.214122
N  -0.117034  4.227500 -0.011011  C -0.415288  6.689541 -0.074820
N   1.783576 -4.062091 -0.136016  H  0.444787  7.045612  0.502491
C  -3.297675  1.454081 -3.435834  H -1.256575  6.616391  0.614052
O  -6.128844  0.007223 -1.098217  H -0.637721  7.430636 -0.844241
O  -3.026950 -2.177578 -3.056706  C  1.082288  4.462693 -2.747379
O  -3.101589  0.011994  1.583416  C  4.062372  0.406156  3.983657
O  -3.534392  1.972819 -4.439775  H  4.295777  0.590392  5.029541
C  -0.143834  1.264312  3.328234  C  2.745827  0.152453  3.606766
H   0.510103  2.014214  2.892149  H  1.972417  0.133116  4.368073
C  -1.516980 -4.411120  2.448994  C  0.798709  4.805443  2.189228
C  -0.228040 -0.572030 -0.387093  H  1.057609 -2.591466 -2.065142
C  -0.081819  1.926038 -4.710544  C  0.618425 -6.160821  0.005798
H  -0.605491  2.029061 -3.753893  H  0.654147 -7.202219 -0.288651
C  -0.042644 -0.070909  2.924127  C  2.872166 -6.111698 -0.993320
C  -0.310471  4.425501  1.412583  H  3.464921 -5.492954 -1.666340
C   3.033896 -3.402663 -0.427794  H  2.508837 -6.990459 -1.530306
C   1.837305  4.971191 -3.958571  H  3.532862 -6.460894 -0.192045
H   1.383084  5.896447 -4.316978  C  4.002523 -4.257534  1.799891
H   1.892089  4.258198 -4.777819  H  3.062471 -4.822034  1.801508
H   2.865867  5.195478 -3.656671  C -1.003401 -4.383625  3.763275
C  -2.897704 -4.347415  2.195411  C  0.990864 -0.524713  1.871028
C  3.433390  -0.086335   1.322540  C  -2.988678  0.211684  0.460932
H  3.197406  -0.300342   0.280672  C  -2.784735  3.840416  1.133778
C  -0.599531   0.648951  -5.387339  H  -2.395559  3.075401  0.450987
H  -0.161487   0.505897  -6.381076  C  -0.461083  3.132166  -5.584245
H  -1.681344   0.717407  -5.523814  H  -0.322877  4.085963  -5.069371
H  -0.391943  -0.245064  -4.793357  H  -1.517935  3.064893  -5.860323
C  3.344714   2.174551  -2.903647  H  0.131295  3.149983  -6.507435
C  -1.046961  1.636068   4.320083  C  0.386694  5.448713  -2.036724
H  -1.083144  2.671532   4.640608  H  0.356614  6.430858  -2.491044
C  3.146159  -2.700036  -1.640904  C  0.571559  5.179966  3.515424
C  -0.070897   5.367413  -0.721647  H  1.412020  5.475127  4.138522
C  4.098980  -3.492950   0.484592  C  -0.886339 -1.001559  3.522397
C  -1.806360  -0.630475   4.499576  H  -0.817202  -2.037761  3.228909
H  -2.450181  -1.390047   4.936920  C  -3.762086  -4.231226  3.286545
C  4.751859   0.151091   1.699159  H  -4.832769  -4.164705  3.112995
H  5.537437   0.114303   0.950144  C  5.428608  -2.149531  -1.034257
C  4.361440  -2.071903  -1.922074  H  6.369084  -1.657619  -1.272448
H  4.477679  -1.511159  -2.845354  C  4.212522  4.136105  -1.500796
C  -3.475368  -4.404241   0.786946  H  4.874111  4.440282  -2.321262
H  -2.709428  -4.811755   0.118999  H  4.719123  4.377940  -0.559296
C  2.221105   4.816320   1.639154  H  3.304547  4.742792  -1.543388
H  2.164386   4.757015   0.546731  C  1.033567  -5.866736  4.083249
C  4.158948   1.576276  -3.868515  H  0.515596  -6.455670  4.849821
H  5.217228   1.439865  -3.669484  H  2.102472  -5.862872  4.327951
C  5.218752   1.879921  -1.210444  H  0.919814  -6.378902  3.122514
H  5.094689   0.794672  -1.292713  C  0.888893  -3.687943  5.326477
H  5.497851  2.112441  -0.178974  H  0.466583  -2.678379  5.347890
H  6.052837   2.185244  -1.853439  H  1.978754  -3.597476  5.375991
C  0.497576  -4.429110   4.044378  H  0.565042  -4.222219  6.227522
H  1.001122  -3.902793   3.227825  C  -1.266399  -6.923691  1.399959
C  -0.390932  -5.797713   0.898128  H  -1.265056  -6.963466  2.492256
42_TS6c.log

SCF (wB97x) = -3920.43353165
E(SCF)+ZPE(0 K) = -3918.851255
H(298 K) = -3918.755751
G(298 K) = -3918.977239
Lowest Frequency = 136.3632 cm⁻¹

W -2.859735 1.273942 -1.496360
Al -0.010165 2.638407 -0.675774
Al 0.328458 -2.907637 2.638407
O -0.621161 -1.879490 -0.125554
O -0.689176 1.331323 -1.766471
O 0.877741 -1.777099 2.118609
O 0.503479 1.550733 0.613920
C -4.780232 1.728825 1.496360
N 0.985805 3.405246 -2.166980
N -0.598824 -4.434696 1.598326
C -3.592054 -0.505140 -2.152247
N -0.377603 4.324311 0.204387
N 1.751421 -3.895540 0.103340
C -3.128475 1.933613 -3.441589
O -5.843661 2.025207 -0.677605
O -4.006415 -1.488982 -2.595214
O -2.980059 0.668237 1.647067
O -3.407623 2.362492 -4.472367
C -0.371862 1.387419 3.608008
H 0.311313 2.139075 3.222183
C -1.520385 -4.295879 2.704950
C -0.371577 -0.533822 -0.184829
C -0.006016 2.259700 -4.767213
H -0.610200 2.731336 -3.986402
C -0.287886 0.067166 3.154406
C -0.480550 4.522510 1.643081
C 2.963460 -3.186829 -0.237015
C 1.463128 5.277921 -3.756061
H 0.711712 5.780822 -4.370941
H 2.010585 4.566416 -4.368472
H 2.164240 6.044425 -3.411369
C -2.891212 4.102726 2.464222
C 2.172817 0.118610 2.502149
C -1.741436 4.533593 2.275356
C 1.423264 2.125446 -4.251538
C 0.300779 0.197385 0.742293
C -1.803794 4.965743 3.600088
H -2.767931 5.005431 4.098394
C 2.356256 1.513917 -5.091906
H 2.032951 1.153873 -6.065595
C 1.704352 -5.206160 -0.131734
C 1.869559 2.615890 -3.005976
C -0.735102 6.790122 0.172893
H 0.169405 7.203383 0.631322
H -1.482465 6.701861 0.958166
C 2.963460 -3.186829 4.214003
H 4.056765 0.794410 5.260933
C 2.510946 0.342584 3.839302
C 1.741074 0.321003 4.600383
C 0.689447 4.862653 2.346338
C 0.901848 -2.491931 -1.825843

