Reducing Hybrid Ligand based Alane and Chasing Aluminum(I): Dialane and unusual transient dialumene

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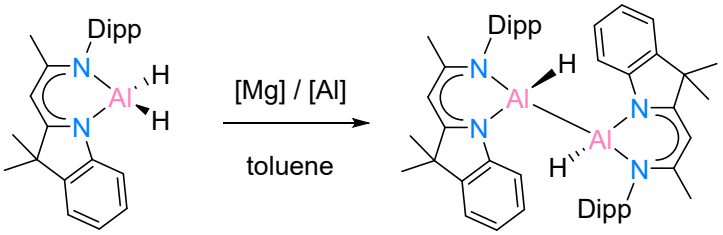
Synthesis and Analytical Data

Compound 2



1 **2,** 23% [Mg], 88% [Al]

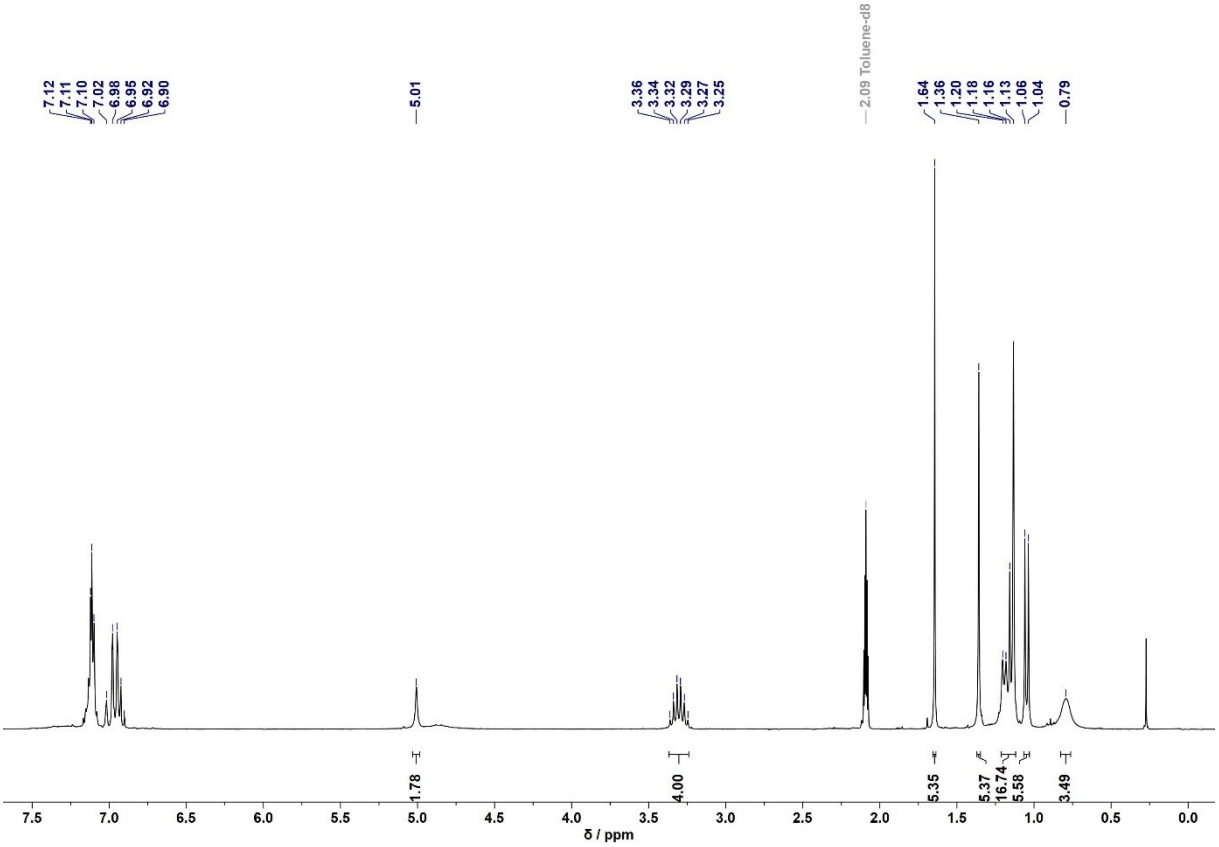


Figure S1: ^{1}H NMR spectrum of **2** in tol-d_8.

