

## Supporting Information







*for*

### **On the competition between six-membered and five-membered NHC towards alane centered ring expansion**

Kajal Balayan,<sup>ab</sup> Himanshu Sharma,<sup>bc</sup> Kumar Vanka,<sup>bc</sup> Sapna Ravindranathan,<sup>bd</sup> Rajesh G.  
Gonnade<sup>bc</sup> and Sakya S. Sen<sup>\*ab</sup>

- a. Inorganic Chemistry and Catalysis Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India. E-mail: ss.sen@ncl.res.in*
- b. Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India.*
- c. Physical and Material Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India.*
- d. Central NMR Facility, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India.*

#### **Contents**

-  General procedures and instrumentation
-  Experimental section with spectroscopic evidences
-  Crystallographic data for the structural analysis
-  Miscellaneous Data
-  Computational details
-  References

## ✚ General procedures and instrumentation

All manipulations and experiments were performed in an inert atmosphere of argon using standard Schlenk techniques and in argon filled MBRAUN glove box. The solvents, toluene and hexane were purified by MBRAUN solvent purification system MB SPS-800 and stored over activated 4 Å molecular sieves prior to use. All chemicals were purchased from Sigma Aldrich and TCI chemicals, and used without further purification. The starting materials 6-SIDipp, 5-IDipp, 5-IDipp·AlH<sub>3</sub> and 6-SIDipp·AlH<sub>3</sub> were synthesized by using literature procedure.<sup>1</sup> Deuterated NMR solvents, benzene-*d*<sub>6</sub>, toluene-*d*<sub>8</sub>, and CDCl<sub>3</sub> were stored over 4 Å molecular sieves at least 48 h prior to use. The <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F NMR spectra were recorded in a Bruker Avance DPX 400 and Bruker Avance DPX 500 spectrometer. NMR spectra were referenced to external SiMe<sub>4</sub> (<sup>1</sup>H and <sup>13</sup>C) and CFC1<sub>3</sub> (<sup>19</sup>F) respectively. Melting points were measured in a sealed glass tube on a Stuart SMP-30 melting point apparatus.

## ✚ Experimental section with spectroscopic evidences

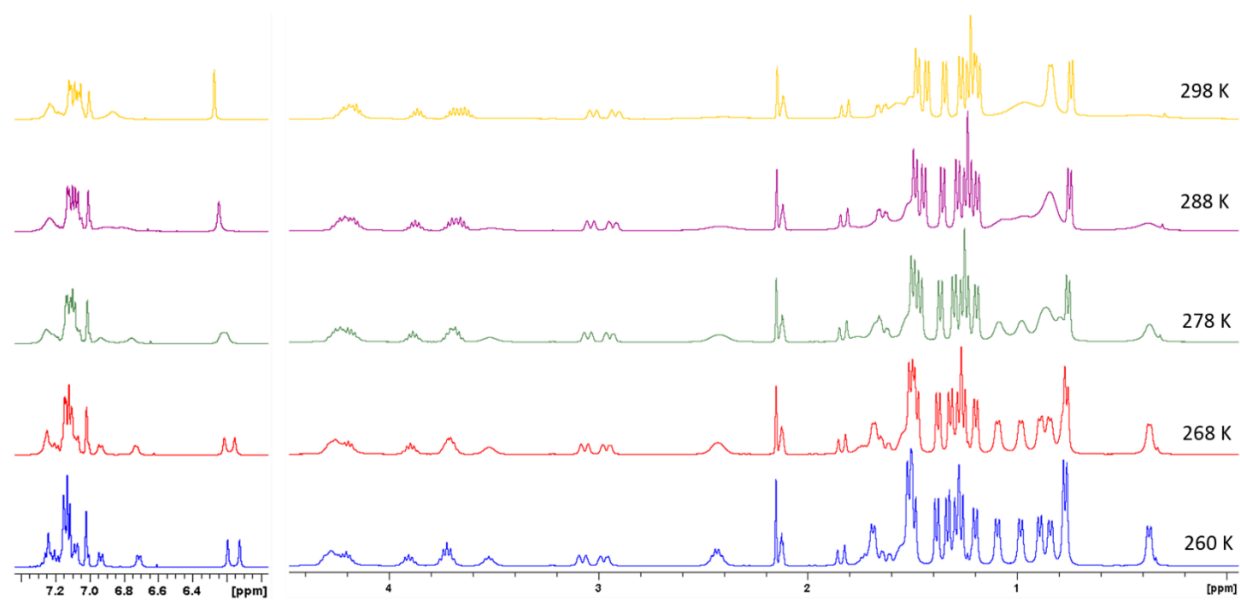
**Synthesis of 2:** Compound **1** (0.200 g, 0.0460 mmol) and IDipp (0.180 g, 0.0464 mmol) were taken together in a Schlenk flask and dissolved in 15 mL toluene at room temperature. The reaction was run for 12 h at 70 °C. After the completion of the reaction, the solution was filtered using a frit. The resulting solution was concentrated to 3 mL and stored it at -4 °C to afford plate shaped colorless crystals of **2** after a day with a yield of 40%.

Melting point: 135 °C.

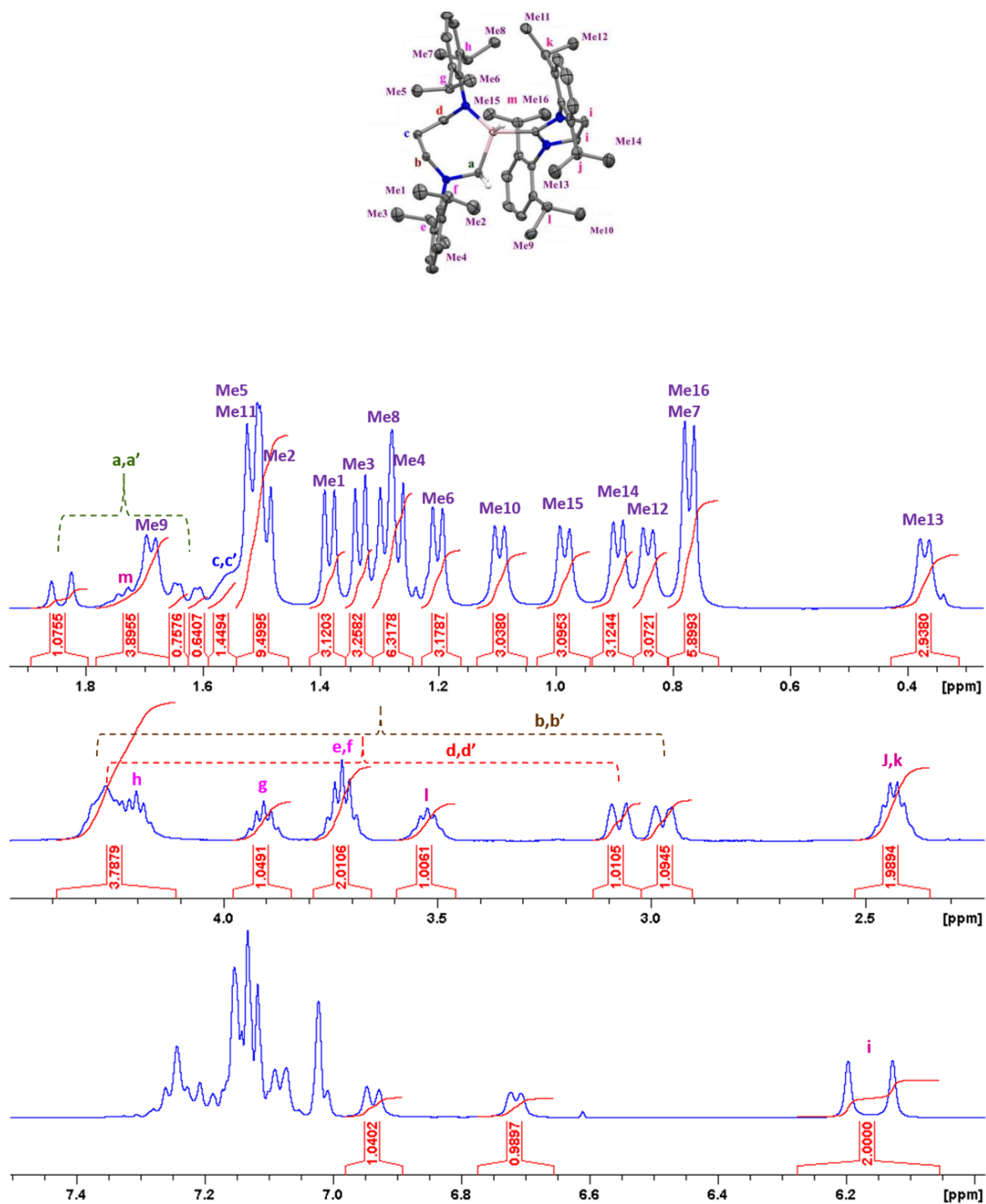
<sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, 298 K, CDCl<sub>3</sub>): 55.8 (CH<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NAI), 55.1 (CH<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NAI), 46.1 (CH<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NAI), 34.8 (CH<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NAI) ppm.

<sup>27</sup>Al{<sup>1</sup>H} NMR (130.38 MHz, 298 K, CDCl<sub>3</sub>): No signal found.

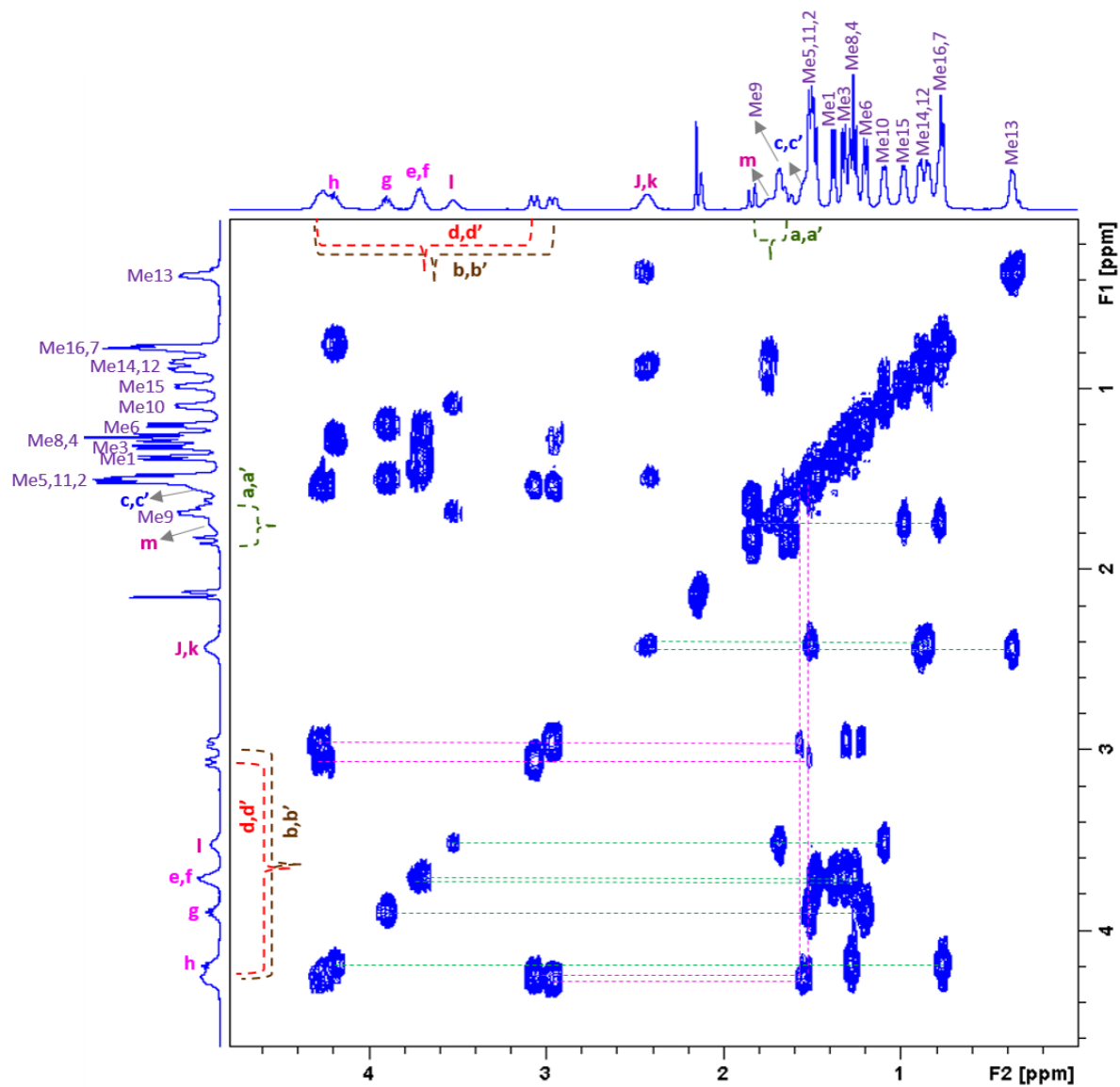
IR (Al-H stretching): 1800.03 cm<sup>-1</sup>.



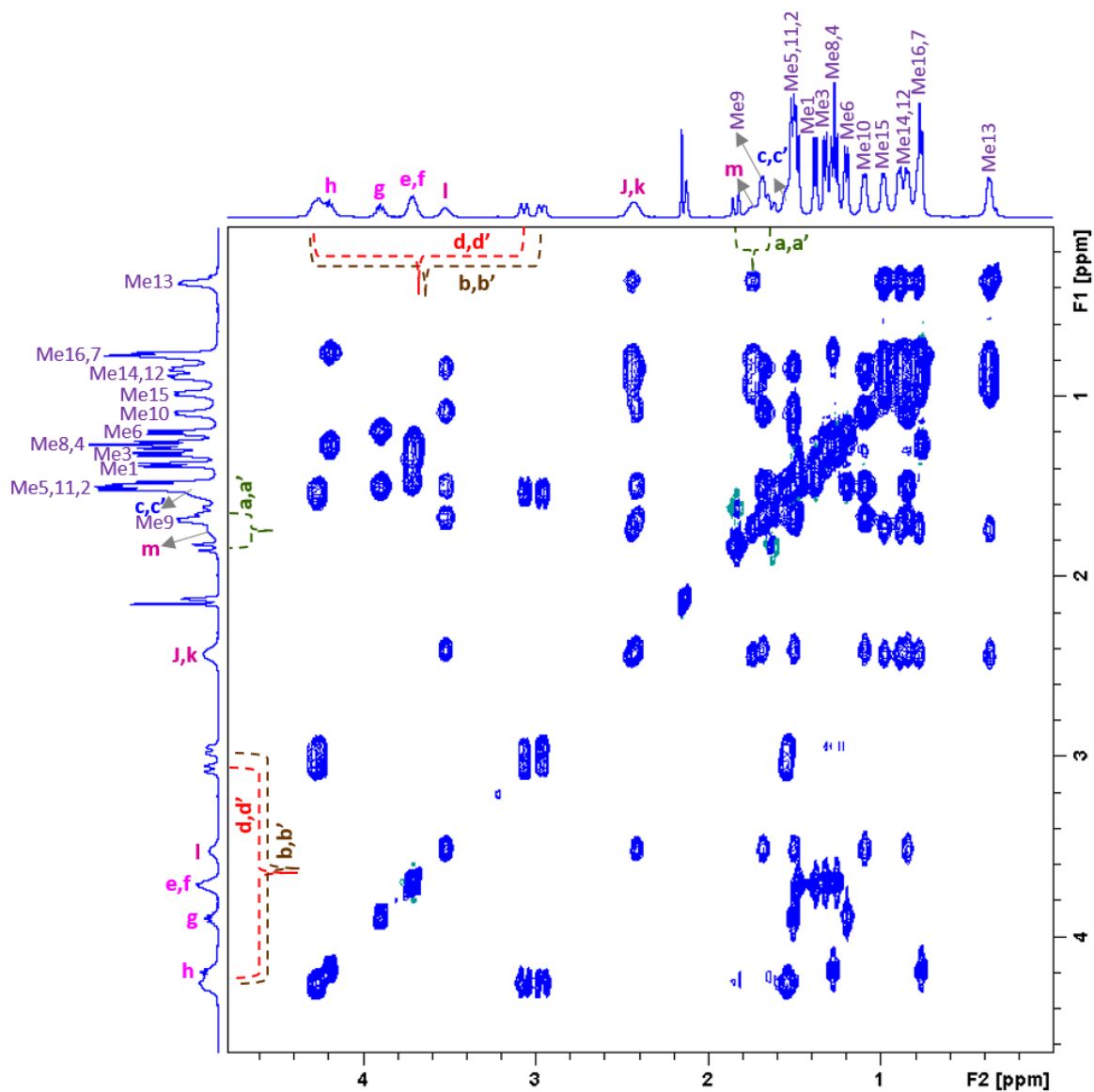
**Figure S1:** Temperature dependence of the  $^1\text{H}$  NMR spectrum of **2** recorded in  $\text{toluene-}d_8$  on a 400 MHz spectrometer.



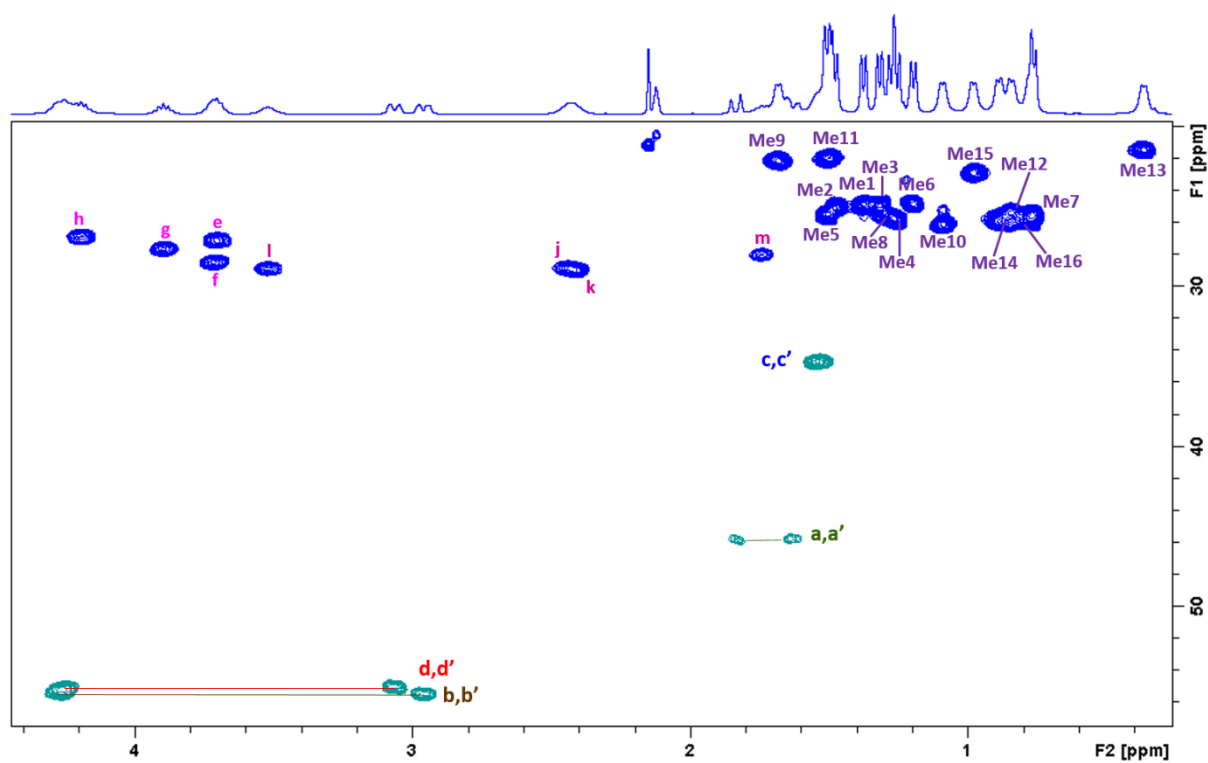
**Figure S2:**  $^1\text{H}$  NMR spectrum of **2** in  $\text{toluene-}d_8$ , recorded at 260 K on a 400 MHz spectrometer. Assignments of aliphatic protons are indicated, with non-equivalent protons of methylene groups connected by braces. Aromatic protons could not be assigned individually due to overlap with residual solvent signal.



