Supporting Information for:

Ring-Expansion and Desulfurisation of Thiophenes with an Aluminium(I) Reagent

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Contents

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_2 and <0.1 ppm H_2O. 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_6D_6 was dried over 3 Å molecular sieves and freeze-pump-thaw degassed thrice before use. All chemicals were purchased from common suppliers (*e.g.* Sigma-Aldrich, Fluorochem, Merck, Alfa Aesar, TCI etc.). Thiophene substrates that were liquids at 25 °C were dried over CaH_2, distilled, and stored over activated 3 Å molecular sieves. [{(ArNCMe)$_2$CH}Al] (**1**, Ar = 2,6-di-isopropylphenyl) was prepared following the literature procedure.[1] NMR Spectra were recorded on Bruker 400 MHz or 500 MHz at 298 K 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, NOESY) spectra.

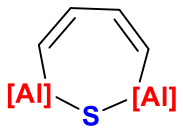
2. Synthetic Procedures

General Procedure

In a glovebox, **1** (50 mg, 0.112 mmol) was dissolved in C_6D_6 (1.2 mL) and transferred to a J-Young NMR tube. To this solution, the relevant thiophene (1.1-10 equivalents) was added. The NMR tube was sealed and heated to 60 °C in an isothermal bath for 32-64 hours during which time the reaction solution turned from orange-red to yellow.

Isolation of 3:

In the reaction, 10 equivalents (90 µL, 1.12 mmol) of thiophene was used. During heating of the reaction solution, a precipitate (**5**) formed and **2a** can be observed at intermediate time points (δ = 4.87 ppm, s, 1H, BDI-C*H*) which is consumed over the course of the reaction. The crude reaction mixture contained both **3** and **4** in an approximately 1:1.4 ratio. In a glovebox, the solution was filtered, and the solvent removed in vacuo. The resulting light-yellow solid was dissolved in toluene. The solution was concentrated to ca. 0.2 mL in volume and cooled to -35 °C for one week resulting in the formation of colourless crystals of **3.** In-situ NMR yield[a] of **3** = 25%, of **4** = 34%.



3

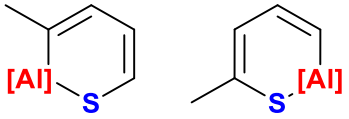
^{1}H NMR 3 (400 MHz, C_6D_6, 298 K): δ 0.93 (d, $^3J_{HH}$ = 6.7 Hz, 12H, Dipp-^{i}Pr-CH_3), 1.03 (d, $^3J_{HH}$ = 6.8 Hz, 12H, Dipp-^{i}Pr-CH_3), 1.17 (d, $^3J_{HH}$ = 6.7 Hz, 12H, Dipp-^{i}Pr-CH_3), 1.22 (d, $^3J_{HH}$ = 6.8 Hz, 12H, Dipp-^{i}Pr-CH_3), 1.39 (s, 12H, BDI-CH_3), 3.09 (hept, $^3J_{HH}$ = 6.8 Hz, 4H, Dipp-^{i}Pr-C*H*), 3.37 (hept, $^3J_{HH}$ = 6.8 Hz, 4H, Dipp-^{i}Pr-C*H*), 4.80 (s, 2H, BDI-C*H*), 6.14 (d, $^3J_{HH}$ = 16.9 Hz, 2H, [Al]C*H*CH), 6.96-7.18 (m, 14H, Dipp-Ar-C*H* and [Al]CHC*H*).

^{13}C{^{1}H} NMR 3 (100.6 MHz, C_6D_6, 298 K): δ 24.5 (BDI-*C*H_3), 24.5 (Dipp-^{i}Pr-*C*H_3), 24.6 (Dipp-^{i}Pr-*C*H_3), 25.2 (Dipp-^{i}Pr-*C*H_3), 27.8 (Dipp-^{i}Pr-*C*H_3), 28.0 (Dipp-^{i}Pr-*C*H), 29.2 (Dipp-^{i}Pr-*C*H), 98.0 (BDI-*C*H), 124.2, 124.6, 126.8 (Ar-*C*), 139.5 ([Al]*C*HCH), 142.4, 143.5, 144.7, 148.6 ([Al]CH*C*H), 169.7 (*C*=N).

^{1}H NMR 4 (400 MHz, C_6D_6, 298 K): δ 1.13 (d, $^3J_{HH}$ = 6.8 Hz, 12H, Dipp-^{i}Pr-CH_3), 1.37 (d, $^3J_{HH}$ = 6.8 Hz, 12H, Dipp-^{i}Pr-CH_3), 1.55 (s, 6H, BDI-CH_3), 3.38 (hept, $^3J_{HH}$ = 6.8 Hz, 4H, Dipp-^{i}Pr-C*H*, overlapping with **3** Dipp-^{i}Pr-C*H*), 4.91 (s, 1H, BDI-C*H*), 6.00 (d, $^3J_{HH}$ = 13.7 Hz, 2H, [Al]C*H*CH), 6.96-7.15 (m, 8H, Dipp-Ar-C*H* and [Al]CHC*H*, overlapping with **3** Dipp-Ar-C*H* and [Al]CHC*H*).

[a] The reaction to calculate the in-situ NMR yield was conducted using 10 mg of **1** in 0.6 mL of C_6D_6 with a capillary containing a 2.92 x10^{-3} M solution of hexamethyldisiloxane in C_6D_6.

Isolation of 2b and 2b':



2b **2b'**

In the reaction, 10 equivalents 2-methylthiophene (109 µL, 1.12 mmol) was added. During the reaction, a precipitate (**5**) formed. The crude reaction mixture contained **2b** and **2b'** in an approximate ratio of 3.4:1 along with other minor products. In a glovebox, the solution was filtered, and the solvent removed in vacuo. The solution was concentrated to ca. 0.2 mL in volume and cooled to -35 °C for two weeks resulting in the formation of colourless crystals which were a 2.5:1 mixture of **2b** and **2b'** respectively. Colourless crystals of **2b** suitable for analysis by single crystal x-ray diffraction were obtained from a concentrated solution of toluene at -35 °C for two weeks. In-situ NMR yield[b] of **2b** = 53%, of **2b'** = 15%.

^{1}H NMR 2b (400 MHz, C_6D_6, 298 K): δ 1.09 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.18-1.24 (m, 12H, Dipp-^{i}Pr-CH_3, overlapping with **2b'** Dipp-^{i}Pr-CH_3), 1.50 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.51 (s, 6H, BDI-CH_3), 2.30 (s, 3H, [Al]CCH_3), 3.16 (hept, $^3J_{HH}$ = 6.8 Hz, 2H , Dipp-^{i}Pr-C*H*), 3.27 (hept, $^3J_{HH}$ = 6.8 Hz, 2H, Dipp-^{i}Pr-C*H*, overlapping with **2b'** Dipp-^{i}Pr-C*H*), 4.86 (s, 1H, BDI-C*H*), 5.92 (dd, $^3J_{HH}$ = 10.0 Hz, 7.1 Hz, 1H, [Al]SCHC*H*), 6.05 (d, $^3J_{HH}$ = 10.0 Hz, 1H, [Al]SC*H*), 6.79 (d, $^3J_{HH}$ = 7.1 Hz, 1H, [Al]CCH$_3$C*H*), 7.01-7.12 (m, 7H, Dipp-Ar-C*H*, overlapping with **2b'** Dipp-Ar-C*H* & [Al]SCCH$_3$C*H*).

^{13}C{^{1}H} NMR (125.7 MHz, C_6D_6, 298 K): δ 23.6 (BDI-*C*H$_3$), 24.6 (Dipp-^{i}Pr-*C*H$_3$), 24.7 (Dipp-^{i}Pr-*C*H$_3$), 24.8 (Dipp-^{i}Pr-*C*H$_3$), 26.1 ([Al]C*C*H$_3$), 28.0 (Dipp-^{i}Pr-*C*H), 29.5 (Dipp-^{i}Pr-*C*H), 98.3 (BDI-*C*H), 121.3 ([Al]S*C*H), 123.4 ([Al]SCH*C*H), 124.4, 124.8 (Dipp-Ar-*C*H, final Dipp-Ar-*C*H overlapping with C_6D_6 solvent signal), 140.2 (Ar-*C*), 143.2 ([Al]CCH$_3$*C*H), 143.6 ([Al]*C*CH$_3$), 143.7, 144.9 (Ar-*C*), 170.9 (*C*=N).

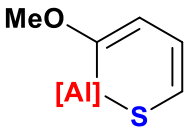
^{1}H NMR 2b' (400 MHz, C_6D_6, 298 K): δ 1.13 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.18-1.24 (m, 12H, Dipp-^{i}Pr-CH_3, overlapping with **2b** Dipp-^{i}Pr-CH_3), 1.33 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.38 (d, $^3J_{HH}$ = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.53 (s, 6H, BDI-CH_3), 2.18 (s, [Al]SCCH_3), 3.27 (hept, $^3J_{HH}$ = 6.8 Hz, 2H, Dipp-^{i}Pr-C*H*, overlapping with **2b** Dipp-^{i}Pr-C*H*), 3.44 (hept, $^3J_{HH}$ = 6.8 Hz, 2H, Dipp-^{i}Pr-C*H*), 4.85 (s, 1H, BDI-C*H*), 5.74 (d, $^3J_{HH}$ = 12.8 Hz, 1H, [Al]C*H*), 6.73 (m, 1H, [Al]SCCH$_3$C*H*), 7.01-7.12 (m, 7H, Dipp-Ar-C*H* & [Al]CHC*H*, overlapping with **2b** Dipp-Ar-C*H*).

^{13}C{^{1}H} NMR (125.7 MHz, C_6D_6, 298 K): δ 23.4 ([Al]SC*C*H$_3$), 24.7 (BDI-*C*H$_3$) 24.7 (Dipp-^{i}Pr-*C*H$_3$), 24.8 (Dipp-^{i}Pr-*C*H$_3$), 25.5 (Dipp-^{i}Pr-*C*H$_3$), 26.4 (Dipp-^{i}Pr-*C*H$_3$), 27.7 (Dipp-^{i}Pr-*C*H), 29.0 (Dipp-^{i}Pr-*C*H), 97.9 (BDI-*C*H), 124.2, 124.7, 127.4 (Dipp-Ar-*C*H), 131.9 ([Al]*C*H, detected indirectly through HSQC), 140.4, 141.9 (Ar-*C*), 145.1 ([Al]S*C*CH$_3$) 145.7 ([Al]SCCH$_3$*C*H), 146.0 (Ar-*C*), 151.3 ([Al]CH*C*H), 170.1 (*C*=N).

[b] The reaction to calculate the in-situ NMR yield was conducted using 5 mg of **1** in 0.6 mL of C_6D_6 with a capillary containing a 2.92 x10^{-3} M solution of hexamethyldisiloxane in C_6D_6.

Isolation of 2c:

In this reaction, 1.1 equivalents of 2-methoxythiophene (12.7 µL, 0.124 mmol) was added. In a glovebox, the solvent was removed in vacuo. Colourless crystals of **2c** suitable for analysis by single crystal x-ray diffraction were obtained from a vapour diffusion of n-pentane into a concentrated solution of toluene (ca. 0.2 mL in volume) at -35 °C for two weeks. In-situ NMR yield[c] of **2c** = 63%.



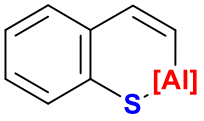
2c

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 1.09 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-C*H*$_3$), 1.24 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-C*H*$_3$), 1.27 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-C*H*$_3$), 1.54 (s, 6H, BDI-C*H*$_3$), 1.55 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-C*H*$_3$), 3.28 (hept, $^{3}J_{HH}$ = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 3.35 (s, 3H, OC*H*$_3$), 3.45 (hept, $^{3}J_{HH}$ = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 4.85 (s, 1H, BDI-C*H*), 5.78-5.89 (m, 2H, [Al]SC*HCH*), 5.93-5.99 (m, 1H, [Al]C(OCH$_3$)C*H*), 7.10 (m, 6H, Dipp-Ar-C*H*).

^{13}C{^{1}H} NMR (125.7 MHz, C_6D_6, 298 K): δ 23.7 (BDI-*C*H$_3$), 24.6 (Dipp-^{i}Pr-*C*H$_3$), 24.9 (Dipp-^{i}Pr-*C*H$_3$), 25.1 (Dipp-^{i}Pr-*C*H$_3$), 26.4 (Dipp-^{i}Pr-*C*H$_3$), 27.9 (Dipp-^{i}Pr-*C*H), 29.6 (Dipp-^{i}Pr-*C*H), 52.8 (O*C*H$_3$), 98.9 (BDI-*C*H), 115.2 ([Al]SCH*C*H), 116.3 ([Al]C(OCH$_3$)*C*H), 121.4 ([Al]S*C*HCH), 124.4, 124.8, 128.4 (Dipp-Ar-*C*H), 140.1, 143.8, 145.2, 171.0 (*C*=N), 176.2 (br, [Al]*C*(OCH$_3$)CH).

[c] The reaction to calculate the in-situ NMR yield was conducted using 5 mg of **1** in 0.6 mL of C_6D_6 with a capillary containing a 2.92 x10^{-3} M solution of hexamethyldisiloxane in C_6D_6.

Isolation of 2d:



2d

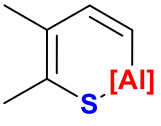
In this reaction, 1.3 equivalents of benzothiophene (19 mg, 0.142 mmol) was added to this solution. In a glovebox, the solvent was removed in vacuo. Colourless crystals of **2d** suitable for analysis by single crystal x-ray diffraction were obtained from a vapour diffusion of hexamethyldisiloxane into a concentrated solution of toluene (ca. 0.2 mL in volume) at room temperature for two weeks. In-situ NMR yield[d] of **2d** = 15%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 1.13 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.15 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.29 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.43 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.53 (s, 6H, BDI-CH_3), 3.38 (hept, $^{3}J_{HH}$ = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 3.51 (hept, $^{3}J_{HH}$ = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 4.85 (s, 1H, BDI-C*H*), 6.27 (d, $^{3}J_{HH}$ = 16.4 Hz, 1H, [Al]C*H*), 6.66-6.75 (m, 2H, [Al]SCCHC*H*C*H*), 6.84-6.87 (m, 1H, [Al]CHCHCC*H*), 6.96-7.03 (m, 6H, Dipp-Ar-C*H*), 7.48-7.51 (m, 1H, [Al]SCC*H*), 7.57 (d, $^{3}J_{HH}$ = 16.4 Hz, 1H, [Al]CHC*H*).

^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 298 K): δ 23.6 (BDI-*C*H_3), 24.8 (Dipp-^{i}Pr-*C*H_3), 25.0 (Dipp-^{i}Pr-*C*H_3), 25.2 (Dipp-^{i}Pr-*C*H_3), 25.9 (Dipp-^{i}Pr-*C*H_3), 28.7 (Dipp-^{i}Pr-*C*H), 29.3 (Dipp-^{i}Pr-*C*H), 98.2 (BDI-*C*H), 123.2 ([Al]SCCH*C*HCH or [Al]SCCHCH*C*H), 124.3 (Dipp-Ar-*C*H), 124.9 (Dipp-Ar-*C*H), 126.1 ([Al]SCCH*C*HCH or [Al]SCCHCH*C*H), 129.3 (Dipp-Ar-*C*H), 134.2 ([Al]CHCHC*C*H), 134.6 ([Al]*C*H, observed indirectly through HSQC), 135.1 ([Al]SC*C*H), 135.8 [Al]CHCH*C*), 136.1 ([Al]S*C*), 139.6, 143.9, 144.8 (Ar-*C*), 154.1 ([Al]CH*C*H), 170.7 (*C*=N).

[d] The reaction to calculate the in-situ NMR yield was conducted using 5 mg of **1** in 0.6 mL of C_6D_6 with a capillary containing a 2.92 x10^{-3} M solution of hexamethyldisiloxane in C_6D_6.

Isolation of 2e:



2e

In this reaction, 2 equivalents of 2,3-dimethylthiophene (25.2 µL**,** 0.225 mmol) was added. In a glovebox, the solvent was removed in vacuo. Colourless crystals of **2e** were obtained from a vapour diffusion of hexamethyldisiloxane into a concentrated solution of toluene (ca. 0.2 mL in volume) at room temperature for two weeks. In-situ NMR yield[e] of **2e** = 29%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 1.14 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.17 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H Dipp-^{i}Pr-CH_3), 1.35 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H Dipp-^{i}Pr-CH_3), 1.51 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H Dipp-^{i}Pr-CH_3). 1.52 (s, 6H, BDI-CH_3), 1.63 (s, 3H, [Al]SC(CH_3)C(CH_3)), 1.98 (s, 3H, [Al]S(CH_3)), 3.34 (hept, , $^{3}J_{HH}$ = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 3.48 (hept, $^{3}J_{HH}$ = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 4.83 (s, 1H, BDI-C*H*), 6.08 (d, $^{3}J_{HH}$ = 16.4 Hz, [Al]C*H*), 7.02-7.13 (m, 7H, Dipp-Ar-C*H* and [Al]CHC*H*).

^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 298 K): δ 23.6 (Dipp-^{i}Pr-*C*H_3), 23.7 ([Al]S(CH_3)C(*C*H_3)), 24.8 (Dipp-^{i}Pr-*C*H_3), 25.0 (Dipp-^{i}Pr-*C*H_3), 25.3 (Dipp-^{i}Pr-*C*H_3), 25.7 (BDI-*C*H_3), 28.6 (Dipp-^{i}Pr-*C*H), 29.1 ([Al]S(*C*H_3)), 29.2 (Dipp-^{i}Pr-*C*H), 98.0 (BDI-C*H*), 124.3 ([Al]SC(CH_3)*C*(CH_3)), 124.3 (Dipp-Ar-*C*H), 124.8 (Dipp-Ar-*C*H, final Dipp-Ar-*C*H overlapping with C_6D_6 solvent signal), 126.9 ([Al]S*C*(CH_3)C(CH_3)), 132.0 ([Al]*C*H, observed indirectly through HSQC), 140.0, 144.0, 144.7 (Ar-*C*), 154.7 ([Al]CH*C*H), 170.3 (*C*=N).

[e] The reaction to calculate the in-situ NMR yield was conducted using 5 mg of **1** in 0.6 mL of C_6D_6 with a capillary containing a 2.92 x10^{-3} M solution of hexamethyldisiloxane in C_6D_6.

3. NMR Spectra

Note: Broad resonances are commonly observed between δ 0-2 ppm in the following ^{1}H NMR spectra due to impurities in starting material **1** and the products being purified from complex mixtures