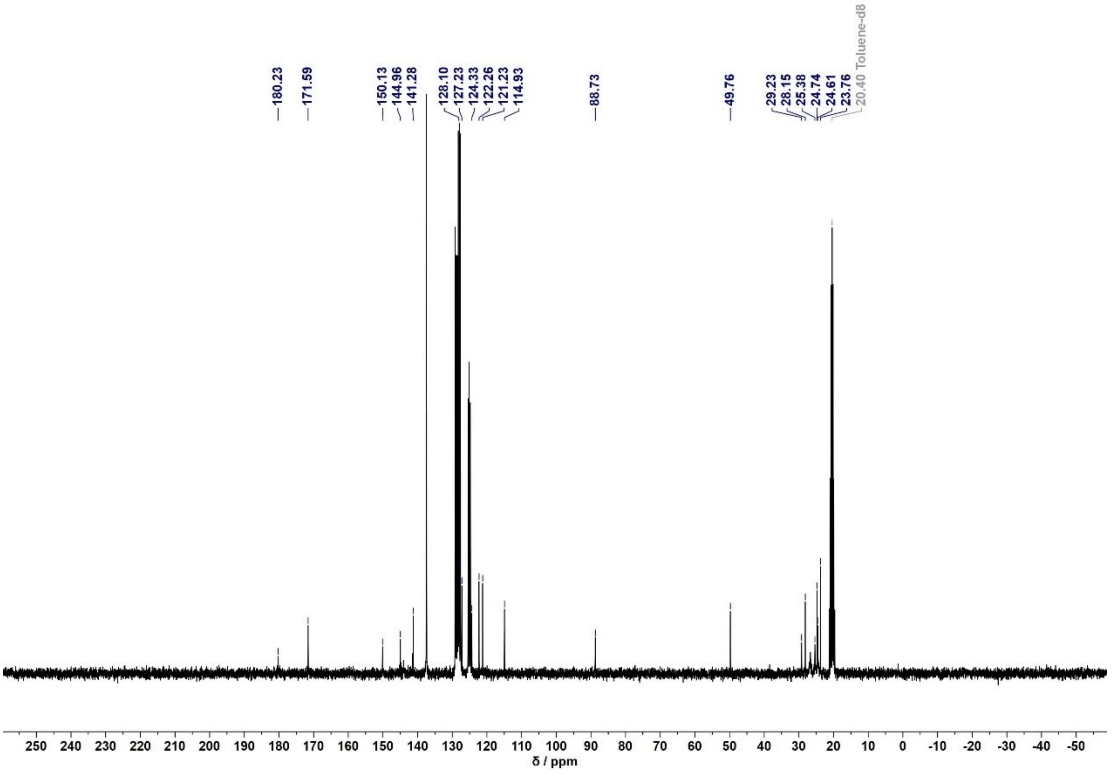


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **2** in tol-d_8.

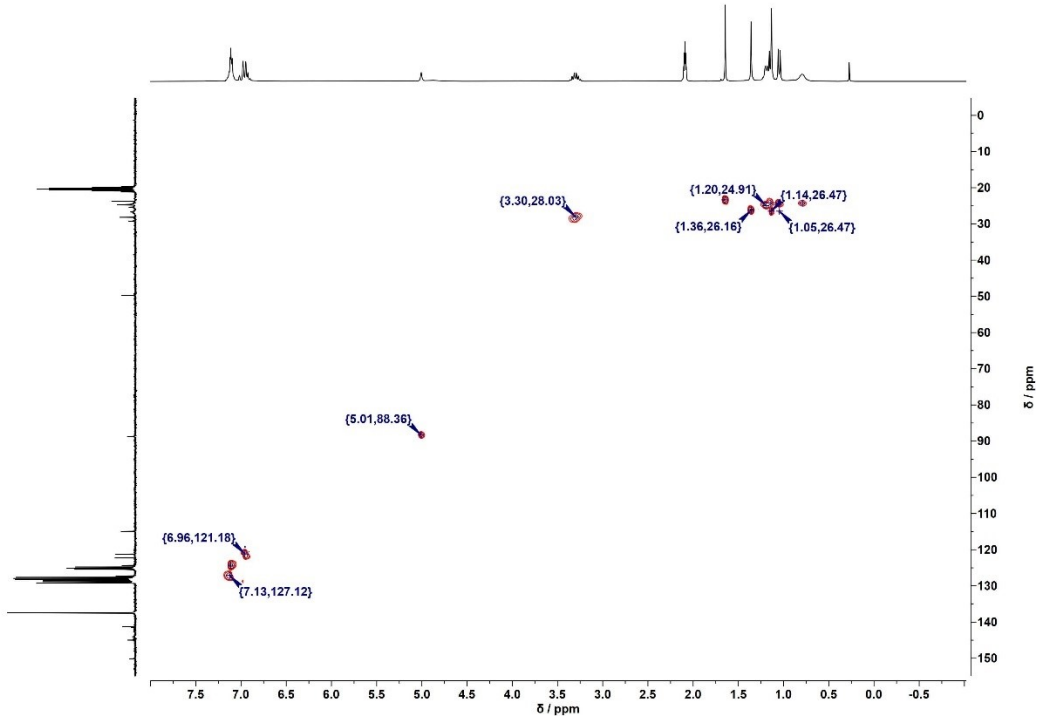


Figure S3: ^{1}H, ^{13}C HSQC spectrum of **2** in tol-d_8.