S211
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 0.629688 | -6.020801| 0.254455 |
| H       | 0.681176 | -7.059454| -0.047650|
| C       | 2.877572 | -5.916891| -0.763911|
| H       | 3.429901 | -5.287071| -1.461113|
| H       | 2.537662 | -6.818702| -1.277073|
| C       | 3.571446 | -6.223937| 0.026975 |
| H       | 4.049427 | -4.015763| 1.943109 |
| H       | 3.161953 | -4.659149| 1.949334 |
| H       | -1.005377| 1.005377 | -4.365973|
| C       | 3.192384 | 0.143035 | 1.549077 |
| H       | 2.958758 | 0.064620 | 0.504871 |
| H       | 0.024666 | 0.311150 | -5.754796|
| H       | -1.590225| 0.987743 | -5.538789|
| H       | -0.729904| 0.297390 | -4.151554|
| C       | 3.207476 | 2.442662 | -2.596132|
| C       | -1.302924| 1.742896 | 4.579238 |
| H       | -1.326905| 2.766235 | 4.938963 |
| C       | 3.000608 | 2.464909 | -1.445212|
| C       | -0.393535| 5.473332 | -0.492051|
| C       | 4.063733 | 3.232724 | 0.636120 |
| C       | -2.131800| -0.506415| 4.628036 |
| C       | -2.812776| -1.263600| 5.008535 |
| C       | 4.508483 | 0.397638 | 1.925188 |
| H       | 5.292779 | 0.382830 | 1.174856 |
| C       | 4.168801 | -1.763201| -1.751680|
| H       | 4.222480 | -1.181351| -2.667494|
| C       | -3.467282| -3.975097| 1.061909 |
| H       | -2.687182| -4.252478| 0.344528 |
| C       | 2.075104 | 4.866143 | 1.712309 |

S212
C     1.782390  -1.257891  -3.318589  N    2.117166  -4.206477  0.049810
H     3.078108   3.894277   3.390379  C    -3.335945   2.384116 -3.556543
H     3.949863   3.772976   1.856745  O    -5.686717   3.052147 -0.873681
H     2.513968   2.771628   2.141296  O    -4.715075  -0.941280 -2.763047
H     2.605305  -1.253048  -4.041546  O    -3.700766   0.333473  1.241383
H     1.828028  -0.323379  -2.748959  O    -3.602102   2.863888 -4.573453
H     0.854436  -1.259275  -3.897907  C    -0.317820   1.090465  3.455267
H    -2.599219   3.056098  -1.278068  H    0.413532   1.841523  3.167560
C    -0.960316   0.034111  -1.427349  C    -1.418125  -4.589101  2.309472
H    -0.880275  -0.646807  -2.275775  C    -0.171011  -0.942352 -0.474162
        C    -0.340084   1.829873 -4.889290
43_Int7c.log
        H   -0.883235   2.309699 -4.072625
        C    -0.274587  -0.191428  2.898338
SCF (wB97x) =  -3920.45365571  C    -0.153552   4.277577  1.581889
E(SCF)+ZPE(0 K)=  -3918.870696  C     3.288381  -3.447311 -0.322761
H(298 K)=  -3918.773909  C     1.223712   4.900291 -4.040828
G(298 K)=  -3919.000625  H     0.443414   5.472677 -4.550452
Lowest Frequency = 8.8956cm^{-1}  H     1.618237   4.150340 -4.721234
        H     2.031304   5.597519 -3.797661
W    -3.080447   1.537199  -1.703129  C    -2.705519  -4.319584  1.813422
Al   -0.305630   2.413266  -0.918316  C     2.217855  -0.076800  2.271649
Al    0.629474  -3.253043   0.774978  C    -1.389246   4.283460  2.265417
O    -0.241708  -2.301561  -0.402525  C     1.119255   1.710029 -4.469986
O    -0.805951   0.837236  -1.954270  C     0.344639  -0.079065  0.518901
O     0.980065  -2.014810   1.934938  C    -1.389533   4.645366  3.612424
O     0.376984   1.209525   0.366199  H    -2.332638   4.680365  4.150061
C    -4.725883   2.478735  -1.201630  C     2.003710  1.084912 -5.351710
N     0.801309   3.053750  -2.402305  H     1.620963   0.689423 -6.289760
N    -0.318471  -4.773485   1.387498  C     2.141955  -5.530261 -0.121693
C    -4.124244  -0.023670  -2.356841  C     1.634130   2.244788 -3.269274
N    -0.128998   4.092842   0.145495  C    -0.312934   6.576544  0.115400
| Atom | X Position | Y Position | Z Position |
|------|------------|------------|------------|
| H    | 0.680493   | 6.969313   | 0.355715   |
| C    | 4.382192   | -3.394152  | 0.559758   |
| H    | -0.88873   | 6.540842   | 1.038350   |
| C    | -2.226021  | -0.787158  | 4.209067   |
| H    | -0.785882  | 7.276089   | -0.577037  |
| C    | -2.973587  | -1.528461  | 4.475693   |
| C    | 0.654178   | 4.338075   | -2.753310  |
| C    | 4.540918   | 0.250908   | 1.670313   |
| C    | 3.870275   | 0.457646   | 3.965579   |
| H    | 5.315012   | 0.258452   | 0.910029   |
| H    | 4.110457   | 0.641112   | 5.009714   |
| H    | 2.561389   | 0.152809   | 3.606272   |
| C    | 4.452557   | -1.489014  | -2.836254  |
| H    | 1.801746   | 0.086348   | 4.377982   |
| C    | -3.013513  | -4.211557  | 0.325907   |
| C    | 1.045525   | 4.589878   | 2.247208   |
| H    | -2.091876  | -4.410842  | -0.230438  |
| H    | 1.216383   | -3.026007  | -1.977528  |
| C    | 2.392686   | 4.641135   | 1.540771   |
| C    | 1.095422   | -6.376918  | 0.266210   |
| H    | 2.217197   | 4.501838   | 0.469544   |
| H    | 1.217418   | -7.428456  | 0.038297   |
| C    | 3.839758   | 1.467142   | -3.861597  |
| C    | 3.368278   | -6.203606  | -0.689748  |
| H    | 4.897612   | 1.366347   | -3.640203  |
| H    | 3.880603   | -5.589923  | -1.430913  |
| C    | 4.886026   | 1.982115   | -1.242691  |
| H    | 3.098877   | -7.163228  | -1.134647  |
| H    | 4.077690   | -6.397516  | 0.123046   |
| H    | 5.161072   | 2.293189   | -0.230986  |
| C    | 4.388244   | -4.122922  | 1.899303   |
| H    | 5.718485   | 2.251730   | -1.903196  |
| H    | 3.578319   | -4.860495  | 1.890459   |
| C    | 0.234573   | -4.926908  | 4.255979   |
| C    | -1.158805  | -4.672195  | 3.691538   |
| H    | 0.909356   | -5.146469  | 3.420643   |
| C    | 0.826223   | -0.616978  | 1.901030   |
| C    | -0.027523  | -6.028489  | 1.020793   |
| C    | 3.227491   | -0.036920  | 1.308322   |
| H    | -3.170114  | 0.749277   | 0.180797   |
| H    | 2.999888   | -0.256184  | 0.264414   |
| C    | -2.706131  | 3.955057   | 1.568510   |
| C    | -0.970106  | 0.452082   | -5.129394  |
| H    | -2.490421  | 3.193099   | 0.816713   |
| H    | -0.514695  | -0.046678  | -5.993082  |
| C    | -0.522379  | 2.684878   | -6.151687  |
| H    | -2.040513  | 0.556085   | -5.334920  |
| H    | -0.116894  | 3.693081   | -6.037368  |
| H    | -0.852271  | -0.200103  | -4.261897  |
| C    | -1.588731  | 2.778021   | -6.381070  |
| C    | 3.000424   | 2.106305   | -2.945127  |
| C    | -0.030904  | 2.222627   | -7.015817  |
| C    | -1.270975  | 1.403447   | 4.419336   |
| C    | 0.040470   | 5.298882   | -1.944383  |
| H    | -1.260925  | 2.390148   | 4.869662   |
| H    | -0.057674  | 6.284643   | -2.384633  |
| C    | 3.293916   | -2.780665  | -1.563683  |
| C    | 0.995654   | 4.892031   | 3.610824   |
| C    | -0.160087  | 5.227518   | -0.556912  |
| H    | 1.918379   | 5.122015   | 4.138819   |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
|    C | -1.250964 | -1.113325 | 3.271262 |
|    H | -1.245096 | -2.106959 | 2.843968 |
|    C | -3.738265 | -4.138970 | 2.736629 |
|    H | -4.740544 | -3.922651 | 2.374922 |
|    C |  5.513671 | -1.958191 | -1.032813 |
|    H |  6.386255 | -1.371187 | -1.310336 |
|    C |  3.864773 |  4.190483 | -1.773577 |
|    H |  5.513671 |  1.958191 |  1.032813 |
|    C | -0.257644 | -6.139233 |  5.195327 |
|    H | -0.345719 | -5.962515 |  6.092360 |
|    H |  1.282084 | -6.342983 |  5.524013 |
|    C | -0.127451 | -7.042720 |  4.709812 |
|    C |  0.775333 | -3.678621 |  4.966373 |
|    H |  0.841481 | -2.832415 |  4.276100 |
|    H |  1.775948 | -3.875245 |  5.368403 |
|    H |  0.125965 | -3.391446 |  5.801561 |
|    C | -0.923455 | -7.154296 |  1.470472 |
|    H | -0.892530 | -7.254181 |  2.559786 |
|    H | -0.611636 | -8.097680 |  1.021505 |
|    H | -1.964084 | -6.953876 |  1.202717 |
|    C | -2.225788 | -4.488794 |  4.570728 |
|    H | -2.048367 | -4.542583 |  5.642333 |
|    C | -0.211793 |  4.941776 |  4.287912 |
|    H | -0.239034 |  5.209898 |  5.341151 |
|    C |  3.590577 |  2.682587 | -1.660164 |
|    H |  2.858677 |  2.529775 | -0.854970 |
|    C |  5.490947 | -2.638566 |  0.176917 |
|    H |  6.347217 | -2.573117 |  0.843437 |
|    C | -3.305222 |  5.155770 |  0.820627 |