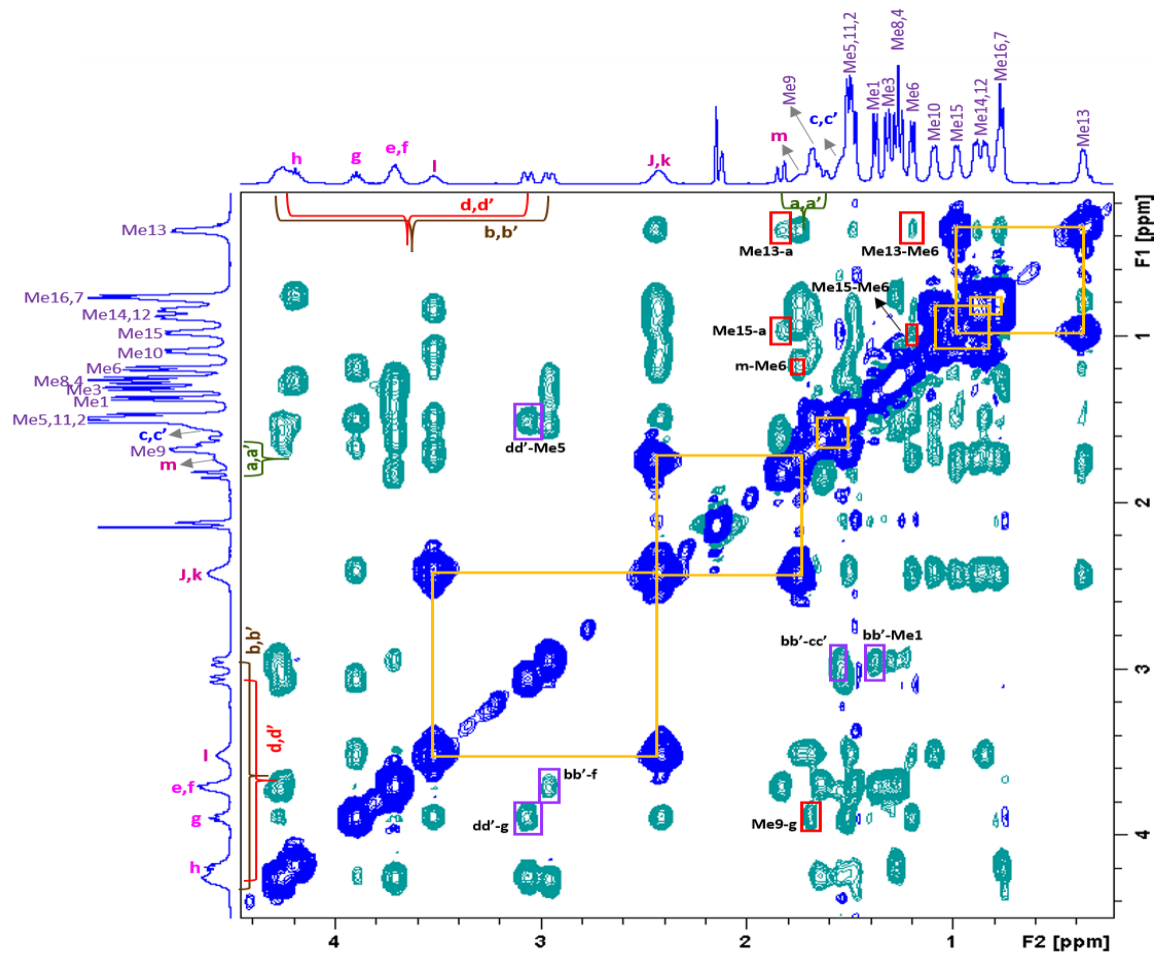
**Figure S3:** Aliphatic region of the COSY spectrum of **2** in toluene-*d*<sub>8</sub>, recorded at 268 K on a 400 MHz spectrometer. Methylene proton J-coupled connections are indicated in magenta while methine to methyl J-coupled connections are shown in green.



**Figure S4:** Aliphatic region of the TQSY spectrum of **2** in toluene- $d_8$ , recorded at 268 K on a 400 MHz spectrometer, showing extended J-coupled connectivities.

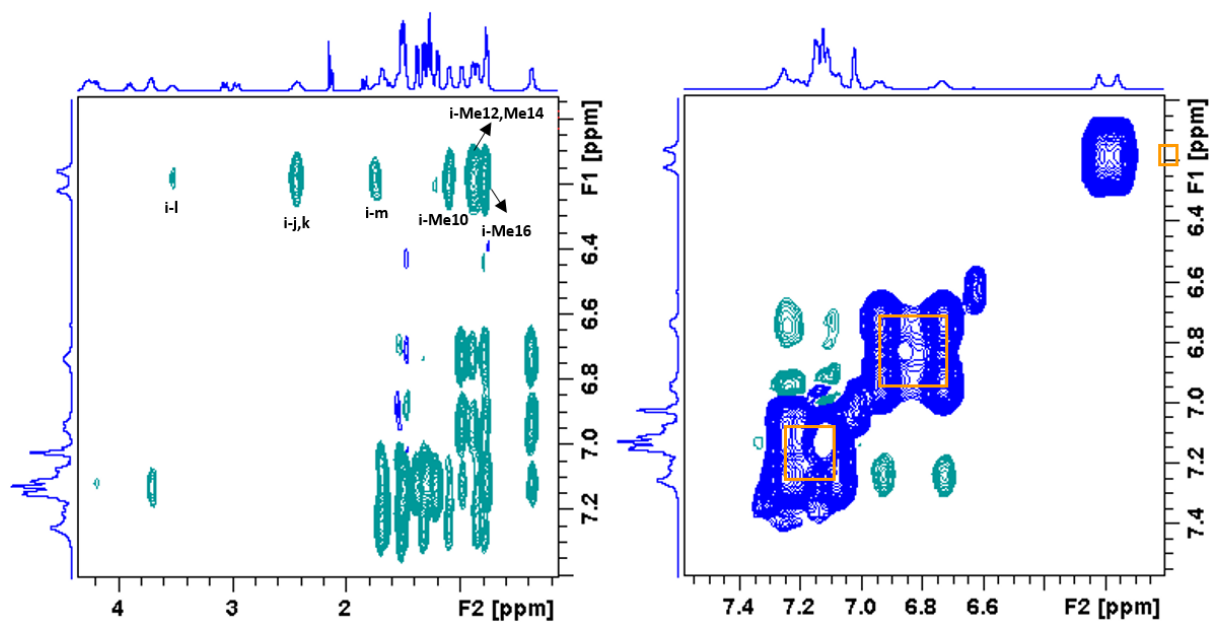


**Figure S5:** Aliphatic region of the  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of **2** in toluene- $d_8$ , recorded at 268 K on a 400 MHz spectrometer.

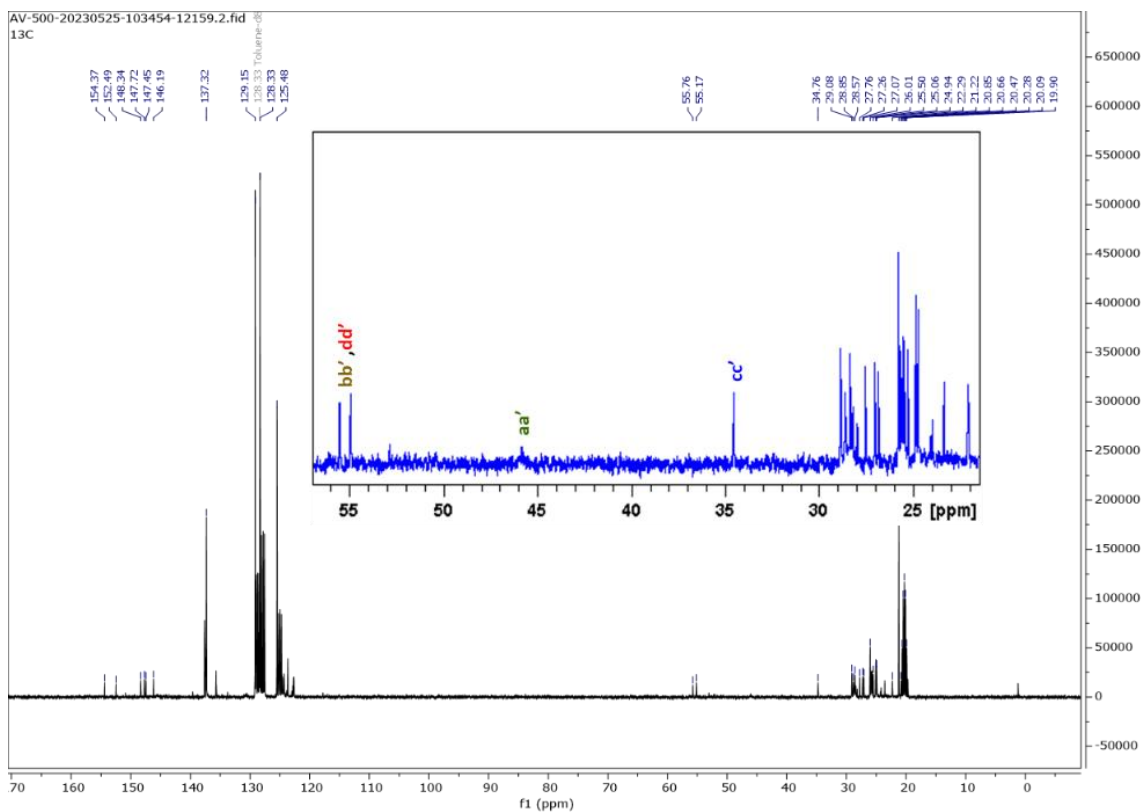


**Figure S6:** Aliphatic region of the ROESY spectrum of **2** in toluene- $d_8$ , recorded at 268 K on a 400 MHz spectrometer. Yellow squares indicate exchange connected protons which show positive cross peaks (**m** to **j**, **i** to **k**, **Me12** to **Me10**, **Me11** to **Me9**, **Me14** to **Me16** etc). Only protons from the 5-IDipp unit shows exchange, indicating this unit flips end-to-end by rotation around the Al-C<sub>IDipp</sub> bond. Negative cross peaks arise from spatial proximity ( $\leq 0.5$  nm) between proton pairs. Cross-peaks marked by red squares show inter-unit proton connections arising due to spatial proximity between the two units of **2** (6-SIDipp and 5-IDipp) while purple squares show spatial connections between protons within 6-SIDipp which were crucial for signal assignments. Flipping of the 5-IDipp unit results in shared spatial proximity cross peaks between exchange connected proton pairs of 5-IDipp and protons in the 6-SIDipp unit.

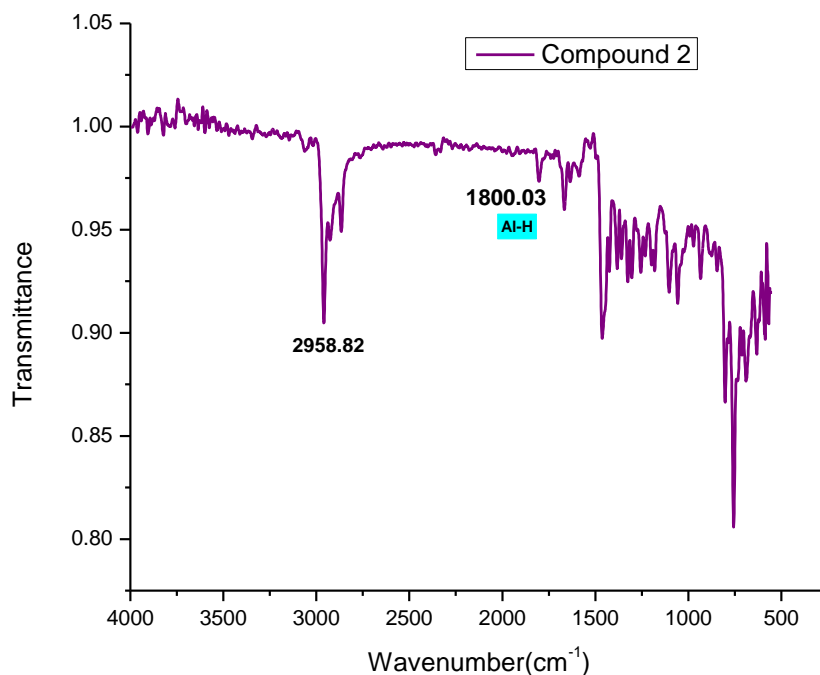




**Figure S7:** Aromatic region of the ROESY spectrum of **2** in toluene- $d_8$ , recorded at 268 K on a 400 MHz spectrometer. Negative cross peaks arising from spatial proximity between protons **i** and aliphatic protons in the 5-IDipp unit are labelled. Yellow squares indicate positive exchange cross peaks connecting aromatic protons of the 5-IDipp. The aromatic protons could not be assigned due to overlap with residual solvent signal.



**Figure S8:**  $^{13}\text{C}\{^1\text{H}\}$  spectrum of **2** in toluene- $d_8$  recorded at 298K on a 400 MHz spectrometer. Aliphatic region is expanded and assignments of methylene carbons are indicated. At 298K several methyl and methine carbon peaks are too broad to be detected, due to rotation around the Al-C bond. Full assignments at 268K are indicated in the HSQC spectrum.



**Figure S9:** IR (ATR) spectrum of **2**.

**Synthesis of 3:** **1** (0.200 g, 0.46 mmol) was dissolved in 10 mL toluene and the solution was cooled to  $-78\text{ }^{\circ}\text{C}$  in a Schlenk flask. After that, a precooled solution of  $\text{CH}_3\text{OTf}$  (0.083 g, 0.50 mmol) in 5 mL toluene was transferred to the flask containing **1** using a cannula. The reaction was run for 30 min at  $-78\text{ }^{\circ}\text{C}$  and slowly allowed to come to room temperature and stirred overnight. The resulting solution was turbid and a white precipitate was isolated by filtration using a cannula and identified as **3**. Colorless crystals of **3** were obtained by concentrating the filtrate part and stored it at  $-4\text{ }^{\circ}\text{C}$  to afford colorless crystals of **3** after one day with a yield of 60%.

The same procedure was followed with TMSOTf.

**Melting point:**  $152\text{ }^{\circ}\text{C}$ .

$^1\text{H NMR}$  (400 MHz, 298 K,  $\text{CDCl}_3$ ): 1.28 (d,  $J = 6.75\text{ Hz}$ , 12 H,  $\text{CH}(\text{CH}_3)_2$ ), 1.41 (d,  $J = 6.63\text{ Hz}$ , 12 H,  $\text{CH}(\text{CH}_3)_2$ ), 2.40 (quintet,  $J = 4.75\text{ Hz}$ , 2 H,  $\text{NCH}_2\text{CH}_2\text{CH}_2\text{N}$ ), 3.03 (sept,  $J = 6.88\text{ Hz}$ , 4 H,  $\text{CH}(\text{CH}_3)_2$ ), 3.56 (t,  $J = 5.25\text{ Hz}$ , 4 H,  $\text{NCH}_2\text{CH}_2\text{CH}_2\text{N}$ ), 7.22-7.24 (m, 4H, Ar-H), 7.42 (t,  $J = 7.75\text{ Hz}$ , 2H, Ar-H) ppm.

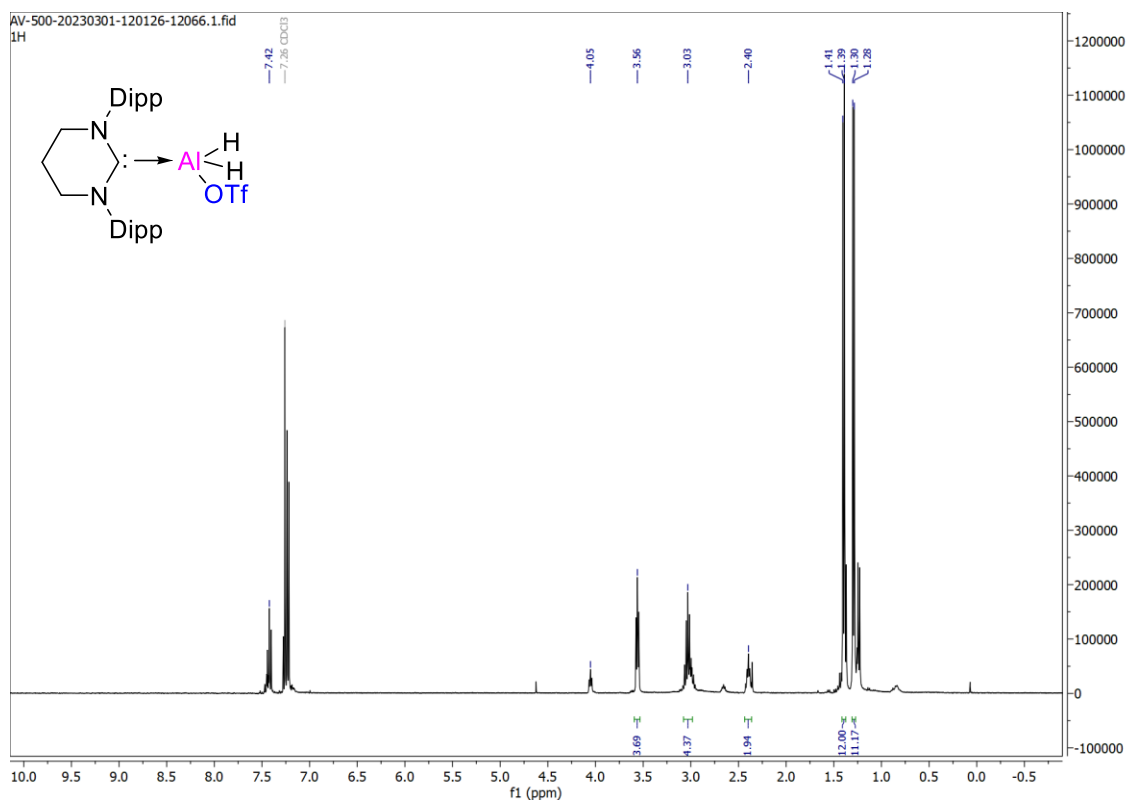
$^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, 298 K,  $\text{CDCl}_3$ ): 19.2 ( $\text{NCH}_2\text{CH}_2$ ), 24.9 ( $\text{CH}(\text{CH}_3)_2$ ), 24.9 ( $\text{CH}(\text{CH}_3)_2$ ), 29.0 ( $\text{CH}(\text{CH}_3)_2$ ), 48.6 ( $\text{NCH}_2$ ), 125.3 (*p*-Ar), 131.5 (*m*-Ar), 135.8 (*o*-Ar), 145.8 (*ipso*-Ar) ppm, NCN signal not observed.

$^{19}\text{F}\{^1\text{H}\}$  NMR (377 MHz, 298 K,  $\text{CDCl}_3$ ): -77.2 (s, 3F,  $\text{AlH}_2\text{OSO}_2\text{CF}_3$ ) ppm.

$^{27}\text{Al}\{^1\text{H}\}$  NMR (130.38 MHz, 298 K,  $\text{CDCl}_3$ ): No signal found.

IR(Al-H stretching):  $1874.26\text{ cm}^{-1}$ .

Elemental analysis: calcd. C, 59.78, H, 7.27, N, 4.81; found C, 57.14, H, 5.91, N, 5.32. The observed values deviate from the calculated one due to the sensitivity of the crystals.