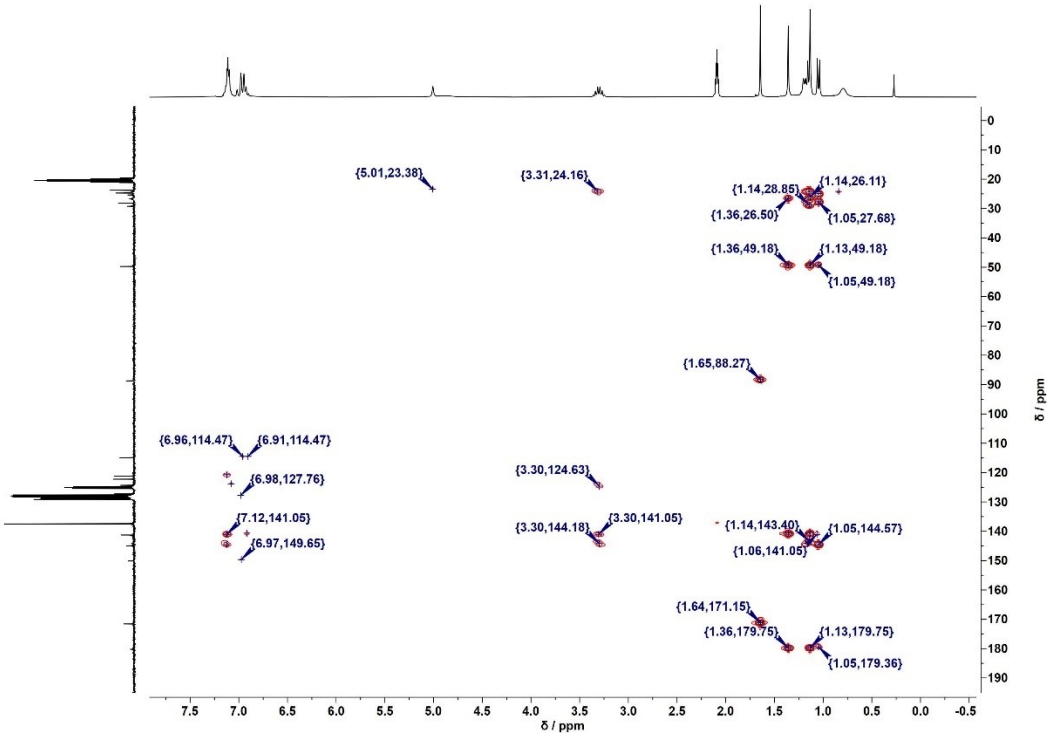


Figure S4: ^{1}H, ^{13}C HMBC spectrum of **2** in tol-d_8.

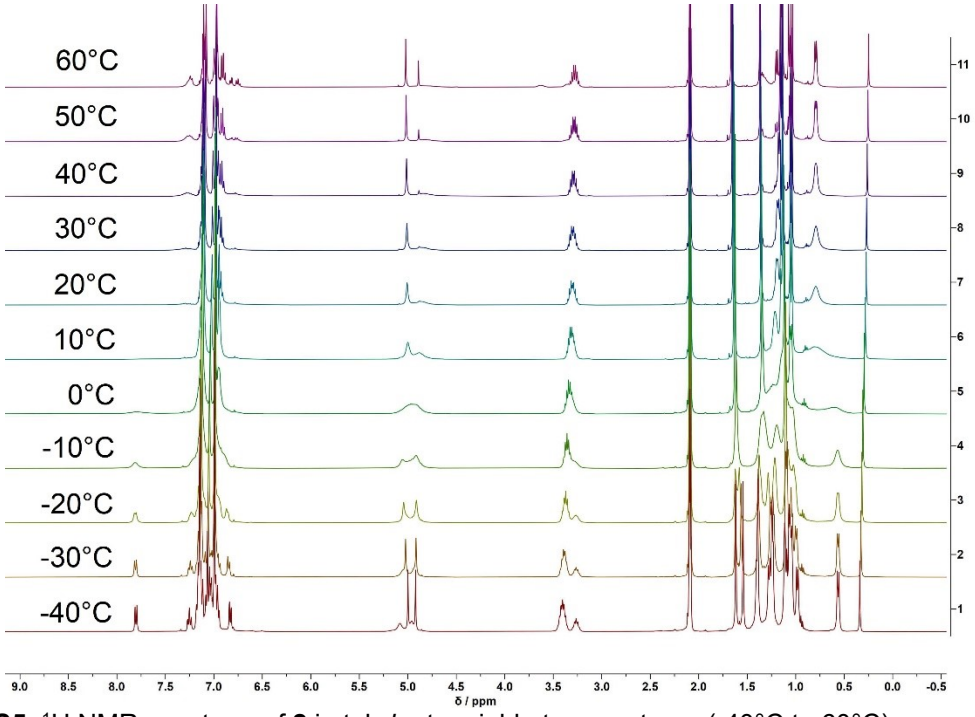


Figure S5: ^{1}H NMR spectrum of **2** in tol-d_8 at variable temperatures (-40°C to 60°C).