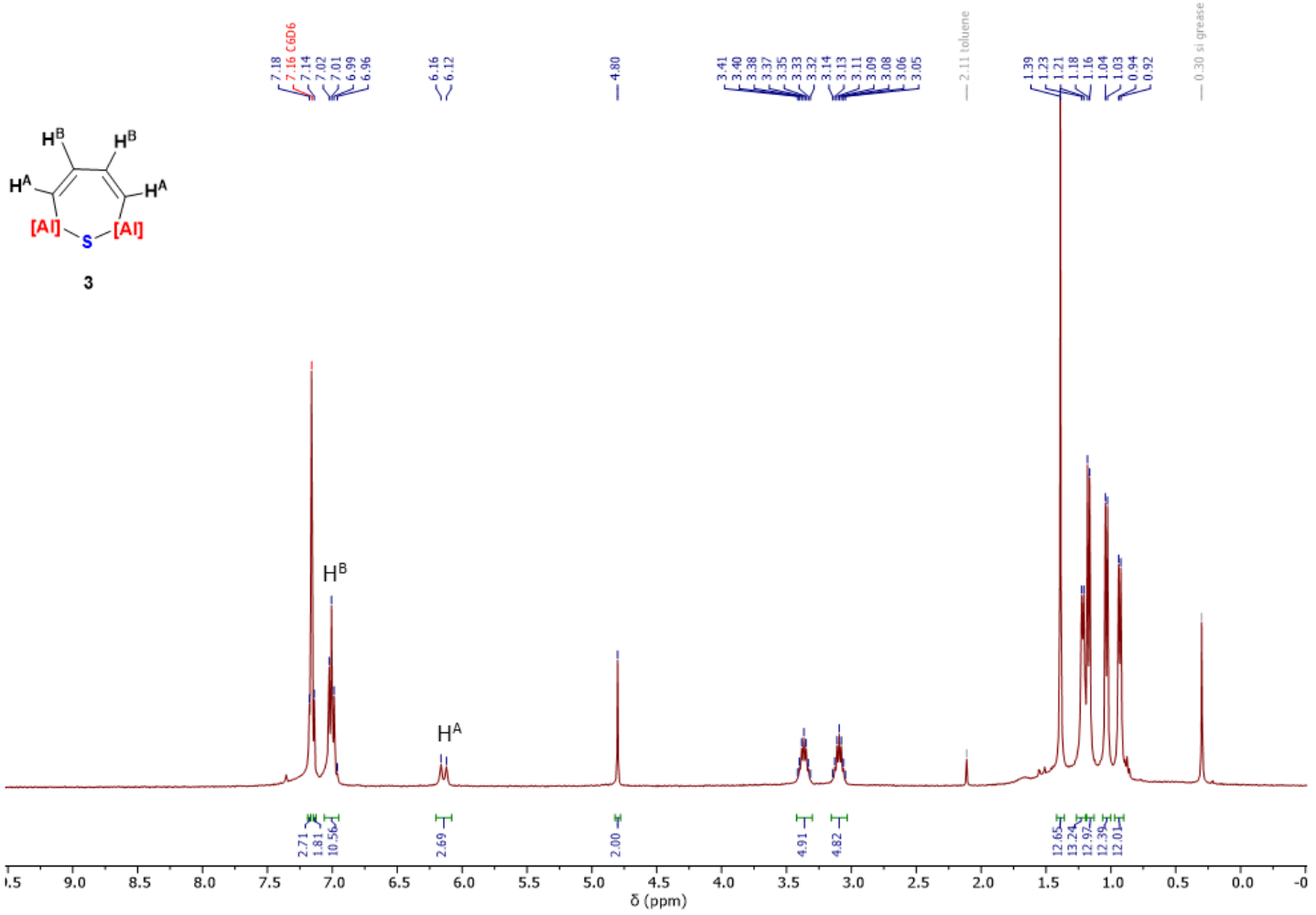


Figure S1: ^{1}H NMR spectrum (400 MHz, C_6D_6) of **3**

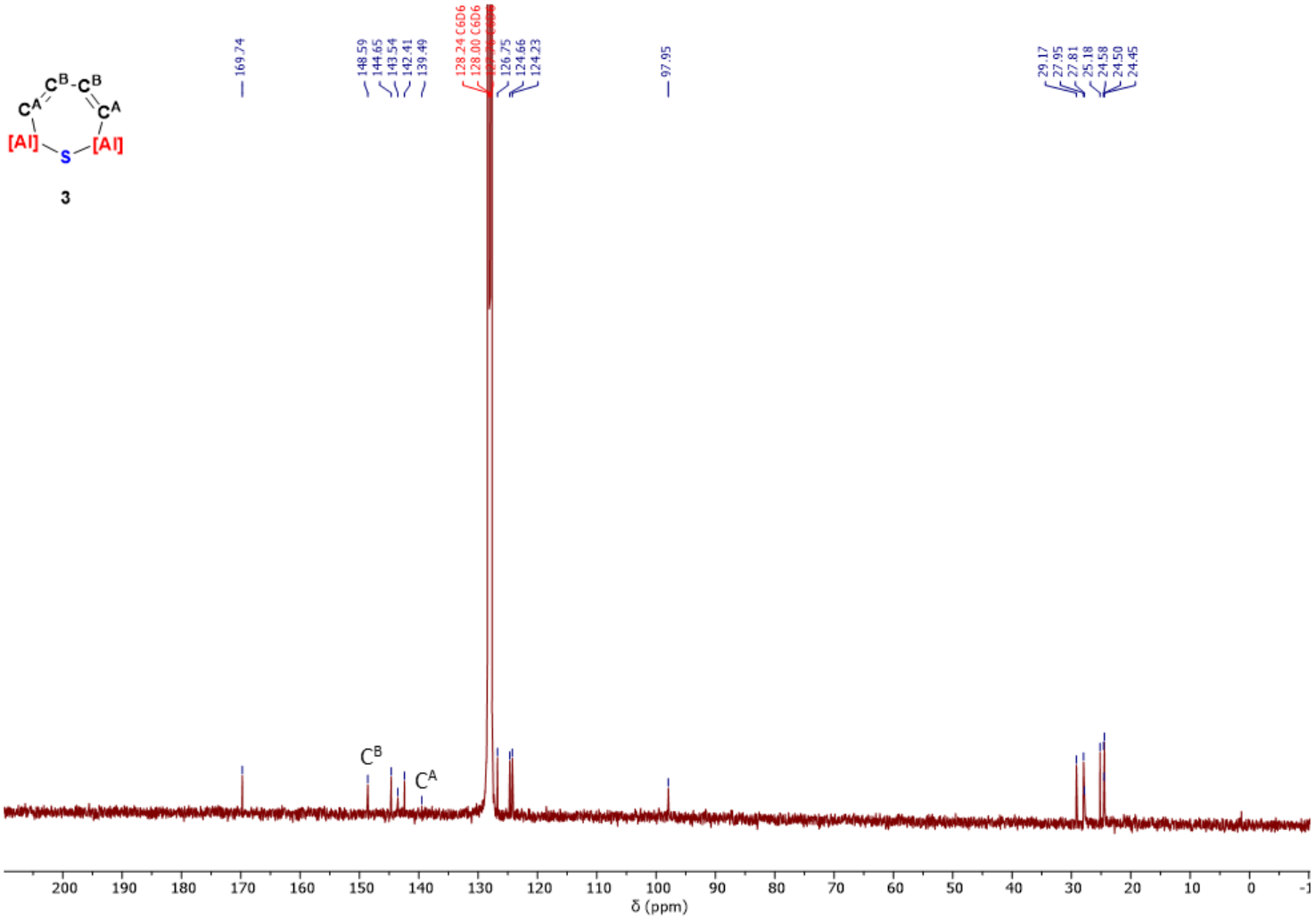


Figure S2: ^{13}C NMR spectrum (100.6 MHz, C_6D_6) of **3**

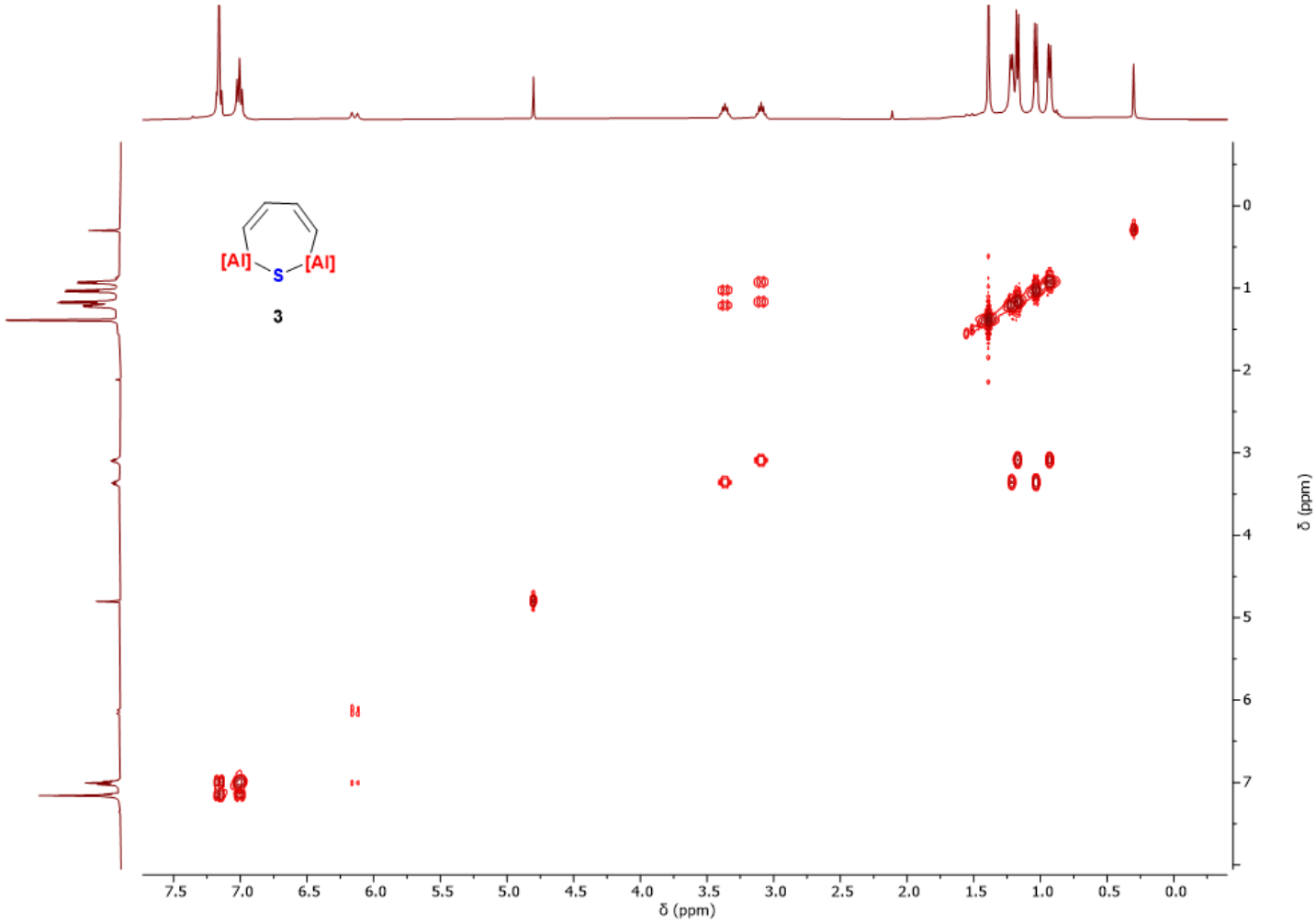


Figure S3: ^{1}H-^{1}H COSY NMR spectrum of **3**

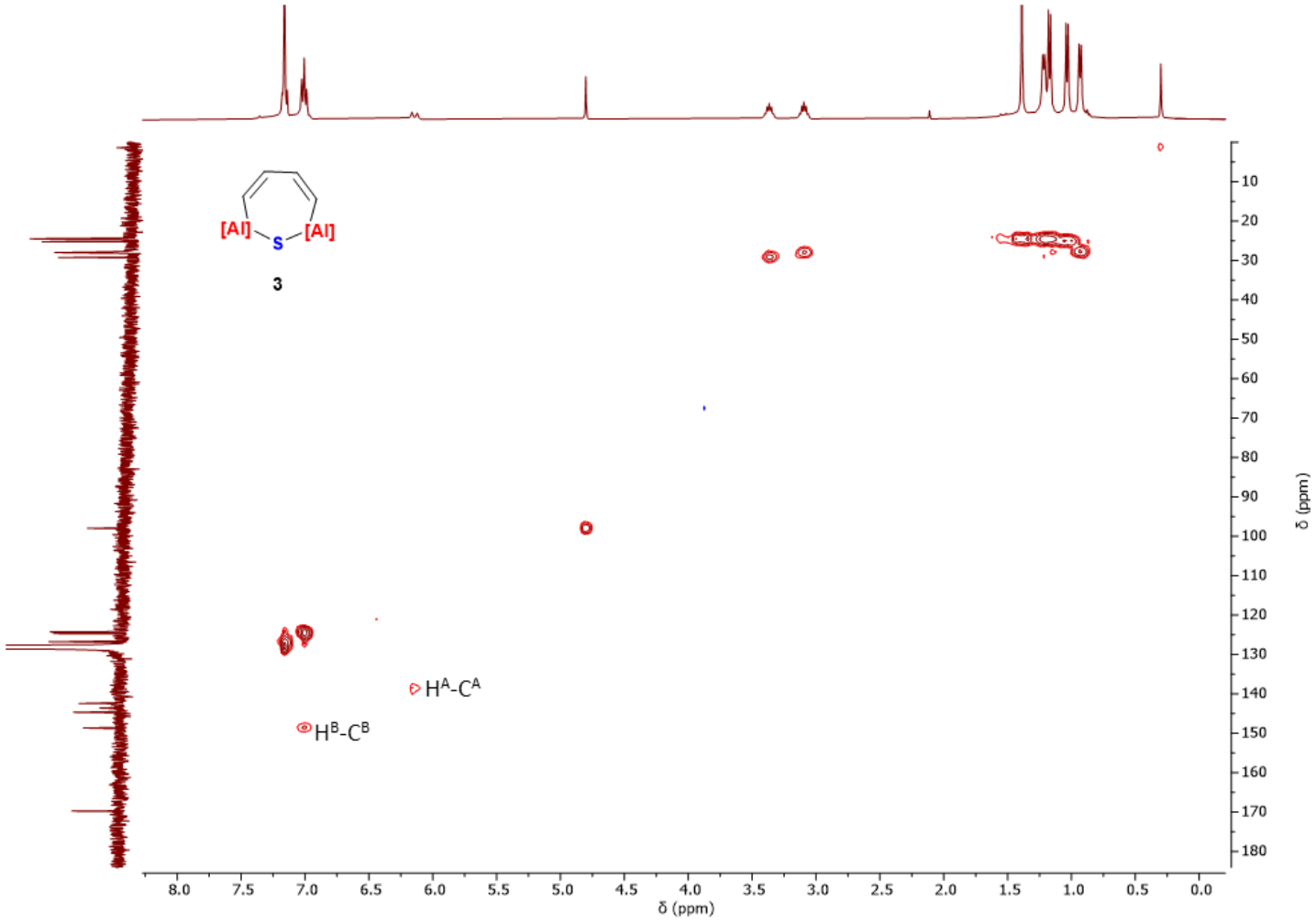


Figure S4: ^{1}H-^{13}C HSQC NMR spectrum of **3**

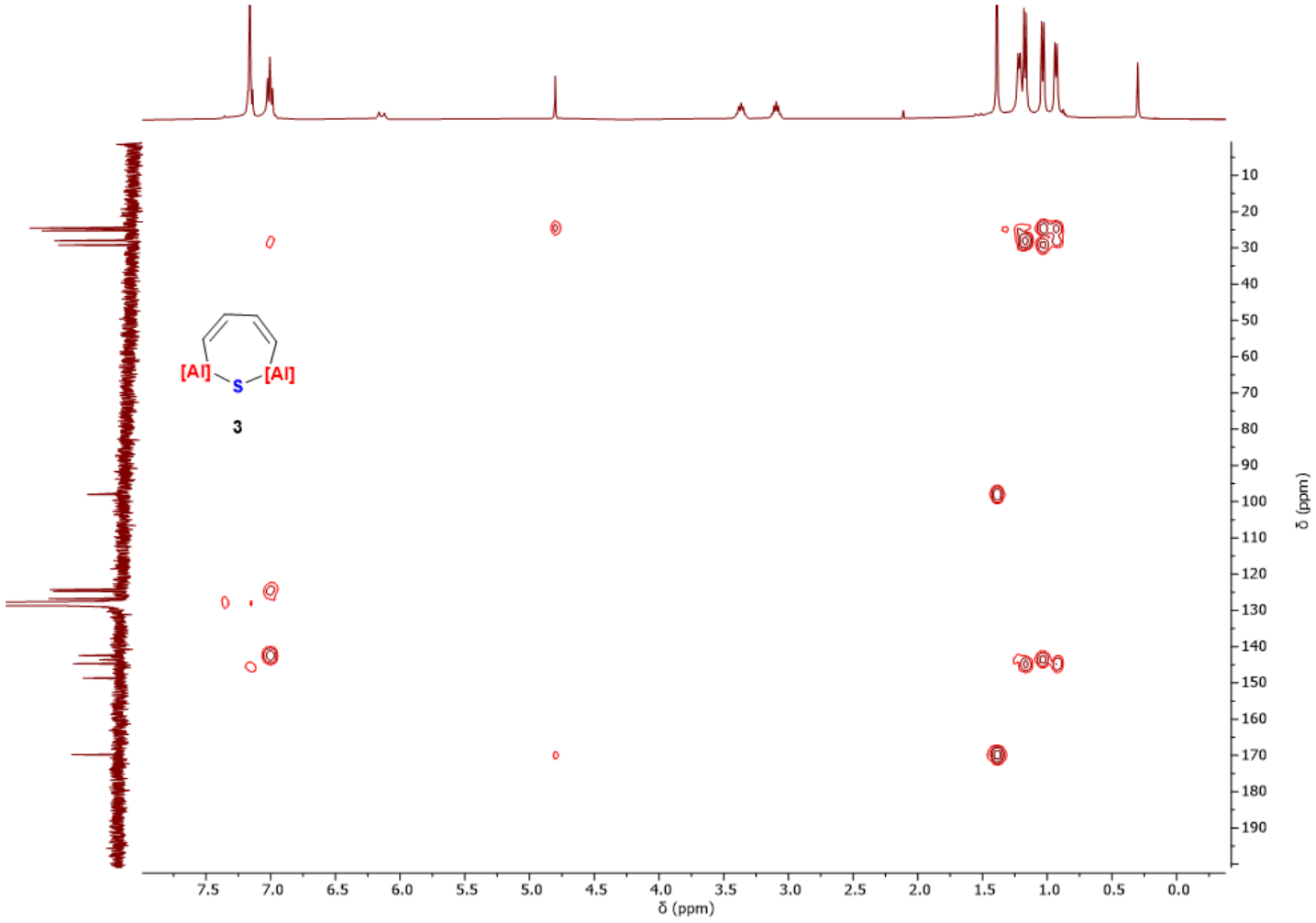


Figure S4: ^{1}H-^{13}C HMBC NMR spectrum of **3**

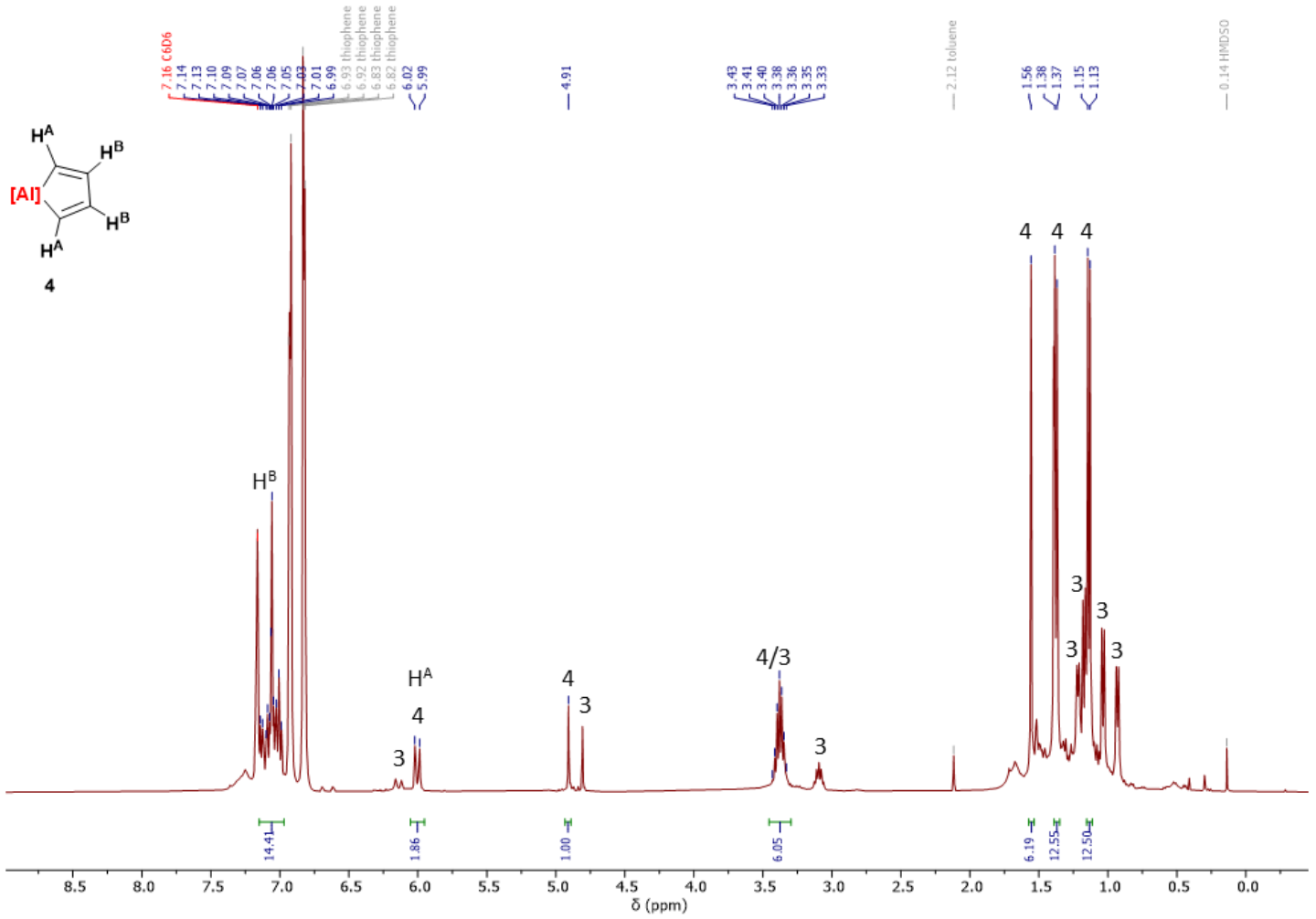


Figure S5: ^{1}H NMR spectrum (400 MHz, C_6D_6) of **4**. Crude mixture at the end of the reaction between **1** and thiophene that also contains **3**.