S216
SCF (wB97x) = -3920.40750919
E(SCF)+ZPE(0 K)= -3918.827153
H(298 K)= -3918.730653
G(298 K)= -3918.956048
Lowest Frequency = -623.5359 cm⁻¹

44_TS7c.log
|   |   |   |   |
|---|---|---|---|
| C | -1.570643 | 3.963644 | 2.119084 |
| H | 3.111474  | -0.111605 | 0.227457 |
| C | 1.372341  | 1.807320  | -4.581221 |
| C | 0.487976  | -0.028690 | 0.587882  |
| H | -0.069579 | -0.109111 | -5.946950 |
| C | -1.598665 | 4.359722  | 3.457351  |
| H | -1.681397 | 0.550754  | -5.645648 |
| C | -2.538527 | 4.299953  | 4.001654  |
| H | -0.702594 | -0.047635 | -4.291590 |
| C | 2.295331  | 1.186627  | -5.427501 |
| C | 1.952668  | 0.799515  | -6.383926 |
| H | -0.028690 | 0.587882  | -0.124802 |
| C | 1.863767  | -5.474598 | -0.124802 |
| C | 1.835276  | 2.320953  | -3.351161 |
| C | -0.926663 | 6.329225  | 0.000716  |
| H | -0.339350 | 6.609871  | 0.878246  |
| H | -1.941618 | 6.117895  | 0.346275  |
| H | -0.958784 | 7.171367  | -0.691095 |
| C | 0.788770  | 4.376480  | -2.787142 |
| C | 4.186378  | 0.312696  | 3.920596  |
| H | 4.254758  | -3.483417 | 0.505226  |
| H | 4.481497  | 0.412884  | 4.961985  |
| C | 2.857796  | 0.052266  | 3.605385  |
| H | -2.818513 | -1.247070 | 4.550128  |
| C | 0.790502  | -6.264231 | 0.312209  |
| C | 0.836115  | -7.316578 | 0.060590  |
| C | 3.016598  | -6.210789 | -0.763620 |
| C | 3.535228  | -5.610854 | -1.511780 |
| H | 2.140042  | -0.069092 | 4.409855  |
| C | 0.825759  | 4.473395  | 2.077918  |
| H | -2.317960 | -3.977615 | 0.120267  |
| H | 1.017965  | -2.815205 | -1.875034 |
| C | 0.790502  | -6.264231 | 0.312209  |
| C | 0.836115  | -7.316578 | 0.060590  |
| C | 3.016598  | -6.210789 | -0.763620 |
| H | 2.140042  | -0.069092 | 4.409855  |
| C | 0.825759  | 4.473395  | 2.077918  |
| H | -2.317960 | -3.977615 | 0.120267  |
| H | 1.017965  | -2.815205 | -1.875034 |
| C | 0.790502  | -6.264231 | 0.312209  |
| C | 0.836115  | -7.316578 | 0.060590  |
| C | 3.016598  | -6.210789 | -0.763620 |
| H | 2.140042  | -0.069092 | 4.409855  |
| C | 0.825759  | 4.473395  | 2.077918  |
| H | -2.317960 | -3.977615 | 0.120267  |
| H | 1.017965  | -2.815205 | -1.875034 |
| C | 0.790502  | -6.264231 | 0.312209  |
| C | 0.836115  | -7.316578 | 0.060590  |
| C | 3.016598  | -6.210789 | -0.763620 |
| H | 2.140042  | -0.069092 | 4.409855  |
| C | 0.825759  | 4.473395  | 2.077918  |
| H | -2.317960 | -3.977615 | 0.120267  |
| H | 1.017965  | -2.815205 | -1.875034 |
| C | 0.790502  | -6.264231 | 0.312209  |
| C | 0.836115  | -7.316578 | 0.060590  |
| C | 3.016598  | -6.210789 | -0.763620 |
| H | 2.140042  | -0.069092 | 4.409855  |
| C | 0.825759  | 4.473395  | 2.077918  |
| H | -2.317960 | -3.977615 | 0.120267  |
| H | 1.017965  | -2.815205 | -1.875034 |
| C | 0.790502  | -6.264231 | 0.312209  |
| C | 0.836115  | -7.316578 | 0.060590  |
| C | 3.016598  | -6.210789 | -0.763620 |
C -2.844099  3.424366  1.490912  H -2.217685 -6.691219  1.499817
H -2.625653  3.201874  0.448920  C -2.050442 -4.311680  4.905744
C -0.196350  2.628721 -6.413874  H -1.778755 -4.400539  5.954991
H  0.307627  3.599012 -6.420345  C -0.459979  4.815011  4.104036
H -1.254772  2.790469 -6.641821  H -0.508944  5.132577  5.142949
H  0.232271  2.037473 -7.231095  C  3.735020  2.752695 -1.669879
C  0.075151  5.284725 -1.998089  H  2.994946  2.566698 -0.879273
H -0.066035  6.271047 -2.421155  C  5.387153 -2.773132  0.104334
C  0.749324  4.837638  3.422943  H  6.266635 -2.769392  0.743384
H  1.649356  5.168532  3.936579  C -4.006563  4.422367  1.522666
C -1.095686 -0.902533  3.323918  H -4.307095  4.657006  2.550529
H -1.222206 -1.842789  2.803511  H -4.875143  3.992246  1.012358
C -3.702439 -3.847025  3.226210  H -3.761366  5.363908  1.020739
H -4.722641 -3.579426  2.961298  C  5.134137  0.42085  2.908435
C  5.403782 -2.058469 -1.084723  H  6.176986  0.614370  3.147745
H  6.295783 -1.509006 -1.377244  C -1.831822  0.606314  5.050537
C  3.974882  4.267877 -1.762096  H -2.512611  0.857474  5.860157
H  4.615573  4.498418 -2.621539  C  3.628722  1.055792 -5.081458
H  4.487915  4.620175 -0.860135  H  4.328623  0.576280 -5.761057
H  3.050920  4.844126 -1.856032  C -3.259168  2.100681  2.142540
C  0.438996 -6.044354  5.262007  H -2.454259  1.360767  2.093440
H -0.089301 -5.888085  6.208891  H -4.131652  1.689263  1.622832
H  1.483722 -6.268153  5.501947  H -3.523070  2.239479  3.197357
H  0.005777 -6.929134  4.782599  C  3.236112  3.716878  2.069876
C  0.973399 -3.583304  5.056262  C  4.148434 -3.274140  3.011817
H  0.984307 -2.719639  4.384432  H  4.973913 -2.552898  3.020294
H  2.004803 -3.798190  5.358390  H  4.171586 -3.828684  3.957768
H  0.405916 -3.315833  5.955147  H  3.212998 -2.709835  2.958223
C -1.169778 -6.957944  1.658297  C -3.654661 -2.371950  0.537188
H -1.039473 -7.093485  2.736511  H -4.549680 -2.143966  1.127904
H -0.958273 -7.903131  1.157499  H -3.905434 -2.219051 -0.517682