**Figure S10:**  $^1\text{H}$  NMR spectrum of **3**.

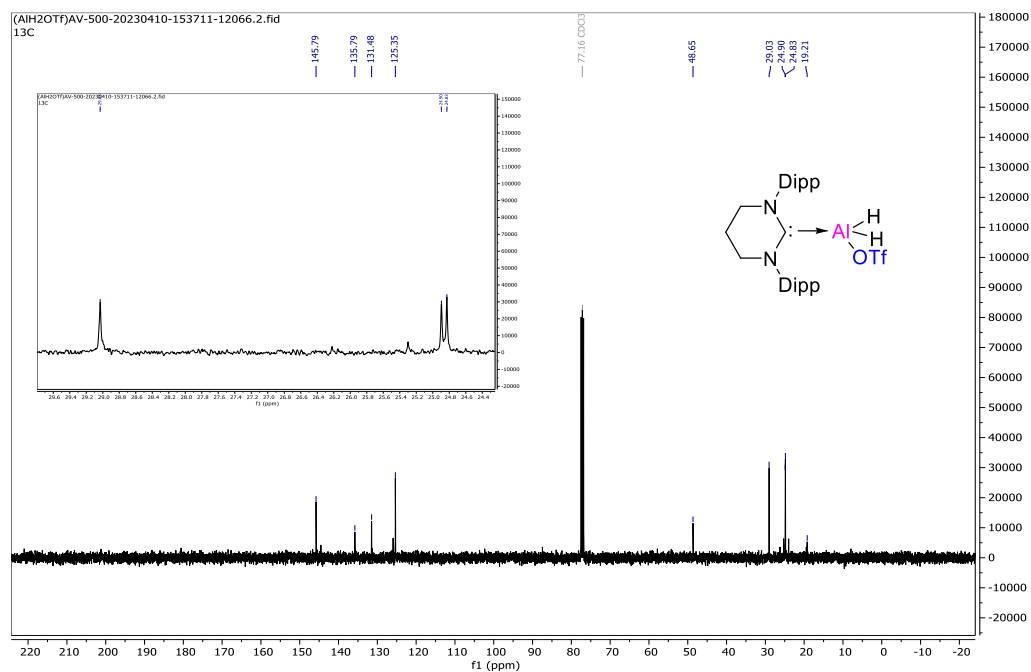


Figure S11:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3**.

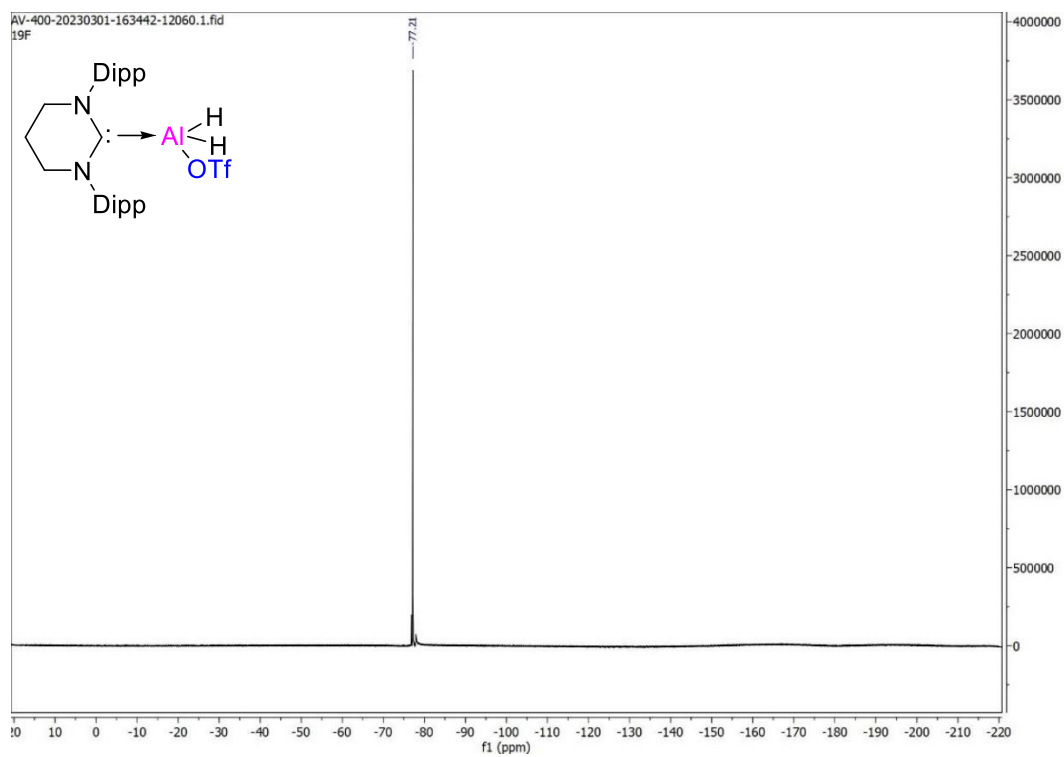


Figure S12:  $^{19}\text{F}\{^1\text{H}\}$  NMR of **3**.

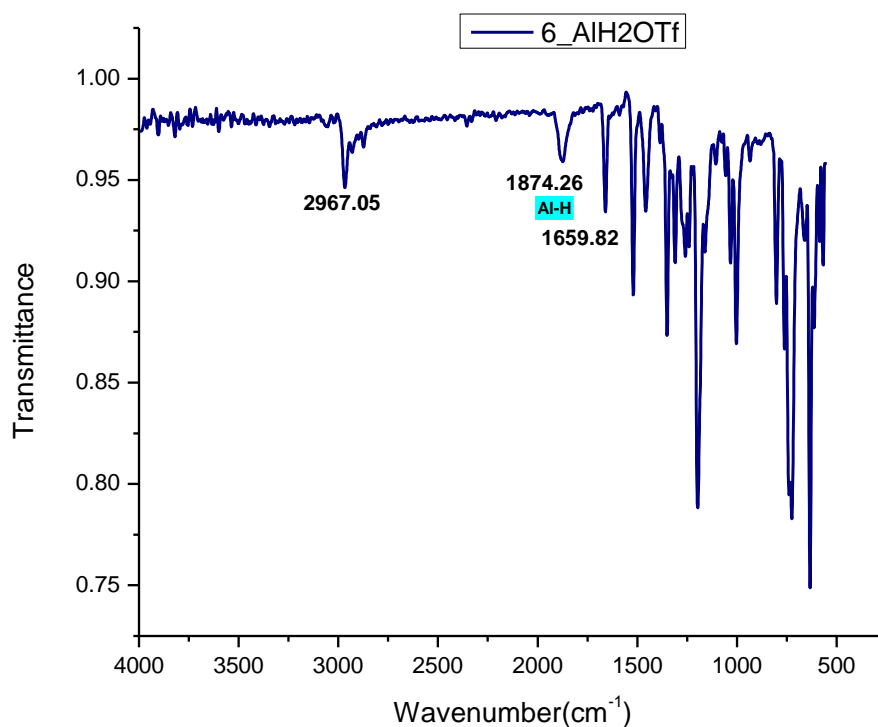


Figure S13: IR (ATR) spectrum of **3**.

### Synthesis of **4**

**1** (0.200 g, 0.46 mmol) and 0.5 equivalent  $I_2$  (0.058 g, 0.23 mmol) were taken in a Schlenk flask and 15 mL toluene was added to the reaction mixture at 0 °C. The reaction was stirred for 1 h at low temperature and another 1 h at room temperature. After the completion of the reaction, the solution was filtered using a frit and the toluene solution was concentrated. Storing the solution at -4 °C yielded colorless crystals of **4** after one day with a yield of 47%. **Melting point:** 148 °C.

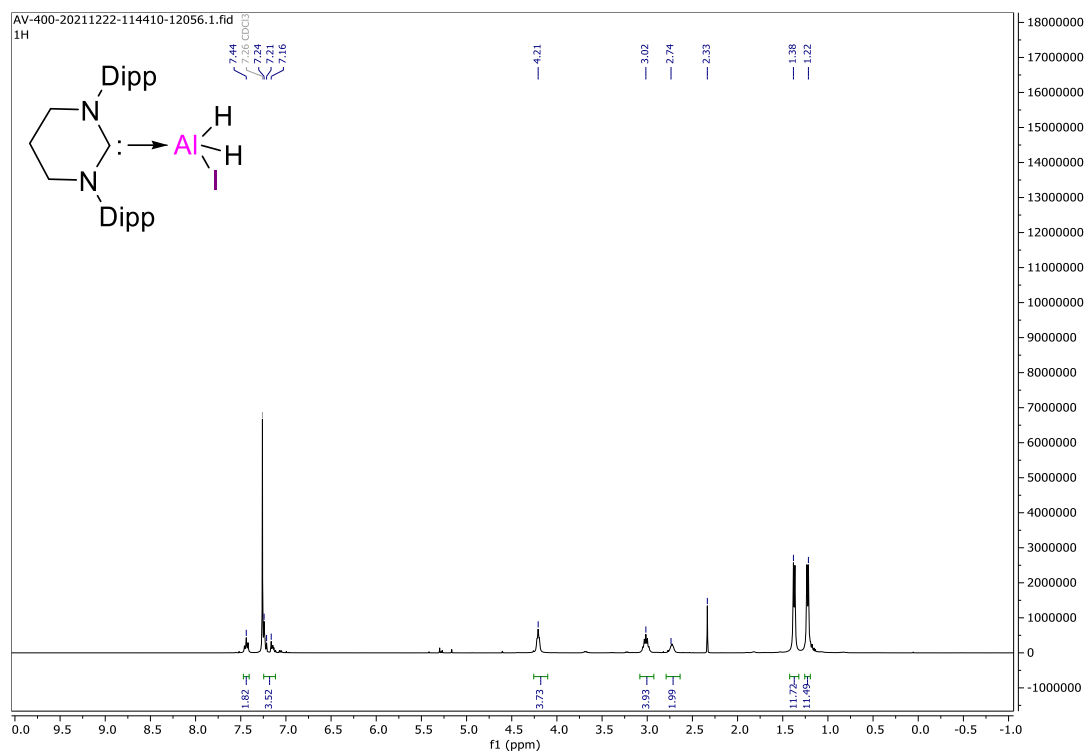
$^1H$  NMR (400 MHz, 298 K,  $CDCl_3$ ): 1.22 (d,  $J = 6.75$  Hz, 12 H,  $CH(CH_3)_2$ ), 1.38 (d,  $J = 6.63$  Hz, 12 H,  $CH(CH_3)_2$ ), 2.74 (quintet,  $J = 4.75$  Hz, 2 H,  $NCH_2CH_2CH_2N$ ), 3.02 (sept,  $J = 6.88$  Hz, 4 H,  $CH(CH_3)_2$ ), 4.21 (t,  $J = 5.25$  Hz, 4 H,  $NCH_2CH_2CH_2N$ ), 7.16-7.24 (m, 4H, Ar-H), 7.44 (t,  $J = 7.75$  Hz, 2H, Ar-H) ppm.

$^{13}C\{^1H\}$  NMR (101 MHz, 298 K,  $CDCl_3$ ): 19.6 ( $NCH_2CH_2$ ), 24.5 ( $CH(CH_3)_2$ ), 26.7 ( $CH(CH_3)_2$ ), 28.9 ( $CH(CH_3)_2$ ), 52.4 ( $NCH_2$ ), 125.6 (*p*-Ar), 130.6 (*m*-Ar), 139.8 (*o*-Ar), 146.2 (*ipso*-Ar) ppm, NCN signal not observed.

$^{27}\text{Al}\{^1\text{H}\}$  NMR (130.38 MHz, 298 K,  $\text{CDCl}_3$ ): 121.9 ppm

IR (Al-H stretching): 1746.62  $\text{cm}^{-1}$ .

Elemental analysis: calcd. C, 60.00, H, 7.55, N, 5.00; found C, 59.12, H, 7.05, N, 5.32



**Figure S14:**  $^1\text{H}$  NMR spectrum of **4**.

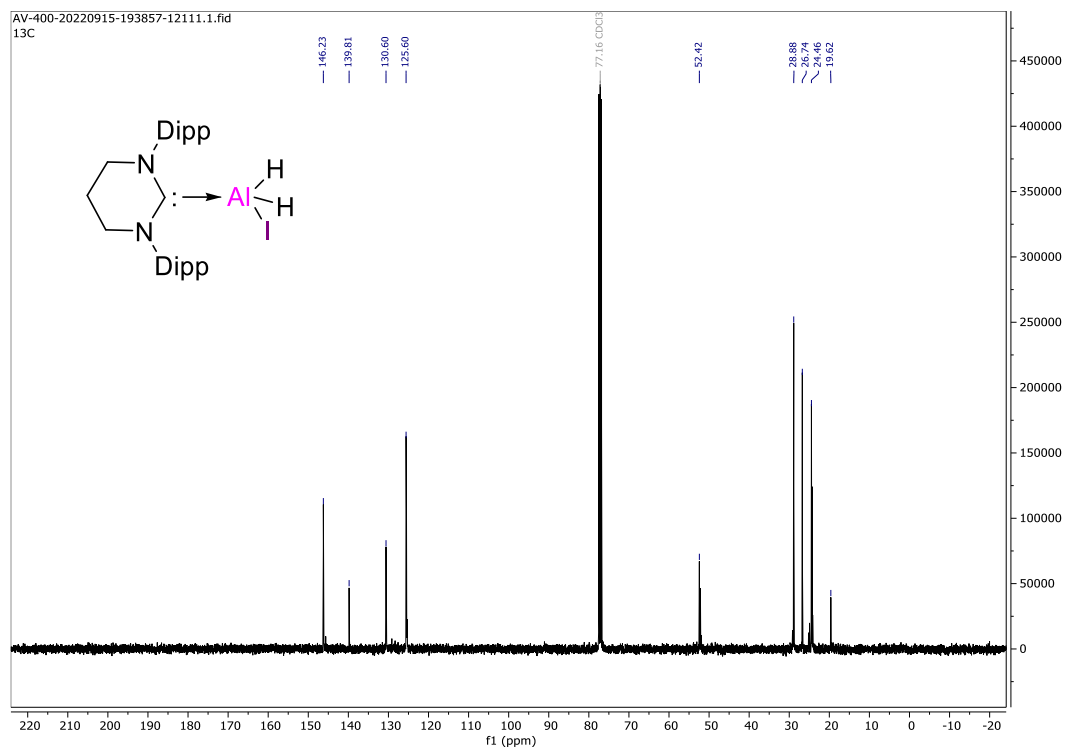


Figure S15:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4.

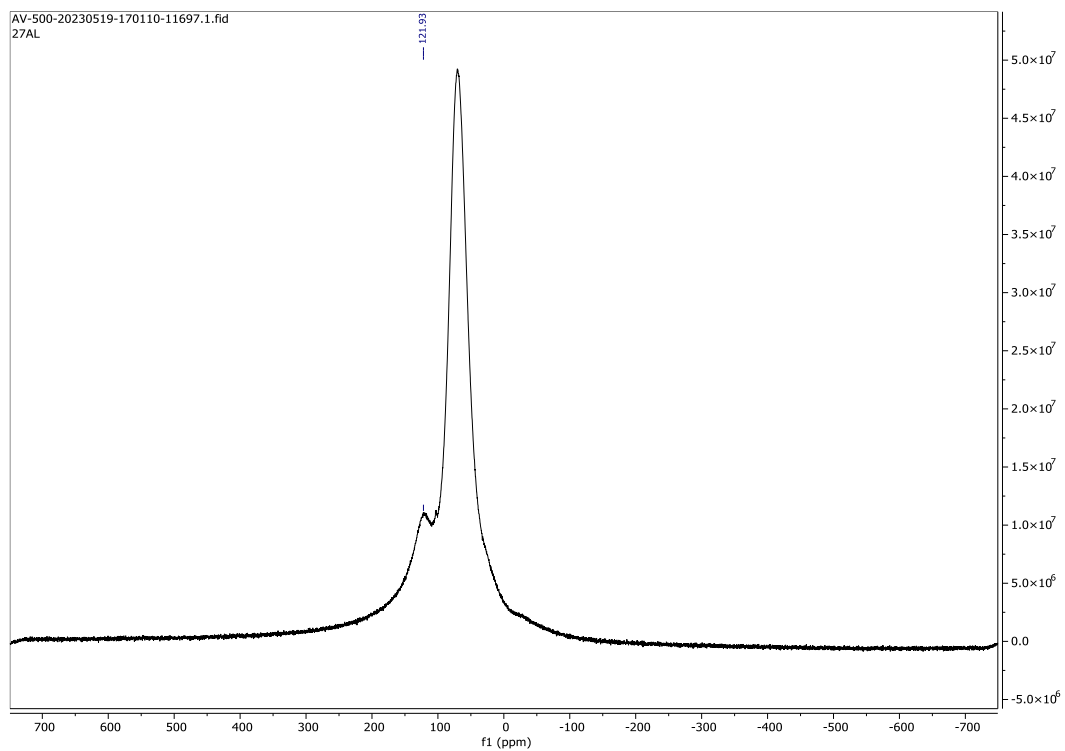
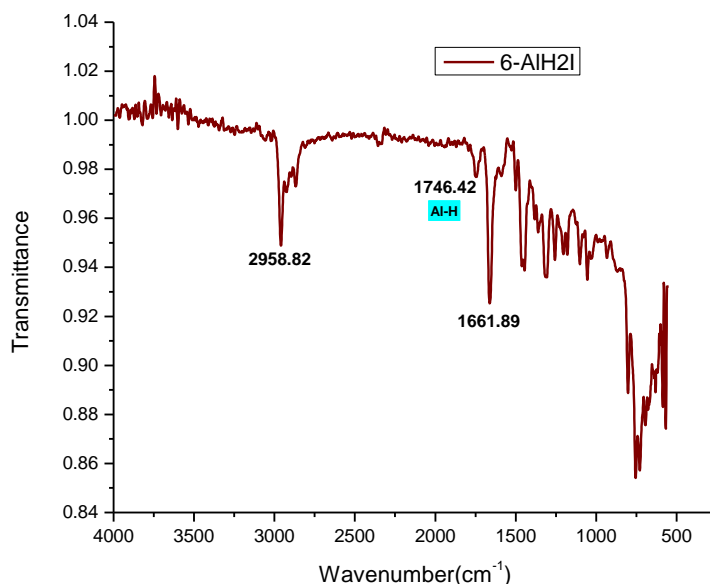


Figure S16:  $^{27}\text{Al}\{^1\text{H}\}$  NMR spectrum of 4.





**Figure S17:** IR (ATR) spectrum of **4**.

### Synthesis of **5**

**1** (0.200 g, 0.46 mmol) was dissolved in 10 mL toluene and the solution was cooled to 0 °C. After that, excess Br<sub>2</sub> (0.047 mL, 0.97 mmol) was added drop by drop to the solution. The reaction was run for 4 h at room temperature giving an orange colored slurry. The orange precipitate was isolated by filtration using a cannula and characterized as **5**. Colorless crystals of **5** were obtained by concentrating the filtrate solution and storing at -4 °C with a yield of 80%.

**Decomposition** at 180 °C.

<sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>): 1.28 (d, J = 6.75 Hz, 12 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.49 (d, J = 6.63 Hz, 12 H, CH(CH<sub>3</sub>)<sub>2</sub>), 2.40 (quintet, J = 4.75 Hz, 2 H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N), 3.27 (sept, J = 6.63 Hz, 4 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.65 (t, J = 5.38 Hz, 4 H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N), 7.24-7.26 (m, 4H, Ar-H), 7.41 (t, J = 7.75 Hz, 2H, Ar-H) ppm.

<sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, 298 K, CDCl<sub>3</sub>): 19.7 (NCH<sub>2</sub>CH<sub>2</sub>), 24.5 (CH(CH<sub>3</sub>)<sub>2</sub>), 26.8 (CH(CH<sub>3</sub>)<sub>2</sub>), 28.9 (CH(CH<sub>3</sub>)<sub>2</sub>), 52.4 (NCH<sub>2</sub>), 125.6 (*p*-Ar), 130.6 (*m*-Ar), 139.8 (*o*-Ar), 146.2 (*ipso*-Ar) ppm, NCN signal not observed.

<sup>27</sup>Al{<sup>1</sup>H} NMR (104.3 MHz, 298 K, CDCl<sub>3</sub>): = 81.1 ppm.

IR: No peak in the region 1740-1900 cm<sup>-1</sup>.

Elemental analysis: calcd. C, 50.10, H, 6.01, N, 4.17; found C, 52.23, H, 6.67, N, 4.78

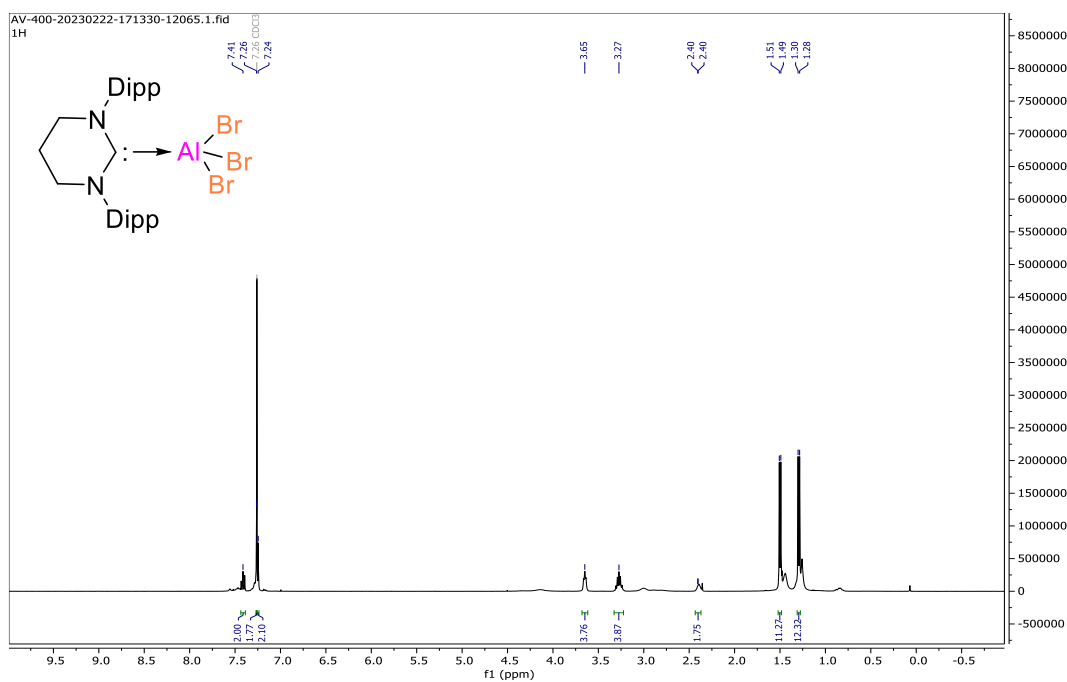


Figure S18:  $^1\text{H}$  NMR spectrum of **5**.

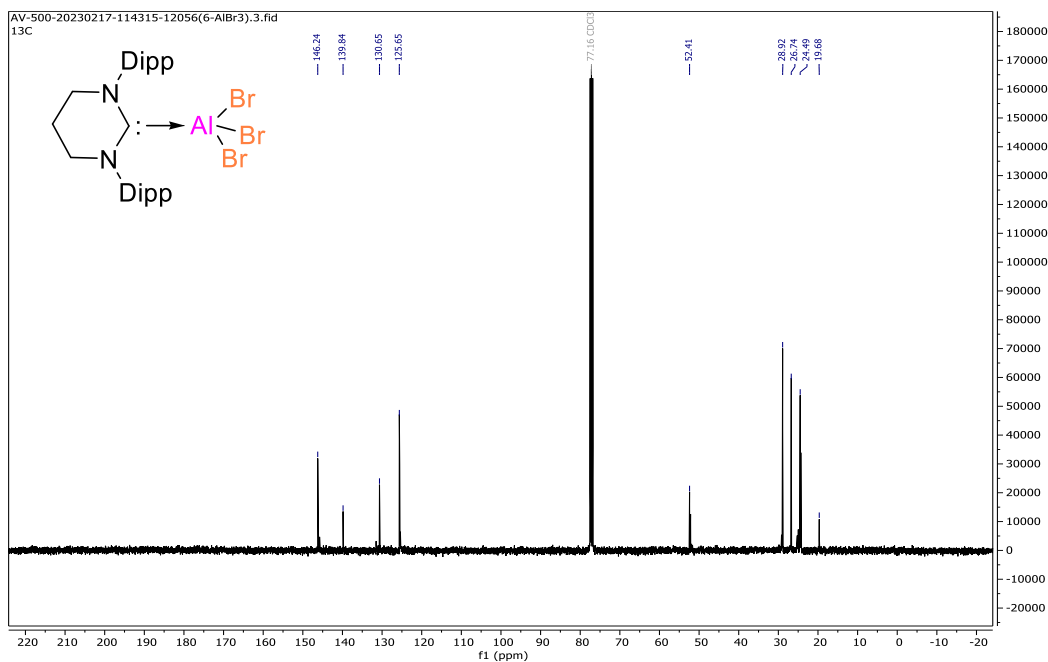
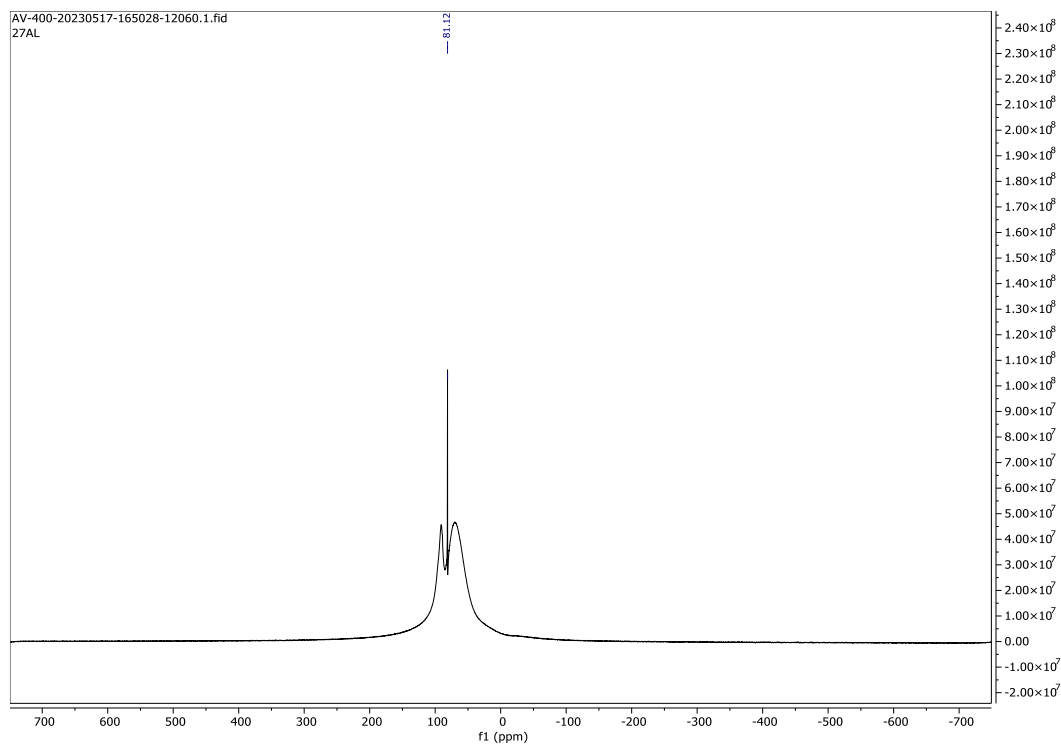
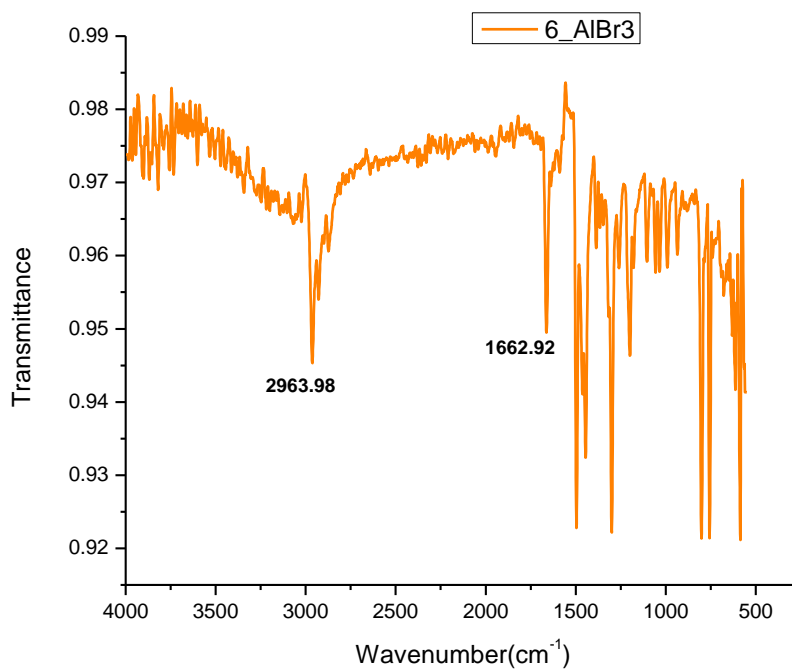


Figure S19:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **5**.



**Figure S20:**  $^{27}\text{Al}\{^1\text{H}\}$  NMR spectrum of **5**.



**Figure S21:** IR (ATR) spectrum of **5**.

## ✚ Crystallographic data for the structural analysis

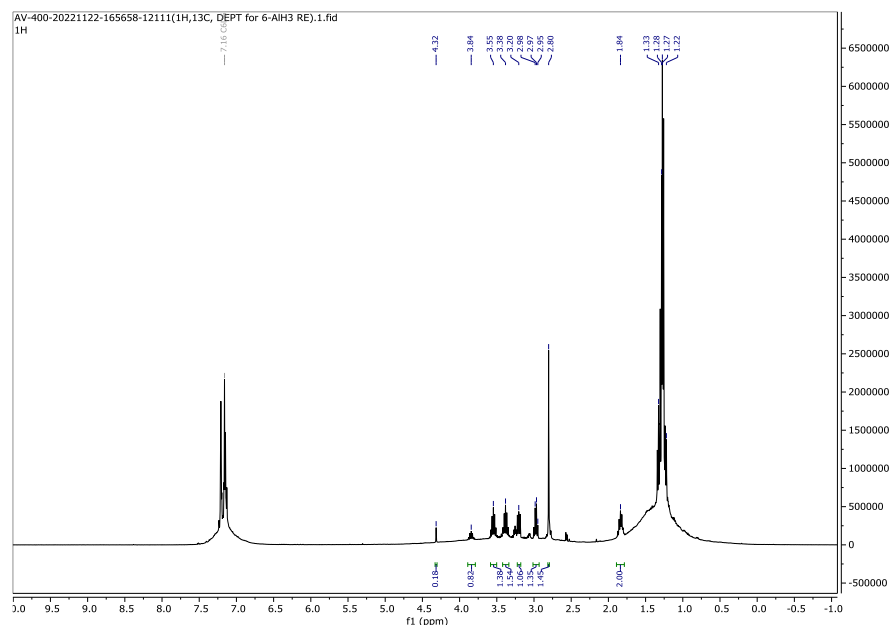
X-ray intensity data measurements were carried out on a Bruker SMART APEX II single crystal X-ray CCD diffractometer with graphite-monochromatized (Mo-K $\alpha$  = 0.71073 Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with  $\omega$  scan width of 0.5° at different settings of  $\phi$  and  $2\theta$  keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2006).<sup>2</sup> All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full-matrix least-squares refinement on  $F^2$ .<sup>3</sup> All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An ORTEPIII<sup>4</sup> view of **2**, **3** and **5** were drawn with 50% probability displacement ellipsoids and H atoms omitted for clarity.

Identification code	6_REAIH3_file001 (2)	AIH2OTf_3 (3)	mo_Kb_AlBr3_5_0ma_a (5)
<b>Empirical formula</b>	C <sub>117</sub> H <sub>165</sub> N <sub>8</sub> Al <sub>2</sub>	C <sub>29</sub> H <sub>42</sub> N <sub>2</sub> O <sub>3</sub> F <sub>3</sub> AlS	C <sub>28</sub> H <sub>40</sub> AlBr <sub>3</sub> N <sub>2</sub>
<b>Formula weight</b>	1737.53	582.68	671.33
<b>Temperature/K</b>	100(2)	100(2)	100(2)
<b>Crystal system</b>	triclinic	orthorhombic	monoclinic
<b>Space group</b>	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<b>a/Å</b>	11.973(3)	10.812(7)	21.7906(14)
<b>b/Å</b>	12.393(3)	16.198(11)	17.5474(11)
<b>c/Å</b>	20.373(4)	17.618(13)	17.0364(12)
<b><math>\alpha</math>/°</b>	99.341(7)	90	90
<b><math>\beta</math>/°</b>	93.667(7)	90	111.758(2)
<b><math>\gamma</math>/°</b>	113.676(7)	90	90
<b>Volume/Å<sup>3</sup></b>	2703.7(10)	3086(4)	6050.1(7)
<b>Z</b>	1	4	8
<b><math>\rho_{\text{calc}}/\text{cm}^3</math></b>	1.067	1.254	1.474
<b><math>\mu/\text{mm}^{-1}</math></b>	0.076	0.183	4.048
<b>F(000)</b>	949.0	1240.0	2720.0
<b>Crystal size/mm<sup>3</sup></b>	0.32 × 0.24 × 0.15	0.15 × 0.12 × 0.09	0.15 × 0.11 × 0.08
<b>Radiation</b>	MoK $\alpha$ ( $\lambda$ = 0.71073)	MoK $\alpha$ ( $\lambda$ = 0.71073)	MoK $\alpha$ ( $\lambda$ = 0.71073)
<b>2<math>\theta</math> range for data collection/°</b>	4.396 to 55.998	4.53 to 57.762	4.784 to 60.23
<b>Index ranges</b>	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -26 ≤ l ≤ 26	-14 ≤ h ≤ 14, -21 ≤ k ≤ 21, -23 ≤ l ≤ 23	-30 ≤ h ≤ 29, -24 ≤ k ≤ 24, -20 ≤ l ≤ 24
<b>Reflections collected</b>	144125	188548	111318

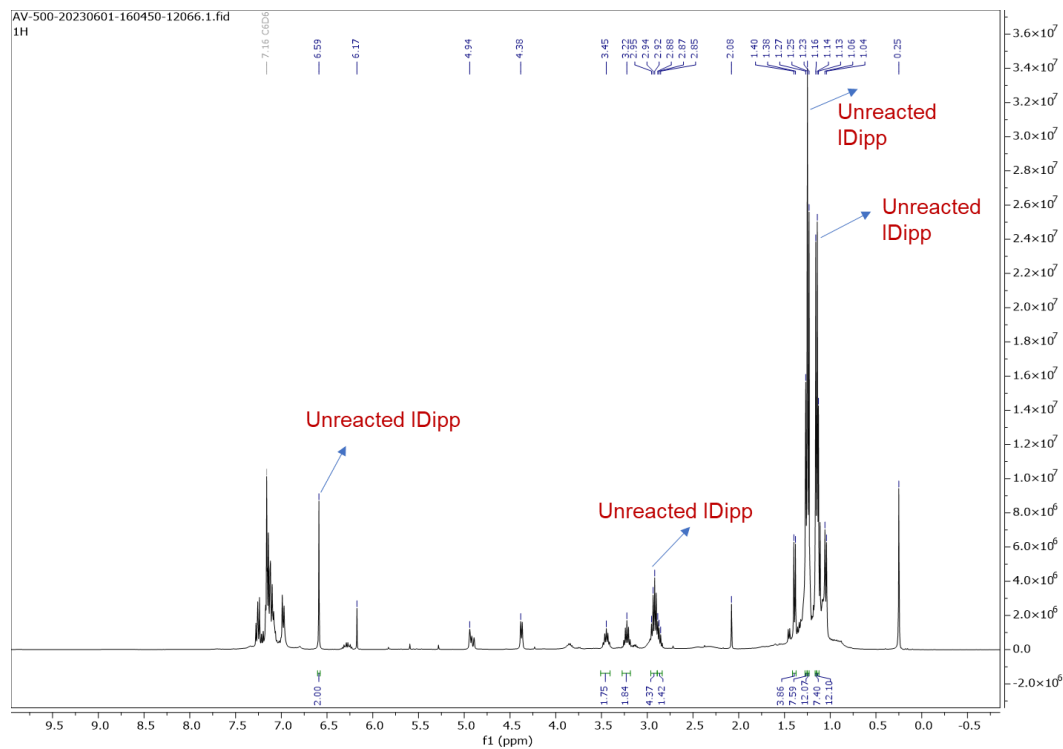
<b>Independent reflections</b>	13033 [ $R_{\text{int}} = 0.0771$ , $R_{\text{sigma}} = 0.0375$ ]	7939 [ $R_{\text{int}} = 0.1607$ , $R_{\text{sigma}} = 0.0629$ ]	17722 [ $R_{\text{int}} = 0.1288$ , $R_{\text{sigma}} = 0.1149$ ]
<b>Data/restraints/parameters</b>	13033/21/597	7939/0/368	17722/0/629
<b>Goodness-of-fit on <math>F^2</math></b>	1.043	1.047	1.009
<b>Final R indexes [<math>I \geq 2\sigma(I)</math>]</b>	$R_1 = 0.0543$ , $wR_2 = 0.1276$	$R_1 = 0.0491$ , $wR_2 = 0.1164$	$R_1 = 0.0633$ , $wR_2 = 0.0994$
<b>Final R indexes [all data]</b>	$R_1 = 0.0719$ , $wR_2 = 0.1393$	$R_1 = 0.0791$ , $wR_2 = 0.1252$	$R_1 = 0.1452$ , $wR_2 = 0.1207$
<b>Largest diff. peak/hole / <math>e \text{ \AA}^{-3}</math></b>	1.27/-0.71	0.59/-0.48	1.96/-1.50
<b>Flack parameter</b>		0.48(3)	
<b>CCDC Number</b>	2249120	2249128	2249125

### ✚ Miscellaneous Data

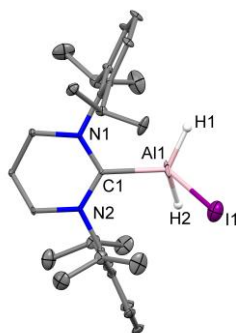
This section provides NMRs of unsuccessful/inconclusive reactions and solid-state structure of compound **4**.



**Figure MS1:**  $^1\text{H}$  NMR of the reaction when **1** was heated at  $80^\circ\text{C}$  for 27 h.



**Figure MS2:**  $^1\text{H}$  NMR of the reaction mixture when **3** was heated in presence of IDipp at 70 °C.



**Figure MS3:** The solid-state structure of **4**.

### ✚ Computational details

All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 7.5.0 suite of programs,<sup>5</sup> using the PBE functional,<sup>6</sup> and def-TZVP basis set<sup>7</sup> for all the atoms. We also used Grimme Dispersion correction (D3)<sup>8</sup> for considering the long-range interactions. The resolution of identity (RI),<sup>9</sup> along with the multipole accelerated resolution of identity (marij)<sup>10</sup> approximations have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent corrections were incorporated with

optimization calculations using the COSMO model,<sup>11</sup> with toluene ( $\epsilon = 2.38$ ) as the solvents. In addition, the intrinsic reaction coordinate (IRC)<sup>12</sup> calculations were done with all the transition states in order to further confirm that they were the correct transition state, yielding the correct reactant and product structures. The values reported are  $\Delta G$  values, with zero-point energy corrections, internal energy, and entropic contributions included through frequency calculations on the optimized minima, with the temperature set to 298.15 K. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition state structures. The conformational search analysis has been done with Grimme's semi-empirical Conformer–Rotamer Ensemble Sampling Tool (CREST)<sup>13</sup> at the xTB-GFN2<sup>14-16</sup> levels of theory.