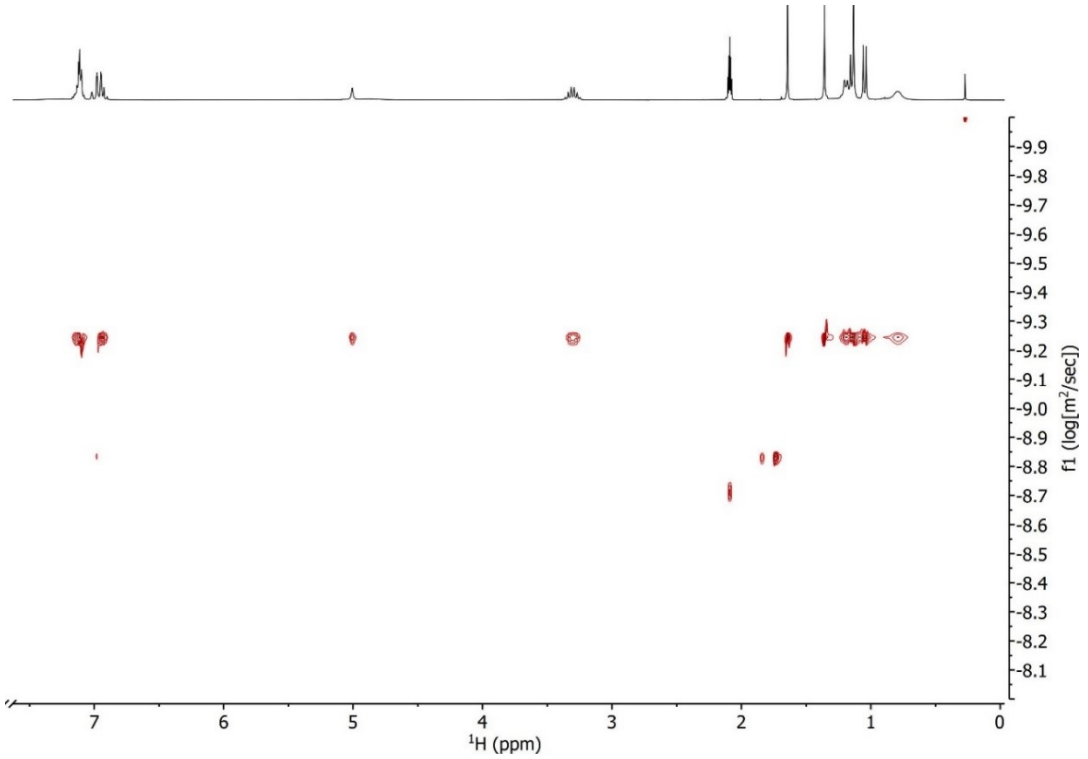


Figure S6: ^{1}H DOSY spectrum of **2** in tol-d_8 at room temperatures (298 K).

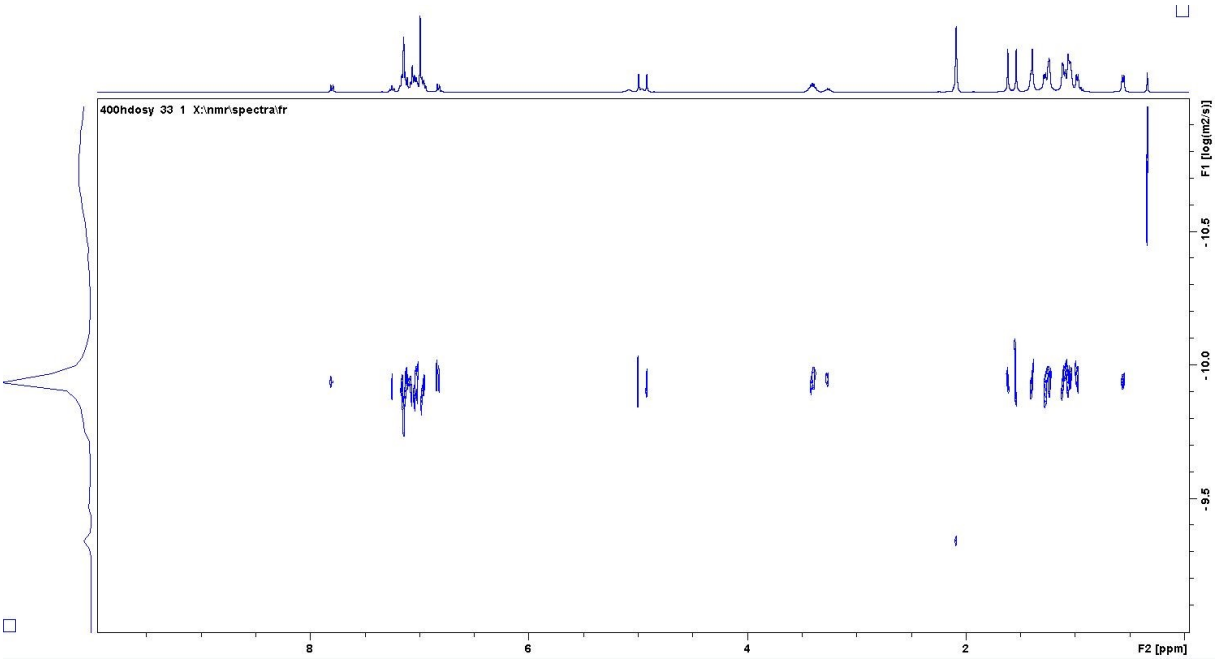


Figure S7: ^{1}H DOSY spectrum of **2** in tol-d_8 at -40℃ (233 K).