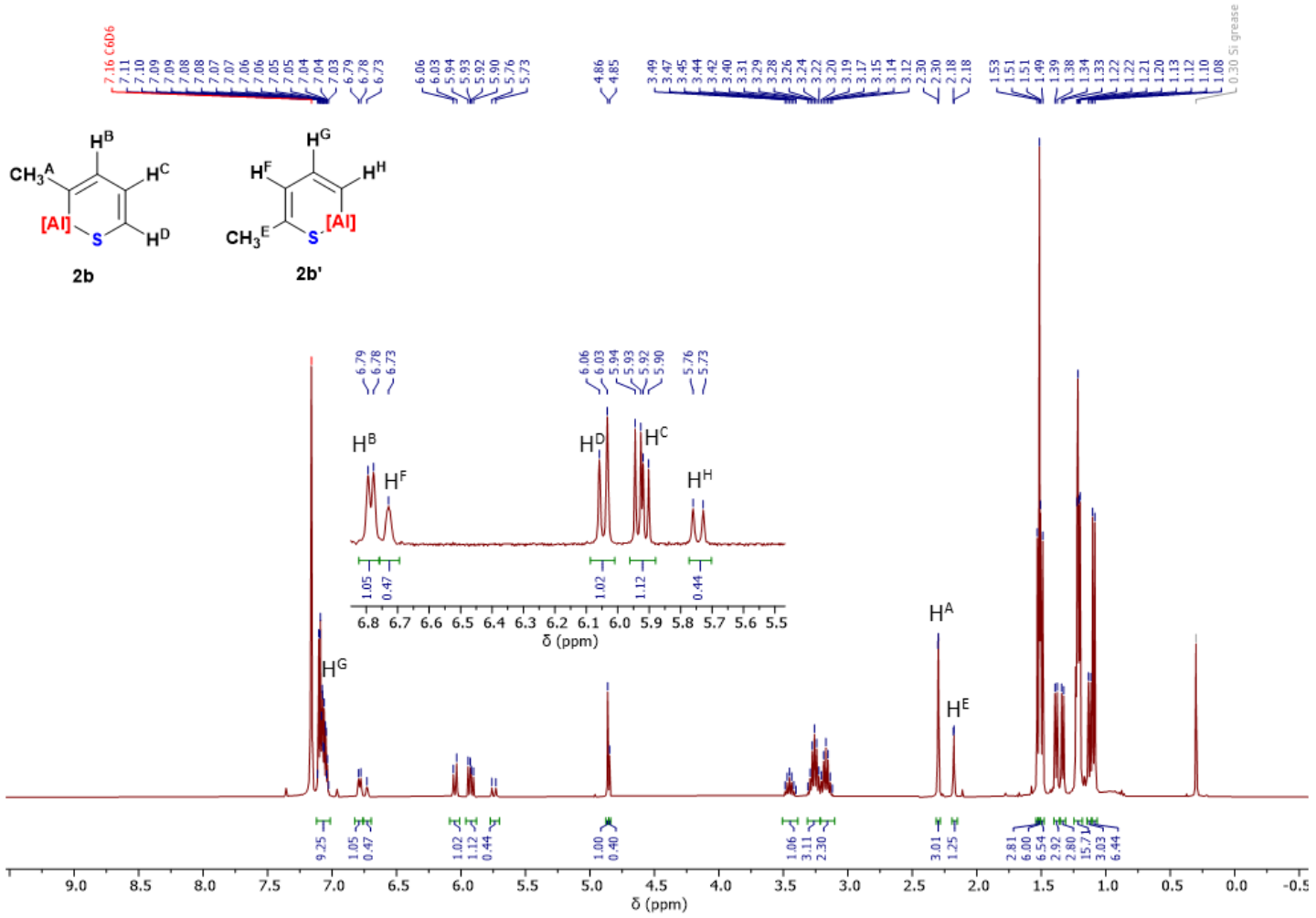


Figure S6: ^{1}H NMR spectrum (400 MHz, C_6D_6) of **2b** and **2b'**

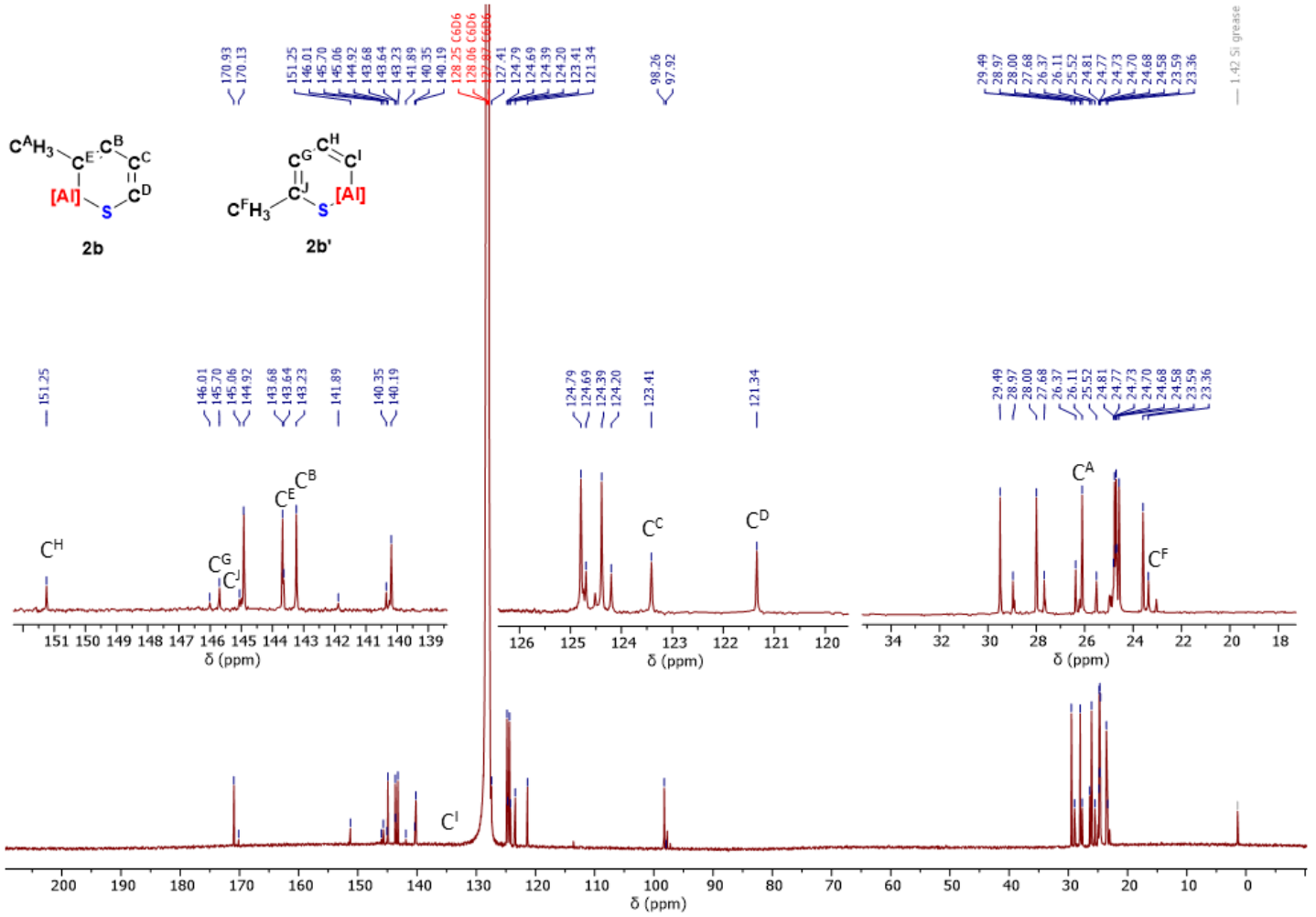


Figure S7: ^{13}C NMR spectrum (125.7 MHz, C_6D_6) of **2b** and **2b'**

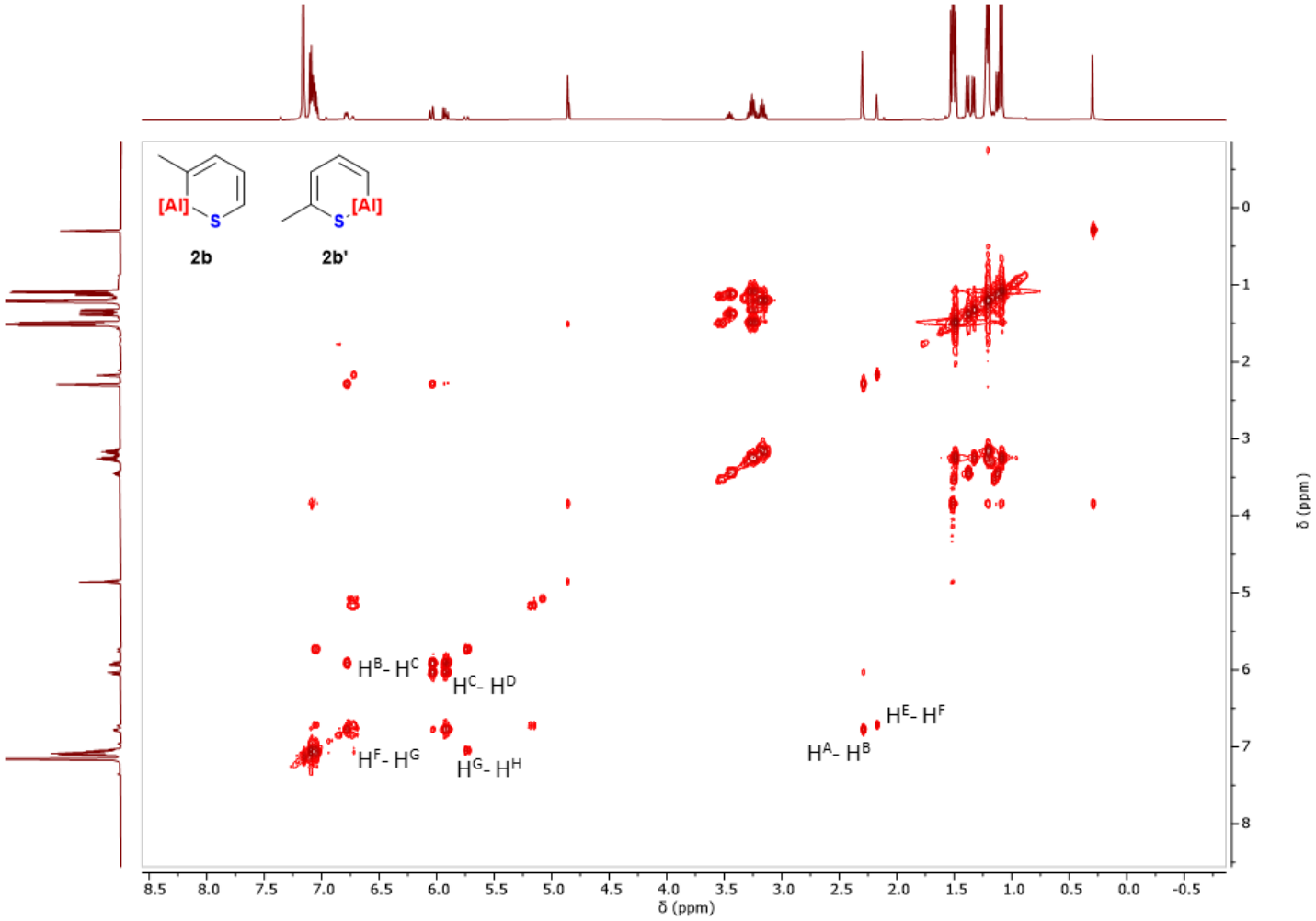


Figure S8: ^{1}H-^{1}H COSY NMR spectrum of **2b** and **2b'**

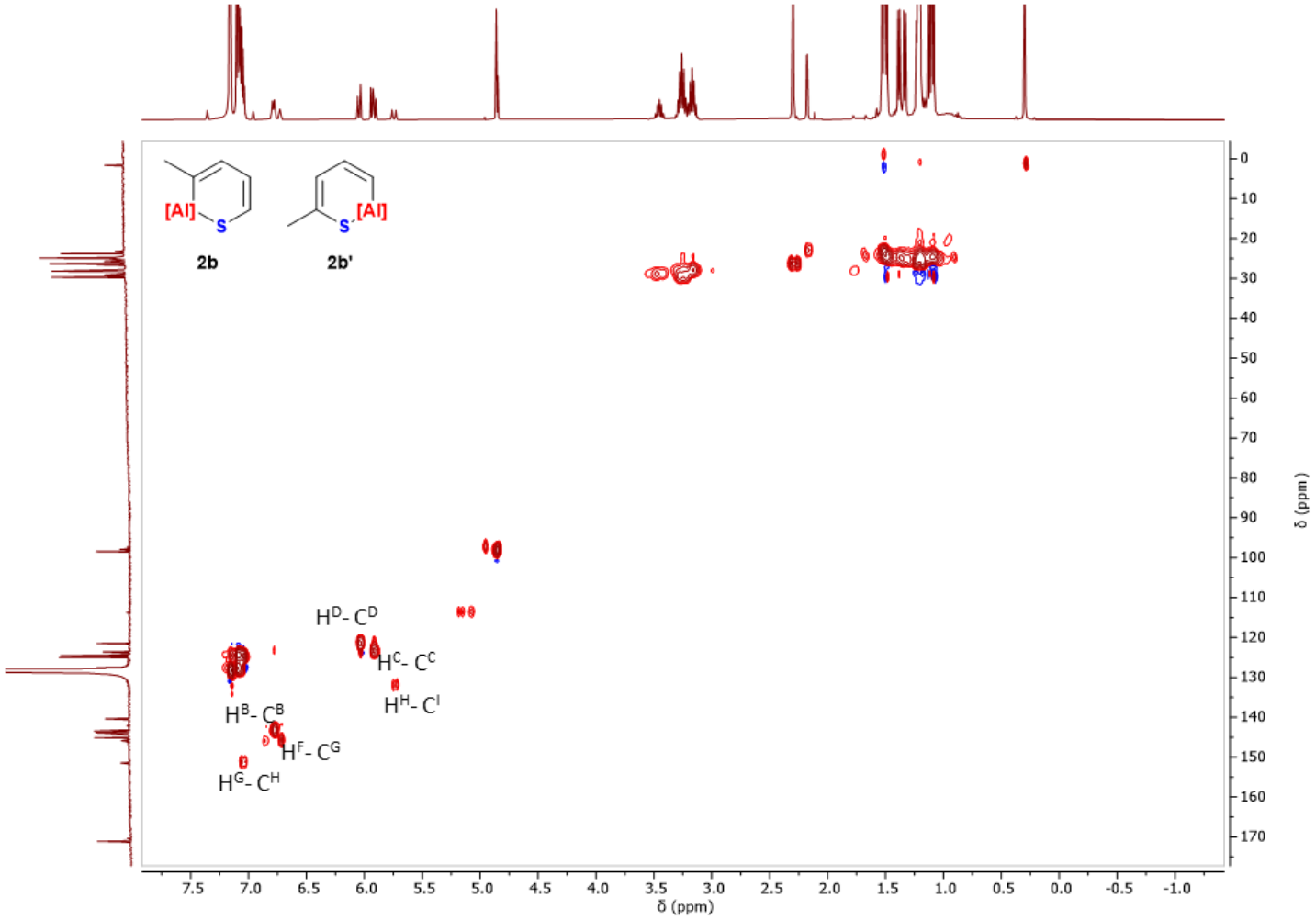


Figure S9: ^{1}H-^{13}C HSQC NMR spectrum of **2b** and **2b'**

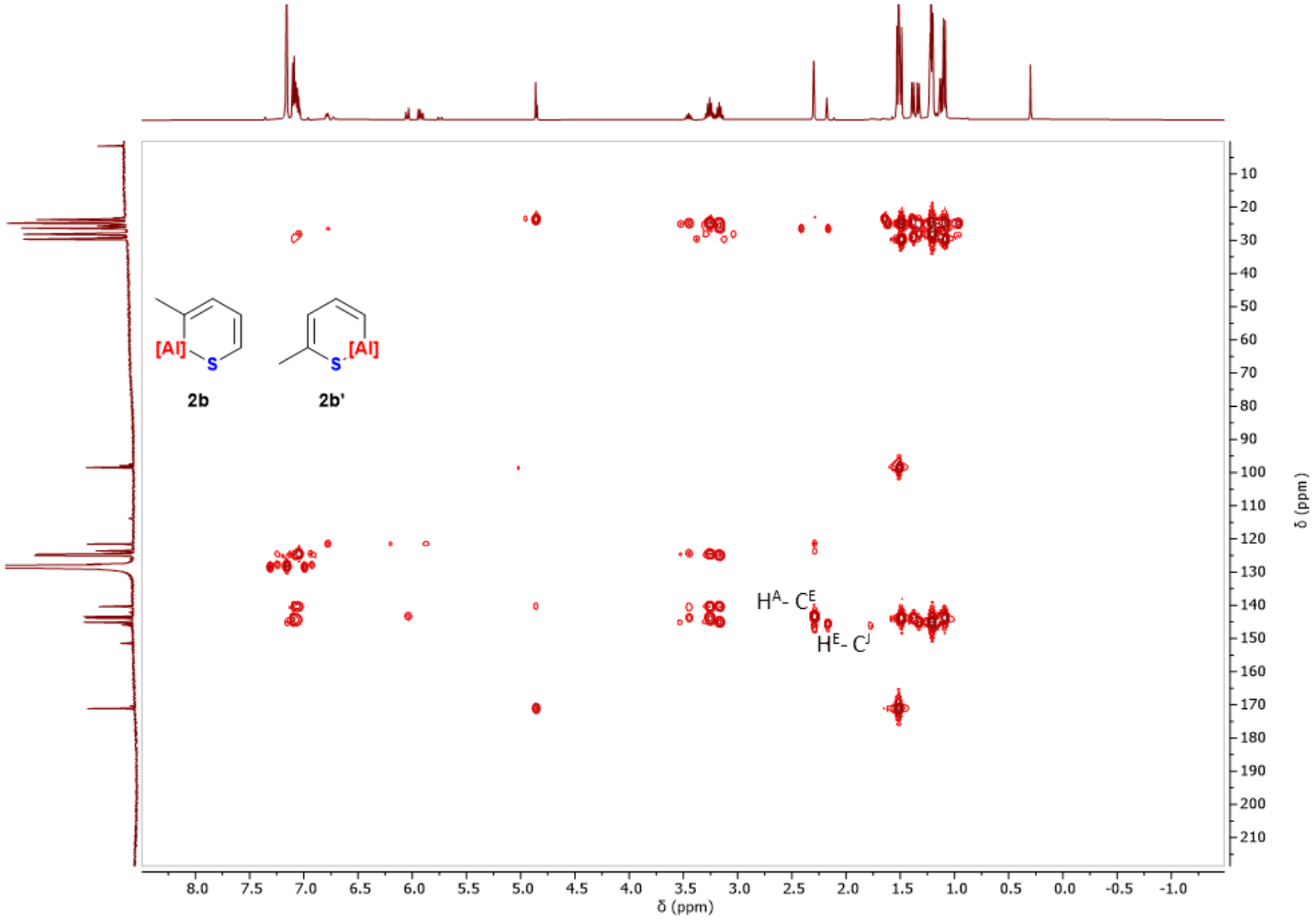


Figure S10: ^{1}H-^{13}C HMBC NMR spectrum of **2b** and **2b'**

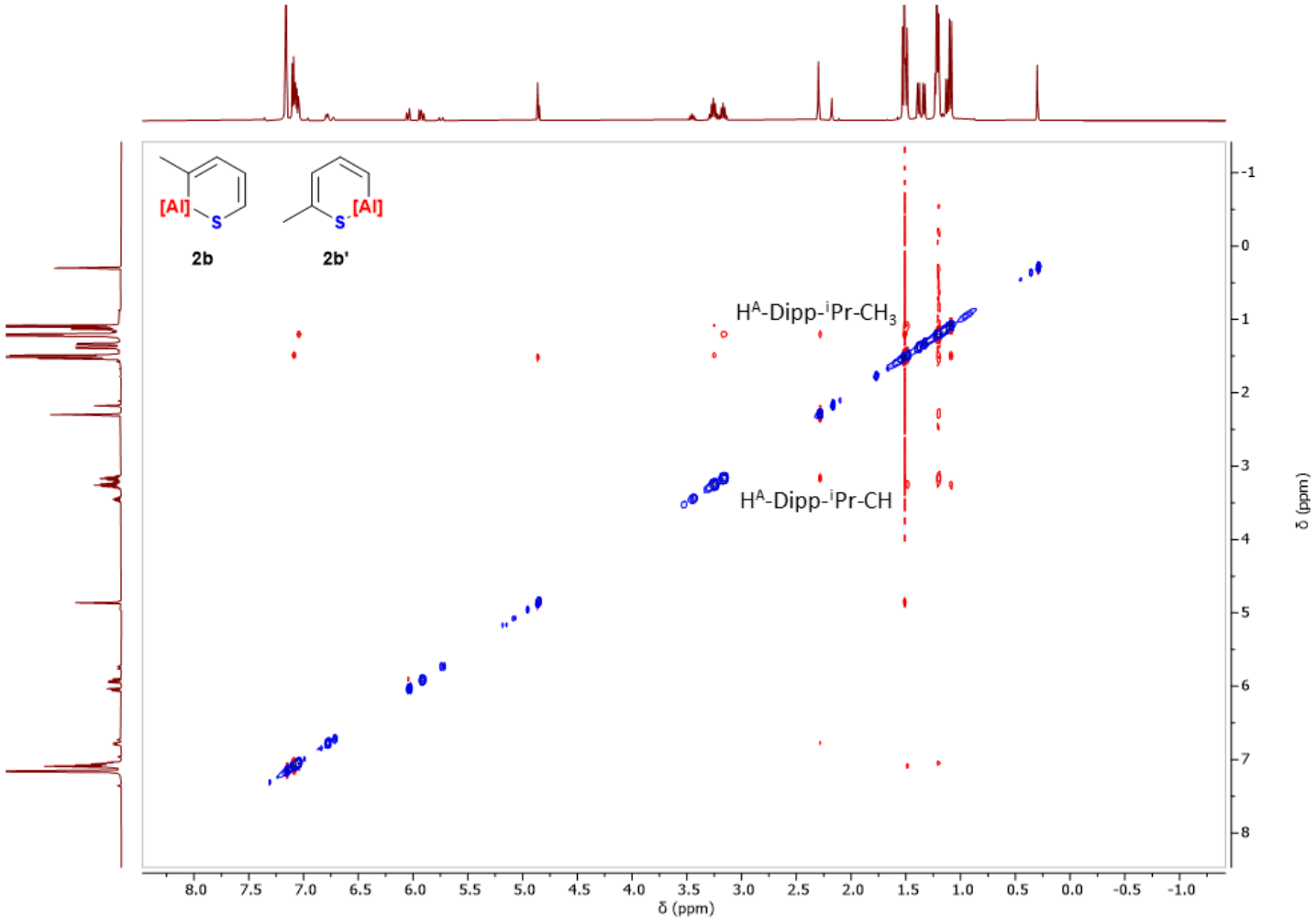


Figure S11: ^{1}H-^{1}H NOESY NMR spectrum of **2b** and **2b'**

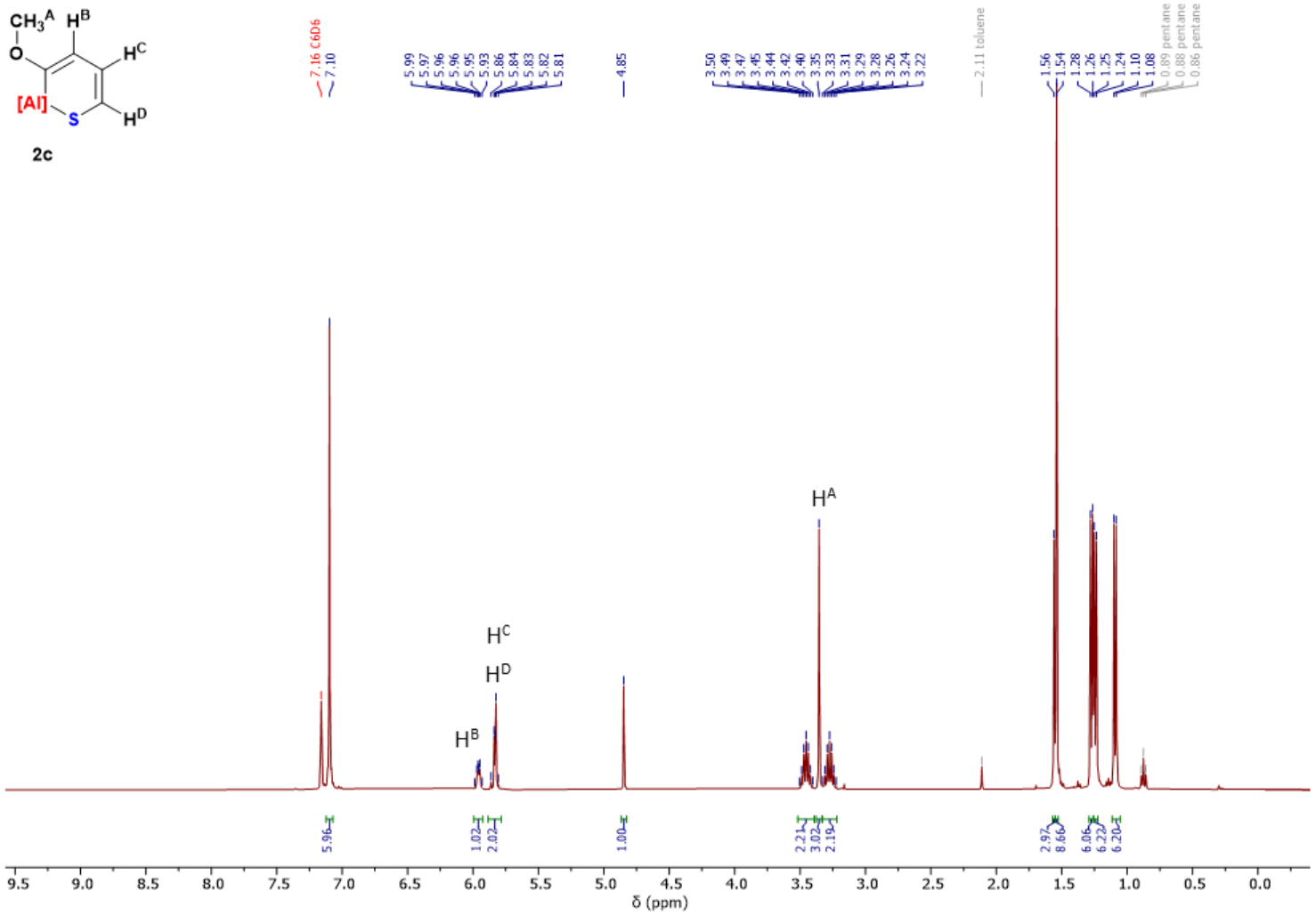


Figure S12: ^{1}H NMR spectrum (400 MHz, C_6D_6) of **2c**

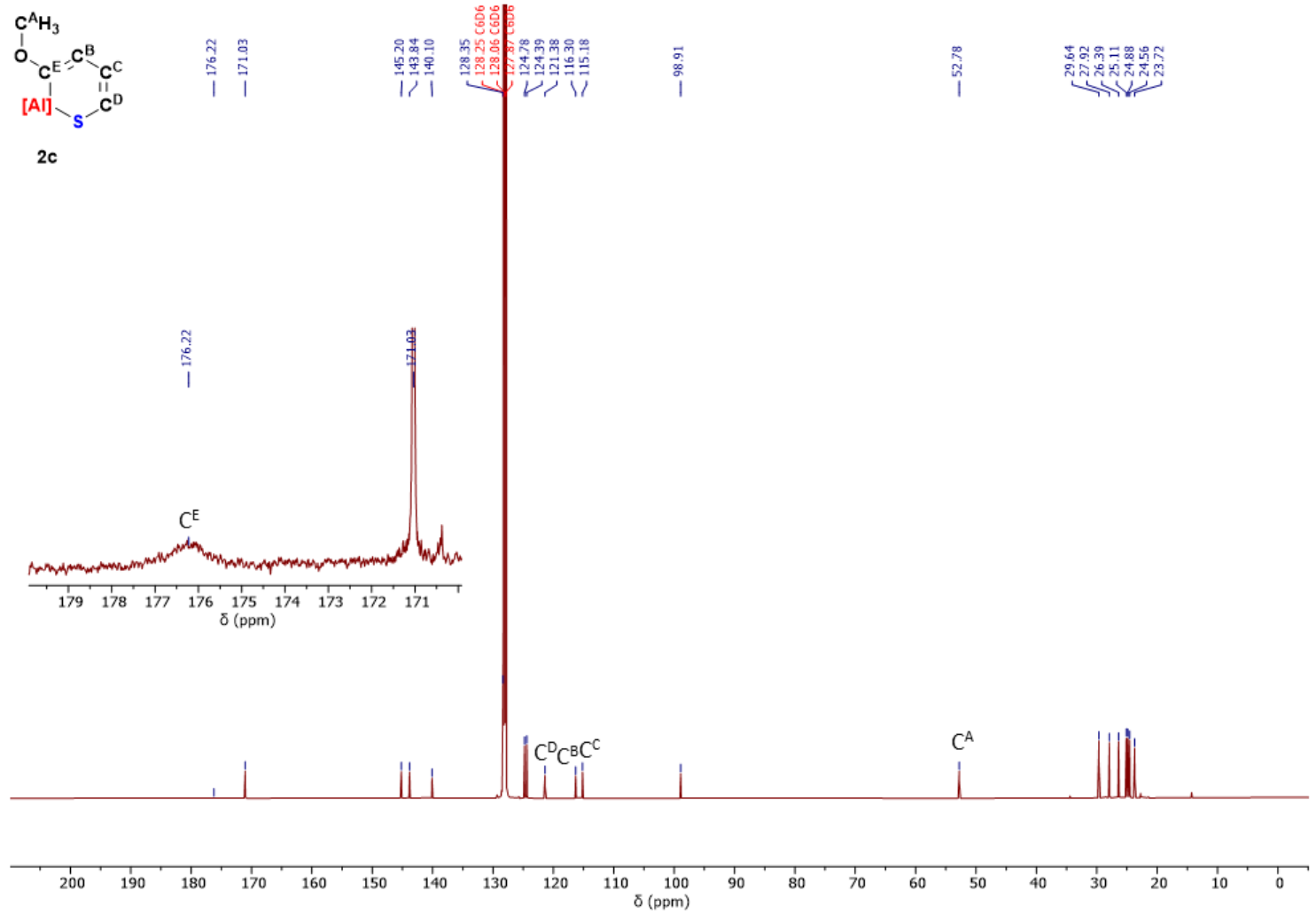


Figure S13: ^{13}C NMR spectrum (125.7 MHz, C_6D_6) of **2c**

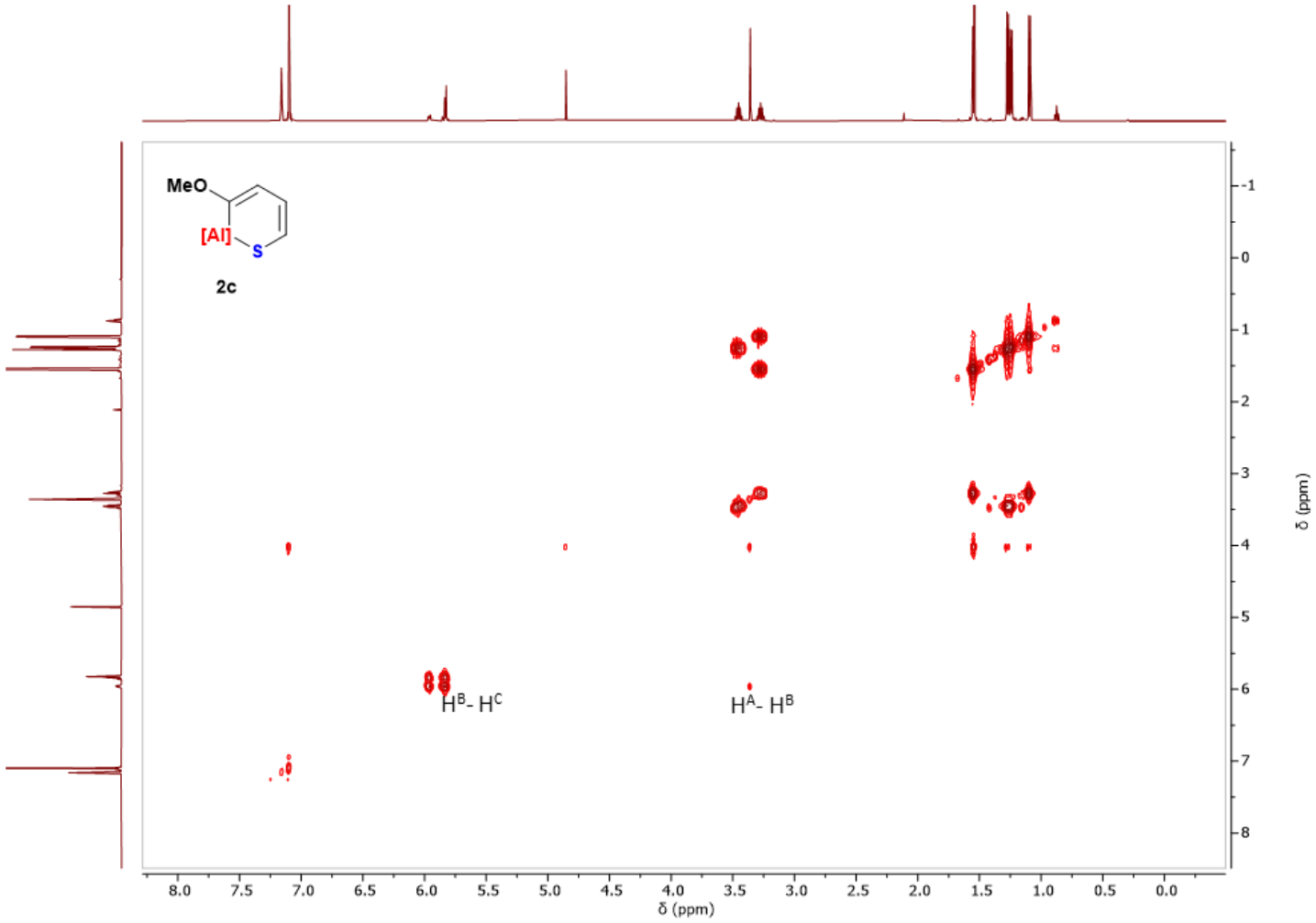


Figure S14: ^{1}H-^{1}H COSY NMR spectrum of **2c**

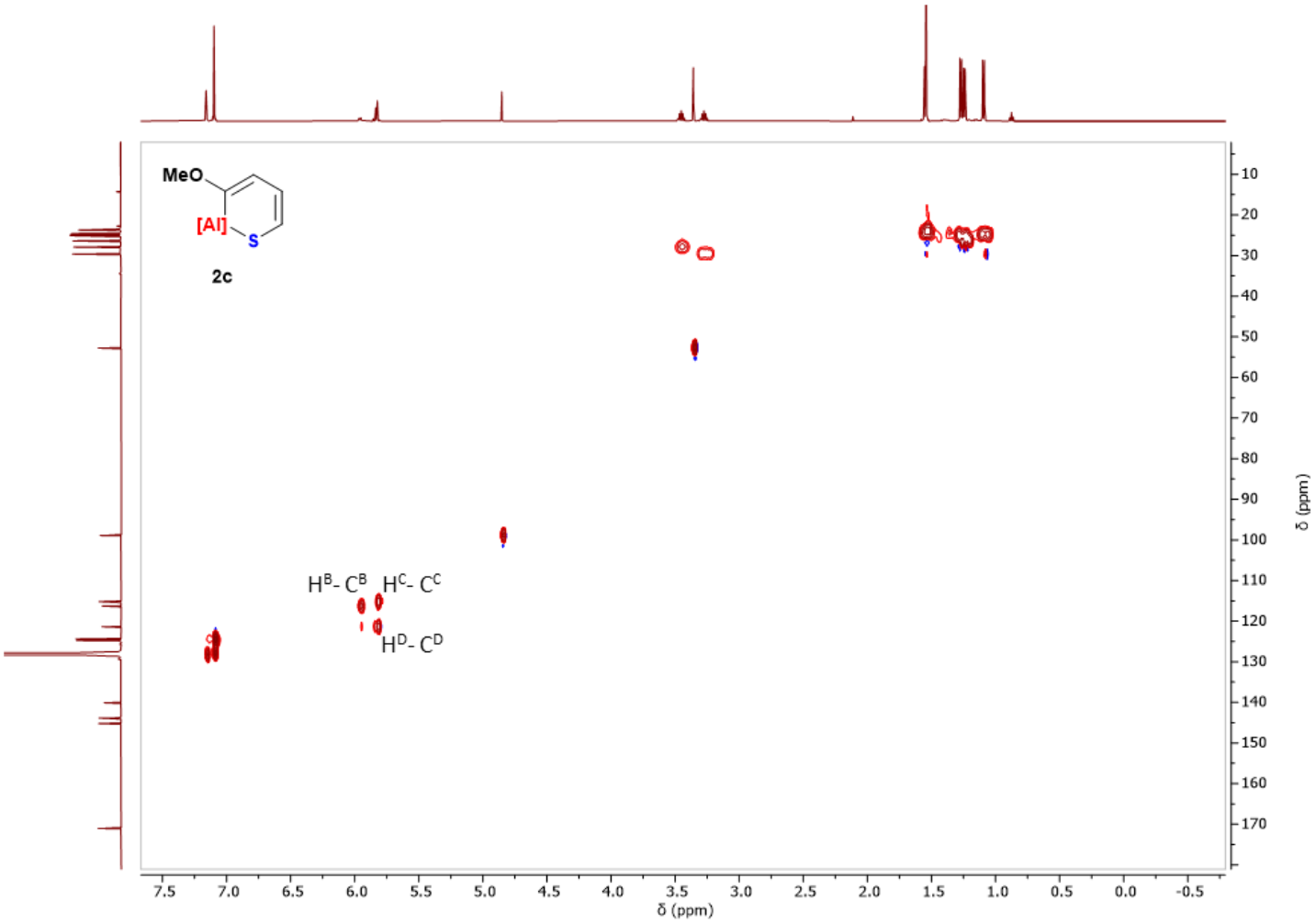


Figure S15: ^{1}H-^{13}C HSQC NMR spectrum of **2c**

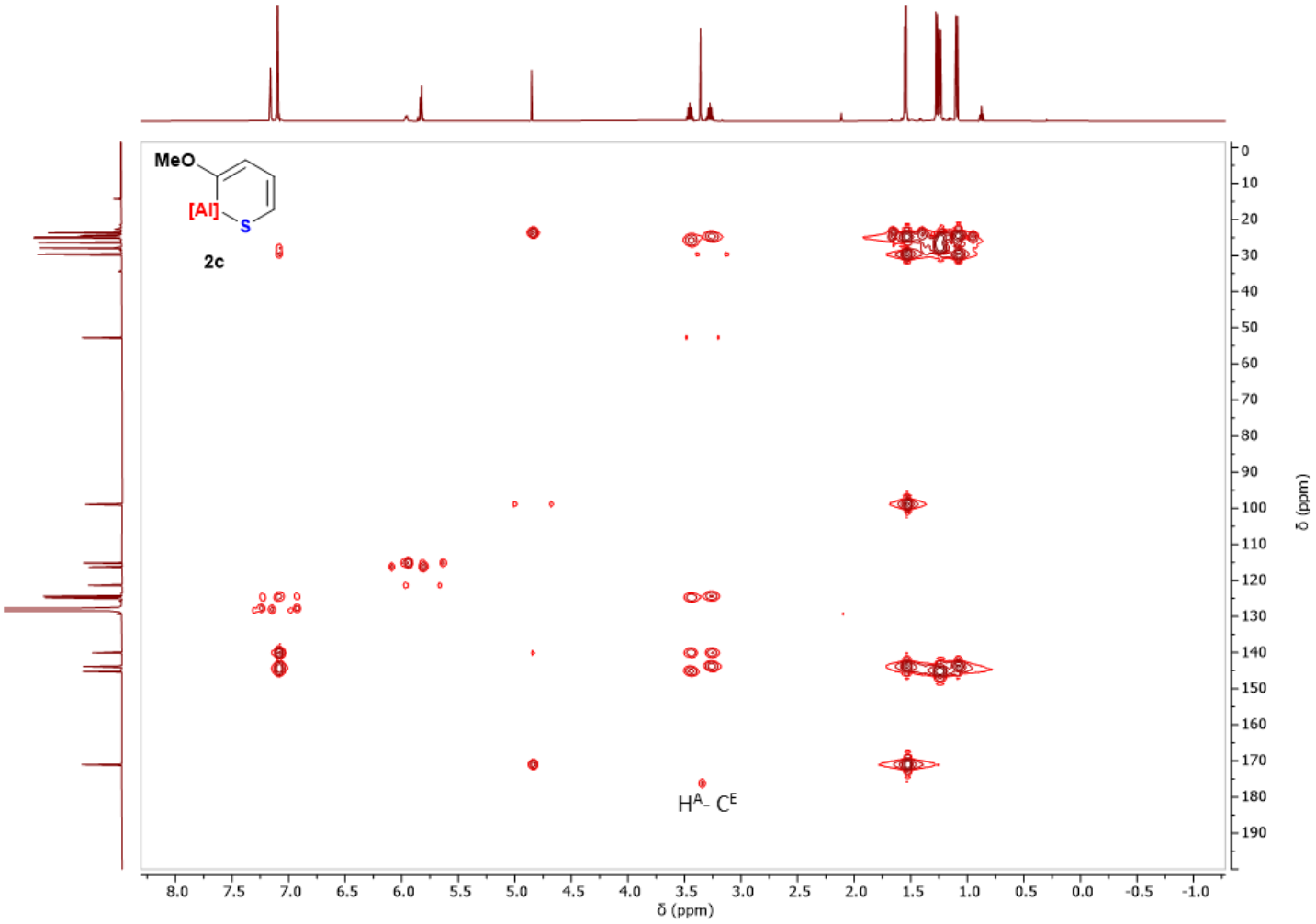


Figure S16: ^{1}H-^{13}C HMBC NMR spectrum of **2c**

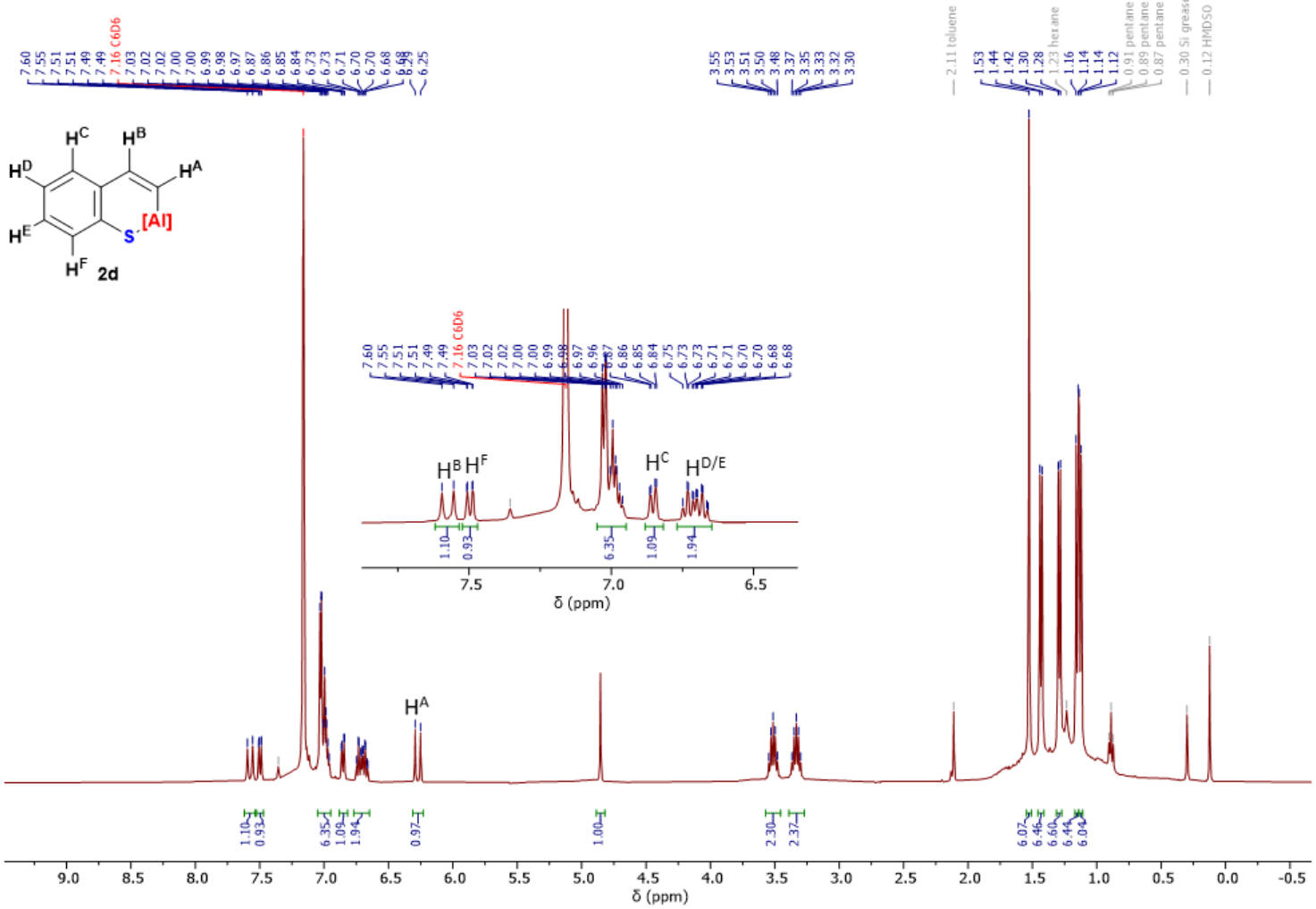


Figure S17: ^{1}H NMR spectrum (400 MHz, C_6D_6) of **2d**

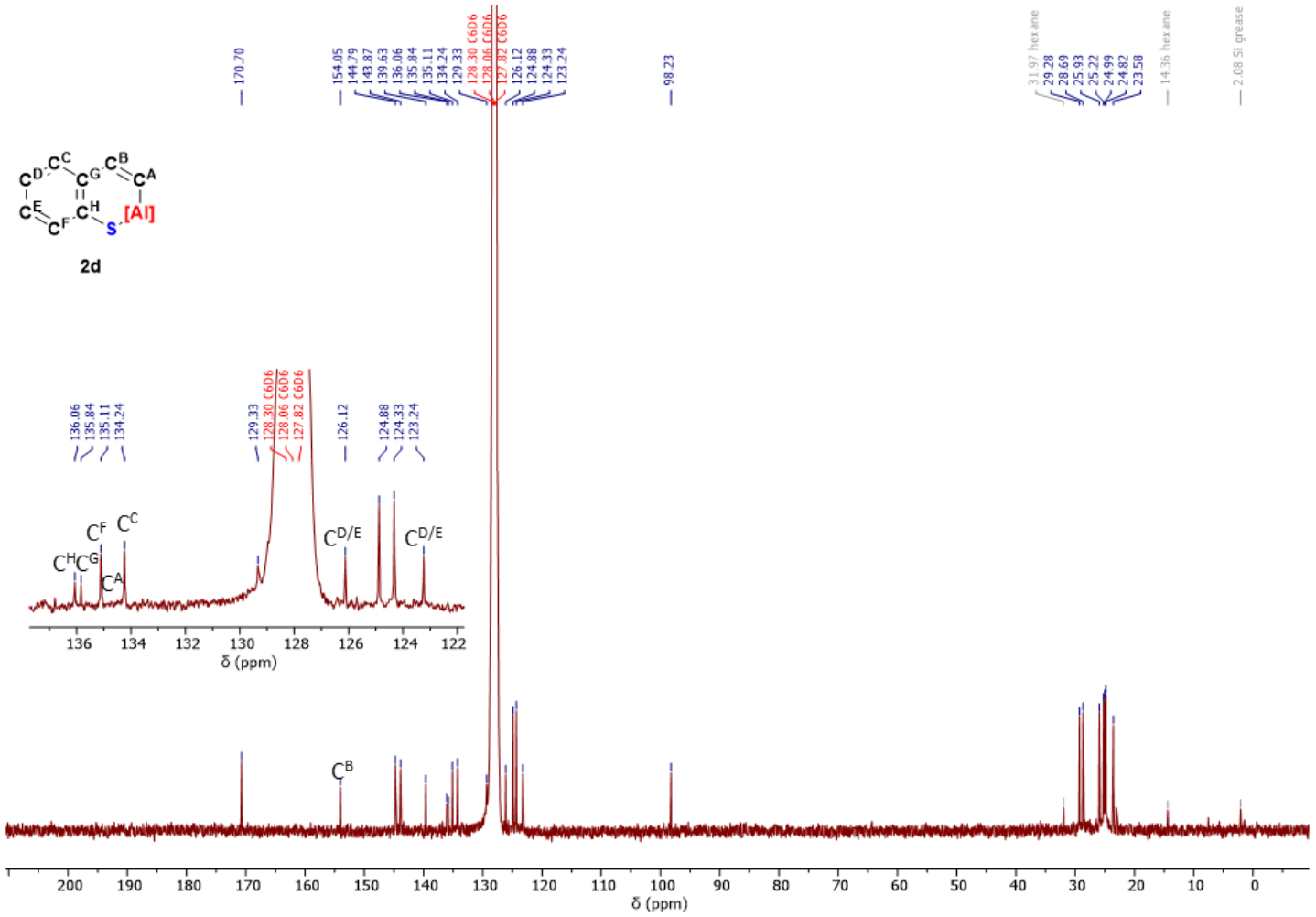


Figure S18: ^{13}C NMR spectrum (100.6 MHz, C_6D_6) of **2d**

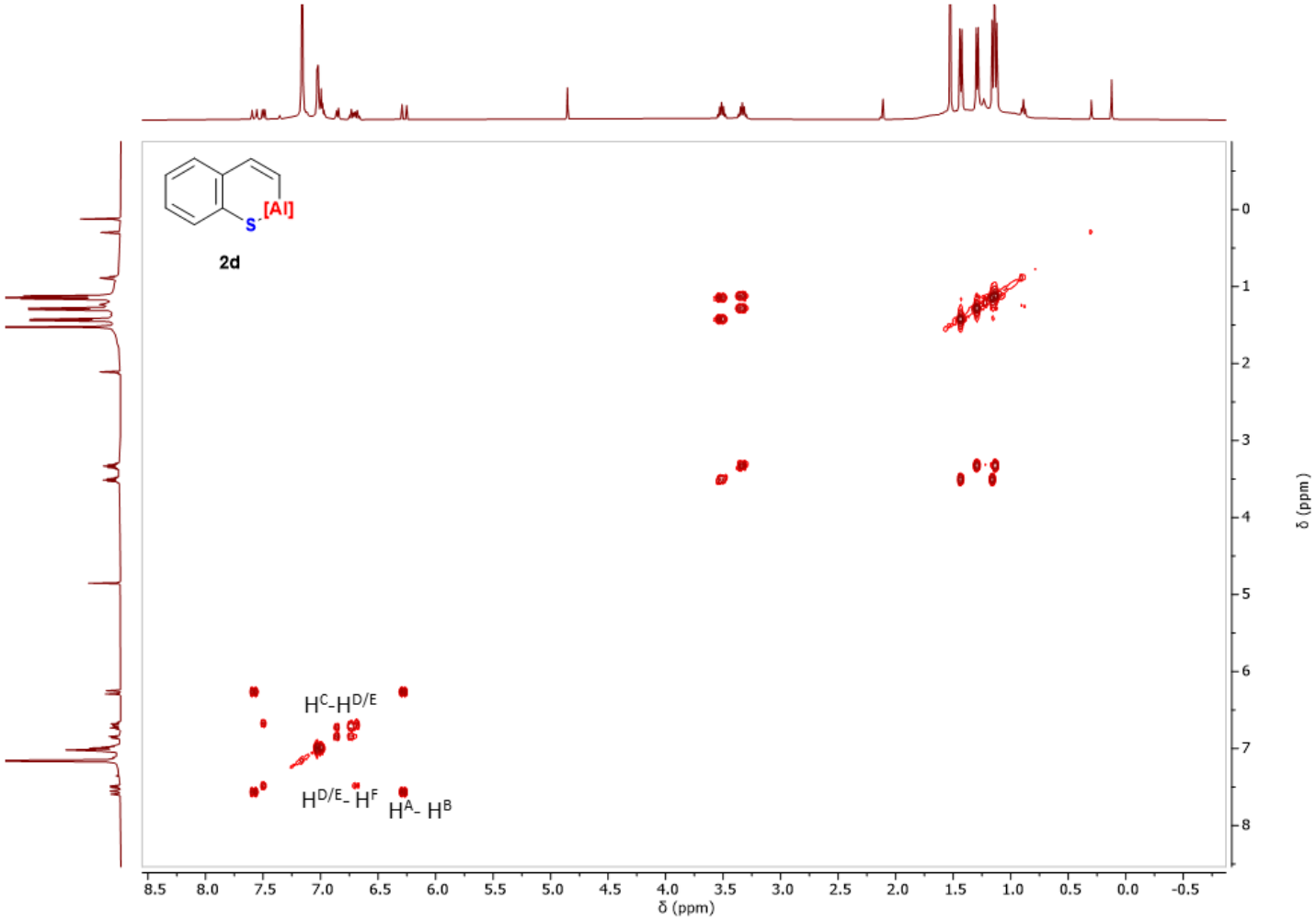


Figure S19: ^{1}H-^{1}H COSY NMR spectrum of **2d**

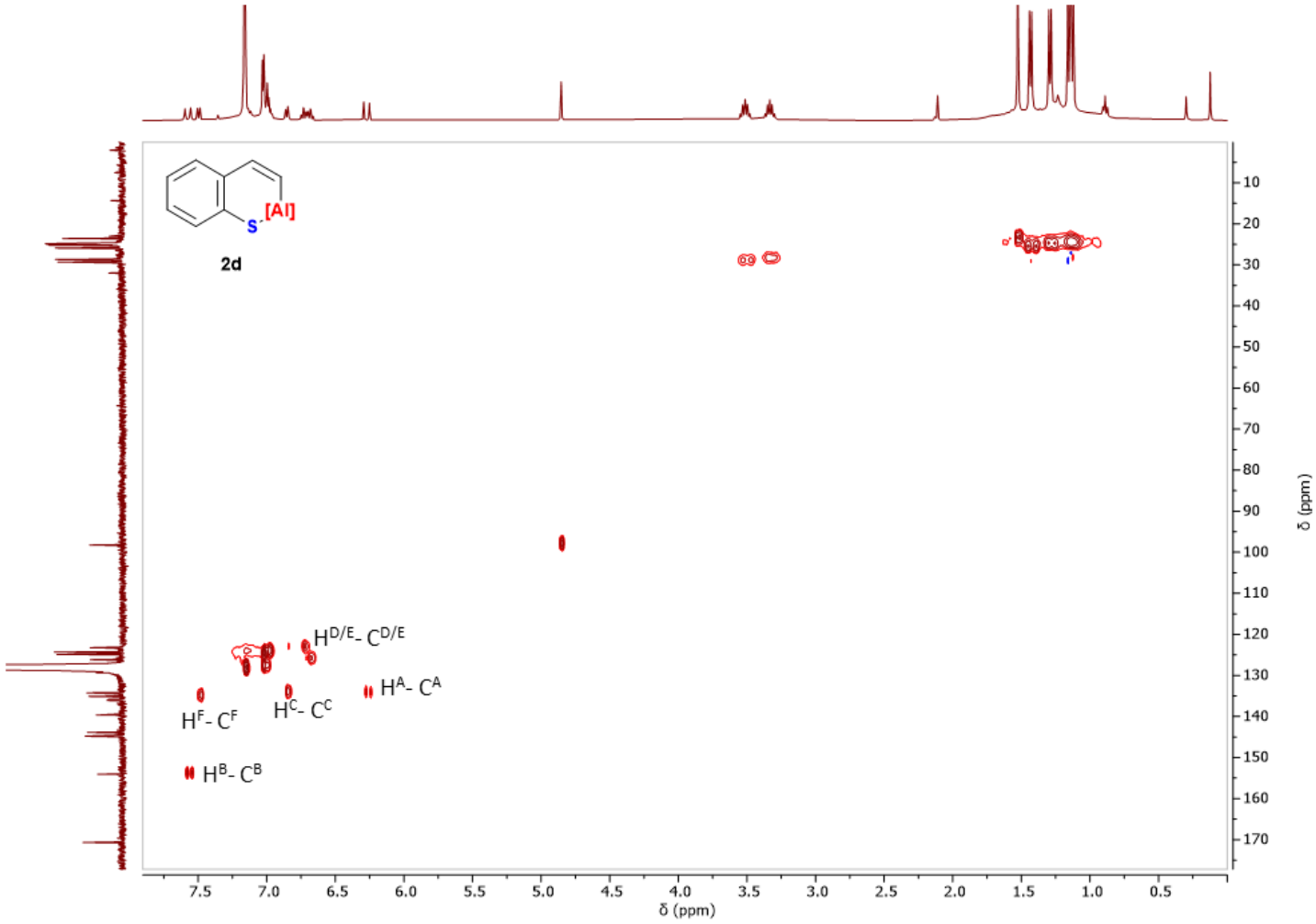


Figure S20: ^{1}H-^{13}C HSQC NMR spectrum of **2d**

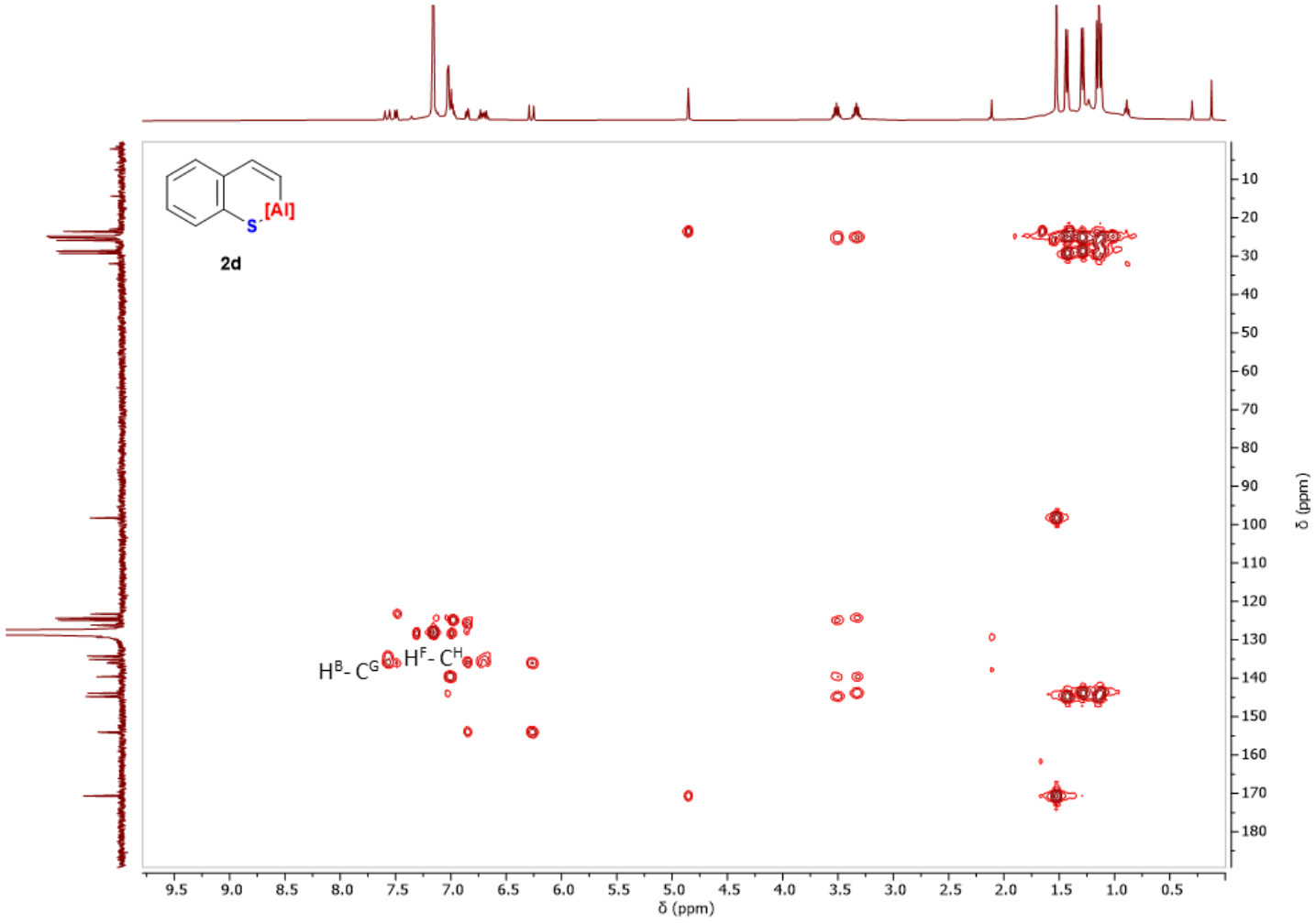


Figure S20: ^{1}H-^{13}C HMBC NMR spectrum of **2d**

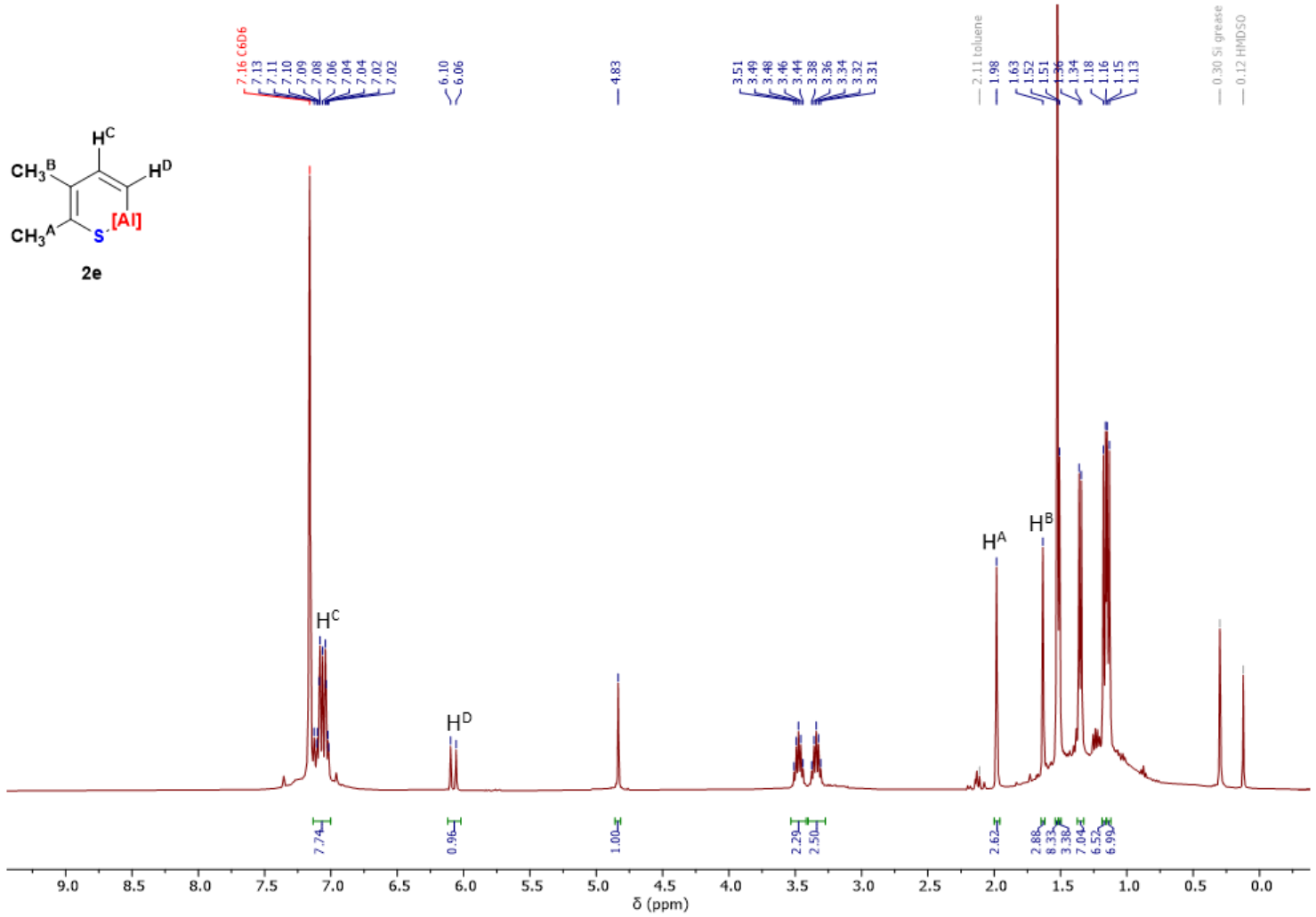


Figure S21: ^{1}H NMR spectrum (400 MHz, C_6D_6) of **2e**

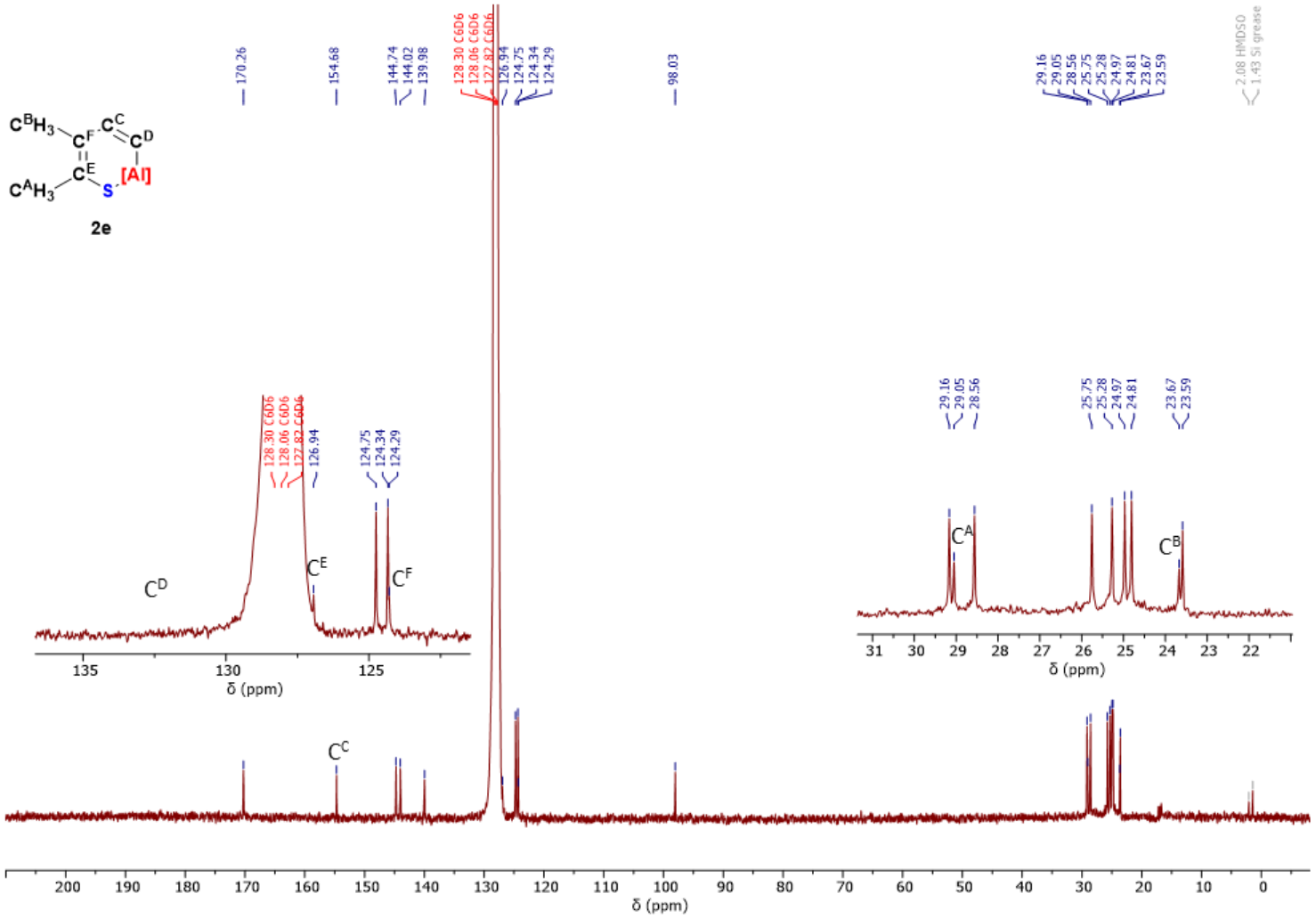


Figure S22: ^{13}C NMR spectrum (100.6 MHz, C_6D_6) of **2e**

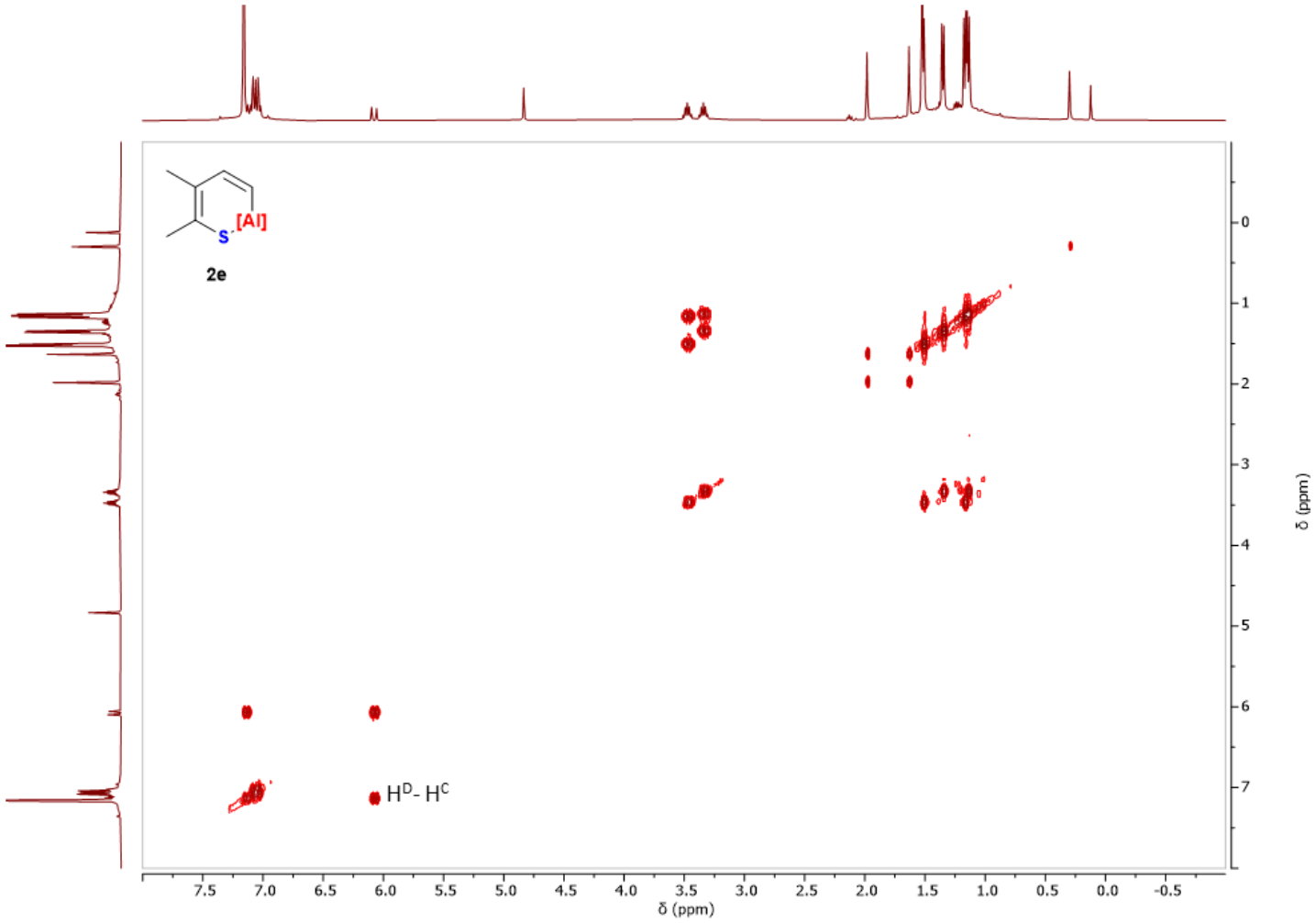


Figure S23: ^{1}H-^{1}H COSY NMR spectrum of **2e**

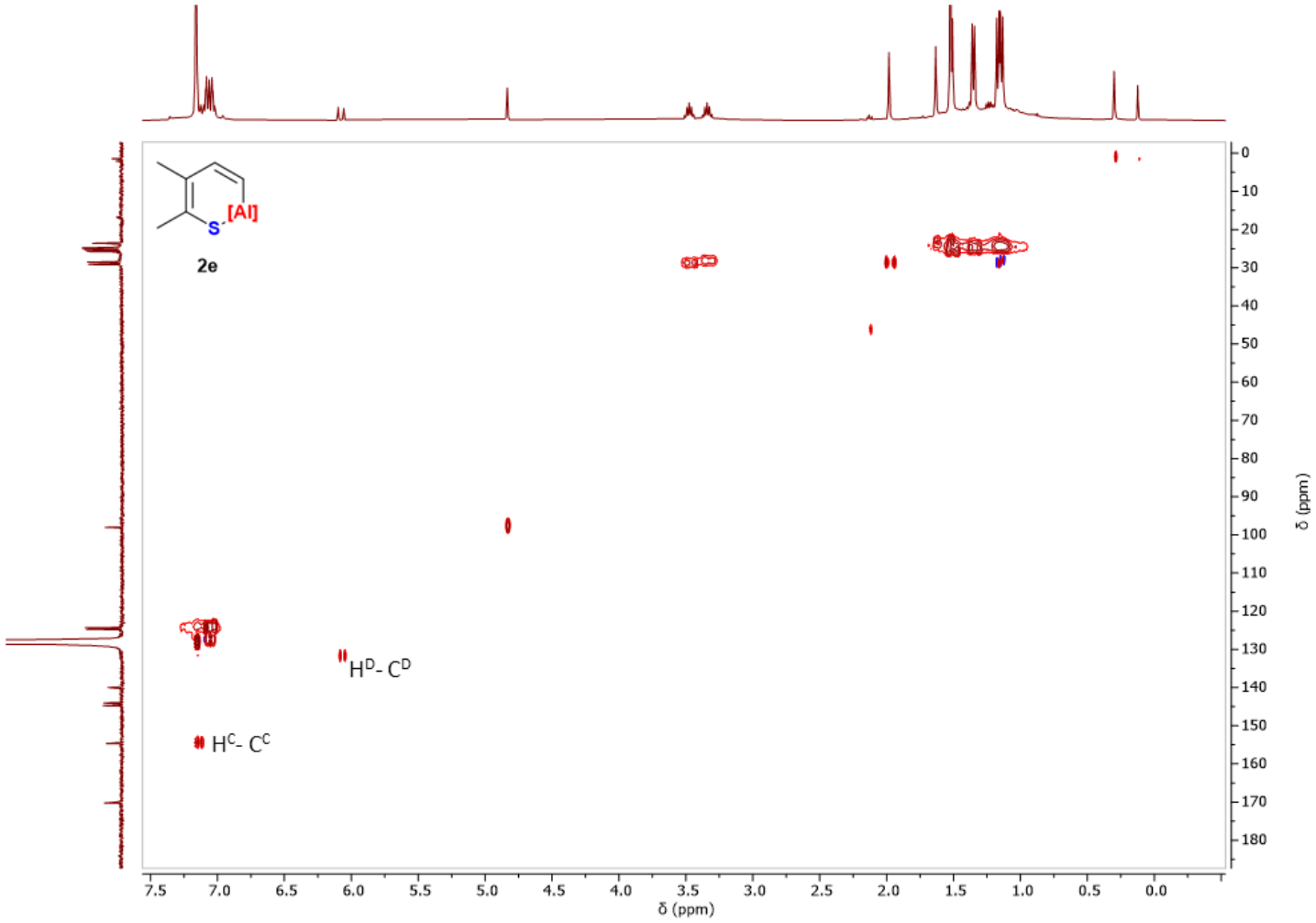


Figure S24: ^{1}H-^{13}C HSQC NMR spectrum of **2e**

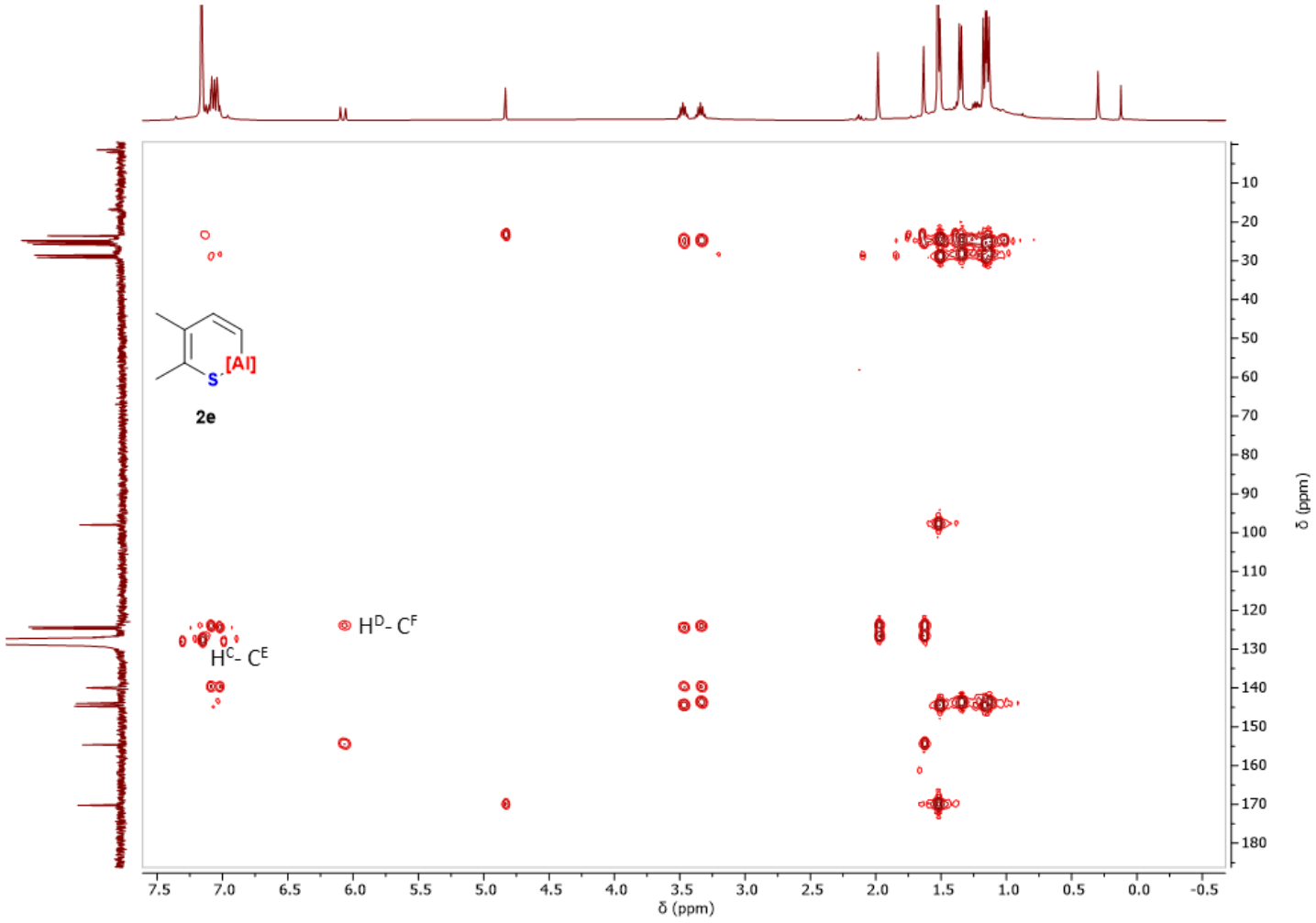


Figure S25: ^{1}H-^{13}C HMBC NMR spectrum of **2e**

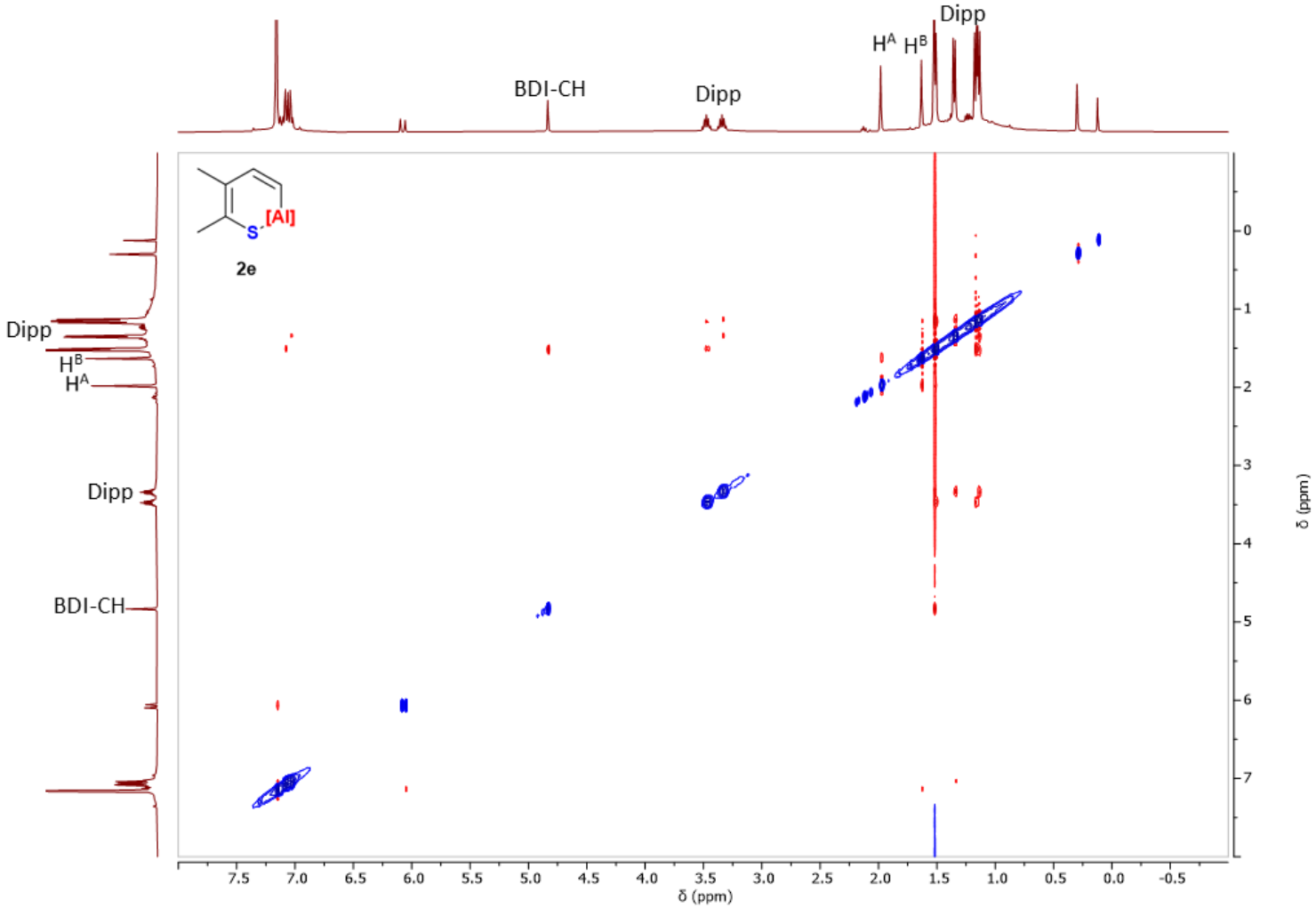


Figure S26: ^{1}H-^{1}H NOESY NMR spectrum of **2e.** The lack of through-space correlations between the H^{A}/H^{B} resonances and the Dipp/BDI-CH resonances indicates **1** inserts into the less sterically hindered C–S bond to give **2e**.

4. X-ray Data

Table S1 provides a summary of the crystallographic data for structures **3**, **2b**, **2c** and **2d**. Data was collected using an Agilent Xcalibur PX Ultra A diffractometer, and the structures were solved and refined using the OLEX2[2], SHELXTL[3] and SHELX-2013[4], program systems. The absolute structure of **3** was determined by use of the Flack parameter [x^+ = –0.05(3)]. CDCC 2293034 t0 2293036 and 2294820.