**Table S1:** The electronic energy (EE), enthalpy(H), entropy (S), Gibb's free energy (G), and imaginary frequency data for all compounds and transition states are provided here.

PBE-D3/def2-TZVP (COSMO $\epsilon=2.38$ ), Temperature 298.15 K						
S.N.	Structure	EE (kcal/mol)	H(kJ/mol)	S(kJ/mol/K)	G(kcal/mol)	Imaginary Frequency
1.	6-SIDipp·AlH <sub>3</sub>	-905792.2005	1725.7	0.91984	346.8964793	No
2.	5-IDipp	-727214.8617	1523.36	0.85711	303.0072242	No
3.	Adduct (A)	-1633027.26	3251.59	1.54788	666.8314091	No
4.	TS1	-1633000.003	3248.12	1.48534	670.4585451	1, at -608.71 cm <sup>-1</sup>
5.	Int 1	-1633022.173	3263.35	1.4798	674.4932836	No
6.	TS2	-1633002.696	3261.5	1.46253	675.2817566	1, at -238.74 cm <sup>-1</sup>
7.	Int2	-1633019.884	3260.1	1.51305	671.3472101	No
8.	TS3	-1633014.097	3254.1	1.45637	673.952105	1, at -300.80 cm <sup>-1</sup>
9.	Product	-1633062.965	3271.43	1.50384	674.7113649	No
10.	TS1a	-1633002.315	3247.31	1.48648	670.1837211	1, at -28.76 cm <sup>-1</sup>
11.	Int 1a	-1633013.743	3263.22	1.46694	675.3785895	No

PBE-D3/def2-TZVP (COSMO $\epsilon=2.38$ ), Temperature 368.15 K						
S.N.	Structure	EE (kcal/mol)	H(kJ/mol)	S(kJ/mol/K)	G(kcal/mol)	Imaginary Frequency
1.	6-SIDipp·AlH <sub>3</sub>	-905792.2005	1771.63	1.05776	330.3495418	No
2.	5-IDipp	-727214.8617	1563.29	0.977	287.6621806	No
3.	Adduct (A)	-1633027.26	3338.37	1.80847	638.7470429	No
4.	TS1	-1633000.003	3334.43	1.74451	643.4330858	1, at -608.71 cm <sup>-1</sup>
5.	Int 1	-1633022.173	3349.63	1.73895	647.5550982	No
6.	TS2	-1633002.696	3347.54	1.72091	648.6428891	1, at -238.74 cm <sup>-1</sup>
7.	Int2	-1633019.884	3346.83	1.77352	643.8441583	No
8.	TS3	-1633014.097	3339.62	1.71315	647.4327948	1, at -300.80 cm <sup>-1</sup>
9.	Product	-1633062.965	3357.7	1.76292	647.3747595	No
10.	TS1a	-1633002.315	3333.71	1.74592	643.1369429	1, at -28.76 cm <sup>-1</sup>
11.	Int 1a	-1633013.743	3349.88	1.72717	648.6513451	No



## References

1. (a) M. Iglesias, D. J. Beetstra, J. C. Knight, L.-L. Ooi, A. Stasch, S. Coles, L. Male, M. B. Hursthouse, K. J. Cavell, A. Dervisi and I. A. Fallis, *Organometallics*, 2008, **27**, 3279-3289. b) A. J. Arduengo III, R. Krafczyk, R. Schmutzler, H. A. Craig, J. R. Goerlich, W. M. Marshall and M. Unverzagt, *Tetrahedron*, 1999, **55**, 14523-14534. c) L. L. Cao, E. Daley, T. C. Johnstone and D. W. Stephan, *Chem. Commun.*, 2016, **52**, 5305-5307. d) J. A. B. Abdalla, I. M. Riddlestone, R. Tirfoin, N. Phillips, J. I. Bates and S. Aldridge, *Chem. Commun.*, 2013, **49**, 5547-5549.
2. APEX3, SAINT-Plus and SADABS; Bruker AXS Inc.: Madison, WI, USA, 2006. (b) Apex CCD and SAINT v8.30C; Bruker AXS Inc.: Madison, WI, USA, 2013.
3. (a) G. M. Sheldrick, A short history of SHELX. *Acta Crystallogr.*, 2008, **A64**, 112-122; (b) L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Crystallogr.*, 2015, **48**, 3-10; (c) L. Krause, R. Herbst-Irmer and D. Stalke, *J. Appl. Crystallogr.*, 2015, **48**, 1907-1913.
4. L. J. Farrugia, *J. Appl. Cryst.*, 1997, **30**, 565-565.
5. TURBOMOLE V7.5.0 2016, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007.
6. M. Ernzerhof and G. E. Scuseria, *J. Chem. Phys.*, 1999, **110**, 5029-5036.
7. A. Schafer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829-5835.
8. S. Grimme, J. Antony, S. Ehrlich, and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
9. K. Eichkorn, O. Treutler, H. Ohm, M. Haser and R. Ahlrichs, *Chem. Phys. Lett.*, 1995, **240**, 283-290.
10. M. Sierka, A. Hogekamp, and R. Ahlrichs, *J. Chem. Phys.*, 2003, **118**, 9136-9148.
11. A. Klamt and G. Schuurmann, *J. Chem. Soc., Perkin Trans. 2*, 1993, 799-805.
12. K. Fukui, *Acc. Chem. Res.*, 1981, **14**, 363-368.
13. P. Pracht, F. Bohle and S. Grimme, *Phys. Chem. Chem. Phys.*, 2020, **22**, 7169 —7192.
14. P. Pracht, E. Caldeweyher, S. Ehlert and S. Grimme, A Robust Non-Self-Consistent Tight-Binding Quantum Chemistry Method for large Molecules, 2019.
15. C. Bannwarth, S. Ehlert and S. Grimme, *J. Chem. Theory Comput.*, 2019, **15**, 1652 -1671.
16. S. Grimme, C. Bannwarth and P. Shushkov, *J. Chem. Theory Comput.*, 2017, **13**, 1989 -2009.



## Optimized cartesian co-ordinates

### 6-SIDipp·AlH<sub>3</sub>

(EE = -1443.493547 Hartree)

N 3.5996249 4.4760616 14.5671395  
N 1.4304826 4.1580389 15.2758734  
C 2.7444283 3.9109392 15.4410205  
C 0.8557909 5.0687085 14.2619473  
H 0.0005672 5.5780684 14.7280665  
H 0.4618751 4.4687365 13.4238799  
C 1.9007972 6.0609743 13.7820848  
H 2.1247720 6.7911697 14.5750434  
H 1.5241498 6.6153981 12.9117124  
C 3.1617731 5.2952113 13.4176326  
H 2.9773138 4.6347100 12.5535820  
H 3.9883284 5.9651008 13.1518857  
C 5.0297043 4.3108721 14.7174165  
C 5.7367841 5.2218470 15.5351282  
C 7.1294152 5.0826083 15.6045795  
H 7.7058962 5.7633468 16.2332956  
C 7.7908647 4.0852006 14.8880400  
H 8.8769838 3.9945007 14.9585491  
C 7.0703550 3.2016304 14.0862310  
H 7.5988719 2.4222854 13.5341113  
C 5.6757537 3.2953216 13.9810201  
C 5.0383490 6.3464713 16.2896527  
H 3.9746363 6.0790758 16.3727443  
C 5.5638175 6.5286800 17.7211401  
H 5.5170615 5.5804251 18.2730066  
H 4.9464614 7.2688952 18.2524317  
H 6.6007233 6.8972929 17.7338724  
C 5.1385395 7.6716634 15.5081370  
H 6.1889088 7.9886069 15.4180673  
H 4.5864838 8.4683379 16.0299761  
H 4.7301121 7.5855643 14.4906513  
C 4.9136211 2.3463415 13.0664409  
H 3.8419136 2.4511785 13.2958076  
C 5.1308438 2.7299581 11.5895890  
H 6.1876199 2.6002314 11.3095216  
H 4.8629176 3.7784135 11.3921624  
H 4.5249682 2.0888046 10.9311931  
C 5.2804949 0.8729102 13.3008179  
H 4.6381333 0.2241314 12.6860626  
H 5.1392832 0.6042957 14.3562765  
H 6.3240210 0.6650695 13.0197722  
C 0.4506252 3.5107765 16.1188748  
C -0.0535382 2.2552956 15.7281395  
C -1.0034466 1.6512283 16.5631339  
H -1.4015802 0.6689330 16.3003627  
C -1.4405994 2.2813873 17.7272464  
H -2.1746980 1.7898346 18.3690193  
C -0.9444274 3.5380493 18.0748239  
H -1.2948799 4.0206591 18.9896442  
C 0.0052788 4.1845614 17.2737408  
C 0.4172615 1.5465939 14.4658889  
H 1.1238561 2.2130087 13.9477439  
C 1.1797912 0.2527781 14.7975763  
H 1.5505324 -0.2190893 13.8746356  
H 0.5267082 -0.4701908 15.3093940  
H 2.0411841 0.4541807 15.4498207

C -0.7521538 1.2755742 13.5035686  
H -1.2915373 2.2021237 13.2552276  
H -1.4774850 0.5739626 13.9431609  
H -0.3816783 0.8300082 12.5682527  
C 0.5535919 5.5465355 17.6772816  
H 1.2161686 5.8952883 16.8703024  
C -0.5676396 6.5873354 17.8360298  
H -1.1770117 6.6658200 16.9227040  
H -0.1403790 7.5785696 18.0501311  
H -1.2412229 6.3286760 18.6665248  
C 1.4120758 5.4493737 18.9501210  
H 2.2385596 4.7362323 18.8207053  
H 0.8079362 5.1164928 19.8078341  
H 1.8411376 6.4328439 19.1966980  
Al 3.5028060 2.6685543 16.9905281  
H 2.2570291 2.0710429 17.8383984  
H 4.3281791 1.5205888 16.1888339  
H 4.4348926 3.6683026 17.8692778

### 5-IDipp

(EE = -1158.908146 Hartree)

N 0.5148367 1.0620825 -0.0417270  
N 0.5367715 -1.0629444 0.0464979  
C -0.3462904 -0.0094202 0.0011466  
C 1.8619789 0.6935210 -0.0223276  
H 2.6684834 1.4182899 -0.0477274  
C 1.8760372 -0.6665597 0.0305805  
H 2.6972589 -1.3744847 0.0580400  
C 0.0727091 2.4305117 -0.0990180  
C -0.0691525 3.0406465 -1.3633103  
C -0.4975827 4.3747558 -1.3947902  
H -0.6212105 4.8786557 -2.3546485  
C -0.7722702 5.0692659 -0.2150294  
H -1.1052916 6.1083231 -0.2612189  
C -0.6248491 4.4407911 1.0201523  
H -0.8476988 4.9926121 1.9360187  
C -0.1969914 3.1068917 1.1054613  
C 0.1627599 2.2542692 -2.6460218  
H 0.8671769 1.4402020 -2.4137187  
C 0.7866786 3.0898770 -3.7712048  
H 1.0352369 2.4402220 -4.6233927  
H 1.7091456 3.5900777 -3.4410502  
H 0.0948855 3.8613876 -4.1423749  
C -1.1560871 1.6007953 -3.1024132  
H -0.9908732 0.9878079 -4.0020500  
H -1.9050151 2.3708481 -3.3435923  
H -1.5626261 0.9541933 -2.3115670  
C -0.0664753 2.4283867 2.4610223  
H 0.3479902 1.4230605 2.2957407  
C -1.4488421 2.2490762 3.1116300  
H -2.1143311 1.6682497 2.4575478  
H -1.9234551 3.2227158 3.3091049  
H -1.3567679 1.7159519 4.0701299  
C 0.8995176 3.1827155 3.3888576  
H 1.8909656 3.2956717 2.9256725  
H 1.0231058 2.6352271 4.3353705  
H 0.5241769 4.1882855 3.6330227  
C 0.1231621 -2.4405633 0.0959790

C -0.0072495 -3.0608030 1.3565854  
C -0.4061011 -4.4042393 1.3798663  
H -0.5204083 -4.9160373 2.3366891  
C -0.6627669 -5.0983267 0.1957608  
H -0.9723309 -6.1448653 0.2356584  
C -0.5273637 -4.4598177 -1.0356172  
H -0.7356016 -5.0114024 -1.9550871  
C -0.1299007 -3.1160218 -1.1126680  
C 0.2050838 -2.2764247 2.6438435  
H 0.8917066 -1.4456239 2.4171219  
C -1.1287605 -1.6546363 3.1010226  
H -1.5483343 -1.0134134 2.3125768  
H -0.9787231 -1.0424416 4.0038020  
H -1.8608567 -2.4423237 3.3370826  
C 0.8450834 -3.1041567 3.7657837  
H 0.1701266 -3.8934537 4.1306982  
H 1.0766831 -2.4541318 4.6224413  
H 1.7795023 -3.5811536 3.4349761  
C -0.0079705 -2.4294714 -2.4650220  
H 0.3565077 -1.4064681 -2.2913454  
C -1.3839972 -2.3123082 -3.1424448  
H -1.2973241 -1.7715110 -4.0971195  
H -2.0888858 -1.7652576 -2.5006292  
H -1.8096031 -3.3055494 -3.3532339  
C 1.0093687 -3.1379879 -3.3740251  
H 0.6862820 -4.1608230 -3.6213389  
H 1.9966085 -3.2029148 -2.8928437  
H 1.1239372 -2.5868368 -4.3196084

### Adduct (A)

(EE = -2602.433881 Hartree)

N 0.5139179 2.4172679 -2.2575400  
N -0.2808320 3.2834570 -0.2941692  
C 0.1022370 2.1870136 -0.9875784  
C -0.3169329 4.6591503 -0.8482648  
H -0.2221851 5.3624792 -0.0112378  
H -1.2995670 4.8390646 -1.3181708  
C 0.7944646 4.8338685 -1.8650097  
H 1.7748194 4.7499126 -1.3695132  
H 0.7362862 5.8247642 -2.3359536  
C 0.6383816 3.7457720 -2.9084826  
H -0.2523856 3.9297201 -3.5339314  
H 1.5055801 3.7056645 -3.5824764  
C 0.7718806 1.3382255 -3.1818965  
C 2.1081839 0.9611924 -3.4362269  
C 2.3450571 0.0046655 -4.4310648  
H 3.3698820 -0.3151518 -4.6354907  
C 1.2904335 -0.5687926 -5.1441116  
H 1.4932932 -1.3310001 -5.9001767  
C -0.0209973 -0.1796702 -4.8795680  
H -0.8418046 -0.6339173 -5.4389424  
C -0.3054655 0.7978574 -3.9127521  
C 3.2705074 1.5473855 -2.6483381  
H 2.8467564 2.2355314 -1.9008823  
C 4.0285025 0.4539918 -1.8774958  
H 3.3340886 -0.1166173 -1.2452772  
H 4.8025160 0.9053390 -1.2372984  
H 4.5250392 -0.2460739 -2.5682132

C	4.2228547	2.3497025	-3.5527730	H	-0.5448865	-0.0468743	5.9562263	H	1.6593784	9.9290467	12.0802229
H	4.7004075	1.6969368	-4.3005635	C	-0.1685511	-1.1784328	4.1555109	H	0.0210302	9.7778669	11.4435907
H	5.0207434	2.8150498	-2.9538501	C	3.2746091	-1.7331155	2.4791616	C	1.1870243	7.9858903	11.1933118
H	3.6932718	3.1482120	-4.0944130	H	2.7719736	-2.2563318	1.6525999	H	0.2619468	7.5727032	10.7551207
C	-1.7392239	1.2663165	-3.7116522	C	4.2572509	-2.7194556	3.1316989	H	1.8220615	8.2737268	10.3417315
H	-1.7422778	1.9828450	-2.8773908	H	4.9984696	-3.0654828	2.3948921	C	3.2112581	6.5953561	11.5087633
C	-2.2616679	1.9950837	-4.9628632	H	3.7333700	-3.6012859	3.5312566	C	4.3451955	7.3845265	11.8335049
H	-2.3160534	1.3103933	-5.8238452	H	4.8029496	-2.2447371	3.9622447	C	5.6144678	6.9746951	11.3953424
H	-1.6095010	2.8364217	-5.2436551	C	4.0065809	-0.5288889	1.8657648	H	6.4910330	7.5751935	11.6511834
H	-3.2731861	2.3911136	-4.7822333	H	4.7312043	-0.8697744	1.1108489	C	5.7725783	5.8307221	10.6183234
C	-2.6660456	0.1122068	-3.3113038	H	4.5559698	0.0393594	2.6329298	H	6.7673458	5.5256950	10.2841542
H	-3.6826270	0.4913408	-3.1206729	H	3.2913357	0.1481493	1.3785031	C	4.6516611	5.0827741	10.2554285
H	-2.2977579	-0.3702322	-2.3964765	C	-1.6334550	-1.5054298	3.9054709	H	4.7808063	4.1974672	9.6294723
H	-2.7312823	-0.6498083	-4.1034333	H	-1.6806582	-2.2396446	3.0881383	C	3.3694509	5.4446428	10.6867688
C	-0.7764551	3.2145904	1.0619273	C	-2.3818756	-0.2501941	3.4301731	C	4.2077943	8.7248299	12.5409138
C	-2.1667951	3.1091639	1.2759392	H	-1.8989837	0.1850083	2.5447857	H	3.1975120	8.7641887	12.9695766
C	-2.6413299	3.2275904	2.5918613	H	-2.3953596	0.5225237	4.2144208	C	5.2011856	8.9154744	13.6920699
H	-3.7139725	3.1472589	2.7834392	H	-3.4235255	-0.4978392	3.1717050	H	5.1293084	8.0913749	14.4111561
C	-1.7681918	3.4436862	3.6556181	C	-2.3094571	-2.1454546	5.1278921	H	4.9953467	9.8581339	14.2232221
H	-2.1567374	3.5340827	4.6728376	H	-1.7828459	-3.0586913	5.4440128	H	6.2417466	8.9589834	13.3337888
C	-0.3945605	3.5257223	3.4232603	H	-3.3480544	-2.4176046	4.8843643	C	4.3418665	9.8745434	11.5241027
H	0.2842787	3.6706897	4.2657307	H	-2.3390411	-1.4555052	5.9852694	H	5.3536210	9.8882236	11.0898615
C	0.4128760	3.4180287	2.1288446	C	-0.8216208	-3.3397296	-1.0028323	H	4.1674105	10.8477392	12.0099643
C	-3.1545892	2.8968630	0.1365025	C	-2.2059729	-3.1566645	-1.2130568	H	3.6267230	9.7700797	10.6950252
H	-2.5712563	2.7127561	-0.7776622	C	-2.6867695	-3.3656954	-2.5122805	C	2.1566894	4.6420794	10.2424121
C	-4.0298322	1.6549577	0.3645343	H	-3.7481082	-3.2264950	-2.7219641	H	1.3819840	4.7992255	11.0092857
H	-4.6976442	1.4995553	-0.4971119	C	-1.8268426	-3.7277262	-3.5521793	C	1.5957806	5.1864930	8.9150934
H	-4.6567915	1.7622728	1.2633985	H	-2.2250082	-3.8733422	-4.5590563	H	2.3330850	5.0703108	8.1047072
H	-3.3976944	0.7633185	0.4706430	C	-0.4634201	-3.8863382	-3.3144034	H	1.3410232	6.2520065	8.9932440
C	-4.0255115	4.1472572	-0.0871894	H	0.0219709	-4.1547353	-4.1374768	H	0.6841878	4.6382061	8.6278857
H	-3.4146754	5.0423443	-0.2782421	C	0.0694428	-3.7005149	-2.0297956	C	2.4213295	3.1367707	10.1054278
H	-4.6522327	4.3507515	0.7956298	C	-3.1324750	-2.7636740	-0.0680261	H	1.4770441	2.6025966	9.9529600
H	-4.6951381	3.9985181	-0.9483786	H	-2.5640034	-2.0664129	0.5668926	H	2.8544875	2.7534040	11.0702697
C	1.6295306	3.5251872	1.8978210	C	-4.3917179	-2.0204245	-0.5287042	H	3.1023036	2.8935205	9.3053289
H	1.8324039	3.0990910	0.9042186	H	-4.1366706	-1.1543358	-1.1525771	C	-0.9769825	6.8566696	14.1209351
C	2.1036890	4.9908332	1.9056410	H	-4.9430173	-1.6527954	0.3497351	C	-1.8520471	6.0640345	13.3277152
H	1.5897495	5.6009612	1.1494242	H	-5.0728021	-2.6750913	-1.0949609	C	-3.0801462	5.6614444	13.8677583
H	3.1851562	5.0432168	1.7034610	C	-3.5265234	-3.9882959	0.7810691	H	-3.7539259	5.0511608	13.2627747
H	1.9207846	5.4519439	2.8895904	H	-4.1009661	-4.7092632	0.1777885	C	-3.4856126	6.0691737	15.1385552
C	2.4270038	2.6996140	2.9151508	H	-4.1566274	-3.6746915	1.6282037	H	-4.4645607	5.7753875	15.5243445
H	2.0587697	1.6669829	2.9418502	H	-2.6486045	-4.5066878	1.1898321	C	-2.6271940	6.8448253	15.9137967
H	2.3586157	3.1218739	3.9299890	C	1.5549576	-3.9088692	-1.7712488	H	-2.9385646	7.1584275	16.9136864
H	3.4912200	2.6825351	2.6341129	H	1.7676079	-3.5642338	-0.7490687	C	-1.3558599	7.2060907	15.4443393
Al	0.0681613	0.0554688	-0.0029763	C	2.4229490	-3.0638073	-2.7112994	C	-1.5445365	5.7609426	11.8692222
H	0.6577636	0.6743528	1.3842730	H	3.4860041	-3.1785998	-2.4473640	H	-0.4598456	5.8694016	11.7357094
H	-1.5451850	-0.0163527	-0.2842470	H	2.1547701	-2.0036916	-2.6239988	C	-1.9267070	4.3399030	11.4327204
H	1.1161351	-0.5568716	-1.0936621	H	2.3014802	-3.3662896	-3.7627869	H	-1.5628623	4.1547917	10.4098561
N	0.4734683	-2.4494191	2.1727615	C	1.9223314	-5.4012354	-1.8545605	H	-3.0175668	4.1890701	11.4239488
N	-0.2992980	-3.2131026	0.3337315	H	1.7415958	-5.7930206	-2.8683064	H	-1.4718541	3.5962062	12.1011505
C	0.0166193	-2.0279936	0.9501290	H	1.3311684	-6.0048501	-1.1496546	C	-2.2456154	6.8031317	10.9755132
C	0.4543810	-3.8375423	2.3062313	H	2.9882152	-5.5475342	-1.6196503	H	-1.9790252	7.8286498	11.2699091
H	0.7788014	-4.3381114	3.2117935					H	-3.3401535	6.7047902	11.0558891
C	-0.0343610	-4.3230039	1.1347229					H	-1.9658228	6.6635517	9.9191895
H	-0.2179456	-5.3380816	0.8017238					C	-0.4047501	7.9393423	16.3807361
C	0.8451309	-1.5989002	3.2736317					H	0.5615442	8.0184479	15.8629107
C	2.2032499	-1.2862436	3.4624346					C	-0.8901520	9.3589260	16.7204612
C	2.5394062	-0.5262172	4.5917092					H	-1.0349206	9.9641392	15.8147286
H	3.5840676	-0.2601368	4.7681291					H	-0.1615808	9.8764777	17.3643750
C	1.5571598	-0.0886063	5.4813154					H	-1.8499331	9.3256203	17.2596257
H	1.8382743	0.5123267	6.3491495					C	-0.1729821	7.1353737	17.6704274
C	0.2162394	-0.4049144	5.2597058					H	0.1808140	6.1190397	17.4431959