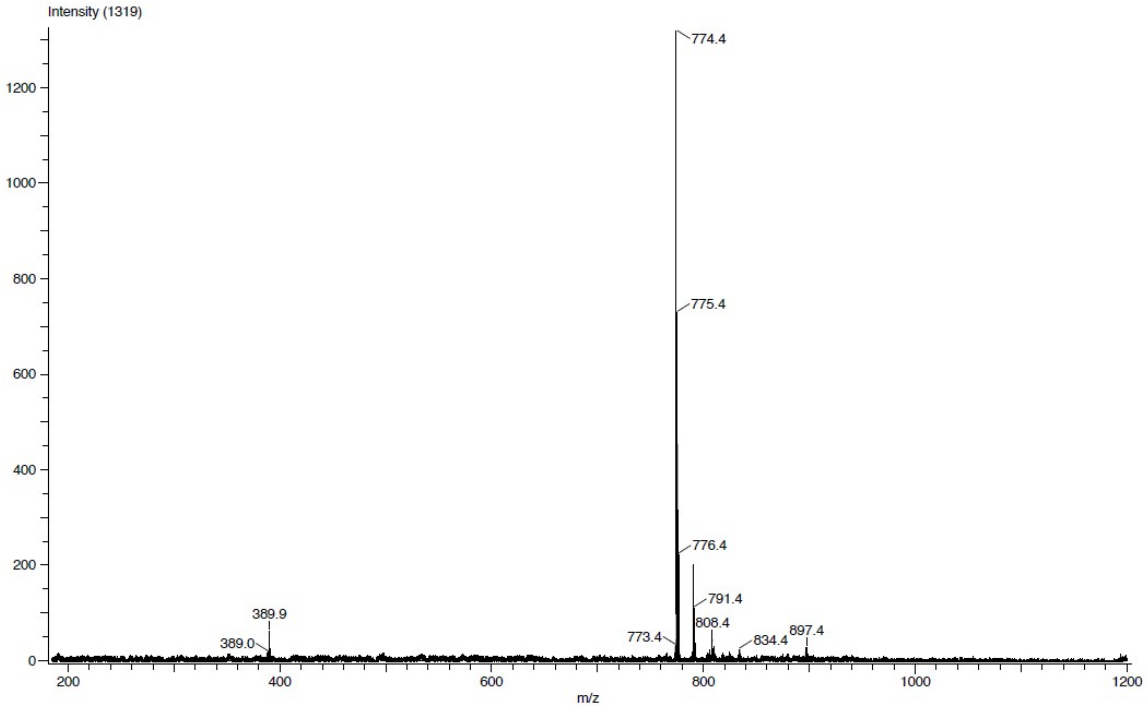


Figure S8: Mass spectrum of **2**.

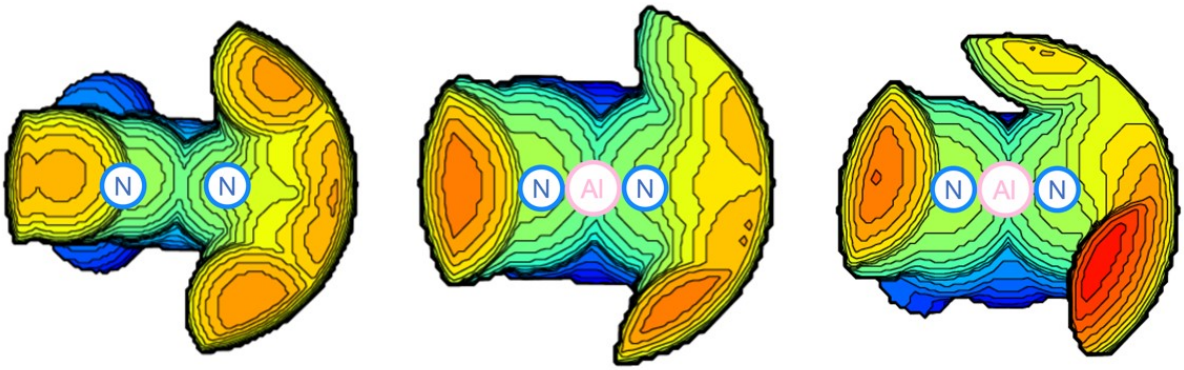
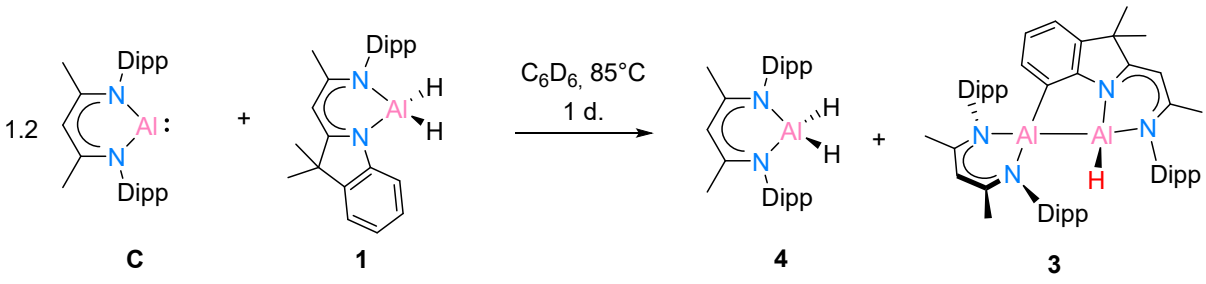