S219
H  -2.874808  -1.652778  0.803324  45_Int8c.log
C  -4.282183  -4.805223  0.341131
H  -3.963251  -5.847132  0.455804  SCF (wB97x) =  -3920.48900748
H  -4.546590  -4.648919  -0.709741  E(SCF)+ZPE(0 K)=  -3918.902422
H  -5.192861  -4.669424  0.935316  H(298 K)=  -3918.805591
C  -3.358898  -3.998695  4.561801  G(298 K)=  -3919.033640
H  -4.107796  -3.857822  5.337026  Lowest Frequency = 16.6080cm⁻¹
C  5.524520  -5.118050  1.971260
H  5.664796  -5.778686  1.108343  W  -3.147444  1.474940  -2.192203
H  5.446011  -5.739601  2.869253  Al  0.083538  2.235007  -0.719923
H  6.431496  -4.512790  2.074931  Al  0.639149  -3.181551  0.949190
C  2.638974  6.031455  1.255643  O  -0.227406  -2.176365  -0.195660
H  1.941833  6.633783  0.663520  O  -1.144601  1.062903  -1.365896
H  3.618985  6.084715  0.769016  O  1.198286  -2.030393  2.108348
H  2.731906  6.496764  2.243539  O  0.949194  1.230700  0.423454
C  1.923300  -2.779910  -2.489687  C  -4.986374  1.562335  -1.518077
C  1.934025  -4.037262  -3.372029  N  0.916772  2.955731  -2.307778
H  2.872589  -4.107727  -3.948011  N  -0.461866  -4.583634  1.594548
H  1.111133  -3.996281  -4.093605  C  -3.830900  1.853228  -3.981045
H  1.812678  -4.955944  -2.791986  N  -0.435540  3.858908  0.069325
C  1.822500  -1.542242  -3.378537  N  1.994666  -4.289775  0.178853
H  3.436932  4.070483  3.087558  C  -3.159079  3.500990  -1.984652
H  4.182422  3.761827  1.517074  O  -6.049474  1.610700  -1.044799
H  2.928852  2.668196  2.126520  O  -4.158652  2.069507  -5.080316
H  2.607516  -1.519208  -4.142226  O  -3.879648  -1.536430  -3.000231
H  1.884917  -0.610224  -2.806229  O  -3.358350  4.642440  -1.952433
H  0.866049  -1.548831  -3.910061  C  0.359538  1.182118  3.696016
H  -2.217427  0.608117  -0.482122  H  1.150018  1.845984  3.359226
C  -0.840066  -0.259316  -1.456683  C  -1.446515  -4.312075  2.618934
H  -1.279940  -1.026689  -2.095657  C  0.029970  -0.837517  -0.239285
C  -0.237425  1.641721  -4.721270
|Atom| X   | Y   | Z   | Atom| X   | Y   | Z   |
|----|-----|-----|-----|----|-----|-----|-----|
| C  | 0.218271 | -0.084898 | 3.123702 | C  | 2.967625 | -6.421772 | -0.594056 |
| C  | -0.529139 | 4.057533 | 1.504039 | H  | 3.560518 | -5.869643 | -1.323664 |
| C  | 3.256529 | -3.679608 | -0.176754 | H  | 2.576330 | -7.330809 | -1.054517 |
| C  | 1.303475 | 4.812257 | -3.929881 | H  | 3.639751 | -6.719198 | 0.219069 |
| H  | 0.585880 | 5.463467 | -4.433967 | C  | 4.257660 | -4.477613 | 2.054091 |
| H  | 1.685914 | 4.080715 | -4.637153 | H  | 3.324921 | -5.052827 | 2.079899 |
| H  | 2.142616 | 5.438505 | -3.608499 | C  | -1.098295 | -4.554532 | 3.962619 |
| C  | -2.707605 | -3.798613 | 2.270395 | C  | 1.187873 | -0.615665 | 2.044674 |
| C  | 2.643432 | -0.206119 | 2.338490 | C  | 3.585849 | -0.152045 | 1.311444 |
| C  | -1.753971 | 3.880204 | 2.170060 | H  | 3.264779 | -0.287156 | 0.279282 |
| C  | 1.245556 | 1.609128 | -4.358479 | C  | -0.297867 | -0.146128 | -5.980806 |
| C  | 0.705934 | -0.103118 | 0.667643 | H  | -1.848470 | 0.300308 | -5.267246 |
| C  | -1.848051 | 4.308133 | 3.493250 | H  | -0.608399 | -0.477124 | -4.270394 |
| H  | -2.792471 | 4.203640 | 4.020242 | C  | 3.145948 | 2.079000 | -2.866740 |
| H  | 1.753918 | 0.601927 | -6.185811 | C  | -0.465315 | 1.584772 | 4.742237 |
| C  | 1.840190 | -5.600131 | -0.017036 | H  | -0.299727 | 2.552149 | 5.203543 |
| C  | 1.774760 | 2.174611 | -3.178935 | C  | 3.356304 | -3.003782 | -1.409516 |
| C  | -1.241435 | 6.189591 | -0.044286 | C  | -0.587699 | 4.979920 | -0.662609 |
| H  | -0.636450 | 6.591638 | 0.773498 | C  | 4.341311 | -3.760059 | 0.713135 |
| H  | -2.213463 | 5.916462 | 0.376270 | C  | -1.674202 | -0.480028 | 4.597145 |
| H  | -1.388555 | 6.965565 | -0.795631 | H  | -2.467336 | -1.145487 | 4.928332 |
| C  | 0.662913 | 4.211268 | -2.696668 | C  | 4.936088 | 0.042933 | 1.595061 |
| C  | 4.437950 | 0.140452 | 3.940086 | H  | 5.657793 | 0.055596 | 0.783609 |
| H  | 4.758687 | 0.246286 | 4.973502 | C  | 4.574244 | -2.397215 | -1.724937 |
| C  | 3.094014 | -0.077059 | 3.656287 | H  | 4.679554 | -1.861577 | -2.664070 |
| H  | 2.386866 | -0.154158 | 4.475901 | C  | -3.087522 | -3.432671 | 0.843147 |
| C  | 0.608189 | 4.549334 | 2.169048 | H  | -2.239230 | -3.656562 | 0.190520 |