**Intl**

**(EE = -2602.425774 Hartree)**

N	1.8954551	6.9436028	11.9415289
N	0.2126527	7.4077359	13.5602531
C	1.4773810	6.7197579	13.3787636
C	0.3009890	8.8557976	13.4142261
H	0.9887710	9.2842761	14.1770486
H	-0.6929819	9.2860636	13.5992063
C	0.8061694	9.2406214	12.0002146

H -1.0974278 7.0430706 18.2585952  
H 0.5760194 7.6292137 18.3078106  
N 1.2424208 2.9978280 16.4210252  
N 3.0984287 4.1004245 16.4253210  
C 1.9281440 3.9664418 15.7221241  
C 1.9697366 2.5588259 17.5224476  
H 1.6011061 1.7832797 18.1812960  
C 3.1332383 3.2580678 17.5300436  
H 3.9846880 3.2279362 18.1989834  
C -0.0124667 2.3745020 16.0438894  
C -1.1419443 2.5637601 16.8657488  
C -2.3398170 1.9480457 16.4710017  
H -3.2361279 2.0889676 17.0766650  
C -2.4024294 1.1625640 15.3254821  
H -3.3473600 0.7023531 15.0291934  
C -1.2546247 0.9460550 14.5639957  
H -1.3110422 0.3075268 13.6826193  
C -0.0300346 1.5303506 14.9089335  
C -1.1013962 3.3301291 18.1818039  
H -0.1903835 3.9478875 18.1946858  
C -1.0341409 2.3501703 19.3707133  
H -0.9437755 2.9022507 20.3183992  
H -0.1859693 1.6548096 19.2989628  
H -1.9516181 1.7435177 19.4157814  
C -2.3012049 4.2705415 18.3590772  
H -2.1578948 4.8974535 19.2515135  
H -3.2367568 3.7085987 18.5005919  
H -2.4227653 4.9246201 17.4882578  
C 1.2335924 1.1849621 14.1328459  
H 1.8686997 2.0827503 14.0956945  
C 0.9719702 0.7909666 12.6763034  
H 0.3903546 1.5672011 12.1599166  
H 0.4394923 -0.1692956 12.5940168  
H 1.9299990 0.6813302 12.1490828  
C 2.0236137 0.0782722 14.8593696  
H 2.2951232 0.3709497 15.8837281  
H 2.9551820 -0.1416711 14.3150978  
H 1.4329773 -0.8493199 14.9143280  
C 4.2881782 4.8364108 16.0430058  
C 5.2474818 4.1700062 15.2499915  
C 6.4674839 4.8254439 15.0360897  
H 7.2274242 4.3476070 14.4158539  
C 6.7335500 6.0631799 15.6163483  
H 7.6977495 6.5478024 15.4495823  
C 5.7637686 6.6961850 16.3909435  
H 5.9780012 7.6734326 16.8268603  
C 4.5104487 6.1072429 16.6064200  
C 5.0244487 2.7738714 14.6896774  
H 3.9444351 2.5735872 14.7136332  
C 5.4620431 2.6541489 13.2233292  
H 4.9954044 3.4362000 12.6099662  
H 5.1544583 1.6751494 12.8254078  
H 6.5552799 2.7250271 13.1132398  
C 5.7286441 1.7179571 15.5625604  
H 6.8180544 1.8768132 15.5648249  
H 5.5318224 0.7084172 15.1710976  
H 5.3784900 1.7502627 16.6043088  
C 3.4614966 6.8191164 17.4456026  
H 2.4996704 6.3153305 17.2727184  
C 3.2904680 8.2876903 17.0274916  
H 2.4765988 8.7533648 17.6016889

H 3.0456053 8.3704810 15.9585159  
H 4.2017733 8.8747539 17.2135199  
C 3.7850138 6.7098740 18.9461846  
H 4.7411023 7.2053193 19.1759576  
H 3.8621268 5.6612833 19.2681434  
H 2.9983311 7.1931392 19.5453561  
H 2.2302633 7.2375016 14.0350825  
Al 1.5333601 4.6929431 13.7783754  
H 2.8732141 4.0542021 13.1316665  
H 0.1906052 3.9036763 13.3882500

## Int2

(EE = -2602.422125 Hartree)

Al -0.3230558 0.0458633 -0.5953897  
N -2.2216211 -0.0007477 -1.0837109  
N -1.5920865 -0.1742016 2.1919915  
C -0.5006617 -0.1905043 1.4580020  
H 0.3143507 -0.7203018 1.9759651  
C -2.8151879 0.5108792 1.6863292  
H -2.4679968 1.3375052 1.0565194  
H -3.3542114 0.9176067 2.5480819  
C -3.7295086 -0.2360416 0.8664124  
H -4.5820446 0.367804 0.5608616  
H -4.1397650 -1.2012713 1.4959297  
C -3.0431003 -0.9778920 -0.3878735  
H -2.4240718 -1.8442719 -0.0831965  
H -3.8392489 -1.3877210 -1.0316808  
C -2.6921365 0.4360593 -2.3362810  
C -2.9060216 1.8242569 -2.5905338  
C -3.4151821 2.2340460 -3.8298244  
H -3.5968220 3.2979928 -4.0061966  
C -3.7113087 1.3185627 -4.8397652  
H -4.1196039 1.6577348 -5.7946142  
C -3.4606601 -0.0355092 -4.6150603  
H -3.6472349 -0.7546391 -5.4184347  
C -2.9333914 -0.4906213 -3.4003779  
C -2.6537144 2.8699636 -1.5134371  
H -2.0919420 2.3577955 -0.7194365  
C -1.7841151 4.0311565 -2.0139174  
H -0.8014635 3.6567208 -2.3351427  
H -1.6266358 4.7744357 -1.2158977  
H -2.2473995 4.5591949 -2.8618805  
C -3.9763770 3.3770635 -0.9139122  
H -4.5827197 3.8961342 -1.6734086  
H -3.7900326 4.0824650 -0.0876864  
H -4.5767329 2.5407395 -0.5241807  
C -2.5394581 -1.9594390 -3.2792939  
H -2.1033699 -2.1041035 -2.2815415  
C -3.7353212 -2.9129666 -3.4352906  
H -4.1820154 -2.8301531 -4.4392141  
H -4.5262522 -2.6947823 -2.7020045  
H -3.4200023 -3.9593550 -3.2965540  
C -1.4305481 -2.3061590 -4.2838458  
H -1.0804463 -3.3402211 -4.1358029  
H -0.5686608 -1.6393621 -4.1559606  
H -1.7792108 -2.2105062 -5.3243139  
C -1.7380600 -0.8993097 3.4513071  
C -1.6863025 -2.3136225 3.4508611  
C -1.9072922 -2.9710011 4.6714514  
H -1.8805502 -4.0622924 4.6942999  
C -2.1702694 -2.2684380 5.8435896

H -2.3487170 -2.8053312 6.7774713  
C -2.1903340 -0.8754826 5.8220079  
H -2.3710101 -0.3265254 6.7483120  
C -1.9686565 -0.1616996 4.6369348  
C -1.4226788 -3.1623142 2.2137908  
H -1.2154596 -2.5020713 1.3618886  
C -0.1769352 -4.0462151 2.3929425  
H 0.0502645 -4.5672744 1.4514183  
H -0.3279890 -4.8073651 3.1734913  
H 0.7017252 -3.4476073 2.6687458  
C -2.6466955 -4.0182915 1.8463823  
H -3.5429285 -3.3995711 1.6978594  
H -2.8703590 -4.7554048 2.6324389  
H -2.4553746 -4.5660774 0.9111901  
C -1.9375770 1.3612127 4.6977080  
H -1.6224977 1.7394090 3.7140371  
C -3.3193234 1.9534564 5.0302543  
H -4.0963671 1.6267793 4.3239333  
H -3.2794261 3.0527507 5.0083254  
H -3.6396381 1.6471858 6.0374219  
C -0.8956762 1.8488429 5.7190354  
H 0.0855466 1.3964250 5.5281283  
H -1.1959500 1.5992613 6.7475791  
H -0.7881172 2.9422457 5.6585491  
N 2.7567872 1.0260657 0.2932494  
N 2.6688696 0.1129115 -1.6439304  
C 1.9359994 0.2546044 -0.4906299  
C 3.9472362 1.3645972 -0.3562279  
H 4.7136024 1.9657555 0.1191947  
C 3.8894966 0.7823475 -1.5810947  
H 4.5952058 0.7701955 -2.4033668  
C 2.5695280 1.3194107 1.6916770  
C 1.7890551 2.4306890 2.0680855  
C 1.7437729 2.7480414 3.4326025  
H 1.1578376 3.6057957 3.7645934  
C 2.4360348 1.9871806 4.3745233  
H 2.3970951 2.2627356 5.4304208  
C 3.1658819 0.8688701 3.9771653  
H 3.6826376 0.2690872 4.7281481  
C 3.2533807 0.5109643 2.6242095  
C 1.0559497 3.2727636 1.0348880  
H 0.8040234 2.6199780 0.1826447  
C 1.9609718 4.3989807 0.5013862  
H 1.4307902 4.9753594 -0.2717300  
H 2.8800297 3.9973935 0.0511257  
H 2.2479648 5.0889573 1.3104697  
C -0.2651145 3.8434563 1.5654046  
H -0.8155688 4.3258681 0.7466639  
H -0.1099875 4.6004012 2.3492657  
H -0.9050135 3.0492158 1.9771807  
C 4.0129799 -0.7405066 2.2020724  
H 4.2483025 -0.6534886 1.1312123  
C 3.1149432 -1.9794332 2.3698010  
H 2.2134728 -1.8991225 1.7463838  
H 2.8006757 -2.0970316 3.4185502  
H 3.6524883 -2.8917010 2.0688809  
C 5.3453977 -0.9178998 2.9434686  
H 5.9761041 -0.0214586 2.8557237  
H 5.8981066 -1.7690584 2.5188215  
H 5.1972256 -1.1264059 4.0136730  
C 2.3128753 -0.6789510 -2.7976437

C 2.4443055 -2.0824508 -2.7157678  
C 2.2932423 -2.8134005 -3.9008758  
H 2.3922036 -3.8998250 -3.8769940  
C 2.0226171 -2.1756964 -5.1120911  
H 1.9164324 -2.7649025 -6.0253611  
C 1.8453158 -0.7947271 -5.1516445  
H 1.5883216 -0.3104067 -6.0955268  
C 1.9727017 -0.0140525 -3.9923855  
C 2.7831560 -2.7778709 -1.4056987  
H 2.4808214 -2.1015381 -0.5940282  
C 1.9935905 -4.0771855 -1.2028739  
H 0.9140914 -3.8870893 -1.2889080  
H 2.1908030 -4.4774703 -0.1964990  
H 2.2769486 -4.8558997 -1.9273530  
C 4.2999101 -3.0150451 -1.2918336  
H 4.6513822 -3.6917483 -2.0863165  
H 4.5470442 -3.4720718 -0.3209337  
H 4.8610045 -2.0727462 -1.3761138  
C 1.7305616 1.4872442 -4.0514204  
H 1.7238288 1.8653825 -3.0178967  
C 0.3494826 1.8016523 -4.6479206  
H 0.1643908 2.8858908 -4.6168329  
H -0.4513827 1.3112783 -4.0788311  
H 0.2763823 1.4817846 -5.6986673  
C 2.8464708 2.2077368 -4.8277138  
H 2.8821857 1.8663539 -5.8739250  
H 3.8364324 2.0278937 -4.3826839  
H 2.6680144 3.2937044 -4.8331564  
H -0.0365769 1.4278735 -1.4393861  
H -0.1273953 -1.6211410 -0.6030666

**Product (2)**

**(EE = -2602.49078 Hartree)**

Al 4.2373594 4.9766851 15.2079875  
H 4.5169737 6.0509264 16.3814519  
N 7.2426526 4.4195445 15.7645218  
N 6.3680605 2.5922129 15.0259196  
N 3.8607423 5.7172773 13.5192256  
N 1.4221992 3.9274825 15.3058157  
C 6.0550298 3.8953557 15.3200421  
C 8.2592033 3.4742070 15.7427997  
H 9.2613729 3.7021249 16.0852754  
C 7.7095135 2.3231220 15.2735949  
H 8.1351389 1.3406260 15.1096134  
C 7.4237739 5.6969813 16.4296136  
C 7.8413041 6.8159391 15.6839221  
C 8.0487251 8.0096123 16.3888135  
H 8.3556742 8.9042452 15.8469189  
C 7.8523767 8.0789009 17.7680682  
H 8.0110311 9.0237374 18.2920783  
C 7.4461713 6.9505410 18.4761588  
H 7.2887216 7.0163433 19.5548192  
C 7.2283906 5.7295179 17.8239966  
C 8.0713073 6.7387495 14.1822799  
H 7.3328353 6.0261971 13.7792754  
C 9.4799197 6.2006117 13.8609358  
H 9.6232137 6.1451196 12.7712261  
H 9.6503913 5.1965192 14.2725388  
H 10.2487714 6.8727839 14.2719715  
C 7.8507234 8.0756503 13.4683244  
H 7.8830758 7.9238097 12.3815360

H 8.6339923 8.8058652 13.7238140  
H 6.8706880 8.5082203 13.7081749  
C 6.7836005 4.5135102 18.6223020  
H 6.6936943 3.6634741 17.9312987  
C 5.3975205 4.7348797 19.2499303  
H 4.6624366 5.0177048 18.4839784  
H 5.4265311 5.5357210 20.0053736  
H 5.0520031 3.8165269 19.7484345  
C 7.8279472 4.1206401 19.6806123  
H 8.8100037 3.9298869 19.2227945  
H 7.5110070 3.2071310 20.2063315  
H 7.9544919 4.9136168 20.4330633  
C 5.4592515 1.5128200 14.6844562  
C 4.8685180 0.7842138 15.7423608  
C 4.1160871 -0.3460965 15.3997334  
H 3.6398954 -0.9299672 16.1880885  
C 3.9483010 -0.7249597 14.0691246  
H 3.3541599 -1.6078689 13.8257949  
C 4.5104248 0.0358262 13.0475937  
H 4.3483111 -0.2584078 12.0104756  
C 5.2823914 1.1728337 13.3302117  
C 5.0141932 1.1946545 17.2026816  
H 5.1886213 2.2812819 17.2199706  
C 3.7438709 0.9321915 18.0272995  
H 2.8480839 1.3363041 17.5359991  
H 3.8396384 1.4127880 19.0121870  
H 3.5874760 -0.1426339 18.2050774  
C 6.2240240 0.5085716 17.8664357  
H 6.0924169 -0.5842428 17.8691971  
H 6.3239854 0.8424207 18.9104800  
H 7.1651994 0.7378340 17.3487354  
C 5.9156672 1.9767490 12.2039671  
H 6.0720617 3.0031448 12.5725378  
C 5.0119155 2.0633162 10.9668545  
H 5.4638884 2.7326752 10.2229605  
H 4.0162676 2.4554320 11.2182985  
H 4.8861422 1.0833738 10.4832107  
C 7.2903422 1.3977407 11.8168146  
H 7.1840242 0.3665364 11.4464083  
H 7.9844162 1.3822318 12.6685057  
H 7.7479437 2.0032325 11.0201148  
C 2.8193310 3.5909014 15.6095331  
H 3.0693173 2.6270129 15.1285852  
H 2.9348481 3.3996473 16.6988330  
C 1.0999616 5.2595637 14.8093642  
H 1.6565780 6.0439110 15.3622897  
H 0.0343134 5.4530963 15.0075321  
C 1.3510778 5.4345160 13.3020689  
H 1.1730485 6.4920640 13.0389914  
H 0.6148997 4.8301848 12.7433696  
C 2.7561032 5.0218216 12.8295419  
H 2.8613856 3.9328095 12.9750242  
H 2.8085425 5.1921551 11.7414069  
C 4.2648524 6.9386309 12.9171234  
C 4.0266085 8.2045225 13.5354218  
C 4.4038939 9.3836511 12.8742613  
H 4.2070739 10.3443827 13.3575003  
C 4.9972070 9.3651075 11.6149581  
H 5.2703518 10.2965850 11.1142256  
C 5.2438332 8.1340723 11.0103429  
H 5.7288904 8.1077353 10.0305866