Figure S9: Calculated buried volumes V_B for the free DNI ligand (left, 50.9%)[1],and that at Al1 of compound **2** (mid, 49.5%) and at Al2 of compound **2** (right, 51.5%) (3.5 Å sphere around Al, the right side of each map is the Dipp group, Dipp = 2,6-diisopropylphenyl).

Compound 3 and 4



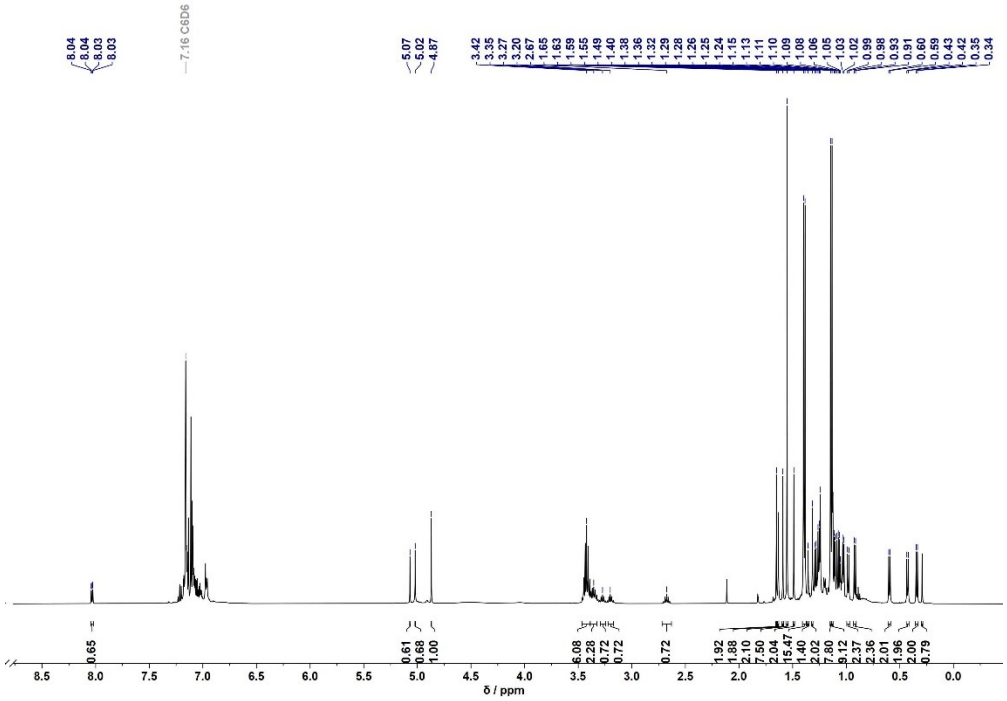


Figure S10: ^{1}H NMR spectrum of **3** and **4** in C_6D_6.