| H  | 1.267171 | -2.873931 | -1.816621 | C  | 1.966748 | 4.682635 | 1.489219 |
| C  | 0.684757 | -6.305860 | 0.351201 | H  | 1.845396 | 4.426757 | 0.431983 |
H  -3.733467  1.206364  1.226594  H  3.105664  3.847899  3.159006
H  -3.037162  1.505962  2.835982  H  3.962150  3.824692  1.611777
C   2.979341  3.693000  2.080993  C   2.664344  2.657312  1.914861
C   4.201830  3.205064  2.835982  H  3.066569  -1.864940  -4.074594
H   5.084541  -2.816784  3.200230  H   2.412823  -0.823629  -2.803027
H   4.169180  -3.988642  4.168918  H   1.325867  -1.689647  -3.909131
H   3.317387  -2.829414  3.120681  H  -1.242929  -0.937975  -1.906089
C  -3.350932  -1.925199  0.734566  C  -0.508176  -0.233729  -1.514165
H  -4.208241  -1.623015  1.348111  H   0.292167  -0.127672  -2.262368
H  -3.574055  -1.657618  -0.302890
H  -2.480191  -1.345463  1.056685  46_TS10.log
C   -4.296076  -4.232721  0.343744
H   -4.115942  -5.312910  0.384691  SCF (wB97x) =  -3920.43472476
H   -4.518665  -3.966998  -0.694989  E(SCF)+ZPE(0 K) =  -3918.858733
H   -5.191442  -4.021833  0.939384  H(298 K)=  -3918.761006
C  -3.322850  -3.847158  4.618024  G(298 K)=  -3918.990921
H  -4.060382  -3.674805  5.397834  Lowest Frequency = -221.7659 cm⁻¹
C   5.414072  -5.465953  2.250841
H   5.508895  -6.162928  1.410669  W  -2.454790  -0.738715  -2.730029
H   5.258664  -6.049859  3.164001  Al  -0.162384  2.934898  -0.489548
H   6.372146  -4.945857  2.357597  Al   0.451631  -2.605100  0.917278
C   2.498153  6.119816  1.543334  O  -0.185247  -1.567967  -0.327136
H   1.786205  6.830111  1.108638  O  -1.089451  1.711958  -1.370011
H   3.436351  6.198070  0.982824  O  1.337813  -1.468839  1.869834
H   2.701688  6.436579  2.572125  O   0.757228  1.841782  0.542608
C   2.192560  -2.964390  -2.395445  C  -3.531495  -1.563993  -4.226067
C   2.099364  -4.252918  -3.226621  N   0.914113  4.122708  -1.506069
H   3.048443  -4.455179  -3.737765  N  -0.670238  -3.489954  2.174137
H   1.321260  -4.149658  -3.990447  C  -4.066867  -0.910995  -1.572969
H   1.842825  -5.125080  -2.620228  N  -1.298758  4.261129  0.265036
C   2.258562  -1.765976  -3.340477  N   1.189829  -4.174046  0.142454
C  0.691000  1.080079  4.910883  H  -0.295676  0.220457  3.213288
H  -0.211724  1.063022  5.517272  C  -2.647567  -1.554659  4.684672
C  4.670372  0.272076  -0.976786  H  -3.595128  -1.025287  4.753257
H  4.921985  0.857374  -1.856538  C  5.110122  -4.373495  -1.446871
C  4.093332  -3.800651  -2.192955  H  6.116386  -4.440591  -1.852435
H  4.308459  -3.418766  -3.188334  C  2.992679  5.857236  0.512912
C  -3.179491  -1.935151  2.259782  H  3.864697  6.382232  0.104981
H  -2.795057  -2.535542  1.427412  H  2.913659  6.115983  1.575248
C  0.047664  4.914408  2.734146  H  2.097157  6.241688  0.014193
H  0.409178  5.025415  1.706261  C  1.132422  -4.957556  4.951212
C  4.612971  3.733231  -1.631616  H  0.795577  -4.976655  5.994374
H  5.477514  3.872239  -0.989997  H  2.122187  -5.427140  4.909538
C  4.284134  3.830349  1.245334  H  0.445744  -5.577335  4.363158
H  4.492287  2.771891  1.059173  C  2.271908  -2.701532  5.130216
H  3.996231  3.938366  2.296058  H  2.276258  -1.667592  4.769289
H  5.210347  4.398069  1.097155  H  3.255931  -3.140765  4.932769
C  1.187434  -3.519042  4.422086  H  2.137668  -2.689445  6.217812
H  1.471889  -3.558127  3.367893  C  -2.168428  -5.319997  2.857133
C  -1.131522  -4.720322  1.942181  H  -1.857958  -5.242149  3.902671
C  -3.059851  1.141800  -3.299991  H  -2.341885  -6.367795  2.610007
C  -4.147824  3.437855  0.236392  H  -3.112480  -4.774850  2.764266
H  -3.568367  3.888244  -0.576453  C  -0.593466  -2.269332  5.693859
C  1.407374  3.625671  -5.628913  H  0.065658  -2.297435  6.557116
H  1.638584  4.695902  -5.602576  C  -3.092676  3.079981  3.884125
H  0.487878  3.492983  -6.207526  H  -3.525349  2.721338  4.814544
H  2.212776  3.128247  -6.179857  C  3.152451  4.339639  0.347067
C  -0.671765  5.943397  -1.331949  H  2.237307  3.854843  0.706029
H  -0.918204  6.929264  -1.706094  C  4.834556  -4.862826  -0.177143
C  -1.831293  3.663139  3.884497  H  5.633753  -5.314703  0.405667
H  -1.290953  3.777933  4.820994  C  -5.407332  4.289267  0.451907
C  0.640143  0.614458  3.604565  H  -6.073997  3.824924  1.186838