Table S1. Crystal Data, Data Collection and Refinement Parameters for the structures of **3**, **2b**, **2c** and **2d**.

Data	3	2b	2c	2d
Formula	$C_{62}H_{86}Al_2N_4S$	$C_{34}H_{47}AlN_2S$	$C_{34}H_{47}AlN_2OS$	$C_{37}H_{47}AlN_2S$
Solvent	-	C_7H_8	0.3 C_5H_{12}	C_7H_8
Formula Weight	937.36	634.91	580.42	670.94
Colour, habit	Colourless needles	Colourless blocks	Yellowish blocks	Colourless needles
Temperature / K	173	173	173	173
Crystal system	Orthorhombic	Triclinic	Monoclinic	Orthorhombic
Space group	*Pca*2$_1$ (no. 29)	*P*–1 (no. 2)	*I*2/*a*	*Pbcm*
***a* / Å**	23.1152(5)	10.4074(4)	27.9297(10)	10.5463(4)
***b* / Å**	13.6692(3)	10.9429(4)	12.4390(4)	22.1504(10)
***c* / Å**	18.0823(4)	17.0594(6)	41.634(2)	17.064(2)
α / deg	90	104.737(3)	90	90
β / deg	90	90.087(3)	104.717(5)	90
γ / deg	90	97.200(3)	90	90
***V* / Å^3**	5713.4(2)	1862.99(12)	13989.8(10)	3986.1(6)
Z	4	2	16	4[f]
***D*$_c$ / g cm^{-3}**	1.132	1.132	1.102	1.118
Radiation used	Cu-Kα	Cu-Kα	Cu-Kα	Cu-Kα
μ / mm^{-1}	1.101	1.209	1.265	1.157
No. of unique reflns				
Measured (*R*$_{int}$)	7346 (0.0575)	7418 (0.0513)	13527 (0.0368)	4049 (0.0564)
Obs, $\|F_o\| > 4\sigma(\|F_o\|)$	5561	5452	9881	2400
Completeness (%)[g]	98.5	100	98.6	99.4
No. of variables	643	418	725	240
***R*$_1$(obs), *wR*$_2$(all)**[h]	0.0522, 0.0963	0.0650, 0.1728	0.0513, 0.1407	0.0963, 0.3128
CDCC code	2293036	2293034	2294820	2293035

[f] The complex has crystallographic C_s symmetry

[g] Completeness to 0.84 Å resolution.

[h] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$

The X-ray Structure of 3

Compound **3** was found to crystallise in a polar space group, and the correct absolute structure was unambiguously determined by use of the Flack parameter [x^+ = –0.05(3)].

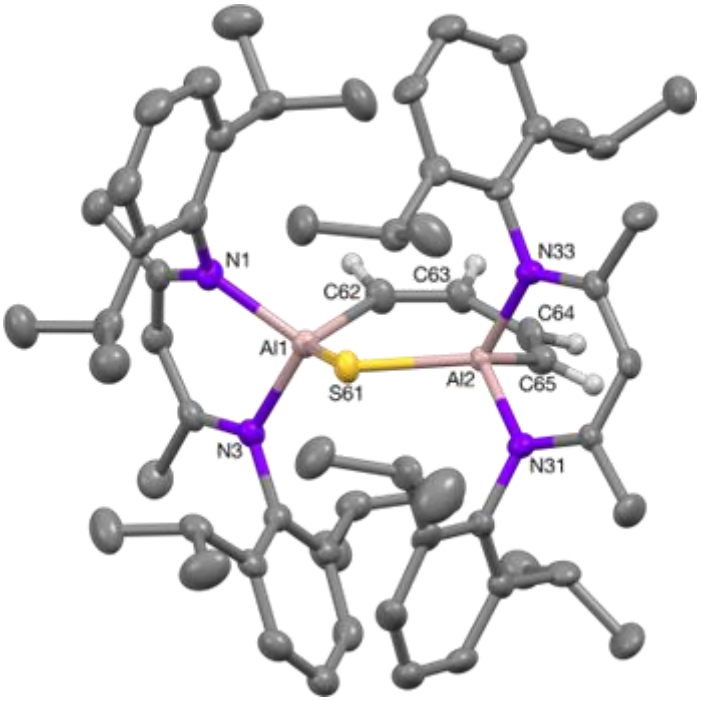


Figure S12: The crystal Structure of **3** (50% probability ellipsoids)

The X-ray Structure of 2b

Inspection of the residual electron density of the structure of 2b reveals the presence of a low occupancy (ca. 14%) secondary component present in addition to the major structure. Though models that give reasonable fits for this electronic density can be constructed, none of them are consistent with either the reactions to get to this point or the other characterisation techniques we have employed. The best approach to this uncertainty would seem to be to just model the major component as the species we know is present (and have characterised through other means), and not include any model of the uncertain secondary component.

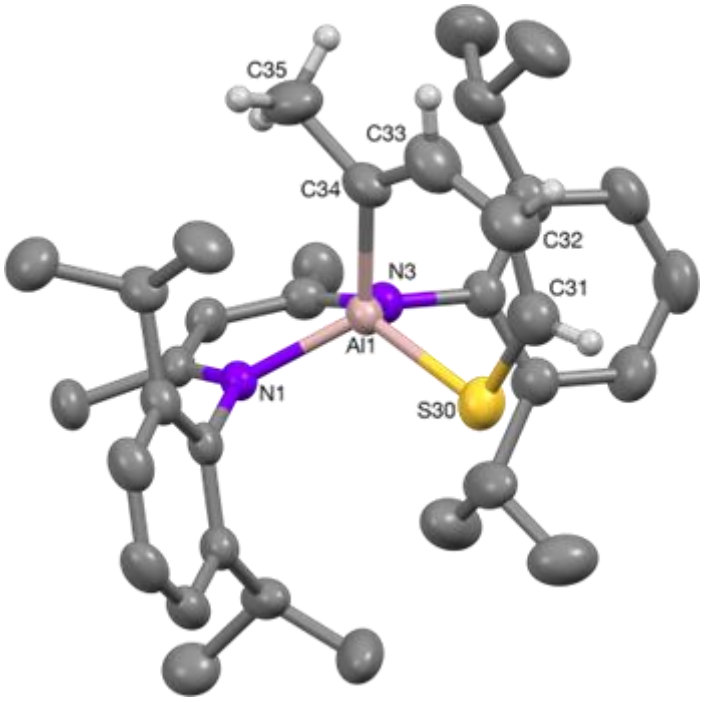


Figure S13: The crystal Structure of **2b** (50% probability ellipsoids)

The X-ray crystal structure of 2c