C 4.9056649 6.9286020 11.6371271  
C 3.3338886 8.3477898 14.8819708  
H 3.1135805 7.3349981 15.2420488  
C 4.2455896 9.0037287 15.9293819  
H 5.1682846 8.4231980 16.0638406  
H 3.7359813 9.0524907 16.9046053  
H 4.5203976 10.0305795 15.6389841  
C 1.9976520 9.0998185 14.7611309  
H 2.1478429 10.1450679 14.4478472  
H 1.4755681 9.1108054 15.7308087  
H 1.3365390 8.6213325 14.0236098  
C 5.2573592 5.6303880 10.9207899  
H 4.9208910 4.8079028 11.5656590  
C 4.5405573 5.5204673 9.5633775  
H 4.8773938 6.3097191 8.8735610  
H 3.4511470 5.6207330 9.6750065  
H 4.7458125 4.5509779 9.0837147  
C 6.7765776 5.4703076 10.7371032  
H 7.0084275 4.5274673 10.2161310  
H 7.2957013 5.4560468 11.7055876  
H 7.2007517 6.2916694 10.1396249  
C 0.4450921 3.2630638 16.1105059  
C -0.2235862 2.1349566 15.5726522  
C -1.1934808 1.4824347 16.3474000  
H -1.7248714 0.6211693 15.9343175  
C -1.4978174 1.9217268 17.6362653  
H -2.2611871 1.4079080 18.2253447  
C -0.8195136 3.0172279 18.1718431  
H -1.0575377 3.3515843 19.1853690  
C 0.1631029 3.6930050 17.4332517  
C 0.0811814 1.6650015 14.1598154  
H 1.0005703 2.1905625 13.8589178  
C 0.3331105 0.1529725 14.0809421  
H 0.6598680 -0.1276706 13.0677492  
H -0.5750169 -0.4275103 14.3084716  
H 1.1196829 -0.1516064 14.7854937  
C -1.0345502 2.0915250 13.1903626  
H -1.1849862 3.1807820 13.2166342  
H -1.9913445 1.6132871 13.4549763  
H -0.7850722 1.8046257 12.1564660  
C 0.8993194 4.8709177 18.0593279  
H 1.6993534 5.1682635 17.3672757  
C -0.0284725 6.0845439 18.2438746  
H -0.4787334 6.3910072 17.2885408  
H 0.5320819 6.9423844 18.6472255  
H -0.8461619 5.8531869 18.9444009  
C 1.5678052 4.4857454 19.3895249  
H 2.2375774 3.6235315 19.2584695  
H 0.8231501 4.2232744 20.1565520  
H 2.1650696 5.3259202 19.7755612

**TS1**

**(EE = -2602.390443 Hartree)**

**(Imaginary frequency = 1, -608.71 cm<sup>-1</sup>)**

N 2.2324136 7.2947322 12.7161137  
N 0.1454582 7.2800860 13.6979750  
C 1.2408178 6.4836068 13.3231730  
C 0.4546693 8.5571700 14.3555337  
H 1.0418298 8.3448588 15.2708523  
H -0.4845701 9.0339821 14.6594871  
C 1.2718216 9.4868385 13.4372676

H	2.0531196	9.9906395	14.0262033	H	-2.5627522	5.3229401	17.2321327	H	2.0967526	7.3156385	17.2995843
H	0.6344635	10.2707488	12.9977857	H	-1.0058000	5.6005366	18.0397538	H	2.4174435	7.3888912	19.0537034
C	1.8847193	8.6570761	12.3057096	N	1.2223058	1.9063563	15.3462312	C	1.5642060	4.7848704	19.6521064
H	1.1571814	8.6151119	11.4710613	N	2.5615081	3.0989774	16.5368287	H	2.2183078	5.1604505	20.4541886
H	2.7925363	9.1296895	11.9082109	C	1.8889766	3.1097808	15.3423224	H	1.6270213	3.6869311	19.6490031
C	3.5122404	6.7753658	12.3441174	C	1.4582956	1.1854886	16.5117475	H	0.5286534	5.0641027	19.8995695
C	4.6300205	7.1358969	13.1356079	H	1.0166608	0.2113285	16.6850524	H	1.8706976	6.0657289	14.6706422
C	5.9030581	6.6872982	12.7553769	C	2.3017822	1.9364673	17.2654397	Al	1.3358665	4.5025816	13.7473663
H	6.7722301	6.9622515	13.3575932	H	2.7615476	1.7528087	18.2293332	H	2.2205559	3.7667281	12.6073815
C	6.0713287	5.8886680	11.6272905	C	0.4784872	1.3431430	14.2361065	H	-0.2255322	4.1716147	14.0143667
H	7.0673280	5.5374528	11.3469851	C	-0.9279434	1.3224106	14.2985503	<b>TS2</b>			
C	4.9639259	5.5350780	10.8552856	C	-1.6140292	0.6965994	13.2482334	<b>(EE = -2602.394734 Hartree)</b>			
H	5.1081535	4.9154586	9.9684053	H	-2.7046401	0.6672698	13.2655115	<b>(Imaginary frequency = 1, -238.74 cm<sup>-1</sup>)</b>			
C	3.6755369	5.9767449	11.1847445	C	-0.9276148	0.1229833	12.1814905	Al	0.1100621	0.5671901	-0.6702607
C	4.4740909	8.0203702	14.3612378	H	-1.4808298	-0.3544742	11.3697350	N	-1.9210930	-0.3685313	-1.3825003
H	3.3946400	8.0896384	14.5627525	C	0.4660193	0.1620256	12.1435728	N	-1.9922864	-0.4403684	1.2930942
C	5.1267637	7.4054843	15.6021442	H	0.9909560	-0.2868097	11.2998603	C	-1.0614484	-0.7614008	0.3178543
H	4.7389067	6.3954600	15.7804378	C	1.2044955	0.7640439	13.1705212	H	-0.8265697	-1.8324262	0.3184816
H	4.9106824	8.0144736	16.4927318	C	-1.7040906	1.9356039	15.4526042	C	-2.4376383	0.9686153	1.2366005
H	6.2212379	7.3374093	15.5038211	H	-1.0070528	2.5718500	16.0176997	H	-1.5343524	1.5966243	1.1996767
C	5.0144442	9.4378156	14.1009452	C	-2.2325990	0.8446942	16.4018910	H	-2.9835140	1.2177350	2.1486284
H	6.0986167	9.4116705	13.9084056	H	-2.7566746	1.3007926	17.2556122	C	-3.3227363	1.2270750	0.0008998
H	4.8422812	10.0850819	14.9751395	H	-1.4211403	0.2159942	16.7966149	H	-3.0069249	2.1722825	-0.4670979
H	4.5336911	9.9056971	13.2293045	H	-2.9432026	0.1851252	15.8800380	H	-4.3756376	1.3507749	0.3039345
C	2.4998401	5.6788185	10.2689661	C	-2.8464060	2.8354928	14.9609977	C	-3.2666568	0.0702360	-1.0088346
H	1.6016512	5.6810940	10.9009391	H	-3.3329868	3.3270445	15.8155521	H	-3.8292459	-0.7723484	-0.5636197
C	2.3506042	6.7867331	9.2084049	H	-3.6185253	2.2600249	14.4283534	H	-3.8326067	0.3413099	-1.9112727
H	3.2281337	6.8056937	8.5424176	H	-2.4660779	3.6185374	14.2916694	C	-1.6775867	-0.6235693	-2.7600129
H	2.2550541	7.7807835	9.6660045	C	2.7265528	0.7476961	13.1440338	C	-1.9045235	0.4375078	-3.7088088
H	1.4574260	6.6088752	8.5892956	H	3.0664000	1.6740076	13.6281725	C	-1.7231033	0.2076868	-5.0759138
C	2.5781791	4.3051311	9.5940961	C	3.3109029	0.7583667	11.7273737	H	-1.9254608	1.0223676	-5.7769569
H	1.6439766	4.1012016	9.0497624	H	2.8849069	1.5766741	11.1321762	C	-1.2309585	-1.0013553	-5.5615940
H	2.7132989	3.5184016	10.3474495	H	3.1357419	-0.1910274	11.1979653	H	-1.0721192	-1.1547940	-6.6311675
H	3.4014847	4.2451242	8.8651261	H	4.3992196	0.9082072	11.7780336	C	-0.9239837	-1.9990738	-4.6429643
C	-1.2115726	6.8230844	13.6870907	C	3.2767010	-0.4537418	13.9371251	H	-0.5036986	-2.9394441	-5.0070076
C	-1.8466971	6.5408288	12.4504432	H	2.9340626	-0.4509506	14.9808833	C	-1.1500649	-1.8513349	-3.2662733
C	-3.2157685	6.2429758	12.4429376	H	4.3774637	-0.4352160	13.9441444	C	-2.2492948	1.8670243	-3.2980267
H	-3.7073432	6.0334489	11.4896686	H	2.9554631	-1.4003260	13.4754070	H	-2.2429052	1.9087131	-2.2045374
C	-3.9673650	6.2358445	13.6163985	C	3.6455279	3.9561363	16.9752964	C	-1.1620965	2.8569950	-3.7525215
H	-5.0382324	6.0235792	13.5866885	C	4.9546486	3.6018652	16.5806612	H	-0.1896155	2.5804235	-3.3232889
C	-3.3291241	6.4779922	14.8299616	C	6.0193484	4.2797677	17.1903604	H	-1.4095942	3.8741242	-3.4089897
H	-3.9046220	6.4273373	15.7573224	H	7.0433229	4.0357364	16.9033557	H	-1.0616867	2.8843270	-4.8483995
C	-1.9528889	6.7374553	14.8934910	C	5.7921631	5.2482282	18.1670717	C	-3.6299481	2.3188738	-3.8038603
C	-1.1024228	6.5586916	11.1257869	H	6.6368100	5.7504741	18.6431525	H	-3.6573893	2.3506248	-4.9045054
H	-0.0574112	6.8127701	11.3402456	C	4.4891157	5.5978231	18.5136613	H	-3.8674073	3.3292767	-3.4349841
C	-1.1111993	5.1661520	10.4734022	H	4.3216099	6.3798441	19.2555989	H	-4.4297536	1.6387403	-3.4751385
H	-0.5312428	5.1740682	9.5381582	C	3.3869378	4.9699773	17.9157099	C	-0.7681090	-3.0308556	-2.3833036
H	-2.1361649	4.8459513	10.2298264	C	5.2203339	2.5557840	15.5086729	H	-1.1705888	-2.8345235	-1.3839417
H	-0.6712236	4.4166780	11.1474158	H	4.3250375	1.9223661	15.4265757	C	-1.3754181	-4.3523881	-2.8860095
C	-1.6500637	7.6336517	10.1735929	C	5.4336235	3.2424993	14.1473178	H	-1.0013491	-4.6126366	-3.8869733
H	-1.6129864	8.6300460	10.6395486	H	4.5566750	3.8314085	13.8433516	H	-2.4724935	-4.2975325	-2.9442446
H	-2.6956403	7.4324997	9.8930513	H	5.6234477	2.4937079	13.3636209	H	-1.1027075	-5.1825831	-2.2169964
H	-1.0538816	7.6656248	9.2484566	H	6.2969073	3.9233524	14.1854229	C	0.7584207	-3.1644583	-2.2551660
C	-1.3022971	6.8410419	16.2679543	C	6.3929234	1.6249782	15.8518017	H	1.0241577	-3.9747056	-1.5572787
H	-0.2199700	6.9558543	16.1195815	H	7.3556172	2.1578293	15.8507183	H	1.2077931	-2.2286539	-1.8994254
C	-1.8244987	8.0426299	17.0726620	H	6.4636706	0.8245292	15.1003223	H	1.2133644	-3.3960811	-3.2312305
H	-1.6637613	8.9919601	16.5412516	H	6.2620730	1.1569064	16.8387785	C	-2.8069530	-1.3165242	-2.1110070
H	-1.3195783	8.1100075	18.0485999	C	1.9725067	5.3764082	18.2912306	C	-3.4815256	-2.4752461	1.6349964
H	-2.9045738	7.9476294	17.2636261	H	1.2982824	4.9679243	17.5237971	C	-4.3768347	-3.1413269	2.4877033
C	-1.4974386	5.5353509	17.0578061	C	1.8078063	6.9032481	18.2775420	H	-4.8980954	-4.0213093	2.1070475
H	-1.0662064	4.6896939	16.5053812	H	0.7598444	7.1733591	18.4684271	C	-4.6329665	-2.7111411	3.7831051



H	-5.3619478	-3.2280415	4.4102977	C	3.9047093	-1.5242299	-0.7864525	H	-1.7089568	5.3990714	-0.3440743
C	-3.9090993	-1.6296518	4.2727815	C	4.2939855	-2.5376222	-1.6754260	C	-3.8811694	3.6862488	0.2750333
H	-4.0518373	-1.3179489	5.3097959	H	4.5874204	-3.5123227	-1.2804091	H	-4.2718849	4.5390015	-0.3023662
C	-2.9743812	-0.9475174	3.4838652	C	4.3017918	-2.3206316	-3.0503404	H	-3.9195968	3.9565355	1.3403209
C	-3.2489083	-3.1238047	0.2787210	H	4.6056011	-3.1217237	-3.7273786	H	-4.5609917	2.8358373	0.1118001
H	-2.6929294	-2.4265673	-0.3577767	C	3.8999313	-1.0886376	-3.5677022	C	-2.1238518	-0.0654322	-4.0140854
C	-2.3913597	-4.3872753	0.4871480	H	3.8831322	-0.9408496	-4.6483000	H	-1.6418305	-0.6545969	-3.2204567
H	-2.2318935	-4.9163618	-0.4605561	C	3.5034689	-0.0418790	-2.7264122	C	-3.4567900	-0.7304116	-4.4093178
H	-2.8883397	-5.0798908	1.1834287	C	3.8850516	-1.7983474	0.7099512	H	-3.9256462	-0.1756772	-5.2380209
H	-1.4072158	-4.1384190	0.9137498	H	3.5369169	-0.8888648	1.2193996	H	-4.1719335	-0.7500255	-3.5753805
C	-4.5467794	-3.4652090	-0.4719612	C	2.8883395	-2.9191416	1.0494771	H	-3.2928838	-1.7662465	-4.7471647
H	-5.2084063	-2.5898948	-0.5485915	H	1.8729650	-2.6567668	0.7204078	C	-1.1672207	-0.0769210	-5.2126861
H	-5.1102231	-4.2748290	0.0154031	H	2.8638189	-3.0971001	2.1347451	H	-0.9271492	-1.1124394	-5.5000393
H	-4.3092210	-3.7988512	-1.4929111	H	3.1670840	-3.8643355	0.5597009	H	-0.2296864	0.4324600	-4.9680264
C	-2.1324683	0.1069898	4.2024079	C	5.2909690	-2.1157932	1.2462774	H	-1.6028560	0.4180066	-6.0946008
H	-1.3910621	0.5062443	3.4960007	H	5.6920521	-3.0372373	0.7978645	C	-1.7252741	-0.2558123	3.6981073
C	-2.9711089	1.2786481	4.7449962	H	5.2606466	-2.2583911	2.3372860	C	-1.6197332	-1.5204940	4.3253309
H	-3.5293360	1.7986799	3.9534878	H	5.9951485	-1.2997856	1.0261059	C	-1.6003292	-1.5554565	5.7263862
H	-2.3221043	2.0177214	5.2371706	C	3.0705417	1.2967452	-3.3042640	H	-1.5143936	-2.5163975	6.2364853
H	-3.7013795	0.9266023	5.4891573	H	2.4802961	1.8123296	-2.5308945	C	-1.6863645	-0.3860516	6.4805388
C	-1.3624080	-0.5443367	5.3683411	C	2.1584613	1.1327376	-4.5278774	H	-1.6622834	-0.4358821	7.5712561
H	-0.8011741	-1.4305973	5.0398462	H	1.7821250	2.1157620	-4.8470177	C	-1.8118165	0.8441132	5.8401015
H	-2.0471164	-0.8634236	6.1676318	H	1.2940184	0.4969617	-4.2930406	H	-1.8956410	1.7539409	6.4368324
H	-0.6524384	0.1725140	5.8097010	H	2.6956908	0.6956855	-5.3832512	C	-1.8449509	0.9353766	4.4402915
N	2.3348881	2.1614194	0.9677256	C	4.2927240	2.1724640	-3.6367242	C	-1.5732799	-2.8240078	3.5370069
N	3.2445426	0.8068748	-0.4304602	H	4.9149139	1.6946524	-4.4094618	H	-1.2623070	-2.5846240	2.5095148
C	2.0355774	1.1085229	0.1429318	H	4.9254172	2.3446105	-2.7533174	C	-0.5613390	-3.8320493	4.1020837
C	3.6810704	2.5021778	0.9133457	H	3.9684889	3.1524704	-4.0183870	H	-0.4655621	-4.6913753	3.4221880
H	4.0994186	3.3032324	1.5113497	H	-0.4156147	2.0933779	-0.7079560	H	-0.8774682	-4.2239056	5.0804241
C	4.2567900	1.6433311	0.0282466	H	0.7928749	-0.0856321	-1.9643056	H	0.4315089	-3.3779186	4.2227969
H	5.2813570	1.5410613	-0.3092456	<b>TS3</b>				C	-2.9722737	-3.4675363	3.4658114
C	1.4001044	2.7565430	1.8931796	<b>(EE = -2602.412904 Hartree)</b>				H	-3.7146703	-2.7874450	3.0266402
C	0.6344760	3.8652662	1.4837357	<b>(Imaginary frequency= 1, -300.80 cm<sup>-1</sup>)</b>				H	-3.3212210	-3.7418852	4.4733861
C	-0.2736540	4.3888751	2.4155341	Al	-0.2120873	0.1426284	-0.3879563	H	-2.9439613	-4.3806800	2.8523035
H	-0.8971065	5.2394632	2.1367533	N	-1.9588410	0.6101386	-1.1004888	C	-2.0840256	2.2822250	3.7779208
C	-0.3896959	3.8439388	3.6932365	N	-1.6986936	-0.2179689	2.2431070	H	-1.7944323	2.2005810	2.7181065
H	-1.1075921	4.2660909	4.3995042	C	-0.5534912	-0.1614437	1.5802587	C	-3.5845150	2.6256935	3.8534360
C	0.4141167	2.7718399	4.0801562	H	0.2796415	-0.0793929	2.2866874	H	-4.1995290	1.8884103	3.3182103
H	0.3288716	2.3757919	5.0927314	C	-3.0049265	-0.3313106	1.5422618	H	-3.7780645	3.6153406	3.4153034
C	1.3348343	2.2043045	3.1898687	H	-3.3203809	0.6871551	1.2649288	H	-3.9188821	2.6485896	4.9023113
C	0.8268268	4.5152398	0.1222998	H	-3.7209956	-0.7134101	2.2809906	C	-1.2528037	3.4118337	4.4041602
H	1.2187399	3.7436496	-0.5572247	C	-2.9453005	-1.2193291	0.2948317	H	-0.1896464	3.1448797	4.4552059
C	1.8645308	5.6511041	0.2188877	H	-3.8062474	-1.9074927	0.2956787	H	-1.5962892	3.6538217	5.4213021
H	2.0361236	6.0958351	-0.7730785	H	-2.0452608	-1.8519752	0.3517138	H	-1.3458738	4.3263779	3.8003946
H	2.8304528	5.2897146	0.6002477	C	-2.9462515	-0.4669138	-1.0454263	N	2.9437073	0.1477021	0.4117547
H	1.5112502	6.4460996	0.8938281	H	-2.8256510	-1.2520955	-1.8207838	N	2.7541269	0.3725552	-1.7102537
C	-0.4816913	5.0271013	-0.4925694	H	-3.9527546	-0.0329798	-1.2075067	C	1.9943530	0.2810751	-0.5737004
H	-0.2959207	5.3804283	-1.5172302	C	-2.2276013	1.6193210	-2.0578737	C	4.2394313	0.1425815	-0.0962919
H	-0.9042602	5.8704063	0.0748529	C	-2.4277165	2.9670099	-1.6300977	H	5.1076077	0.0414049	0.5441316
H	-1.2260307	4.2200975	-0.5449664	C	-2.7161549	3.9670671	-2.5685016	C	4.1202069	0.2853507	-1.4392285
C	2.2289522	1.0386945	3.5984161	H	-2.8701169	4.9931982	-2.2226240	H	4.8617264	0.3474671	-2.2268067
H	3.1594645	1.1208022	3.0145854	C	-2.8375559	3.6815366	-3.9269843	C	2.6855857	0.0994943	1.8268819
C	1.5874020	-0.3138948	3.2448722	H	-3.0703601	4.4725051	-4.6438927	C	2.5055496	1.3210328	2.5071003
H	1.3133009	-0.3701929	2.1829187	C	-2.6574806	2.3665616	-4.3542566	C	2.2091525	1.2511894	3.8754983
H	0.6767015	-0.4735542	3.8321643	H	-2.7483492	2.1350539	-5.4187835	H	2.0439236	2.1711988	4.4374364
H	2.2839850	-1.1350588	3.4692787	C	-2.3424560	1.3368188	-3.4567000	C	2.1198727	0.0220307	4.5282009
C	2.6310244	1.0770851	5.0794070	C	-2.4463443	3.3355058	-0.1555485	H	1.8599042	-0.0127146	5.5878713
H	3.0641529	2.0486579	5.3586322	H	-2.1201118	2.4375848	0.3885280	C	2.3686826	-1.1648713	3.8375786
H	3.3798752	0.2968974	5.2799552	C	-1.4696486	4.4659100	0.1909722	H	2.3350853	-2.1117697	4.3763902
H	1.7753959	0.8807462	5.7427806	H	-0.4412129	4.1740243	-0.0634600	C	2.6676743	-1.1563715	2.4671443
C	3.5307937	-0.2849552	-1.3381629	H	-1.4995853	4.6855349	1.2703822	C	2.6870677	2.6566474	1.7996947