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H  -5.965355  4.379901  -0.485873  C  -0.226231  6.327170  3.271488
H  -5.171606  5.296311  0.811681  H  -0.987559  6.850511  2.683378
C   5.556537  -0.677562  -0.486375  H   0.690179  6.927554  3.249375
H   6.510746  -0.844297  -0.979769  H  -0.577375  6.285370  4.308856
C   1.896266  1.536682  5.445736  C   1.705666 -3.138342  -2.600718
H   1.943155  1.885928  6.474389  C   1.531273 -3.967043  -3.880076
C   4.802925  3.331998  -2.948375  H   2.418366 -3.904964  -4.521364
H   5.809358  3.181078  -0.485873  H   0.676068 -3.596094  -4.456538
C  -4.529268  2.033350  -0.223302  H   1.356294 -5.025317  -3.660803
H  -3.636257  1.438414  -0.426779  C   2.002777 -1.677085  -2.945616
H  -5.118362  2.080474  -1.145417  H   0.892317  4.120774  4.587351
H  -5.128026  1.511015  0.531099  H   2.066768  4.860742  3.500287
C   1.160752  4.243541  3.533388  H   1.398511  3.256596  3.129725
C   4.359684  -4.860517  2.770303  H   2.977216 -1.567492  -3.437021
H   5.351313  -5.267675  2.544339  H   2.007218 -1.053501  -2.047444
H   4.097479  -5.194040  3.780360  H   1.240008 -1.290558  -3.627951
H   4.437943  -3.768596  2.782458  H  -0.905434 -0.313239  -3.830777
C  -3.113154  -0.464428  1.838241  C  -1.101804  0.391663  -1.290556
H  -3.450179  0.190131  2.650774  H  -1.021239 -1.101539  -3.982711
H  -3.755690  -0.295043  0.974358  H  -2.093107 -0.166455  1.571386  47_int1prima.log
C  -4.637166  -2.343598  2.502037  H  -4.729258  -3.380871  2.842103  SCF (wB97x)=  -3920.43497524
H  -5.207204  -2.234450  1.573940  E(SCF)+ZPE(0 K)=  -3918.858619
H  -5.110313  -1.706810  3.258248  H(298 K)=  -3918.760312
C  -1.823480  -1.632653  5.796105  G(298 K)=  -3918.991716
H  -2.129194  -1.183213  6.737745  Lowest Frequency = 14.0235 cm^-1
C   3.240272  -6.870408  1.756407  H   2.433230  -7.239889  1.116266  W  -2.463967 -0.716267  -2.765334
H   3.064246  -7.250697  2.768933  H  -0.168323  2.952876  -0.529373
H   4.181441  -7.298883  1.392342  Al  0.441541  -2.586134  0.880587
| Element | X       | Y       | Z       | Element | X       | Y       | Z       |
|---------|---------|---------|---------|---------|---------|---------|---------|
| O       | -0.194085 | -1.548515 | -0.363771 | C       | 2.383441 | 3.322376 | -3.351134 |
| O       | -1.092128 | 1.730613 | -1.413221 | C       | 0.666843 | 0.520214 | 0.477867  |
| O       | 1.324137  | -1.449680 | 1.836218  | C       | -3.806645 | 3.002702 | 2.678742  |
| O       | 0.750353  | 1.860700 | 0.504669  | H       | -4.813449 | 2.591399 | 2.700657  |
| C       | -3.490006 | -1.566966 | -4.283104 | C       | 3.680617 | 3.094663 | -3.817391 |
| N       | 0.905324  | 4.139916 | -1.548506 | H       | 3.826870 | 2.748125 | -4.837254 |
| N       | -0.680744 | -3.475897 | 2.133950  | C       | 0.432269 | -5.263576 | 0.026659  |
| C       | -4.092748 | -0.896539 | -1.632485 | C       | 2.222214 | 3.772352 | -2.09701  |
| N       | -1.302779 | 4.278406 | 0.228080  | C       | -2.510911 | 6.433926 | 0.219244  |
| N       | 1.182778  | -4.151756 | 0.102401  | H       | -3.412217 | 6.335967 | -0.396447 |
| C       | -1.942273 | -2.577931 | -2.073408 | H       | -2.163908 | 7.466060 | 0.142953  |
| O       | -4.076049 | -2.043632 | -5.164836 | H       | -2.786838 | 6.217941 | 1.251566  |
| O       | -5.065777 | -1.052172 | -1.012429 | C       | 0.480422 | 5.374042 | -1.877442 |
| O       | -3.480321 | 2.209861 | -3.605965 | C       | 5.201040 | -1.402091 | 0.626050  |
| O       | -1.744329 | -3.660763 | -1.718181 | H       | 5.881297 | -2.150726 | 1.024989  |
| C       | 2.963134  | 1.088724 | 3.311161  | C       | 3.968460 | -1.200807 | 1.230634  |
| H       | 3.873742  | 1.069292 | 2.719758  | H       | 3.677156 | -1.783647 | 2.100037  |
| C       | -1.074215 | -2.809198 | 3.356717  | C       | -1.244073 | 4.134875 | 2.662500  |
| C       | -0.181382 | -0.185465 | -0.354342 | H       | 0.762509 | -3.122711 | -2.095688 |
| C       | 1.203943  | 3.053144 | -4.274730 | C       | -0.688512 | -5.495990 | 0.828964  |
| H       | 0.305894  | 3.494815 | -3.829699 | H       | -1.212960 | -6.429020 | 0.664214  |
| C       | 1.772593  | 0.609943 | 2.771459  | C       | 0.775311 | -6.330374 | -0.982832 |
| C       | -1.967226 | 3.946163 | 1.469274  | H       | 1.850546 | -6.480650 | -1.088689 |
| C       | 2.519058  | -4.189885 | -0.451836 | H       | 0.388134 | -6.002922 | -1.955065 |
| C       | 1.298847  | 6.221839 | -2.820601 | H       | 0.298518 | -7.278044 | -0.728179 |
| H       | 2.335034  | 6.296220 | -2.479988 | C       | 3.292874 | -5.316501 | 1.729773  |
| H       | 0.875774  | 7.223845 | -2.894731 | H       | 2.317925 | -4.951813 | 2.067254  |
| H       | 1.321552  | 5.776912 | -3.818695 | C       | -0.197628 | -2.836986 | 4.459053  |
| C       | -2.302783 | -2.133606 | 3.424394  | C       | 1.694092 | -0.154036 | 1.435560  |
| C       | 3.062283  | -0.257943 | 0.730845  | C       | 3.431723 | 0.489870 | -0.384591 |
| C       | -3.277928 | 3.441823 | 1.462658  | H       | 2.757796 | 1.236752 | -0.793597 |
| Atoms | Coordinates |
|-------|-------------|
| C 0.964011 1.544008 -4.378892 | H -3.575471 3.894769 -0.603324 |
| H 1.838189 1.038335 -4.806385 | C 1.382213 3.656325 -5.673383 |
| H 0.101268 1.341280 -5.023323 | H 1.626408 4.723501 -5.641215 |
| H 0.768595 1.105278 -3.395931 | H 0.459533 3.538114 -6.250085 |
| C 3.325807 3.941800 -1.167736 | H 2.180028 3.152910 -6.229915 |
| C 3.010236 1.557958 4.626389 | C -0.677115 5.962542 -1.367512 |
| H 3.953836 1.911210 5.035237 | H -0.923097 6.949280 -1.739700 |
| C 2.786546 -3.690974 -1.737290 | C -1.815403 3.677548 3.849631 |
| C -1.461716 5.488410 -0.307627 | H -1.269834 3.792198 4.783114 |
| C 3.545225 -4.758321 0.333886 | C 0.617623 0.640541 3.562921 |
| C 0.661760 1.105942 4.869566 | H -0.317848 0.252606 3.164581 |
| H -0.245507 1.094469 5.469302 | C -2.671042 -1.544145 4.636987 |
| C 4.665322 0.278460 -1.004142 | H -3.621209 -1.019127 4.702814 |
| H 4.918876 0.858016 -1.887131 | C 5.108724 -4.347917 -1.473100 |
| C 4.095138 -3.772165 2.221162 | H 6.116254 -4.415137 -1.875471 |
| H 4.314415 -3.388472 3.219252 | C 3.001478 5.864964 0.457524 |
| C -3.200660 -1.940079 2.213958 | H 3.874237 6.384798 0.044601 |
| H -2.815122 -2.546465 1.386489 | H 2.928804 6.125831 1.519786 |
| C 0.053994 4.934774 2.690130 | H 2.105572 6.253220 -0.037468 |
| H 0.411311 5.044764 1.660640 | C 1.117443 -4.933167 4.918698 |
| C 4.600673 3.725218 -1.690059 | H 0.777281 -4.950602 5.960809 |
| H 5.468946 3.857904 -1.052133 | H 2.108103 -5.401169 4.881213 |
| C 4.284986 3.832892 1.188675 | H 0.433646 -5.555341 4.329818 |
| H 4.486081 2.772575 1.005466 | C 2.252680 -2.675039 5.096488 |
| H 4.002035 3.946358 2.240193 | H 2.255723 -1.641455 4.734549 |
| H 5.213957 4.394588 1.034835 | H 3.238082 -3.112465 4.901808 |
| C 1.171637 -3.495626 4.386742 | H 2.115966 -2.662167 6.183769 |
| H 1.459261 -3.536369 3.333457 | C -2.174196 -5.311320 2.812906 |
| C -1.137944 -4.707344 1.900441 | H -1.868545 -5.228370 3.859427 |
| C -3.091295 1.161865 -3.316965 | H -2.339805 -6.360919 2.568031 |
| C -4.151665 3.449085 0.214523 | H -3.121559 -4.772864 2.714433 |
$\text{SCF (wB97x) } = -3920.42527802$