The asymmetric unit was found to contain what appeared to be disordered pentane solvent that could not be satisfactorily modelled. The solvent was removed using OLEX2's BYPASS function. 27 electrons per asymmetric unit were removed corresponding to 0.6 pentane molecules.

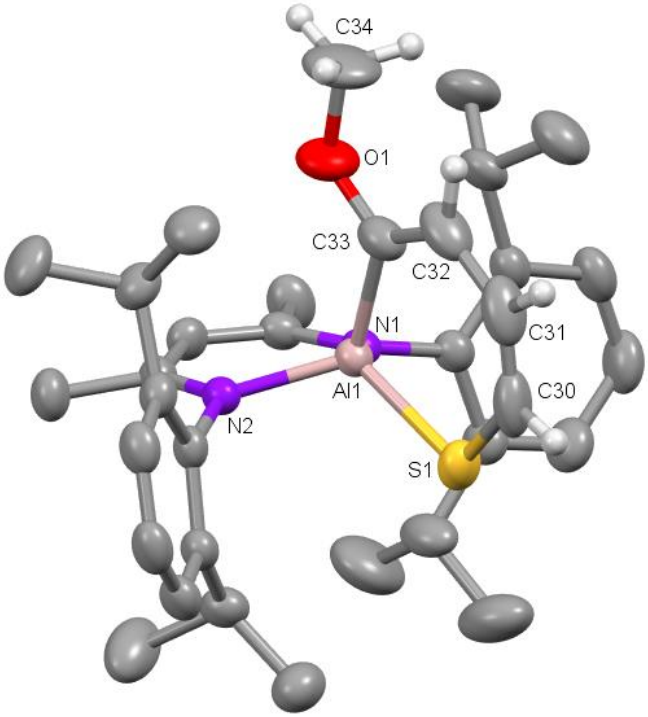


Figure S14: The crystal Structure of **2c** (50% probability ellipsoids)

The X-ray crystal structure of 2d

The structure of **2d** was found to sit across a mirror plane that passes through C2, Al1, and all of the atoms of the thiophene ligand (S21 to C29), and bisects the N1···N1A vector. However, inspection of thermal ellipsoid plots clearly show that almost all of the atoms have markedly stretched ellipsoids with their major axes perpendicular to the mirror plane, suggesting that the molecule might not actually have mirror symmetry, and that the apparent mirror may be an average across the whole crystal. However, neither of the two standard approaches to such an issue (dropping to a lower symmetry space group that removes the mirror plane, or constructing one complete molecule at 50% occupancy that is slightly shifted away from, and no longer has to "obey", the mirror plane) produced satisfactory results, so the original model was retained. The C30-based included toluene solvent molecule was found to be disordered across a mirror plane, and two unique orientations were identified of *ca*. 30 and 20% occupancy (with two further orientations of the same occupancies being generated by operation of the mirror plane). The geometries of the two unique orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and all of the atoms were refined isotropically.

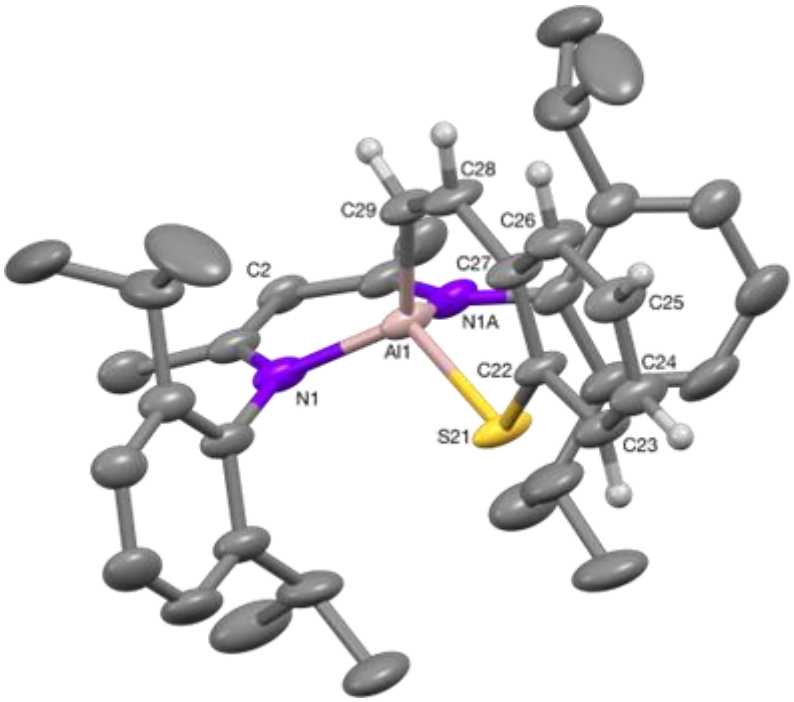


Figure S15: The crystal Structure of **2b** (50% probability ellipsoids)

5. **Computational Details**

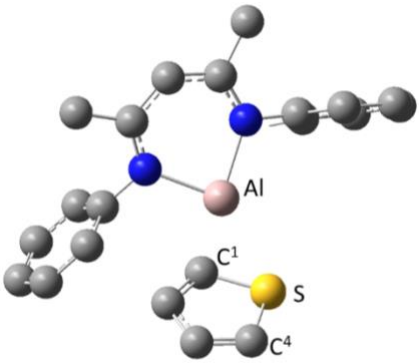
Geometry optimisations, single point corrections and NICS calculations were performed with the Gaussian 16 (Revision C.01) [5] program package using the M06L[6] functional and ultrafine integrations grid (keyword int=ultrafine). The ωB97XD exchange-correlation functional were also employed to assess differences in performance arising from the level of theory.[7] The graphical user interface used to visualise various properties of compounds and stationary points was GaussView 5.0.9.[8]

Geometry optimisation calculations were performed without symmetry constraints (keyword nosymm). Aluminium atoms were described with Stuttgart SDDAll RECPs and associated basis sets and the 6-31G** basis set was used for all other atoms.[9–18] Frequency analyses for all stationary points were performed to confirm the nature of the structures as minima (no imaginary frequencies) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations followed by full geometry optimisations on final points were used to connect transition state 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.