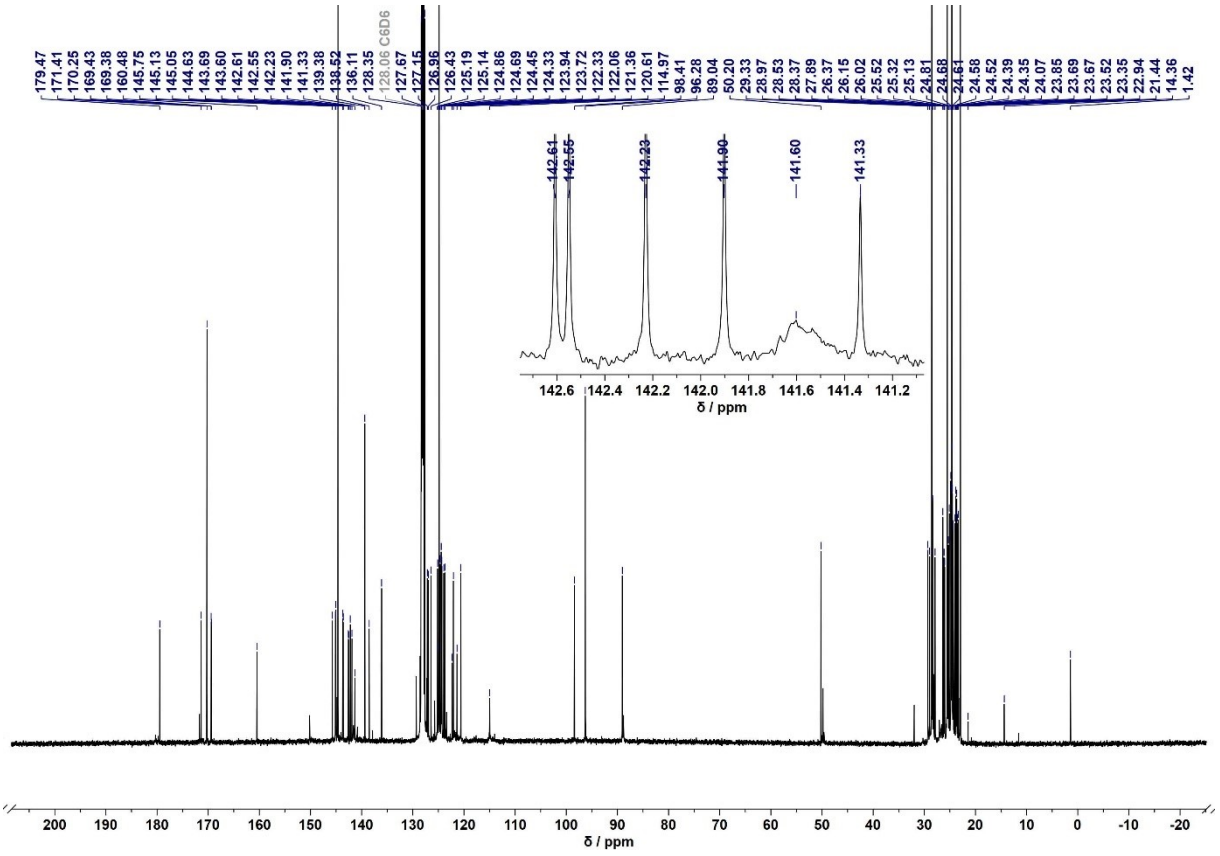


Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum of **3** and **4** in C_6D_6.

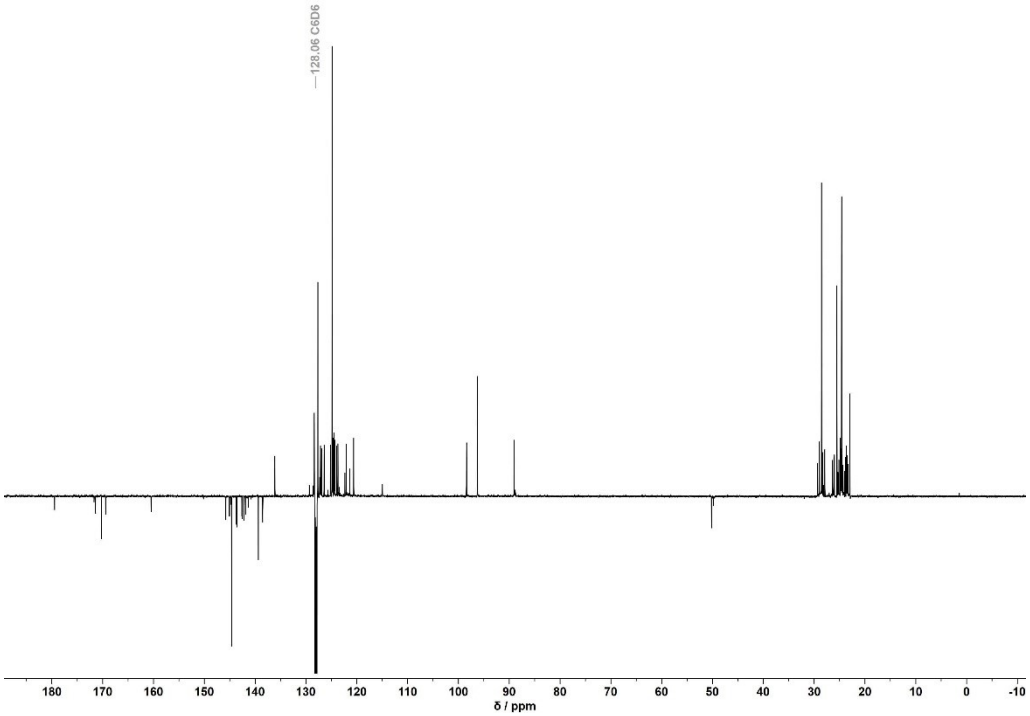


Figure S12: $^{13}C\{^{1}H\}$ APT NMR spectrum of **3** and **4** in C_6D_6.