$E(\text{SCF})+\text{ZPE (0 K)} = -3918.847533$

$H(298 \text{ K}) = -3918.750599$

$G(298 \text{ K}) = -3918.977922$

Lowest Frequency $= -23.9830 \text{ cm}^{-1}$

W $-2.489624$ $-0.569049$ $-2.935212$

Al $-0.134956$ $2.879970$ $-0.541731$

Al $0.452137$ $-2.684240$ $0.725842$

O $-0.244667$ $-1.636765$ $-0.491696$

O $-1.102713$ $1.707940$ $-1.438082$

O $1.356938$ $-1.573544$ $1.688067$

O $0.772470$ $1.746693$ $0.438448$

C $-3.570671$ $-1.186637$ $-4.524187$

N $0.922460$ $4.024725$ $-1.621310$

N $-0.703387$ $-3.590459$ $1.960226$

C $-3.326257$ $-1.947787$ $-1.766337$

N $-1.173812$ $4.226813$ $0.313412$

N $1.292930$ $-4.245605$ $0.033611$

C $-1.229589$ $-2.080427$ $-3.488280$

C $1.189478$ $2.645160$ $-4.258467$

H $0.260253$ $2.896480$ $-3.733333$

H $1.782332$ $0.482131$ $2.653778$

C $-1.717476$ $3.961946$ $1.631591$

H $2.682646$ $-4.314705$ $-0.376140$

C $1.215181$ $6.065059$ $-2.984027$

H $2.244331$ $6.236912$ $-2.655228$

H $0.725537$ $7.027610$ $-3.132834$

H $1.273274$ $5.543593$ $-3.941951$

C $-2.454701$ $-2.331707$ $3.172239$

C $3.073481$ $-0.327318$ $0.592635$

C $-3.026151$ $3.473549$ $1.784161$

C $2.366849$ $3.146353$ $-3.433289$

C $0.667500$ $0.410340$ $0.378080$

C $-3.440673$ $3.108085$ $3.067398$

C $-4.443902$ $2.711770$ $3.205880$

C $3.653380$ $3.021008$ $-3.966450$

C $3.774142$ $2.625813$ $-4.972082$

C $0.551035$ $-5.362228$ $-0.095689$

C $2.232925$ $3.676375$ $-2.139631$

C $-2.334212$ $6.409425$ $0.327713$

C $-3.288386$ $6.311937$ $-0.202195$

C $-1.973358$ $7.429332$ $0.182868$

C $-2.520370$ $6.236444$ $1.387850$

C $0.463749$ $5.241577$ $-1.966887$

C $5.238992$ $-1.411684$ $0.434564$

C $5.932148$ $-2.168408$ $0.792318$

C $3.994244$ $-1.282845$ $1.035905$

C $3.708852$ $-1.930780$ $1.859463$

C $-0.889280$ $4.206114$ $2.743907$

H $1.088919$ $-3.560381$ $-2.323864$

H $-0.624827$ $-5.590753$ $0.620452$

H $-1.134382$ $-6.526259$ $0.424952$
|   | X     | Y     | Z     |   | X     | Y     | Z     |
|---|-------|-------|-------|---|-------|-------|-------|
| H | 1.928065 | -5.401785 | 4.852764 | H | -5.016220 | 1.603834 | 1.314301 |
| H | 0.325930 | -5.541711 | 4.115537 | C | 1.580173 | 4.274071 | 3.349118 |
| C | 2.055870 | -2.687991 | 5.138227 | C | 4.225705 | -4.847714 | 2.995087 |
| H | 2.078188 | -1.637111 | 4.831295 | H | 5.216638 | -5.296625 | 2.868810 |
| H | 3.057766 | -3.106336 | 4.998861 | H | 3.873981 | -5.128934 | 3.992766 |
| H | 1.837308 | -2.733596 | 6.211316 | H | 4.343453 | -3.759283 | 2.969902 |
| C | -2.179400 | -5.476015 | 2.552538 | C | -3.433948 | -0.881794 | 1.412038 |
| H | -2.029664 | -5.247853 | 3.610099 | H | -3.759916 | -0.180370 | 2.189066 |
| H | -2.174359 | -6.557309 | 2.409847 | H | -4.140980 | -0.824279 | 0.580414 |
| H | -3.167406 | -5.096474 | 2.272923 | H | -2.454864 | -0.550788 | 1.047724 |
| C | -0.812508 | -2.205061 | 5.427710 | C | -4.785622 | -2.811732 | 2.269204 |
| H | -0.176121 | -2.143208 | 6.305260 | H | -4.781466 | -3.783126 | 2.775444 |
| C | -2.608897 | 3.262988 | 4.166283 | H | -5.346697 | -2.913052 | 1.334941 |
| H | -2.950659 | 2.967306 | 5.154781 | H | -5.332400 | -2.111486 | 2.911096 |
| C | 3.246379 | 4.381329 | 0.112955 | C | -2.077487 | -1.635162 | 5.464750 |
| H | 2.342599 | 3.908400 | 0.514484 | H | -2.429633 | -1.142541 | 6.367735 |
| C | 4.955342 | -4.950243 | 0.131698 | C | 3.127313 | -6.863806 | 1.973347 |
| H | 5.686369 | -5.376031 | 0.814287 | H | 2.348754 | -7.235848 | 1.300336 |
| C | -5.203741 | 4.385469 | 0.927293 | H | 2.875498 | -7.195869 | 2.986939 |
| H | -5.802741 | 4.027684 | 1.772133 | H | 4.075253 | -7.334915 | 1.687996 |
| H | -5.863866 | 4.441549 | 0.055486 | C | 0.250923 | 6.402806 | 3.121665 |
| H | -4.866980 | 5.397657 | 1.171496 | H | -0.545157 | 6.928370 | 2.583402 |
| C | 5.582682 | -0.595246 | -0.640536 | H | 1.179387 | 6.969756 | 2.989545 |
| H | 6.549332 | -0.705817 | -1.125556 | H | -0.003106 | 6.415920 | 4.187672 |
| C | 1.842364 | 1.424635 | 5.297379 | C | 2.102607 | -3.416198 | -2.707133 |
| H | 1.869128 | 1.773406 | 6.327014 | C | 2.235839 | -4.219611 | -4.007979 |
| C | 4.772282 | 3.395036 | -3.241339 | H | 3.188058 | -4.014047 | -4.510120 |
| H | 5.762612 | 3.313391 | -3.681687 | H | 1.428898 | -3.952008 | -4.694632 |
| C | -4.571848 | 2.019609 | 0.403796 | H | 2.187735 | -5.299083 | -3.826040 |
| H | -3.774654 | 1.348547 | 0.073694 | C | 2.275997 | -1.920762 | -2.980028 |
| H | -5.341924 | 2.034539 | -0.370693 | H | 1.391749 | 4.187269 | 4.423737 |
| Atom | X     | Y     | Z     | Atom | X     | Y     | Z     |
|------|-------|-------|-------|------|-------|-------|-------|
| C    | -3.30 | 3.30  | 3.30  | H    | -1.93 | 3.02  | 3.02  |
| O    | -0.12 | -0.12 | -0.12 | H    | -1.29 | -0.03 | -0.03 |
| H    | -0.21 | -0.01 | -0.01 | C    | 3.06  | 0.31  | 0.81  |
| O    | -1.05 | 1.70  | 0.44  | C    | 1.31  | 0.31  | 0.44  |
| O    | 1.28  | -1.45 | 1.90  | C    | 0.78  | 0.84  | 0.50  |
| C    | -3.76 | -1.55 | -0.48 | N    | 0.96  | 4.12  | 1.55  |
| N    | -0.73 | 3.44  | 2.22  | C    | 1.89  | -2.60 | 1.71  |
| N    | 1.13  | 4.26  | 0.17  | N    | 1.11  | 0.93  | 0.19  |
| C    | -1.11 | -0.92 | -4.27 | N    | 1.39  | 6.20  | 2.82  |
| C    | 2.49  | 4.86  | 3.22  | O    | -4.52 | -1.97 | -4.81 |
| H    | 1.75  | 3.27  | 2.95  | O    | -1.61 | -3.71 | -1.88 |
| H    | 3.31  | -1.68 | -3.27 | O    | -4.91 | -1.19 | -0.74 |
| H    | 2.03  | -1.02 | -2.09 | O    | -0.43 | -1.12 | 5.20  |
| H    | 1.61  | -1.62 | -3.79 | C    | 2.98  | 1.11  | 3.32  |
| H    | -1.93 | 1.02  | -3.93 | C    | 3.88  | 1.07  | 2.71  |
| C    | -1.13 | 0.39  | -1.40 | C    | -1.08 | -2.78 | 3.45  |
| H    | 2.04  | -1.33 | -2.09 |