H	2.5097087	2.4892329	0.7279102	C	1.8150337	8.3203150	11.5335653	Al	0.1562784	6.6955431	15.3839044
C	4.1361650	3.1513672	1.9718561	H	1.1400199	7.8945301	10.7710035	H	-0.3039894	7.8233520	16.4430246
H	4.2853113	4.0911725	1.4188164	H	2.8417003	8.1681999	11.1864243	H	-1.0271344	5.8367678	14.6945766
H	4.8642866	2.4180858	1.5965613	C	2.4981661	6.4153276	12.9590135	N	2.1147715	5.8205622	17.5988012
H	4.3602999	3.3393349	3.0334889	C	3.8616052	6.6205022	13.2731801	N	0.1600409	4.6515049	17.2700055
C	1.6860931	3.7256583	2.2457934	C	4.6904847	5.4947210	13.3749388	C	1.2738955	5.3016724	16.4740089
H	1.8071266	4.6282110	1.6282375	H	5.7395308	5.6281129	13.6451125	C	1.3074186	5.9026109	18.7464067
H	1.8346711	4.0240999	3.2946577	C	4.1999204	4.2155205	13.1290858	H	1.6721685	6.3737658	19.6519326
H	0.6585236	3.3634944	2.1162689	H	4.8588927	3.3493082	13.2134473	C	0.1698433	5.2018920	18.5587407
C	2.9448572	-2.4446191	1.6999390	C	2.8672382	4.0416975	12.7626735	H	-0.6079680	4.9703956	19.2765896
H	3.6374264	-2.1934403	0.8807915	H	2.5033086	3.0406612	12.5293238	C	3.4458738	6.2827038	17.5968063
C	1.6692741	-3.0134496	1.0513886	C	1.9875074	5.1282513	12.6591780	C	4.5325261	5.3881571	17.3558426
H	1.1982059	-2.3071315	0.3524205	C	4.4693695	8.0062492	13.4420333	C	5.8399296	5.8566540	17.5230120
H	0.9291364	-3.2721554	1.8214940	H	3.6435446	8.7328653	13.4938137	H	6.6756940	5.1779055	17.3467418
H	1.9108961	-3.9296596	0.4904450	C	5.2765779	8.1365119	14.7383349	C	6.1044513	7.1521005	17.9756127
C	3.6351647	-3.5115978	2.5613753	H	4.6888695	7.8327928	15.6101654	H	7.1334607	7.4809489	18.1354527
H	4.5268869	-3.1145135	3.0684477	H	5.5954468	9.1792277	14.8852700	C	5.0412899	8.0207213	18.2053474
H	3.9468673	-4.3536065	1.9264464	H	6.1821802	7.5135822	14.7140878	H	5.2461563	9.0470290	18.5212552
H	2.9587455	-3.9189322	3.3285048	C	5.3635730	8.3652566	12.2374361	C	3.7137479	7.6294184	17.9795383
C	2.3384492	0.5888948	-3.0769028	H	6.2341900	7.6932221	12.1976810	C	4.2876539	3.9078463	17.1031763
C	2.4619786	-0.4914165	-3.9715406	H	5.7373453	9.3959361	12.3334710	H	3.4385554	3.8119963	16.4097551
C	2.3627268	-0.2085658	-5.3412548	H	4.8398908	8.2809404	11.2741808	C	3.8976866	3.2195890	18.4271181
H	2.4592859	-1.0201976	-6.0653225	C	0.5772562	4.8991234	12.1294111	H	3.6900404	2.1510003	18.2639454
C	2.1267110	1.0900549	-5.7872206	H	-0.0403480	5.7562422	12.4281636	H	3.0048132	3.6793987	18.8712838
H	2.0551815	1.2935555	-6.8576629	C	0.5996415	4.8347651	10.5889871	H	4.7252699	3.2985654	19.1495240
C	1.9280887	2.1245567	-4.8710364	H	1.1668492	3.9552265	10.2461626	C	5.4671284	3.1698722	16.4576177
H	1.6904442	3.1236310	-5.2366025	H	1.0664406	5.7251376	10.1435093	H	5.1530886	2.1560679	16.1680267
C	2.0321024	1.9031438	-3.4910383	H	-0.4255925	4.7519216	10.1959795	H	6.3144244	3.0625769	17.1522095
C	2.6669502	-1.9206475	-3.4910121	H	-0.0999377	3.6517176	12.7088351	H	5.8254035	3.6845187	15.5550804
H	2.7385406	-1.9027967	-2.3935300	H	-1.1292196	3.5789409	12.3301753	C	2.6196080	8.6856793	18.0770890
C	1.4405007	-2.7818486	-3.8400614	H	-0.1580952	3.6977711	13.8031599	H	1.6553758	8.2062933	17.8537192
H	0.5361686	-2.3627832	-3.3763348	H	0.4201133	2.7253352	12.4224482	C	2.8437553	9.7731541	17.0094138
H	1.5776578	-3.8064998	-3.4616421	C	-1.4967497	9.0385842	13.9413364	H	2.7847700	9.3463280	15.9971589
H	1.2868065	-2.8388486	-4.9287005	C	-2.5665111	8.3894938	13.2780964	H	3.8300705	10.2491342	17.1173678
C	3.9649848	-2.5344080	-4.0395147	C	-3.8703329	8.6370845	13.7295682	H	2.0801332	10.5593584	17.0920843
H	3.9403747	-2.6100653	-5.1372227	H	-4.7082290	8.1377555	13.2388078	C	2.5256508	9.3095662	19.4789478
H	4.1062667	-3.5492380	-3.6380463	C	-4.1147504	9.5102088	14.7851182	H	2.3642741	8.5422875	20.2501742
H	4.8434793	-1.9320393	-3.7637907	H	-5.1379734	9.6910424	15.1209816	H	1.6876479	10.0214018	19.5293584
C	1.8610749	3.0407055	-2.4899822	C	-3.0493702	10.1486155	15.4156622	H	3.4458599	9.8560261	19.7392832
H	1.4139813	2.6136814	-1.5766416	H	-3.2501122	10.8306470	16.2435263	C	-0.7962269	3.7381487	16.7752978
C	0.9046577	4.1300847	-2.9884511	C	-1.7246122	9.9342901	15.0108629	C	-2.1820774	4.0739332	16.7385114
H	0.7018581	4.8421931	-2.1760603	C	-2.3780945	7.4756733	12.0732200	C	-3.0753705	3.1579452	16.1717289
H	-0.0578887	3.7107734	-3.3097096	H	-1.2986112	7.3512080	11.9042853	H	-4.1365266	3.4131623	16.1269186
H	1.3371384	4.7024719	-3.8242371	C	-2.9657977	6.0748879	12.3112078	C	-2.6435847	1.9446502	15.6309163
C	3.2200224	3.6568829	-2.1029092	H	-2.7638650	5.4285491	11.4433187	H	-3.3589345	1.2627277	15.1659482
H	3.7056393	4.1027343	-2.9849640	H	-4.0572813	6.1181641	12.4450717	C	-1.2965272	1.5993099	15.7252587
H	3.9076389	2.9147577	-1.6737684	H	-2.5227818	5.6108694	13.2024694	H	-0.9627157	0.6243497	15.3598385
H	3.0738287	4.4523878	-1.3560323	C	-2.9826310	8.1023695	10.8020485	C	-0.3679902	2.4583871	16.3257457
H	-0.0492221	1.6187298	0.5521628	H	-2.5848945	9.1101226	10.6082187	C	-2.7211321	5.3802386	17.3073387
H	-0.0720985	-1.3039533	-1.2238034	H	-4.0758396	8.1912699	10.8916244	H	-1.8665296	6.0534331	17.4713510
<b>Int1a</b>				H	-2.7663400	7.4726876	9.9258753	C	-3.6755943	6.1069489	16.3505615
<b>(EE = -2602.41234 Hartree)</b>				C	-0.6016434	10.6823753	15.7138946	H	-3.1919416	6.2841690	15.3820787
N	1.6440459	7.5757585	12.7997279	H	0.3433791	10.1896500	15.4416629	H	-3.9536082	7.0865042	16.7674491
N	-0.1646849	8.8984207	13.3712462	C	-0.5387533	12.1529136	15.2567640	H	-4.6042964	5.5395361	16.1830308
C	0.6391783	7.8444797	13.6606727	H	-0.4308750	12.2496227	14.1664749	C	-3.4102311	5.1382866	18.6645293
C	0.0700376	9.8681997	12.2745783	H	0.3152064	12.6636254	15.7275879	H	-4.3096497	4.5151709	18.5359607
H	-0.1664443	10.8666646	12.6667998	H	-1.4558577	12.6891545	15.5462577	H	-3.7214271	6.0925853	19.1173114
H	-0.6416213	9.6624236	11.4588202	C	-0.7366152	10.6152172	17.2436741	H	-2.7523959	4.6185332	19.3766713
C	1.4953884	9.7860766	11.7662056	H	-0.7625454	9.5703174	17.5816587	C	1.0362090	1.9490765	16.6151063
H	2.1981257	10.2109934	12.4997846	H	-1.6457376	11.1262481	17.5944273	H	1.5845012	2.7680116	17.0973565
H	1.5943671	10.3582249	10.8339721	H	0.1175786	11.1150536	17.7232401	C	1.8060959	1.5297936	15.3562419

H	2.8172240	1.1813389	15.6184693	H	-0.7472949	-0.5460339	-2.8726469	C	-2.9074379	0.9742400	3.1881311
H	1.9098402	2.3695601	14.6567033	H	-0.5784129	-1.8536529	-4.0538371	C	0.4848020	-0.7607206	3.8322459
H	1.2960458	0.7086809	14.8283492	C	-0.6765218	3.4130154	-0.7785818	H	0.5309820	-1.1060164	2.7887840
C	0.9765596	0.7924974	17.6302156	C	-1.9417381	3.4916904	-1.3978588	C	0.1944727	-1.9831855	4.7225380
H	0.4415795	-0.0754320	17.2147285	C	-2.9404040	4.2369542	-0.7564864	H	1.0004928	-2.7272952	4.6260424
H	0.4578332	1.1020290	18.5493105	H	-3.9269316	4.3182149	-1.2182661	H	-0.7492344	-2.4715019	4.4400983
H	1.9920356	0.4645899	17.9029368	C	-2.6987946	4.8652704	0.4635343	H	0.1259306	-1.6877032	5.7814236
H	1.8204728	4.5450975	15.8856281	H	-3.4917459	5.4385670	0.9486863	C	1.8539375	-0.1549134	4.1585938
<b>TS1a</b>				C	-1.4539148	4.7404232	1.0765110	H	2.6426807	-0.8962109	3.9612778
<b>(EE = -2602.394127 Hartree)</b>				H	-1.2794193	5.2197906	2.0418777	H	1.9392098	0.1394794	5.2165841
<b>(Imaginary frequency = 1, -28.76 cm<sup>-1</sup>)</b>				C	-0.4108156	4.0326596	0.4630106	H	2.0513097	0.7250068	3.5302849
N	1.9640133	1.3308001	-2.2213653	C	-2.2373064	2.8191991	-2.7299917	C	-4.1572327	0.7971663	2.3365151
N	0.4344228	2.8932244	-1.5448295	H	-1.3524496	2.2264386	-3.0065828	H	-4.0242513	-0.1029230	1.7207782
C	0.8558792	1.6118570	-1.4917550	C	-3.4137341	1.8390012	-2.6088298	C	-4.3344109	1.9663944	1.3622966
C	1.0494647	3.9237405	-2.4158705	H	-3.5706418	1.3141449	-3.5638774	H	-3.4621203	2.0462485	0.7027711
H	0.7733674	4.9066308	-2.0159887	H	-4.3492345	2.3628577	-2.3569857	H	-4.4515799	2.9244315	1.8912033
H	0.6168670	3.8454500	-3.4286979	H	-3.2034173	1.0913537	-1.8285986	H	-5.2259167	1.8109562	0.7350258
C	2.5517755	3.7235195	-2.4611712	C	-2.4880797	3.8550915	-3.8408369	C	-5.4063433	0.5892579	3.2095118
H	2.9773794	3.8677495	-1.4561731	H	-1.6461059	4.5562657	-3.9440831	H	-5.2849892	-0.2657450	3.8918097
H	3.0235965	4.4508214	-3.1362717	H	-3.3908332	4.4483535	-3.6284180	H	-6.2869164	0.4003212	2.5768494
C	2.8081383	2.3130587	-2.9491333	H	-2.6361991	3.3516519	-4.8085296	H	-5.6194883	1.4779287	3.8237184
H	2.6018442	2.2253320	-4.0304679	C	0.9712426	4.0126300	1.1016786	C	-1.2240829	-3.2300338	-0.4783168
H	3.8558826	2.0184950	-2.7969329	H	1.5575003	3.2329422	0.5938091	C	-2.0945967	-3.3449935	-1.5809798
C	2.4479720	-0.0158444	-2.4394633	C	1.6839579	5.3658789	0.9133277	C	-1.6558816	-4.0998372	-2.6808283
C	3.5259963	-0.4897460	-1.6651662	H	1.7630868	5.6536361	-0.1452335	H	-2.3084839	-4.2098892	-3.5494681
C	4.0452948	-1.7525478	-1.9751120	H	2.7015625	5.3244255	1.3311714	C	-0.3995015	-4.6998302	-2.6834070
H	4.8717022	-2.1531390	-1.3832689	H	1.1367868	6.1675127	1.4336842	H	-0.0687705	-5.2695006	-3.5549867
C	3.5094534	-2.5160880	-3.0123236	C	0.9216907	3.6340930	2.5864677	C	0.4404004	-4.5772322	-1.5739975
H	3.9131375	-3.5087173	-3.2239538	H	0.4151552	2.6714932	2.7204610	H	1.4222756	-5.0512664	-1.5913860
C	2.4585420	-2.0145517	-3.7775662	H	0.3962615	4.3915734	3.1881376	C	0.0429947	-3.8548227	-0.4438033
H	2.0486400	-2.6193700	-4.5886526	H	1.9438193	3.5446796	2.9862938	C	-3.4888946	-2.7302734	-1.5833266
C	1.9275858	-0.7416611	-3.5283363	Al	0.0681613	0.0554688	-0.0029763	H	-3.5465167	-2.0325978	-0.7347571
C	4.0936013	0.3043680	-0.4975666	H	0.6063094	0.9650541	1.2285297	C	-3.7770239	-1.9112834	-2.8487540
H	3.5199981	1.2407833	-0.4215045	H	-1.9388085	-0.0338757	-0.3528713	H	-3.0463710	-1.1025648	-2.9593987
C	3.9063274	-0.4440509	0.8328959	H	0.9250113	-1.1332142	-0.6647525	H	-4.7780335	-1.4584250	-2.7817673
H	2.8486773	-0.6972293	0.9905399	N	-1.9225105	-1.0503792	2.2495122	H	-3.7524417	-2.5331363	-3.7569644
H	4.2394850	0.1831309	1.6738642	N	-1.6680293	-2.5053319	0.6798736	C	-4.5602877	-3.8211672	-1.3980494
H	4.4914096	-1.3760073	0.8496219	C	-1.2203477	-1.2515275	1.0736113	H	-4.5535017	-4.5209176	-2.2487830
C	5.5721513	0.6660801	-0.7204636	C	-2.8225427	-2.0881609	2.5162325	H	-5.5627663	-3.3705370	-1.3381540
H	6.1980058	-0.2385358	-0.7622592	H	-3.4710784	-2.0794422	3.3844611	H	-4.3953487	-4.4096462	-0.4841832
H	5.9434407	1.2923266	0.1050969	C	-2.6608408	-3.0001993	1.5282211	C	0.9127280	-3.7820281	0.8036452
H	5.7210657	1.2172915	-1.6613125	H	-3.1366135	-3.9586211	1.3587029	H	0.7855491	-2.7692910	1.2163069
C	0.7980777	-0.1891752	-4.3840537	C	-1.8139608	0.0905232	3.1126099	C	2.4056747	-3.9667180	0.5220381
H	0.7589003	0.8990527	-4.2195248	C	-0.6578663	0.2414677	3.9106846	H	2.9824484	-3.7619078	1.4365354
C	1.0249927	-0.4147317	-5.8866759	C	-0.6282060	1.3171516	4.8055308	H	2.7455416	-3.2753954	-0.2596228
H	0.9827524	-1.4825765	-6.1484567	H	0.2488696	1.4667536	5.4368220	H	2.6431113	-4.9962803	0.2098369
H	2.0013681	-0.0250738	-6.2117158	C	-1.6972155	2.2114413	4.8977755	C	0.4333671	-4.7948331	1.8613744
H	0.2405920	0.0949036	-6.4664955	H	-1.6462210	3.0488720	5.5973661	H	0.5267636	-5.8243767	1.4814002
C	-0.5539760	-0.7604487	-3.9341909	C	-2.8193965	2.0442334	4.0921074	H	-0.6152391	-4.6262894	2.1425065
H	-1.3713221	-0.3273826	-4.5321468	H	-3.6474924	2.7534077	4.1636520	H	1.0437843	-4.7106591	2.7737977