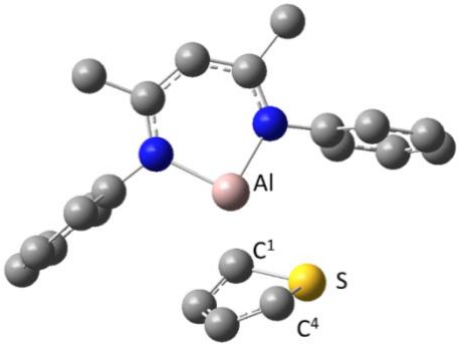
Single point corrections were performed using the 6-311+G** basis set to describe all atoms.[19,20] Solvent corrections were applied using the SMD solvation model in benzene[21] and dispersion corrections were applied using the Grimme's D3 (GD3) correction.[22]

Natural Bond Orbital analysis was carried in NBO 6.0[23] with the M06L[6] functional and 6-311+G**[19,20] basis set describing all atoms. Relevant NPA charges and Wiberg Bond Indices are tabulated (Tables S6-S9)

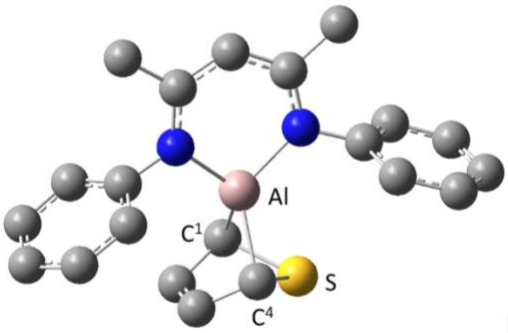
Mechanism Stationary Points: Insertion of 1 into thiophene



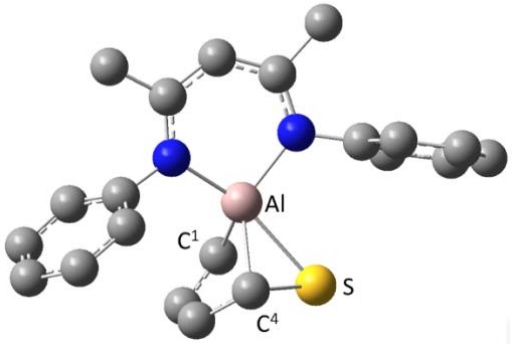
Int-1



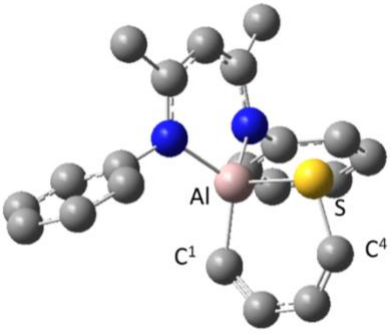
TS-1



Int-2



TS-2

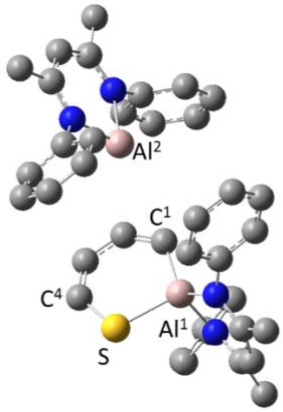


2a

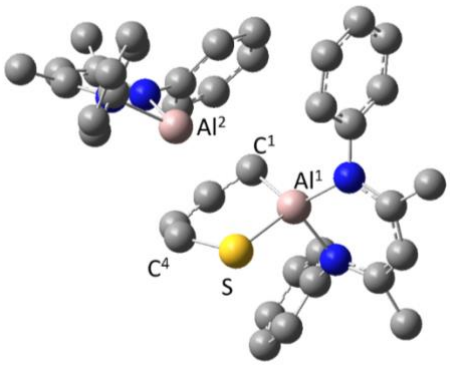
	Int-1	**TS-1**	**Int-2**	**TS-2**	**2a**
Al–S	3.98	2.94	2.60	2.46	2.30
C^1–S	1.72	1.80	1.87	2.46	3.36
C^4–S	1.72	1.75	1.87	1.88	1.74
Al–C^1	3.74	2.27	2.04	2.00	1.92
Al–C^4	4.07	2.91	2.04	2.07	3.17

Table S2: Selected distances between atoms (in Å) for **Int-1** to **2a**

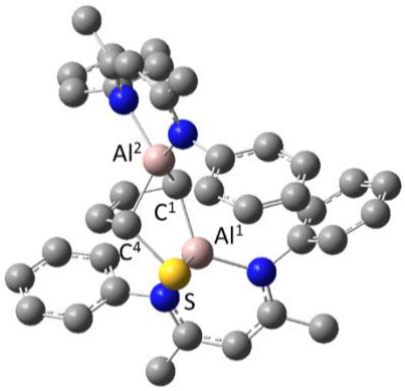
Mechanism Stationary Points: Insertion of 1 into 2a



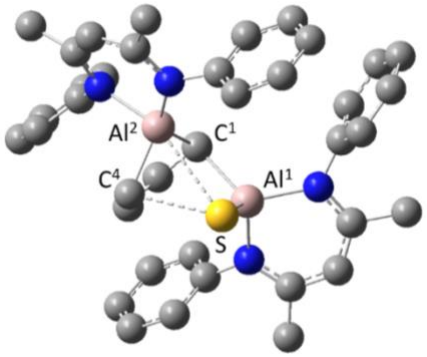
Int-3



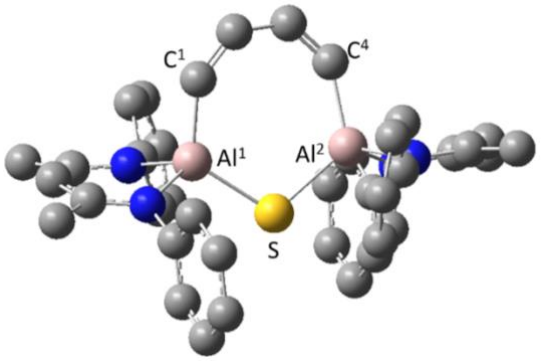
TS-3



Int-4



TS-4



3

	Int-3	**TS-3**	**Int-4**	**TS-4**	**3**
Al^1–S	2.31	2.28	2.27	2.18	2.25
Al^2–S	5.94	3.74	3.19	3.09	2.25
Al^2–C^1	4.47	2.70	2.06	2.08	3.92
Al^2–C^4	5.55	2.86	2.01	1.96	1.96
Al^1–C^1	1.93	1.93	1.99	2.10	1.96
C^4–S	1.75	1.76	1.91	2.74	3.65

Table S3: Selected distances between atoms (in Å) for **Int-3** to **3**

Nucleus-Independent Chemical Shift calculations (NICS):

NICS(0) and NICS(1) calculations were carried out on the optimised geometries of **2a**, **3** and **4** inspecting the ring systems containing Al–C and C–Al–S bonds. All atoms were described using the 6-311+G** basis set. Overall, the small NICS values observed indicate that there is essentially no degree of aromaticity present in the rings and that the thiophene substrate has been dearomatized due to the insertion of **1**. These results are analogous to those obtained from the insertion of **1** into furans.[24]

	Isotropic Shielding Tensor (ppm)
2a	0.21
3	-0.12
4	-3.68

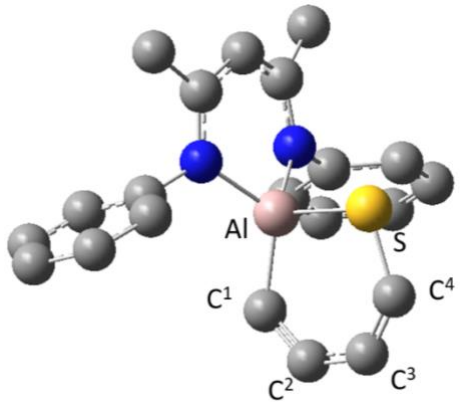
Table S4: Isotropic shielding tensor values for 'dummy atom' in NICS(0) calculation

	Isotropic Shielding Tensor (ppm)
2a	1.81, 1.87
3	0.48, 0.92
4	-0.76, 0.33

Table S5: Isotropic shielding tensor values for 'dummy atoms' in NICS(1) calculation

NBO Analysis:

The NPA charges and Wiberg Bond Indices were inspected (M06L) for the pathway of the double insertion of **1** into thiophene.

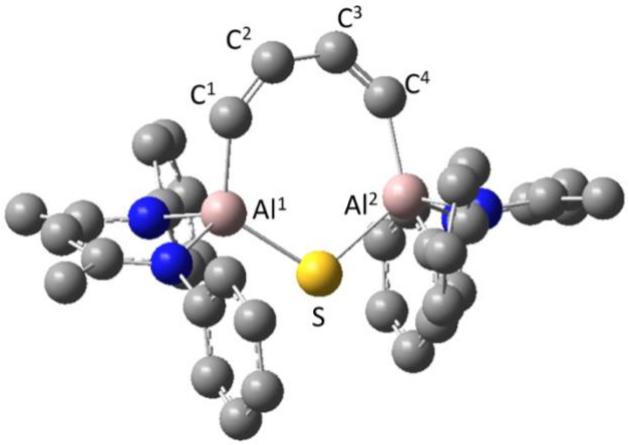


	Thiophene	Int-1	TS-1	Int-2	TS-2	2a
Al–C^1	-	0.02	0.33	0.46	0.47	0.77
Al–C^4	-	0.01	0.31	0.43	0.37	-
Al–S	-	-	-	-	0.36	0.82
C^1–S	1.22	1.21	1.04	0.98	0.55	-
C^4–S	1.22	1.22	1.12	0.98	1.00	1.09
C^1–C^2	1.62	1.60	1.27	1.07	1.33	1.34
C^2–C^3	1.29	1.28	1.51	1.80	1.54	1.08
C^3–C^4	1.62	1.62	1.38	1.08	1.24	1.30

Table S6: Wiberg Bond Indices on stationary points on pathway for the single insertion of **1** into thiophene

	Thiophene	1	Int-1	TS-1	Int-2	TS-2	2a
Al	-	0.78	0.79	1.19	1.81	1.75	1.72
S	0.42	-	0.45	0.34	0.18	-0.13	-0.27
C^1	-0.41	-	-0.41	-0.74	-0.87	-0.61	-0.85
C^4	-0.41	-	-0.39	-0.44	-0.88	-0.82	-0.31

Table S7: NPA charges on stationary points on pathway for the single insertion of **1** into thiophene



	2a	Int-3	TS-3	Int-4	TS-4	3
Al^1–C^1	0.77	0.57	0.45	0.42	0.31	0.50
Al^1–S	0.82	0.66	0.56	0.67	0.82	0.67
Al^2–C^1	-	0.01	0.26	0.41	0.36	-
Al^2–C^4	-	0.00	0.21	0.34	0.37	0.50
Al^2–S	-	0.01	0.12	0.09	0.18	0.67
C^4–S	1.09	1.18	1.12	0.93	0.28	-
C^1–C^2	1.34	1.80	1.51	1.16	1.44	1.87
C^2–C^3	1.08	1.17	1.31	1.68	1.33	1.11
C^3–C^4	1.30	1.71	1.48	1.10	1.53	1.87

Table S8: Wiberg Bond Indices on stationary points on pathway for the insertion of **1** into **2a**

	2a	1	Int-3	TS-3	Int-4	TS-4	3
Al^1	1.72	-	1.73	1.86	1.83	1.83	1.82
Al^2	-	0.78	0.79	1.14	1.99	1.99	1.82
S	-0.27	-	-0.27	-0.32	-0.44	-0.96	-1.08
C^1	-0.85	-	-0.83	-1.01	-1.42	-1.28	-0.81
C^4	-0.31	-	-0.31	-0.40	-0.94	-0.70	-0.81

Table S9: NPA charges on stationary points on pathway for the insertion of **1** into **2a**

Basis Set Testing for the Energy Barrier to TS-3

Noting that the energy barrier to TS-3 is higher than expected for a process that occurs at 60 °C, basis set convergence was explored with this system with the results reported in table S10. The results are consistent across computational approaches.

	Basis Set	**Dispersion**	**Solvent**	**2a ΔG** kcal/mol	**Int-3 ΔG** kcal/mol	**TS-3 ΔG** kcal/mol	**Energy Barrier (ΔG)** kcal/mol
M06L	6-311+G**	GD3	Smd, benzene	-42.9	-30.4	-8.1	34.7
M06L	6-31G** (SDDAll, Al)	No	No	-36.3	-23.6	-4.4	31.9

Table S10: ΔG values of 2a, Int-3 and TS-3 calculated using varying basis sets.

XYZ coordinates

1.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1240.602498

H(298 K)= -1240.566154

G(298 K)= -1240.668856

Lowest Frequency = 18.2971cm-1

Al	-0.000671	-0.029378	-1.011722
N	-1.404006	0.002256	0.454570
N	1.400870	-0.043074	0.455190
C	-1.253342	0.036406	1.783807
C	-0.002395	-0.029122	2.407569
H	-0.002666	-0.032317	3.491791
C	1.249247	-0.082569	1.784337
C	-2.465535	0.143367	2.664178
H	-3.067193	1.016584	2.391434
H	-2.189978	0.219563	3.716927
H	-3.122847	-0.723876	2.538064
C	2.462177	-0.176048	2.665052
H	3.103350	0.704355	2.546805
H	3.080008	-1.035630	2.385323
H	2.187121	-0.265797	3.716870
C	-2.734749	0.054398	-0.077138
C	-3.251356	1.283698	-0.526631
C	-4.517328	1.292994	-1.119602
H	-4.926579	2.236789	-1.475394
C	-5.253112	0.125804	-1.263161
H	-6.234177	0.152310	-1.729217
C	-4.730483	-1.079640	-0.807367
H	-5.310682	-1.991921	-0.921812
C	-3.471502	-1.141184	-0.209204
C	-2.488663	2.587564	-0.385130
H	-1.547530	2.377299	0.140870
C	-2.134505	3.171128	-1.752067
H	-1.539104	2.465359	-2.341674
H	-1.558604	4.096480	-1.644603
H	-3.037875	3.406059	-2.326421
C	-3.266823	3.603385	0.450102
H	-3.516851	3.213030	1.441882
H	-4.207532	3.882281	-0.037619
H	-2.685564	4.520860	0.586679
C	-2.892217	-2.468920	0.243043
H	-2.160005	-2.263499	1.034707
C	-3.938441	-3.414359	0.824165
H	-4.528052	-2.937940	1.614110
H	-3.457295	-4.300513	1.248861
H	-4.637580	-3.769190	0.059447
C	-2.137228	-3.142460	-0.903563
H	-1.353866	-2.489850	-1.311541
H	-2.818289	-3.380490	-1.728268
H	-1.665447	-4.074416	-0.573218
C	2.733549	-0.058310	-0.074201
C	3.285533	-1.270655	-0.527480
C	4.552125	-1.241825	-1.118586
H	4.988152	-2.172384	-1.477494
C	5.255141	-0.053870	-1.256111
H	6.237262	-0.050845	-1.720673
C	4.698161	1.134373	-0.795984
H	5.252612	2.063186	-0.905342
C	3.436859	1.157932	-0.199891
C	2.559734	-2.595801	-0.391707
H	1.615291	-2.414358	0.138574
C	2.216741	-3.180236	-1.761128
H	1.600043	-2.487738	-2.344383
H	1.667437	-4.122151	-1.657455
H	3.124363	-3.386575	-2.339824
C	3.368845	-3.595062	0.434033
H	3.612662	-3.204041	1.427128
H	4.314661	-3.845132	-0.059400
H	2.813534	-4.528901	0.567397
C	2.821142	2.467670	0.257027
H	2.087117	2.239203	1.040752
C	3.839369	3.433599	0.854169
H	4.433352	2.965591	1.645833
H	3.333492	4.304847	1.280997
H	4.536485	3.810679	0.098308

C 2.060463 3.131797 -0.891364

H 1.294915 2.464918 -1.310095

H 2.742577 3.390712 -1.708888

H 1.565510 4.050789 -0.558363

C4H4S.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -552.898908

H(298 K)= -552.893886

G(298 K)= -552.926133

Lowest Frequency = 457.8435cm-1

C -0.006233 -1.235513 -0.000010

C -1.269291 -0.709880 0.000002

C -1.269291 0.709880 0.000007

C -0.006233 1.235513 -0.000013

S 1.191086 0.000000 0.000006

H 0.290022 -2.274944 -0.000015

H -2.165567 -1.319569 0.000005

H -2.165567 1.319569 0.000014

H 0.290022 2.274944 -0.000020

Int-1.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1793.509772

H(298 K)= -1793.467931

G(298 K)= -1793.582148

Lowest Frequency = 22.9566cm-1

H 1.362184 -0.674713 -3.365179

C 1.830792 0.305644 -3.478497

H 2.807370 0.165340 -3.957041

H 1.205777 0.884917 -4.166793

C 1.985587 1.041869 -2.145175

H 1.002077 1.035495 -1.649824

C 2.360825 2.496006 -2.417969

H 2.605446 3.044034 -1.502793

H 1.531249 3.013098 -2.912863

C -1.594908 -1.762350 -1.407577

C -2.840294 -2.085743 -2.184524

H -3.601836 -2.545632 -1.546038

H -2.628099 -2.765617 -3.010927

H -3.292866 -1.172543 -2.585011

H -1.429894 0.347637 -2.822618

H -0.884746 1.966857 -3.260875

H -2.608248 1.575930 -3.321632

C -1.839196 1.884968 -1.312056

C -1.932549 3.404747 -1.277794

H -2.057639 3.787448 -0.259893

H -2.769751 3.775782 -1.879827

C -4.171470 1.861501 -0.310644

H -4.288556 2.894831 -0.623762

C -5.206747 1.238594 0.376484

H -6.124087 1.781482 0.586713

C -5.053668 -0.068827 0.813941

H -5.851020 -0.542658 1.382342

C -3.885028 -0.788282 0.552206

H -5.808186 -2.692824 1.501713

C -4.949799 -3.059793 0.928889

H -4.752347 -4.081187 1.268389

C -2.859671 -0.157708 -0.179738

C -2.980506 1.188994 -0.590878

H -0.914513 1.612822 -0.772127

H -2.875979 -2.665992 0.623088

C -3.718293 -2.180640 1.130337

C -3.358764 -2.086519 2.613856

H -2.446597 -1.498006 2.764647

H -3.200650 -3.080827 3.044915

H -4.163439 -1.599779 3.176716

C 0.877057 2.647005 3.255538

C 2.072170 2.268361 2.708021

H 2.860714 1.781910 3.271793

H 3.024244 2.346513 0.708414

H 0.532305 2.519563 4.271796

C 1.023134 3.168975 0.845821

H 0.813350 3.517619 -0.157015

Al	-0.142682	-0.348285	0.883290
N	-1.631179	-0.844191	-0.437720
H	-5.256394	-3.107022	-0.121594
H	-1.023084	3.846430	-1.699339
C	-1.683209	1.409314	-2.757293
C	-0.419976	-2.443348	-1.758694
H	-0.519593	-3.232758	-2.495283
C	0.884165	-2.120756	-1.363043
C	2.010500	-2.911653	-1.968009
H	1.644660	-3.632873	-2.700528
H	2.549735	-3.456467	-1.184481
H	2.749440	-2.263841	-2.448965
H	1.918534	-2.680623	1.248559
C	2.925095	-2.361385	1.548955
C	2.833260	-1.819076	2.975397
H	2.131284	-0.980158	3.034618
H	2.495007	-2.596220	3.668791
H	3.812753	-1.466801	3.320896
C	3.840647	-3.583492	1.498637
H	3.941479	-3.983230	0.484185
H	3.454878	-4.382702	2.139146
H	4.848783	-3.342043	1.853385
C	3.374637	-1.273715	0.594349
C	2.515446	-0.710937	-0.367185
C	2.948676	0.348463	-1.197359
C	2.158879	2.569981	1.323917
C	4.275302	0.771480	-1.095719
H	4.629294	1.575210	-1.736327
C	5.142548	0.207534	-0.165521
H	6.168477	0.558129	-0.094118
C	4.683832	-0.789896	0.682062
H	5.353647	-1.215166	1.427216
N	1.157143	-1.145350	-0.487055
H	3.224852	2.573624	-3.087654
S	-0.155484	3.365850	2.084464

TS-1.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1793.485044

H(298 K)= -1793.444171

G(298 K)= -1793.554623

Lowest Frequency = -170.8271cm-1

H	-2.002628	-2.077225	-2.498473
C	-2.207517	-2.874064	-1.777986
H	-3.237886	-3.214471	-1.933746
H	-1.540740	-3.709141	-2.017525
C	-1.998755	-2.409919	-0.335088
H	-0.989952	-1.977237	-0.283005
C	-2.043020	-3.603046	0.612911
H	-1.956924	-3.299247	1.661483
H	-1.221866	-4.292725	0.390736
C	1.249597	0.346158	-2.149848
C	2.437687	0.283678	-3.066764
H	3.102369	1.136867	-2.891058
H	2.133107	0.294332	-4.114050
H	3.039437	-0.610989	-2.880168
H	1.529883	-2.266525	-2.301843
H	1.137022	-3.865527	-1.669736
H	2.826355	-3.429081	-1.962842
C	1.968506	-2.528474	-0.173954
C	2.147163	-3.688888	0.798359
H	2.278299	-3.342070	1.828499
H	3.014753	-4.307512	0.543134
C	4.294921	-1.760621	0.477256
H	4.533271	-2.789151	0.734064
C	5.250720	-0.769169	0.669111
H	6.230164	-1.025577	1.063288
C	4.941018	0.549634	0.372894
H	5.680032	1.328775	0.548871
C	3.690358	0.906317	-0.139976
H	5.412365	3.106100	-0.706645
C	4.452962	3.057406	-1.233131
H	4.159926	4.086344	-1.463553
C	2.742132	-0.111829	-0.348663
C	3.027732	-1.454204	-0.018886
H	1.007926	-2.050033	0.055915

H	2.430031	2.437025	-0.925580
C	3.383581	2.370420	-0.385689
C	3.207379	3.100967	0.946301
H	2.403113	2.650954	1.538851
H	2.960869	4.155805	0.784941
H	4.130174	3.057004	1.536641
C	0.412840	1.265244	3.346237
C	-0.942552	0.916697	3.513080
H	-1.677196	1.603713	3.920591
H	-2.240281	-0.698249	2.805128
H	0.902114	2.132792	3.772407
C	-0.109597	-0.808312	2.201003
H	-0.056436	-1.862089	1.926694
Al	0.062392	0.742216	0.536675
N	1.427756	0.201888	-0.830396
H	4.630085	2.537379	-2.180569
H	1.271770	-4.345622	0.771403
C	1.862082	-3.045920	-1.609138
C	-0.006252	0.557960	-2.740476
H	-0.012972	0.702153	-3.814887
C	-1.258067	0.480241	-2.113675
C	-2.485129	0.580192	-2.973355
H	-2.239825	0.511970	-4.034194
H	-2.984497	1.540900	-2.798749
H	-3.217981	-0.193012	-2.725943
H	-2.327494	2.591928	-0.728107
C	-3.226544	2.540245	-0.100207
C	-2.906137	3.253814	1.212728
H	-2.035828	2.804412	1.703962
H	-2.686313	4.312336	1.038636
H	-3.754535	3.196741	1.905317
C	-4.358912	3.252498	-0.838301
H	-4.629009	2.741794	-1.768643
H	-4.073412	4.279587	-1.085922
H	-5.264700	3.308049	-0.224564
C	-3.544071	1.078693	0.145092
C	-2.665366	0.044963	-0.225484
C	-2.969089	-1.307815	0.046220
C	-1.237783	-0.300985	2.935433
C	-4.180963	-1.602047	0.672345
H	-4.433815	-2.637567	0.885576
C	-5.061239	-0.591036	1.044745
H	-5.995708	-0.838140	1.540908
C	-4.737608	0.733303	0.786572
H	-5.422267	1.523869	1.087845
N	-1.385715	0.336318	-0.792040
H	-2.971605	-4.175387	0.509263
S	1.366318	-0.159724	2.998079

Int-2.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1793.514480

H(298 K)= -1793.473999

G(298 K)= -1793.582779

Lowest Frequency = 33.5946cm-1

Al	0.022039	-0.255465	-0.517144
S	-1.180017	-0.211994	-2.801574
N	1.417549	-0.237000	0.828014
N	-1.425390	-0.237767	0.763078
C	1.240464	-0.455903	2.134504
C	-0.028659	-0.609600	2.706434
H	-0.052277	-0.796024	3.773770
C	-1.271369	-0.454911	2.080570
C	2.427412	-0.545694	3.047941
H	2.139318	-0.370660	4.085512
H	3.211498	0.162226	2.767482
H	2.874015	-1.544987	2.990790
C	-2.484355	-0.512411	2.962640
H	-2.201906	-0.557950	4.014835
H	-3.094699	-1.391236	2.730579
H	-3.130816	0.355807	2.803484
C	2.725498	0.056847	0.315752
C	3.021590	1.404246	0.020201
C	4.244188	1.690080	-0.587691
H	4.493273	2.720795	-0.826196
C	5.140302	0.676373	-0.909027