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| SCF (wB97x) | -3920.43311639 |
|-------------|----------------|
| E(SCF)+ZPE(0 K) | -3918.856982 |
| H(298 K) | -3918.759214 |
| G(298 K) | -3918.989230 |
| Lowest Frequency | -122.9899cm^-1 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -2.617215    | -1.476110    | 4.776893     |
| H       | -3.547832    | -0.919673    | 4.861141     |
| C       | 5.050751     | -4.555346    | -1.359839    |
| H       | 6.055779     | -4.672241    | -1.757249    |
| C       | 3.002571     | 5.862033     | 0.477113     |
| H       | 3.867865     | 6.393198     | -0.062892    |
| C       | 5.050751     | -4.555346    | -1.359839    |
| H       | 6.055779     | -4.672241    | -1.757249    |
| C       | 1.081680     | -4.943680    | 5.105884     |
| H       | 0.803377     | -4.872992    | 6.163907     |
| H       | 2.051925     | -5.450148    | 5.047514     |
| C       | 0.342290     | -5.579754    | 4.605559     |
| C       | 2.277325     | -2.706220    | 5.064968     |
| H       | 2.299231     | -1.712961    | 4.604725     |
| H       | 3.243541     | -3.191972    | 4.890398     |
| H       | 2.168767     | -2.583894    | 6.148402     |
| C       | -2.271591    | -5.239940    | 2.892902     |
| H       | -1.932279    | -5.211594    | 3.932388     |
| H       | -2.497218    | -6.270325    | 2.616661     |
| H       | -3.191955    | -4.650557    | 2.843268     |
| C       | -0.577135    | -2.261888    | 5.755595     |
| H       | 0.090092     | -2.322806    | 6.611294     |
| C       | -3.123978    | 3.167611     | 3.800193     |
| H       | -3.571796    | 2.835540     | 4.733268     |
| C       | 3.182401     | 4.344477     | 0.328665     |
| H       | 2.271150     | 3.851170     | 0.687217     |
| C       | 4.733268     | -0.503461    | -0.103439    |
| H       | 5.498065     | -5.562513    | 0.478507     |
| C       | -5.397806    | 4.312055     | 0.320810     |
| H       | -6.073512    | 3.857043     | 1.053058     |
| H       | -5.944571    | 4.389590     | -0.624939    |
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50_Int1aprima.log

SCF (wB97x) = -3920.43645857
E(SCF)+ZPE(0 K) = -3918.858565
H(298 K) = -3918.760955
G(298 K) = -3918.987935
Lowest Frequency = 16.6896 cm⁻¹
| atom | x    | y    | z    | atom | x    | y    | z    |
|------|------|------|------|------|------|------|------|
| C    | 1.437397 | 3.584158 | -5.91428 | C    | 1.437397 | 3.584158 | -5.91428 |
| H    | 1.978237 | 4.525013 | -5.771327 | H    | 1.978237 | 4.525013 | -5.771327 |
| H    | 0.537299 | 3.790651 | -6.502917 | H    | 0.537299 | 3.790651 | -6.502917 |
| H    | 2.074994 | 2.925830 | -6.514032 | C    | -0.326748 | 5.800679 | -1.651689 |
| C    | -0.637668 | 6.712163 | -2.148840 | H    | 1.978237 | 4.525013 | -5.771327 |
| C    | -0.473453 | 5.476947 | 3.855912 | C    | -0.152799 | -0.018522 | 3.662917 |
| H    | 0.157138 | 6.090624 | 4.495684 | C    | -0.152799 | -0.018522 | 3.662917 |
| C    | 3.473290 | -2.690034 | 4.141666 | C    | 0.157138 | 6.090624 | 4.495684 |
| H    | 3.972821 | 5.402502 | -0.515995 | C    | 5.192401 | -3.355885 | -1.564139 |
| H    | 4.911660 | 5.494475 | -1.073940 | C    | -0.604195 | -0.954209 | 3.354747 |
| H    | 4.090896 | 5.939049 | 0.431481 | C    | 3.972821 | 5.402502 | -0.515995 |
| H    | 3.189883 | 5.908078 | -1.090337 | C    | 4.911660 | 5.494475 | -1.073940 |
| C    | 0.891621 | -5.303804 | 4.399769 | C    | 4.090896 | 5.939049 | 0.431481 |
| C    | 1.485725 | -3.022380 | 5.289912 | C    | 3.189883 | 5.908078 | -1.090337 |
| C    | 4.911660 | 5.494475 | -1.073940 | C    | 0.891621 | -5.303804 | 4.399769 |
| H    | 1.437397 | 3.584158 | -5.91428 | C    | 1.485725 | -3.022380 | 5.289912 |
| H    | 1.957585 | -5.555560 | 4.454866 | H    | 1.310042 | -1.944926 | 5.206188 |
| H    | 0.461594 | -5.871924 | 3.568020 | C    | 1.310042 | -1.944926 | 5.206188 |
| C    | 3.645887 | 3.922208 | -0.267279 | C    | 0.461594 | -5.871924 | 3.568020 |
| H    | 2.674720 | 3.870687 | 0.240098 | C    | 4.976949 | -3.922002 | -0.317919 |
| C    | -0.326748 | 5.800679 | -1.651689 | H    | 2.674720 | 3.870687 | 0.240098 |
| H    | -0.637668 | 6.712163 | -2.148840 | C    | -0.473453 | 5.476947 | 3.855912 |
| C    | -0.473453 | 5.476947 | 3.855912 | H    | -0.637668 | 6.712163 | -2.148840 |
| C    | 0.157138 | 6.090624 | 4.495684 | C    | -0.473453 | 5.476947 | 3.855912 |
| H    | 0.326748 | 5.800679 | -1.651689 | C    | 0.157138 | 6.090624 | 4.495684 |
| H    | 0.637668 | 6.712163 | -2.148840 | C    | -0.473453 | 5.476947 | 3.855912 |
| H    | 0.157138 | 6.090624 | 4.495684 | C    | 0.157138 | 6.090624 | 4.495684 |
| H    | -0.637668 | 6.712163 | -2.148840 | C    | -0.473453 | 5.476947 | 3.855912 |
| H    | -0.637668 | 6.712163 | -2.148840 | C    | -0.473453 | 5.476947 | 3.855912 |
| H    | 0.157138 | 6.090624 | 4.495684 | C    | 0.157138 | 6.090624 | 4.495684 |
| H    | 0.157138 | 6.090624 | 4.495684 | C    | 0.157138 | 6.090624 | 4.495684 |
| H    | -0.637668 | 6.712163 | -2.148840 | C    | -0.473453 | 5.476947 | 3.855912 |

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| Element | X       | Y       | Z       | Element | X       | Y       | Z       |
|---------|---------|---------|---------|---------|---------|---------|---------|
| C       | -5.048995 | -3.921748 | 1.911638 | C       | 1.082115  | -3.686647 | -3.613976 |
| H       | -4.901206 | -4.903847 | 2.374210 | H       | 1.881560  | -4.126677 | -4.223216 |
| H       | -5.555118 | -4.067980 | 0.952136 | H       | 0.324216  | -3.281906 | -4.291061 |
| H       | -5.730392 | -3.355765 | 2.556397 | H       | 0.610963  | -4.484903 | -3.033603 |
| C       | -2.756266 | -2.637198 | 5.328417 | C       | 2.014312  | -1.358702 | -3.564886 |
| H       | -3.239391 | -2.313198 | 6.246881 | H       | 2.274912  | 5.810962  | 3.911048  |
| C       | 4.271192  | -6.057508 | 1.701065 | H       | 3.308261  | 5.919070  | 2.485906  |
| H       | 4.017334  | -6.769436 | 0.908539 | H       | 2.495255  | 4.390518  | 2.876054  |
| H       | 4.030944  | -6.522898 | 2.663227 | H       | 2.705369  | -1.624756 | -4.374196 |
| H       | 5.355786  | -5.905646 | 1.673368 | H       | 2.480734  | -0.563211 | -2.971693 |
| C       | 1.095544  | 7.438359  | 1.955725 | H       | 1.118061  | -0.954268 | -4.035091 |
| H       | 0.303411  | 7.774800  | 1.279338 | H       | -2.376482 | 1.587392  | -3.160796 |
| H       | 2.040669  | 7.860398  | 1.596366 | H       | -2.958955 | 1.396616  | -3.667312 |
| H       | 0.894362  | 7.861869  | 2.946272 | C       | 1.636608  | -2.572953 | -2.713224 |
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