H	6.080651	0.916480	-1.397326
C	4.834023	-0.640871	-0.598540
H	5.540566	-1.430951	-0.845298
C	3.630434	-0.978923	0.026615
C	2.050936	2.514056	0.382132
H	1.035103	2.100239	0.320476
C	2.102677	3.698885	-0.573784
H	3.035540	4.265816	-0.479481
H	1.285398	4.394072	-0.355895
H	2.005779	3.380595	-1.616313
C	2.257031	2.973633	1.826483
H	2.071407	2.165820	2.541459
H	1.576399	3.794679	2.075171
H	3.282006	3.329721	1.981846
C	3.349956	-2.431644	0.362412
H	2.434070	-2.473556	0.964238
C	4.484975	-3.038892	1.187643
H	5.404490	-3.121699	0.598228
H	4.224383	-4.047884	1.522365
H	4.721579	-2.436784	2.071055
C	3.101054	-3.269005	-0.890768
H	2.213798	-2.926970	-1.428578
H	2.955913	-4.322390	-0.629577
H	3.953307	-3.210902	-1.577787
C	-2.758894	0.031385	0.286565
C	-3.656546	-1.025484	0.058049
C	-4.933432	-0.714528	-0.415484
H	-5.635602	-1.522201	-0.611150
C	-5.313812	0.598290	-0.650756
H	-6.311865	0.820466	-1.017941
C	-4.408138	1.629134	-0.429270
H	-4.706682	2.653374	-0.633451
C	-3.117050	1.371175	0.033452
C	-3.265896	-2.479590	0.238352
H	-2.313075	-2.515024	0.781372
C	-3.044712	-3.138713	-1.123288
H	-3.975970	-3.150197	-1.700884
H	-2.708272	-4.174612	-1.009098
H	-2.302328	-2.593519	-1.711739
C	-4.294794	-3.269164	1.045638
H	-4.513604	-2.804688	2.013073
H	-3.938336	-4.286592	1.234002
H	-5.244651	-3.356359	0.507397
C	-2.123729	2.501183	0.240602
H	-1.140431	2.124575	-0.071618
C	-1.996696	2.910080	1.709131
H	-2.969529	3.197666	2.124928
H	-1.326355	3.771259	1.809169
H	-1.584988	2.107249	2.328981
C	-2.418610	3.720283	-0.625027
H	-2.569922	3.444918	-1.673296
H	-1.584855	4.427626	-0.577617
H	-3.311816	4.258048	-0.287433
C	0.074506	0.998455	-2.118608
H	-0.223123	2.037902	-2.256762
C	1.341873	0.538367	-2.773043
H	2.157870	1.208710	-3.028368
C	1.384027	-0.807538	-2.821811
H	2.236423	-1.403867	-3.132483
C	0.146185	-1.394127	-2.204104
H	-0.085690	-2.435530	-2.424994

TS-2.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1793.489985

H(298 K)= -1793.449585

G(298 K)= -1793.558270

Lowest Frequency = -403.7446cm-1

Al	-0.007320	-0.440323	-0.468556
S	-1.247676	-0.678660	-2.531857
N	1.391083	0.079833	0.806534
N	-1.446357	-0.139217	0.783174
C	1.219630	0.227720	2.121670
C	-0.037943	0.137773	2.734347
H	-0.052901	0.253806	3.812061
C	-1.281359	0.028958	2.109874

C	2.388359	0.500269	3.023874
H	3.201806	1.013841	2.507231
H	2.792209	-0.443656	3.406503
H	2.080324	1.092754	3.887490
C	-2.488235	0.174093	2.992933
H	-2.216538	0.043692	4.041468
H	-3.277366	-0.534903	2.730601
H	-2.927891	1.171808	2.881020
C	2.691034	0.274398	0.229249
C	2.928589	1.483268	-0.461714
C	4.149925	1.638821	-1.118753
H	4.351773	2.560632	-1.657308
C	5.108540	0.631735	-1.103236
H	6.048912	0.766904	-1.630388
C	4.864590	-0.539531	-0.401828
H	5.621816	-1.320972	-0.377817
C	3.663093	-0.742148	0.283623
C	1.900150	2.599021	-0.455197
H	0.907718	2.129263	-0.479063
C	1.990554	3.510873	-1.672215
H	2.885368	4.142933	-1.645870
H	1.127048	4.182050	-1.708575
H	2.012466	2.940263	-2.606136
C	1.975294	3.419857	0.833403
H	1.786075	2.808222	1.720595
H	1.229906	4.222895	0.823638
H	2.962832	3.881396	0.948622
C	3.484747	-2.023973	1.076773
H	2.519311	-1.977379	1.595782
C	4.589457	-2.169829	2.126840
H	5.559917	-2.345110	1.649642
H	4.392634	-3.024085	2.782595
H	4.695565	-1.277152	2.750442
C	3.466174	-3.264053	0.184864
H	2.635229	-3.239308	-0.522683
H	3.377951	-4.171927	0.790542
H	4.393312	-3.342938	-0.394507
C	-2.798713	-0.038712	0.292878
C	-3.503825	-1.207177	-0.042416
C	-4.817961	-1.076325	-0.493642
H	-5.381374	-1.969104	-0.753559
C	-5.410938	0.172542	-0.628893
H	-6.433502	0.254473	-0.986656
C	-4.688010	1.316819	-0.318875
H	-5.148900	2.293265	-0.446090
C	-3.374503	1.236558	0.148723
C	-2.868541	-2.577456	0.081057
H	-1.780633	-2.438077	0.067069
C	-3.214397	-3.492584	-1.088777
H	-4.272417	-3.776735	-1.088928
H	-2.635334	-4.419748	-1.028989
H	-2.992161	-3.015993	-2.048140
C	-3.227867	-3.239546	1.411594
H	-2.879004	-2.653368	2.267791
H	-2.778309	-4.235175	1.487900
H	-4.313530	-3.356217	1.508571
C	-2.577761	2.502399	0.408101
H	-1.762603	2.265630	1.105184
C	-3.404019	3.616787	1.042200
H	-4.161594	4.005704	0.353701
H	-2.761786	4.459143	1.317052
H	-3.923692	3.279573	1.945240
C	-1.930447	2.982471	-0.891865
H	-1.306688	2.201393	-1.340319
H	-1.306675	3.867204	-0.718893
H	-2.695406	3.244784	-1.631099
C	0.363750	0.283134	-2.378693
H	0.277608	1.285443	-2.793652
C	1.532866	-0.476960	-2.759015
H	2.354695	-0.014654	-3.306158
C	1.511151	-1.802615	-2.388832
H	2.167791	-2.548261	-2.830547
C	0.456910	-2.107030	-1.481894
H	0.109180	-3.141214	-1.409335

2a.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1793.582874

H(298 K)= -1793.541847

G(298 K)= -1793.652893

Lowest Frequency = 14.2534cm-1

Al	0.014198	-0.630669	-0.334541
N	-1.435248	0.022425	0.739617
N	1.403213	0.195680	0.710199
C	-1.271847	0.201850	2.059227
C	-0.009910	0.285169	2.663171
H	-0.003764	0.404993	3.740219
C	1.236971	0.398046	2.023952
C	-2.481776	0.339516	2.933628
H	-3.131472	1.152470	2.596317
H	-2.205335	0.516530	3.973314
H	-3.088367	-0.571833	2.880992
C	2.411061	0.798517	2.864915
H	3.151405	-0.006347	2.907442
H	2.104755	1.043290	3.882170
H	2.925730	1.661251	2.430038
C	-2.727440	0.288860	0.164252
C	-3.006998	1.607825	-0.248862
C	-4.263857	1.883108	-0.790989
H	-4.495900	2.900537	-1.099021
C	-5.216473	0.884266	-0.943199
H	-6.188418	1.116127	-1.369801
C	-4.915664	-0.412597	-0.552480
H	-5.654922	-1.200514	-0.681490
C	-3.678074	-0.736629	0.010418
C	-1.999222	2.730876	-0.099117
H	-1.034434	2.285387	0.171208
C	-2.389984	3.686597	1.028272
H	-3.370470	4.138699	0.839433
H	-1.661592	4.499511	1.121147
H	-2.440420	3.177767	1.996090
C	-1.805943	3.495470	-1.405639
H	-1.478185	2.835007	-2.214972
H	-1.053634	4.281978	-1.281094
H	-2.729600	3.985476	-1.731402
C	-3.398177	-2.171983	0.398986
H	-2.436719	-2.204394	0.924687
C	-3.265193	-3.039339	-0.852680
H	-4.218835	-3.089146	-1.392122
H	-2.968651	-4.059627	-0.588864
H	-2.510753	-2.645209	-1.540895
C	-4.465865	-2.738082	1.332910
H	-4.595263	-2.126748	2.232539
H	-4.198904	-3.750644	1.650367
H	-5.442297	-2.799204	0.839392
C	2.688632	0.466775	0.118269
C	3.743726	-0.459218	0.230630
C	4.980798	-0.123143	-0.327565
H	5.801814	-0.832480	-0.246360
C	5.172544	1.078048	-0.991166
H	6.143501	1.322517	-1.412944
C	4.106688	1.956808	-1.139580
H	4.252040	2.881333	-1.690219
C	2.850132	1.668873	-0.604023
C	3.578576	-1.834041	0.845628
H	2.583055	-1.897450	1.301517
C	4.622230	-2.136459	1.919952
H	5.632319	-2.170883	1.496907
H	4.429610	-3.112777	2.374830
H	4.634852	-1.391424	2.722258
C	3.648841	-2.893198	-0.256857
H	2.945611	-2.681760	-1.067344
H	3.409220	-3.884721	0.140232
H	4.656909	-2.932062	-0.686923
C	1.695105	2.634433	-0.792183
H	0.786394	2.029815	-0.926848
C	1.843058	3.499839	-2.038437
H	2.648886	4.234388	-1.933014
H	0.923520	4.062295	-2.221807
H	2.052844	2.896088	-2.926549
C	1.478192	3.511310	0.442601

H	2.388205	4.071990	0.685679
H	1.194551	2.925153	1.322918
H	0.678292	4.239494	0.264256
C	-0.000615	-0.382911	-2.242492
H	-0.082935	0.597598	-2.719719
C	0.103385	-1.426510	-3.112150
H	0.097497	-1.209883	-4.184728
C	0.223670	-2.837579	-2.826698
H	0.298942	-3.481927	-3.701399
C	0.250180	-3.493541	-1.638000
H	0.340768	-4.577702	-1.661079
S	0.158082	-2.896671	-0.003949

Int-3.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -3034.191701

H(298 K)= -3034.114508

G(298 K)= -3034.301504

Lowest Frequency = 14.9137cm-1

Al	-2.562928	-0.796475	0.323526
N	-2.185590	-1.954932	-1.160968
N	-4.466977	-0.661095	-0.011094
C	-3.139237	-2.744435	-1.690457
C	-4.497971	-2.644785	-1.370623
H	-5.149216	-3.372561	-1.840477
C	-5.138242	-1.601960	-0.681800
C	-2.765790	-3.757540	-2.734034
H	-2.579635	-3.272395	-3.697609
H	-3.569030	-4.482792	-2.871466
H	-1.842423	-4.281760	-2.475663
C	-6.634196	-1.544036	-0.757189
H	-7.023494	-2.284190	-1.456771
H	-6.973925	-0.549637	-1.062990
H	-7.079339	-1.727675	0.224816
C	-0.918589	-1.944494	-1.852545
C	-0.828585	-1.203762	-3.046979
C	0.357508	-1.264674	-3.781524
H	0.440928	-0.689780	-4.702757
C	1.430806	-2.023590	-3.340750
H	2.350568	-2.060624	-3.920195
C	1.340353	-2.708505	-2.135478
H	2.202656	-3.260296	-1.771891
C	0.177616	-2.683614	-1.361392
C	-5.198808	0.447357	0.545414
C	-5.909569	0.311307	1.754602
C	-6.637477	1.410404	2.220419
H	-7.189753	1.314008	3.153080
C	-6.656981	2.612076	1.530556
H	-7.234607	3.451650	1.907440
C	-5.913463	2.743489	0.364648
H	-5.908714	3.694265	-0.160843
C	-5.166663	1.679020	-0.143202
C	-1.712071	0.911747	0.606153
H	-1.562157	1.660710	-0.176987
C	-1.329645	1.324102	1.844143
H	-0.941700	2.343500	1.944350
C	-1.313225	0.585785	3.086771
H	-0.939680	1.138902	3.949484
C	-1.636919	-0.707755	3.339519
H	-1.495073	-1.076993	4.353641
S	-2.281426	-1.947564	2.295539
Al	2.622415	0.363444	0.075572
N	3.270657	2.313708	0.166544
N	4.437383	-0.137712	0.874048
C	4.453635	2.822019	0.502636
C	5.492137	2.028130	1.009357
H	6.414670	2.540612	1.258458
C	5.492957	0.636061	1.166120
C	4.726425	4.283782	0.287216
H	4.805897	4.487721	-0.787451
H	5.659784	4.594054	0.759748
H	3.912517	4.913132	0.656703
C	6.774521	0.006976	1.638749
H	7.184166	-0.652201	0.866083
H	6.614018	-0.624795	2.514935
H	7.522272	0.763686	1.881152

C	2.199567	3.170656	-0.228493
C	1.909983	3.320281	-1.595962
C	0.728722	3.974827	-1.956265
H	0.481295	4.085183	-3.011454
C	-0.129761	4.474631	-0.988163
H	-1.051048	4.971897	-1.279226
C	0.199444	4.362132	0.360810
H	-0.476245	4.779871	1.101548
C	1.366448	3.714970	0.775460
C	4.618474	-1.557394	0.974644
C	4.383407	-2.237751	2.190455
C	4.631532	-3.614453	2.222802
H	4.457924	-4.148454	3.155468
C	5.064664	-4.308077	1.102899
H	5.253250	-5.376580	1.159569
C	5.216187	-3.635306	-0.102532
H	5.508999	-4.192520	-0.987480
C	4.986526	-2.260297	-0.199357
C	3.765127	-1.628007	3.445501
H	3.819818	-2.430598	4.195287
C	4.472518	-0.430760	4.077860
H	5.515870	-0.652416	4.322369
H	4.450738	0.462376	3.448291
H	3.970256	-0.171674	5.016087
C	2.277234	-1.336533	3.242015
H	1.720732	-2.232357	2.950815
H	1.828130	-0.940457	4.160019
H	2.107070	-0.593320	2.452814
C	5.065527	-1.561672	-1.552481
H	4.168516	-0.916630	-1.618390
C	6.288939	-0.660247	-1.737075
H	6.284118	0.211954	-1.080998
H	7.216072	-1.219220	-1.562176
H	6.323855	-0.286852	-2.766314
C	4.999666	-2.528318	-2.730433
H	5.923126	-3.111146	-2.827120
H	4.168755	-3.235357	-2.650588
H	4.878163	-1.967130	-3.662273
C	2.858069	2.815336	-2.667005
H	3.730383	2.379982	-2.161486
C	3.353348	3.962081	-3.547440
H	3.824560	4.756474	-2.959513
H	4.083297	3.604381	-4.280887
H	2.526270	4.417341	-4.104061
C	2.227985	1.716551	-3.518561
H	1.810525	0.916378	-2.897230
H	1.414687	2.117514	-4.135711
H	2.967251	1.271341	-4.195785
C	1.770962	3.656535	2.247620
H	2.770815	4.115890	2.310285
C	0.857086	4.485242	3.144532
H	1.256313	4.510184	4.162182
H	0.756951	5.518307	2.798744
H	-0.149523	4.053528	3.204238
C	1.911114	2.242596	2.833214
H	1.085313	1.591677	2.531996
H	2.844756	1.756051	2.540372
H	1.907634	2.286222	3.928716
C	0.128981	-3.389102	-0.018392
H	-0.285024	-2.664732	0.696957
C	1.504752	-3.783050	0.500416
H	2.199317	-2.935300	0.504638
H	1.422494	-4.155792	1.526514
H	1.958178	-4.585806	-0.094271
C	-0.787665	-4.613898	0.006315
H	-1.836561	-4.365582	-0.170652
H	-0.476210	-5.354327	-0.741130
H	-0.736922	-5.094582	0.988397
C	-1.943621	-0.295636	-3.532713
H	-2.804138	-0.406188	-2.861220
C	-1.487600	1.161791	-3.468455
H	-2.298744	1.838037	-3.761654
H	-1.147248	1.440087	-2.464392
H	-0.650761	1.336762	-4.153889
C	-2.414013	-0.635647	-4.945590
H	-1.603754	-0.520932	-5.674273
H	-2.783937	-1.662570	-5.025628
H	-3.226117	0.031777	-5.253024

C	-5.868666	-0.937145	2.613865
H	-5.292982	-1.707296	2.085614
C	-5.143574	-0.633267	3.926739
H	-4.979185	-1.550872	4.500796
H	-4.170594	-0.166864	3.754310
H	-5.740094	0.049240	4.544181
C	-7.259818	-1.490133	2.925894
H	-7.841371	-0.778962	3.523292
H	-7.847955	-1.711267	2.029782
H	-7.181675	-2.413234	3.508410
C	-4.368124	1.853692	-1.421272
H	-3.497771	1.187451	-1.362569
C	-5.174787	1.428295	-2.648649
H	-6.105992	2.001727	-2.724782
H	-4.603394	1.597498	-3.568887
H	-5.435247	0.364637	-2.615835
C	-3.829907	3.271527	-1.582555
H	-4.625153	3.992911	-1.800331
H	-3.310195	3.601801	-0.676897
H	-3.118649	3.319309	-2.412825

TS-3.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -3034.166639

H(298 K)= -3034.091086

G(298 K)= -3034.270969

Lowest Frequency = -177.1928cm-1

Al	-1.731938	-0.902566	0.581165
N	-1.773146	-2.608890	-0.271091
N	-3.662946	-0.753812	0.823450
C	-2.786333	-3.472059	-0.041149
C	-3.972411	-3.124572	0.606430
H	-4.683839	-3.929097	0.757003
C	-4.439727	-1.830499	0.909609
C	-2.682149	-4.879490	-0.553783
H	-2.860559	-4.913456	-1.633837
H	-3.422046	-5.519973	-0.071754
H	-1.683586	-5.295602	-0.395934
C	-5.880789	-1.723829	1.312981
H	-6.498990	-2.393520	0.710666
H	-6.264504	-0.706152	1.225259
H	-5.994343	-2.036620	2.356477
C	-0.781925	-3.027710	-1.227018
C	-1.112222	-2.993720	-2.595699
C	-0.183998	-3.486435	-3.516817
H	-0.423447	-3.456100	-4.578284
C	1.035199	-3.998013	-3.097906
H	1.745500	-4.385698	-3.823871
C	1.361329	-3.983240	-1.746580
H	2.328433	-4.361845	-1.429621
C	0.475539	-3.490331	-0.785048
C	-4.192273	0.568857	1.025806
C	-4.425047	1.072442	2.320286
C	-4.849580	2.399960	2.443792
H	-5.030910	2.798638	3.439859
C	-5.033042	3.209723	1.335198
H	-5.354572	4.240771	1.456011
C	-4.801781	2.695509	0.064814
H	-4.944372	3.334140	-0.801998
C	-4.379866	1.378548	-0.116336
C	-0.996470	0.705234	-0.191314
H	-1.125897	0.969585	-1.245747
C	-0.915963	1.811257	0.656028
H	-0.972932	2.802766	0.223066
C	-0.443315	1.757360	1.986210
H	-0.146248	2.698235	2.451473
C	-0.085406	0.612282	2.691571
H	0.459419	0.764082	3.621349
S	-0.862594	-0.971090	2.691847
Al	1.633276	0.625725	0.403497
N	1.873509	2.473113	-0.603450
N	3.651516	0.761107	0.957472
C	2.982106	3.226568	-0.579970
C	4.050456	3.041925	0.308146
H	4.798817	3.826671	0.310603
C	4.408104	1.867080	0.975747

C	3.180149	4.317879	-1.603054
H	3.227938	3.877479	-2.605607
H	4.113841	4.852474	-1.423153
H	2.363861	5.043589	-1.635179
C	5.782657	1.848763	1.593207
H	6.442045	1.183031	1.023609
H	5.778408	1.458053	2.613297
H	6.223765	2.846921	1.597758
C	0.973109	2.762086	-1.690950
C	1.039484	1.915925	-2.824375
C	0.164607	2.120593	-3.892648
H	0.209866	1.449886	-4.749188
C	-0.720968	3.185193	-3.889285
H	-1.387979	3.356422	-4.730013
C	-0.729649	4.049191	-2.805043
H	-1.388588	4.913328	-2.834891
C	0.082718	3.867235	-1.676781
C	4.315585	-0.430838	1.412137
C	4.415898	-0.768795	2.775945
C	5.216450	-1.866111	3.124598
H	5.306116	-2.119192	4.180226
C	5.882618	-2.623990	2.176857
H	6.507785	-3.459065	2.480791
C	5.720755	-2.319604	0.831031
H	6.204160	-2.938847	0.080599
C	4.935064	-1.240602	0.427354
C	3.656487	-0.147675	3.943384
H	4.340151	-0.222558	4.802991
C	3.216334	1.311906	3.882183
H	4.045537	2.002632	3.709214
H	2.466512	1.494342	3.109309
H	2.766983	1.582719	4.844170
C	2.462474	-1.061979	4.242246
H	2.794702	-2.072458	4.501398
H	1.859668	-0.679302	5.074166
H	1.810865	-1.150175	3.366107
C	4.711830	-0.974399	-1.051901
H	3.662214	-0.654679	-1.148495
C	5.600658	0.143498	-1.601949
H	5.370740	1.120056	-1.167805
H	6.657297	-0.077738	-1.408231
H	5.479439	0.232802	-2.686990
C	4.872989	-2.220370	-1.918061
H	5.921294	-2.529239	-2.000798
H	4.302390	-3.069760	-1.528469
H	4.520358	-2.017348	-2.935287
C	2.088823	0.830842	-2.975622
H	2.708426	0.826572	-2.071472
C	3.020736	1.131491	-4.150666
H	3.549755	2.082122	-4.023836
H	3.773113	0.341760	-4.256247
H	2.467362	1.184101	-5.094977
C	1.474357	-0.555311	-3.131197
H	0.801011	-0.796698	-2.300242
H	0.901424	-0.638097	-4.062808
H	2.252156	-1.326541	-3.158547
C	-0.053167	4.987552	-0.624401
H	0.252638	5.896005	-1.171122
C	-1.515062	5.231141	-0.204684
H	-1.600847	6.216128	0.264778
H	-2.221924	5.197892	-1.036750
H	-1.851961	4.495577	0.533117
C	0.785930	4.948647	0.652255
H	0.683381	4.000886	1.183231
H	1.851499	5.113541	0.489878
H	0.440004	5.744495	1.319864
C	0.867140	-3.424537	0.678569
H	0.561198	-2.431223	1.037065
C	2.369646	-3.503043	0.894548
H	2.896066	-2.786274	0.259225
H	2.619228	-3.257382	1.931996
H	2.774437	-4.502516	0.689487
C	0.157214	-4.454467	1.556746
H	-0.927278	-4.319043	1.574842
H	0.372097	-5.476634	1.220941
H	0.507463	-4.361037	2.590047
C	-2.401733	-2.376982	-3.106404
H	-3.055464	-2.168691	-2.249781

C	-2.100324	-1.042742	-3.790181
H	-3.021681	-0.572292	-4.151937
H	-1.599627	-0.339367	-3.114297
H	-1.441555	-1.188926	-4.655003
C	-3.163714	-3.295096	-4.059567
H	-2.596207	-3.482351	-4.977743
H	-3.386443	-4.268054	-3.610168
H	-4.114633	-2.839414	-4.354325
C	-4.244823	0.261882	3.588627
H	-3.842749	-0.722812	3.318906
C	-3.243941	0.926378	4.534222
H	-3.022699	0.269714	5.381448
H	-2.303306	1.155541	4.029543
H	-3.651410	1.860972	4.937704
C	-5.576928	0.075355	4.319763
H	-5.956812	1.038813	4.678881
H	-6.354200	-0.358881	3.685035
H	-5.451785	-0.570904	5.194637
C	-4.162269	0.826466	-1.511989
H	-3.303234	0.142139	-1.467657
C	-5.364349	0.001706	-1.975887
H	-6.272817	0.614418	-1.999856
H	-5.199376	-0.390616	-2.986412
H	-5.554312	-0.852435	-1.318049
C	-3.824093	1.907823	-2.529271
H	-4.685444	2.550794	-2.743469
H	-3.002593	2.542692	-2.180845
H	-3.515392	1.460443	-3.478672

Int-4.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -3034.209128

H(298 K)= -3034.134838

G(298 K)= -3034.310272

Lowest Frequency = 9.5723cm-1

Al	-1.232163	-1.050418	0.510127
N	-1.356545	-2.832125	-0.217811
N	-3.202216	-0.903633	0.826625
C	-2.373596	-3.679397	0.032999
C	-3.544434	-3.295301	0.679923
H	-4.270464	-4.079485	0.857357
C	-3.977308	-1.986699	0.948661
C	-2.296959	-5.105562	-0.435131
H	-2.245306	-5.168553	-1.526156
H	-3.167464	-5.668994	-0.097547
H	-1.392245	-5.596580	-0.068525
C	-5.421394	-1.847380	1.338515
H	-5.952932	-2.789445	1.200644
H	-5.920326	-1.068619	0.755029
H	-5.516023	-1.553202	2.386546
C	-0.419032	-3.305513	-1.197142
C	-0.754214	-3.111425	-2.551820
C	0.050282	-3.708059	-3.527307
H	-0.194287	-3.567291	-4.578872
C	1.114660	-4.517582	-3.164655
H	1.708929	-5.015378	-3.926329
C	1.438024	-4.680366	-1.820905
H	2.291724	-5.299503	-1.565380
C	0.718927	-4.046126	-0.802105
C	-3.862571	0.362774	1.029619
C	-4.131532	0.843622	2.326151
C	-4.773095	2.081393	2.446650
H	-4.975178	2.468951	3.443386
C	-5.152464	2.817305	1.335067
H	-5.649323	3.776492	1.454947
C	-4.882041	2.324965	0.063296
H	-5.165219	2.910317	-0.807176
C	-4.231397	1.103617	-0.113922
C	-0.336522	0.407302	-0.492927
H	-0.437478	0.463357	-1.579109
C	-1.126105	1.489636	0.169891
H	-1.867968	2.057115	-0.389226
C	-0.924717	1.732882	1.498813
H	-1.515120	2.473516	2.037560
C	0.198155	1.007216	2.149431
H	0.449237	1.415384	3.129290

S	-0.154309	-0.839922	2.487538
Al	1.319013	1.138960	0.483920
N	1.603601	2.847522	-0.496822
N	3.248042	0.918213	0.834652
C	2.723592	3.578329	-0.455967
C	3.871768	3.182177	0.237318
H	4.696141	3.885258	0.237772
C	4.150175	1.911043	0.750994
C	2.822448	4.855910	-1.244762
H	2.789211	4.652059	-2.319709
H	3.754715	5.377487	-1.024199
H	1.984480	5.529588	-1.047579
C	5.580100	1.665064	1.157347
H	6.004437	0.830135	0.590517
H	5.674413	1.386602	2.209845
H	6.187922	2.552496	0.977396
C	0.686508	3.192957	-1.552305
C	0.872628	2.521669	-2.786215
C	0.013741	2.806422	-3.847288
H	0.146956	2.284537	-4.793471
C	-0.972981	3.774289	-3.721744
H	-1.625151	4.008767	-4.558862
C	-1.111884	4.451130	-2.520612
H	-1.865067	5.231871	-2.438850
C	-0.314920	4.172845	-1.399142
C	3.776640	-0.330240	1.320191
C	4.012610	-0.547757	2.692376
C	4.669784	-1.736803	3.044647
H	4.873269	-1.915846	4.098963
C	5.097859	-2.655278	2.103710
H	5.627195	-3.552267	2.414104
C	4.846972	-2.421520	0.756923
H	5.183822	-3.142333	0.017962
C	4.171436	-1.275863	0.343047
C	3.690709	0.353474	3.891484
H	4.622072	0.346752	4.481372
C	3.333836	1.825547	3.699532
H	4.127111	2.416106	3.236951
H	2.425149	1.966158	3.112007
H	3.152272	2.262299	4.687102
C	2.622120	-0.308987	4.768346
H	2.879762	-1.342815	5.014735
H	2.506412	0.243581	5.706600
H	1.654483	-0.334121	4.260107
C	3.903846	-1.038214	-1.135964
H	2.893246	-0.604377	-1.218292
C	4.888057	-0.058083	-1.782197
H	4.791884	0.967976	-1.417976
H	5.920685	-0.387760	-1.615237
H	4.727904	-0.032397	-2.866290
C	3.907151	-2.324518	-1.950859
H	4.921157	-2.723986	-2.069842
H	3.285780	-3.097630	-1.497665
H	3.514184	-2.139682	-2.955330
C	2.042957	1.580656	-3.039218
H	2.569269	1.411061	-2.092434
C	3.037714	2.237026	-4.001736
H	3.434311	3.178101	-3.608945
H	3.889379	1.576074	-4.193466
H	2.563391	2.455353	-4.965263
C	1.636057	0.212415	-3.582057
H	1.058180	-0.367969	-2.855669
H	1.042673	0.294676	-4.499674
H	2.530695	-0.370506	-3.830331
C	-0.621700	5.037868	-0.169015
H	-0.523161	6.072715	-0.538994
C	-2.088153	4.880283	0.259414
H	-2.341747	5.627418	1.018656
H	-2.788339	5.002680	-0.571587
H	-2.272464	3.894879	0.694439
C	0.258487	4.942100	1.076208
H	0.257066	3.937611	1.504150
H	1.296452	5.233357	0.907434
H	-0.143381	5.622943	1.834015
C	1.213072	-4.092499	0.645503
H	1.396887	-3.040172	0.928706
C	2.529591	-4.849435	0.792996
H	3.313968	-4.487060	0.125191

H	2.903433	-4.740690	1.814466
H	2.390705	-5.920878	0.601966
C	0.259677	-4.659513	1.703614
H	-0.684063	-4.122459	1.789471
H	0.047961	-5.719560	1.518455
H	0.746486	-4.596498	2.681422
C	-2.003528	-2.357960	-2.983586
H	-2.478691	-1.936841	-2.089694
C	-1.694975	-1.195205	-3.923977
H	-2.626813	-0.737681	-4.276109
H	-1.109059	-0.415490	-3.428669
H	-1.137263	-1.521955	-4.809487
C	-3.016618	-3.301211	-3.636329
H	-2.590415	-3.791046	-4.519362
H	-3.352413	-4.084978	-2.950934
H	-3.904867	-2.748970	-3.960962
C	-3.752909	0.110455	3.601468
H	-3.321888	-0.861940	3.330618
C	-2.692262	0.876320	4.392477
H	-2.449598	0.341948	5.316629
H	-1.768292	0.987533	3.825646
H	-3.060379	1.872237	4.668870
C	-4.964086	-0.112569	4.512943
H	-5.324900	0.838397	4.921063
H	-5.813486	-0.581932	4.007417
H	-4.689509	-0.743660	5.363766
C	-3.900688	0.601567	-1.508906
H	-2.920770	0.105731	-1.448249
C	-4.907561	-0.438163	-2.003636
H	-5.926325	-0.033213	-1.990154
H	-4.680976	-0.728312	-3.036566
H	-4.896799	-1.351648	-1.400025
C	-3.760027	1.724645	-2.529648
H	-4.726515	2.180943	-2.773586
H	-3.091694	2.517798	-2.177037
H	-3.341804	1.337269	-3.464327

TS-4.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -3034.202345

H(298 K)= -3034.128703

G(298 K)= -3034.301472

Lowest Frequency = -78.9270cm-1

Al	0.298272	-1.547964	-0.449354
N	-0.832780	-2.911402	0.373708
N	1.907895	-2.717535	-0.467693
C	-0.564755	-4.227317	0.278386
C	0.627845	-4.746203	-0.230293
H	0.682871	-5.825455	-0.302813
C	1.808404	-4.052961	-0.512804
C	-1.557711	-5.243317	0.775190
H	-1.743621	-5.114225	1.846134
H	-1.185367	-6.254373	0.607892
H	-2.531582	-5.140841	0.291871
C	3.007129	-4.895939	-0.843945
H	2.824077	-5.943274	-0.600821
H	3.906580	-4.562142	-0.320692
H	3.227342	-4.832387	-1.914148
C	-2.104710	-2.632072	0.992484
C	-2.105506	-2.470742	2.394964
C	-3.332183	-2.445075	3.061570
H	-3.357503	-2.328973	4.141470
C	-4.518509	-2.570266	2.355492
H	-5.469940	-2.571299	2.881482
C	-4.496880	-2.674533	0.971093
H	-5.444152	-2.745879	0.449809
C	-3.302704	-2.697283	0.236765
C	3.239996	-2.178847	-0.528349
C	3.901072	-1.990681	-1.756419
C	5.178428	-1.420383	-1.732742
H	5.694815	-1.254972	-2.676288
C	5.792656	-1.060246	-0.542216
H	6.783325	-0.613862	-0.550908
C	5.139130	-1.284378	0.664590

H	5.625341	-1.009450	1.596883
C	3.862884	-1.847536	0.696276
C	0.637154	0.220822	0.606161
H	0.499913	0.128161	1.687694
C	1.995941	0.503061	0.250817
H	2.805977	0.403550	0.974125
C	2.321873	0.851752	-1.072923
H	3.357883	0.759474	-1.399133
C	1.270038	1.250238	-1.897139
H	1.456255	1.424772	-2.955161
S	-0.380489	-0.788979	-2.378687
Al	-0.194555	1.636263	-0.663700
N	0.464964	3.397131	0.147417
N	-1.948348	2.357973	-0.995239
C	-0.155061	4.565737	0.014756
C	-1.390286	4.698745	-0.641605
H	-1.770147	5.708417	-0.744641
C	-2.246292	3.677776	-1.040821
C	0.448386	5.824764	0.580822
H	0.737174	5.690252	1.626714
H	-0.254116	6.656681	0.512720
H	1.365178	6.106577	0.054262
C	-3.619587	4.103984	-1.487030
H	-4.393295	3.764846	-0.790601
H	-3.879186	3.670795	-2.457700
H	-3.676750	5.190506	-1.561617
C	1.730476	3.431302	0.820067
C	1.757992	3.029032	2.177438
C	2.975257	3.039984	2.858288
H	3.012016	2.727752	3.898208
C	4.139470	3.459019	2.227233
H	5.080891	3.480440	2.769251
C	4.088090	3.865239	0.904655
H	4.998693	4.216967	0.424066
C	2.903098	3.852166	0.154188
C	-3.117860	1.517671	-0.935207
C	-3.777091	1.041008	-2.084824
C	-5.015833	0.416240	-1.881417
H	-5.574058	0.076641	-2.751040
C	-5.562794	0.231195	-0.620810
H	-6.527510	-0.259362	-0.513191
C	-4.879511	0.683010	0.498116
H	-5.304075	0.543678	1.490793
C	-3.667738	1.356004	0.358265
C	-3.369876	1.221631	-3.550347
H	-4.205056	1.791745	-3.994334
C	-2.090966	1.985880	-3.888182
H	-2.090694	3.022854	-3.544521
H	-1.205989	1.485471	-3.485597
H	-1.983576	2.007491	-4.977809
C	-3.332190	-0.131465	-4.274103
H	-4.260090	-0.698183	-4.155904
H	-3.174692	0.023009	-5.346379
H	-2.505943	-0.740973	-3.894428
C	-3.043009	1.983654	1.595134
H	-2.125249	2.508939	1.306911
C	-3.971886	3.030793	2.210697
H	-4.206993	3.831655	1.502085
H	-4.919427	2.585506	2.534061
H	-3.505946	3.491695	3.088351
C	-2.651530	0.933806	2.625958
H	-3.506068	0.320632	2.933645
H	-1.891474	0.252875	2.225925
H	-2.241563	1.413244	3.523608
C	0.487573	2.617483	2.902590
H	-0.156428	2.110511	2.174222
C	-0.305538	3.816664	3.427973
H	-0.728279	4.419749	2.618851
H	-1.144579	3.474428	4.045486
H	0.319183	4.467244	4.051296
C	0.745662	1.631660	4.036522
H	1.347227	0.777320	3.705425
H	1.265610	2.099030	4.880269
H	-0.202402	1.245150	4.422882
C	3.079143	4.362639	-1.287655
H	3.534770	5.357592	-1.150001
C	4.114499	3.531206	-2.064917
H	4.510934	4.118629	-2.899126

H	4.956903	3.206644	-1.449191
H	3.651600	2.636100	-2.488244
C	1.883861	4.567776	-2.217616
H	1.310764	3.649365	-2.367254
H	1.190144	5.346442	-1.898347
H	2.266467	4.872626	-3.197299
C	-3.370828	-2.722162	-1.298128
H	-3.048109	-1.715265	-1.615802
C	-4.790645	-2.945078	-1.820782
H	-5.509938	-2.205434	-1.468574
H	-4.784995	-2.892566	-2.913368
H	-5.162238	-3.940106	-1.544163
C	-2.477146	-3.706620	-2.064583
H	-1.411058	-3.514754	-1.965025
H	-2.686369	-4.749247	-1.797693
H	-2.699321	-3.603423	-3.131200
C	-0.806953	-2.334383	3.180875
H	-0.117970	-1.738074	2.562860
C	-0.994164	-1.600290	4.506567
H	-0.019904	-1.346615	4.936099
H	-1.567207	-0.675470	4.396430
H	-1.511764	-2.227208	5.241575
C	-0.112444	-3.669136	3.468120
H	-0.800049	-4.367028	3.961076
H	0.285304	-4.150590	2.571478
H	0.730824	-3.509902	4.149717
C	3.305339	-2.371082	-3.099059
H	2.353654	-2.888899	-2.922613
C	2.996327	-1.138479	-3.946971
H	2.656599	-1.438362	-4.943546
H	2.202435	-0.542676	-3.494676
H	3.890871	-0.514357	-4.071089
C	4.240278	-3.301382	-3.877008
H	5.138411	-2.767814	-4.208031
H	4.578749	-4.160207	-3.288359
H	3.742593	-3.679844	-4.775083
C	3.168858	-2.114043	2.021530
H	2.088164	-1.978461	1.861985
C	3.389744	-3.562013	2.468734
H	4.460948	-3.790152	2.516482
H	2.969342	-3.730895	3.465438
H	2.920437	-4.281280	1.791862
C	3.589670	-1.166278	3.140719
H	4.616132	-1.357864	3.473337
H	3.528659	-0.111313	2.849084
H	2.942493	-1.309936	4.013116

3.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -3034.296369

H(298 K)= -3034.219789

G(298 K)= -3034.401602

Lowest Frequency = 23.6685cm-1

Al	-0.717370	1.644100	-0.673775
Al	0.717370	-1.644103	-0.673769
N	-0.084017	3.347952	0.034692
C	-0.778245	4.479532	-0.156203
C	-2.123777	4.494758	-0.534469
H	-2.572831	5.472697	-0.661874
C	-3.007329	3.404873	-0.566950
N	-2.612056	2.126560	-0.501315
C	-0.116270	5.806563	0.079658
H	0.281558	5.884565	1.095774
H	-0.811922	6.629100	-0.089503
H	0.742519	5.930421	-0.589223
C	-4.469082	3.740034	-0.645192
H	-4.859141	3.544559	-1.648140
H	-4.637106	4.793357	-0.418089
H	-5.059701	3.128359	0.041871
C	1.156649	3.473167	0.750271
C	1.126395	3.382010	2.155287
C	2.318894	3.579409	2.855084
H	2.309706	3.524421	3.942122
C	3.513985	3.821491	2.188639
H	4.434885	3.954695	2.750834
C	3.526735	3.888410	0.801697

H	4.462561	4.075021	0.278422
C	2.352397	3.737749	0.060195
C	-0.161542	3.125095	2.913620
H	-0.919644	2.813138	2.184985
C	-0.014904	1.993787	3.925848
H	0.722336	2.228539	4.702700
H	0.293779	1.068586	3.429979
H	-0.969929	1.809594	4.431753
C	-0.669633	4.400058	3.588015
H	-1.586315	4.202969	4.154212
H	-0.896051	5.186385	2.860205
H	0.073854	4.798673	4.288355
C	2.384644	3.854012	-1.448344
H	1.347906	3.938020	-1.797641
C	3.142734	5.089465	-1.928254
H	2.757681	6.013049	-1.482684
H	3.071531	5.185247	-3.016225
H	4.207995	5.028688	-1.679760
C	2.976144	2.592912	-2.068322
H	2.860053	2.598426	-3.157632
H	2.490302	1.688043	-1.685593
H	4.043911	2.509858	-1.837297
C	-3.638044	1.118668	-0.450571
C	-4.350836	0.762883	-1.614415
C	-5.372985	-0.183074	-1.495398
H	-5.930414	-0.468575	-2.385733
C	-5.669173	-0.779063	-0.278792
H	-6.461268	-1.520855	-0.211596
C	-4.941621	-0.432718	0.853051
H	-5.170255	-0.910276	1.801485
C	-3.926587	0.524546	0.796897
C	-4.046899	1.331402	-2.989164
H	-3.313515	2.140839	-2.877532
C	-5.292333	1.888408	-3.682086
H	-5.991124	1.084567	-3.938693
H	-5.019858	2.386522	-4.617660
H	-5.844580	2.605481	-3.067108
C	-3.419886	0.262336	-3.883106
H	-2.521784	-0.165456	-3.434625
H	-3.142175	0.682540	-4.856202
H	-4.131131	-0.554108	-4.059442
C	-3.204290	0.962452	2.057146
H	-2.165877	1.175896	1.779720
C	-3.148709	-0.123797	3.120055
H	-4.135877	-0.349046	3.541742
H	-2.511155	0.194698	3.951154
H	-2.731492	-1.047935	2.711783
C	-3.800045	2.249659	2.630546
H	-3.677712	3.103440	1.955597
H	-3.303872	2.508886	3.573373
H	-4.870051	2.132688	2.840562
N	0.084017	-3.347953	0.034706
C	0.778245	-4.479533	-0.156187
C	2.123776	-4.494760	-0.534455
H	2.572831	-5.472700	-0.661857
C	3.007328	-3.404875	-0.566940
N	2.612056	-2.126562	-0.501309
C	0.116271	-5.806563	0.079680
H	0.811923	-6.629101	-0.089479
H	-0.742520	-5.930424	-0.589200
H	-0.281556	-5.884561	1.095797
C	4.469082	-3.740036	-0.645183
H	4.859140	-3.544564	-1.648131
H	4.637106	-4.793358	-0.418077
H	5.059701	-3.128359	0.041879
C	-1.156648	-3.473165	0.750285
C	-1.126393	-3.382002	2.155301
C	-2.318893	-3.579398	2.855099
H	-2.309704	-3.524406	3.942137
C	-3.513984	-3.821481	2.188656
H	-4.434884	-3.954682	2.750851
C	-3.526734	-3.888406	0.801714
H	-4.462561	-4.075017	0.278440
C	-2.352396	-3.737749	0.060211
C	0.161544	-3.125084	2.913633
H	0.919646	-2.813132	2.184996
C	0.014908	-1.993770	3.925854
H	-0.293774	-1.068572	3.429981

H	0.969933	-1.809576	4.431759
H	-0.722333	-2.228517	4.702708
C	0.669634	-4.400044	3.588035
H	1.586317	-4.202953	4.154230
H	0.896051	-5.186375	2.860229
H	-0.073852	-4.798654	4.288378
C	-2.384643	-3.854018	-1.448327
H	-1.347906	-3.938029	-1.797625
C	-3.142736	-5.089473	-1.928232
H	-4.207997	-5.028693	-1.679739
H	-2.757684	-6.013055	-1.482658
H	-3.071532	-5.185259	-3.016202
C	-2.976143	-2.592920	-2.068310
H	-2.860053	-2.598439	-3.157620
H	-2.490300	-1.688051	-1.685585
H	-4.043910	-2.509864	-1.837285
C	3.638044	-1.118670	-0.450570
C	4.350835	-0.762889	-1.614416
C	5.372985	0.183066	-1.495402
H	5.930414	0.468563	-2.385739
C	5.669175	0.779059	-0.278799
H	6.461271	1.520851	-0.211606
C	4.941623	0.432720	0.853046
H	5.170258	0.910280	1.801478
C	3.926588	-0.524543	0.796896
C	4.046896	-1.331412	-2.989163
H	3.313514	-2.140851	-2.877527
C	5.292330	-1.888418	-3.682085
H	5.019855	-2.386534	-4.617658
H	5.844579	-2.605489	-3.067106
H	5.991121	-1.084577	-3.938694
C	3.419881	-0.262349	-3.883106
H	4.131124	0.554095	-4.059445
H	2.521779	0.165442	-3.434624
H	3.142168	-0.682556	-4.856200
C	3.204291	-0.962444	2.057147
H	2.165877	-1.175886	1.779722
C	3.148713	0.123810	3.120052
H	2.511159	-0.194681	3.951153
H	2.731499	1.047948	2.711777
H	4.135882	0.349057	3.541737
C	3.800043	-2.249649	2.630551
H	4.870050	-2.132681	2.840565
H	3.677708	-3.103433	1.955606
H	3.303870	-2.508872	3.573380
S	0.000000	0.000001	0.674720
C	-0.259635	1.630434	-2.581713
H	-0.214967	2.662976	-2.961451
C	-0.011149	0.732008	-3.560819
H	0.167387	1.125909	-4.569553
C	0.011143	-0.732023	-3.560816
H	-0.167394	-1.125928	-4.569548
C	0.259632	-1.630445	-2.581706
H	0.214963	-2.662989	-2.961440

4.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -1395.353837

H(298 K)= -1395.313699

G(298 K)= -1395.423166

Lowest Frequency = 21.6055cm-1

Al	-0.028309	-0.681282	-0.484922
N	1.411222	-0.204312	0.710313
N	-1.427347	-0.026032	0.673062
C	1.234435	-0.039836	2.027344
C	-1.274220	0.107224	1.994928
C	3.552533	-1.057165	-0.160438
C	2.716814	0.029449	0.158137
C	-0.028735	0.004003	2.633742
C	-2.705532	0.245149	0.075537
C	0.005609	-0.055073	-2.356412
C	-1.769666	2.519363	-0.607689
H	-0.823737	1.969114	-0.708133
C	-2.885625	1.490801	-0.565331
C	3.147534	-2.496568	0.086376
H	2.095098	-2.506249	0.393312

C	4.812577	-0.785998	-0.701276
H	5.471382	-1.618373	-0.940433
C	3.123291	1.357740	-0.085260
C	-3.724008	-0.726274	0.085729
C	-0.154989	-2.508658	-2.417312
C	-0.155311	-2.568705	-1.067013
C	4.388051	1.574570	-0.634345
H	4.709274	2.595418	-0.832773
C	-4.944321	-0.408493	-0.518284
H	-5.739047	-1.151927	-0.519755
C	-0.079419	-1.185275	-3.093841
C	-4.125196	1.758728	-1.147846
H	-4.287146	2.713078	-1.640576
C	2.221475	2.548031	0.182728
H	1.320599	2.194052	0.700231
C	3.974593	-3.116607	1.212657
H	5.040857	-3.125057	0.958217
H	3.670181	-4.152240	1.395045
H	3.866884	-2.567526	2.153903
C	5.234248	0.515100	-0.935809
H	6.217215	0.703861	-1.358324
C	2.429564	0.175748	2.907050
H	3.238196	-0.519134	2.663056
H	2.166822	0.071675	3.960397
H	2.839107	1.181037	2.758061
C	-3.541813	-2.110437	0.677815
H	-2.563654	-2.147302	1.174650
C	-5.152810	0.822945	-1.119604
H	-6.109820	1.051393	-1.580493
C	3.260626	-3.334343	-1.184861
H	2.680144	-2.896645	-2.001226
H	2.881615	-4.346778	-1.011593
H	4.302099	-3.424553	-1.514226
C	-2.467593	0.409010	2.851266
C	-1.872510	3.456157	-1.805456
H	-1.988787	2.902688	-2.742005
H	-0.970294	4.069656	-1.885437
H	-2.718865	4.146110	-1.714505
C	-1.685171	3.324813	0.690169
H	-2.626367	3.851502	0.886849
H	-0.890705	4.077741	0.625346
H	-1.464543	2.692531	1.555570
C	-3.541881	-3.166226	-0.428536
H	-4.510113	-3.185469	-0.942218
H	-3.367242	-4.164094	-0.012125
H	-2.764476	-2.968165	-1.171071
C	1.776857	3.180830	-1.135710
H	2.638719	3.559984	-1.696581
H	1.101950	4.025259	-0.954739
H	1.259461	2.456644	-1.772693
C	-4.620912	-2.445964	1.708042
H	-4.701679	-1.693878	2.499412
H	-4.416074	-3.411551	2.180726
H	-5.606681	-2.520940	1.235817
C	2.888180	3.596592	1.071372
H	3.236797	3.176666	2.020355
H	2.189270	4.407426	1.301402
H	3.756269	4.046295	0.576921
H	-0.036651	0.103191	3.712998
H	-2.169962	0.678913	3.864997
H	-3.066664	1.219645	2.425926
H	-3.128022	-0.462457	2.907970
H	-0.101410	-1.184209	-4.187619
H	-0.207326	-3.393229	-3.059989
H	0.045844	0.897751	-2.881352
H	-0.207695	-3.546563	-0.590141

5.log

SCF (M06L) = SCF

E(SCF)+ZPE(0 K)= -3277.815142

H(298 K)= -3277.741269

G(298 K)= -3277.918124

Lowest Frequency = 9.5626cm-1

Al	0.006812	-1.442156	0.455665
S	-0.031463	0.515239	1.624125
N	1.442779	-2.680433	0.882713

C	1.277300	-3.773463	1.644751
C	0.028676	-4.234836	2.064063
H	0.031316	-5.111151	2.700353
C	-1.220137	-3.810175	1.605947
N	-1.402414	-2.723809	0.835038
C	2.463811	-4.592918	2.062296
H	3.124772	-4.818035	1.221293
H	2.144591	-5.528662	2.521930
H	3.070307	-4.045580	2.789708
C	-2.387361	-4.680467	1.972249
H	-3.081011	-4.153442	2.631809
H	-2.049107	-5.583807	2.480401
H	-2.965000	-4.966928	1.088611
C	2.761807	-2.506083	0.328034
C	3.017888	-3.053564	-0.946070
C	4.320454	-2.983877	-1.442785
H	4.538819	-3.417091	-2.416897
C	5.332093	-2.358763	-0.724477
H	6.336038	-2.297514	-1.136966
C	5.056875	-1.815363	0.522510
H	5.851558	-1.333942	1.089344
C	3.782138	-1.907696	1.089869
C	1.953764	-3.789528	-1.739542
H	0.980301	-3.584530	-1.276565
C	1.870666	-3.321405	-3.188644
H	1.640829	-2.253555	-3.243489
H	1.077018	-3.865081	-3.713460
H	2.803616	-3.507141	-3.733360
C	2.183209	-5.300693	-1.666267
H	3.175570	-5.565734	-2.049378
H	1.441902	-5.837930	-2.267185
H	2.111165	-5.677827	-0.640441
C	3.566110	-1.420883	2.509679
H	2.571087	-1.747879	2.836406
C	4.608483	-1.991679	3.474411
H	4.705760	-3.080255	3.410848
H	4.353333	-1.734555	4.507120
H	5.600027	-1.570755	3.274559
C	3.598035	0.098608	2.581861
H	4.580499	0.476348	2.280966
H	3.406701	0.437737	3.606194
H	2.843805	0.548890	1.931852
C	-2.743558	-2.558845	0.326979
C	-3.745030	-2.005936	1.146600
C	-5.049668	-1.955244	0.644332
H	-5.831600	-1.508274	1.255447
C	-5.364952	-2.490282	-0.595520
H	-6.390178	-2.465441	-0.956215
C	-4.363545	-3.046195	-1.383830
H	-4.613409	-3.442532	-2.364354
C	-3.035348	-3.069914	-0.956437
C	-3.475289	-1.495954	2.550549
H	-2.451261	-1.774678	2.828654
C	-4.437632	-2.088611	3.582674
H	-4.145992	-1.781919	4.591833
H	-4.479312	-3.182266	3.564710
H	-5.459101	-1.727296	3.420289
C	-3.573822	0.023181	2.599252
H	-2.900704	0.494952	1.879808
H	-3.314931	0.399845	3.595244
H	-4.595642	0.345646	2.373815
C	-1.947101	-3.651607	-1.841959
H	-1.039177	-3.062506	-1.661221
C	-2.254713	-3.522738	-3.329003
H	-3.072018	-4.183385	-3.640722
H	-1.375374	-3.802555	-3.916944
H	-2.521235	-2.496927	-3.596479
C	-1.628543	-5.109072	-1.500475
H	-1.189144	-5.224021	-0.504544
H	-0.907169	-5.515149	-2.218704
H	-2.529823	-5.732032	-1.550803
Al	-0.006793	1.442148	-0.455683
S	0.031496	-0.515247	-1.624144
N	-1.442761	2.680397	-0.882797
C	-1.277273	3.773429	-1.644828
C	-0.028640	4.234841	-2.064067
H	-0.031267	5.111157	-2.700355
C	1.220160	3.810208	-1.605885

N	1.402422	2.723832	-0.834986
C	-2.463790	4.592836	-2.062448
H	-3.124814	4.817931	-1.221490
H	-2.144580	5.528591	-2.522068
H	-3.070217	4.045469	-2.789896
C	2.387384	4.680523	-1.972135
H	3.081019	4.153537	-2.631746
H	2.049127	5.583896	-2.480227
H	2.965040	4.966924	-1.088490
C	-2.761798	2.506035	-0.328147
C	-3.017919	3.053548	0.945937
C	-4.320491	2.983825	1.442633
H	-4.538889	3.417059	2.416729
C	-5.332092	2.358641	0.724332
H	-6.336039	2.297357	1.136811
C	-5.056837	1.815224	-0.522639
H	-5.851493	1.333758	-1.089474
C	-3.782096	1.907597	-1.089984
C	-1.953834	3.789572	1.739408
H	-0.980357	3.584608	1.276445
C	-1.870729	3.321482	3.188520
H	-1.640807	2.253651	3.243391
H	-1.077136	3.865234	3.713343
H	-2.803706	3.507150	3.733212
C	-2.183339	5.300726	1.666101
H	-3.175713	5.565737	2.049199
H	-1.442056	5.838004	2.267014
H	-2.111300	5.677842	0.640268
C	-3.566034	1.420794	-2.509791
H	-2.571011	1.747815	-2.836495
C	-4.608402	1.991584	-3.474534
H	-4.705703	3.080157	-3.410956
H	-4.353231	1.734478	-4.507242
H	-5.599940	1.570636	-3.274701
C	-3.597923	-0.098695	-2.582001
H	-4.580386	-0.476469	-2.281143
H	-3.406549	-0.437794	-3.606336
H	-2.843698	-0.548970	-1.931980
C	2.743545	2.558887	-0.326867
C	3.745070	2.006027	-1.146455
C	5.049689	1.955380	-0.644136
H	5.831664	1.508451	-1.255226
C	5.364903	2.490412	0.595737
H	6.390117	2.465611	0.956469
C	4.363442	3.046264	1.384020
H	4.613249	3.442595	2.364561
C	3.035262	3.069938	0.956572
C	3.475398	1.496054	-2.550422
H	2.451379	1.774771	-2.828570
C	4.437778	2.088732	-3.582499
H	4.146170	1.782070	-4.591676
H	4.479463	3.182387	-3.564499
H	5.459240	1.727407	-3.420091
C	3.573945	-0.023080	-2.599128
H	2.900773	-0.494864	-1.879742
H	3.315139	-0.399742	-3.595144
H	4.595749	-0.345536	-2.373611
C	1.946959	3.651591	1.842049
H	1.039032	3.062534	1.661194
C	2.254446	3.522585	3.329107
H	3.071761	4.183161	3.640951
H	1.375073	3.802395	3.917001
H	2.520888	2.496735	3.596511
C	1.628477	5.109087	1.500633
H	1.189175	5.224104	0.504665
H	0.907046	5.515142	2.218818
H	2.529769	5.732019	1.551079

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