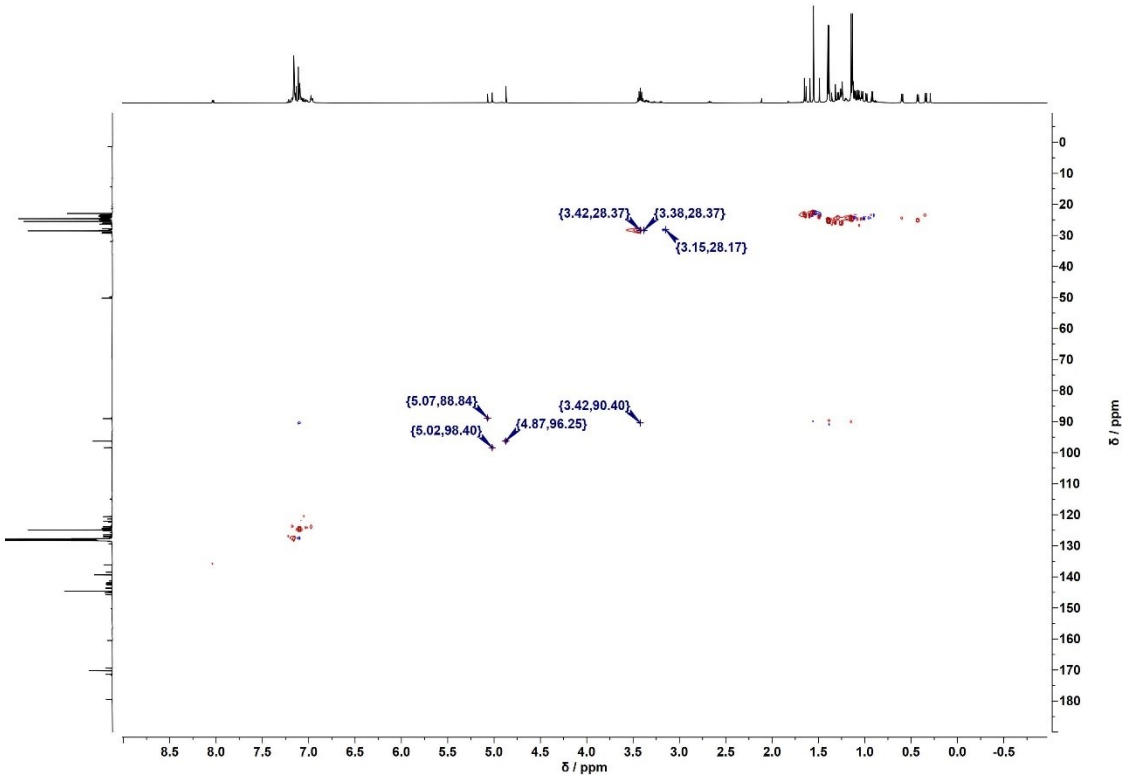


Figure S13: ^{1}H, ^{13}C HSQC spectrum of **3** and **4** in C_6D_6.

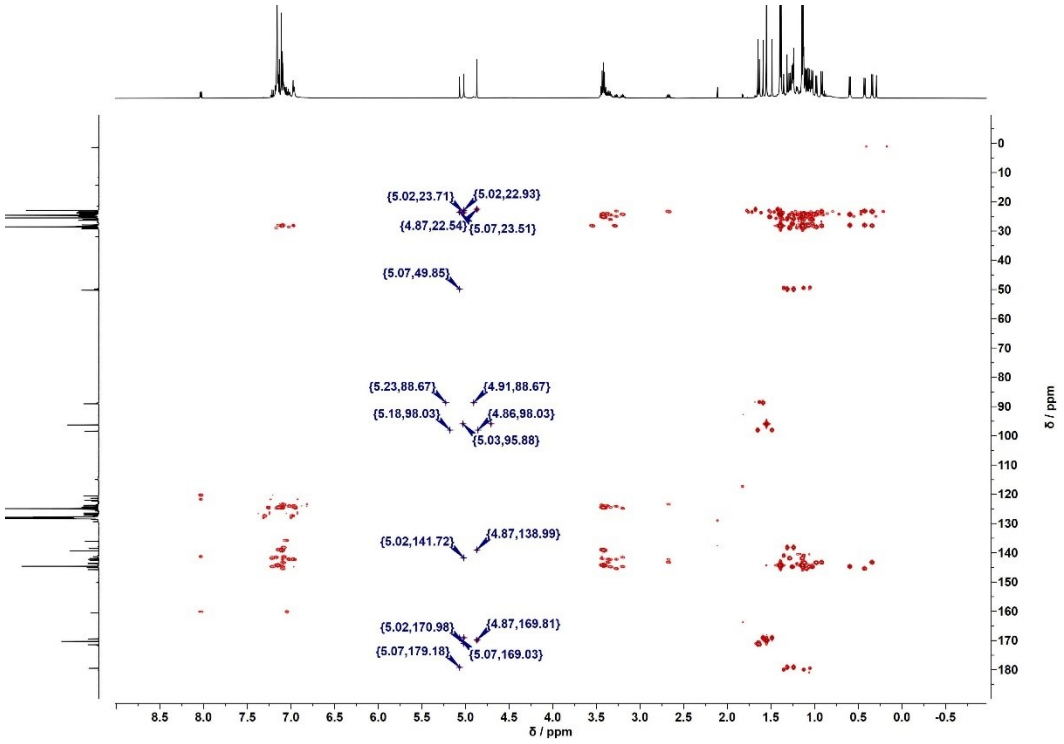


Figure S14: ^{1}H, ^{13}C HMBC spectrum of **3** and **4** in C_6D_6.

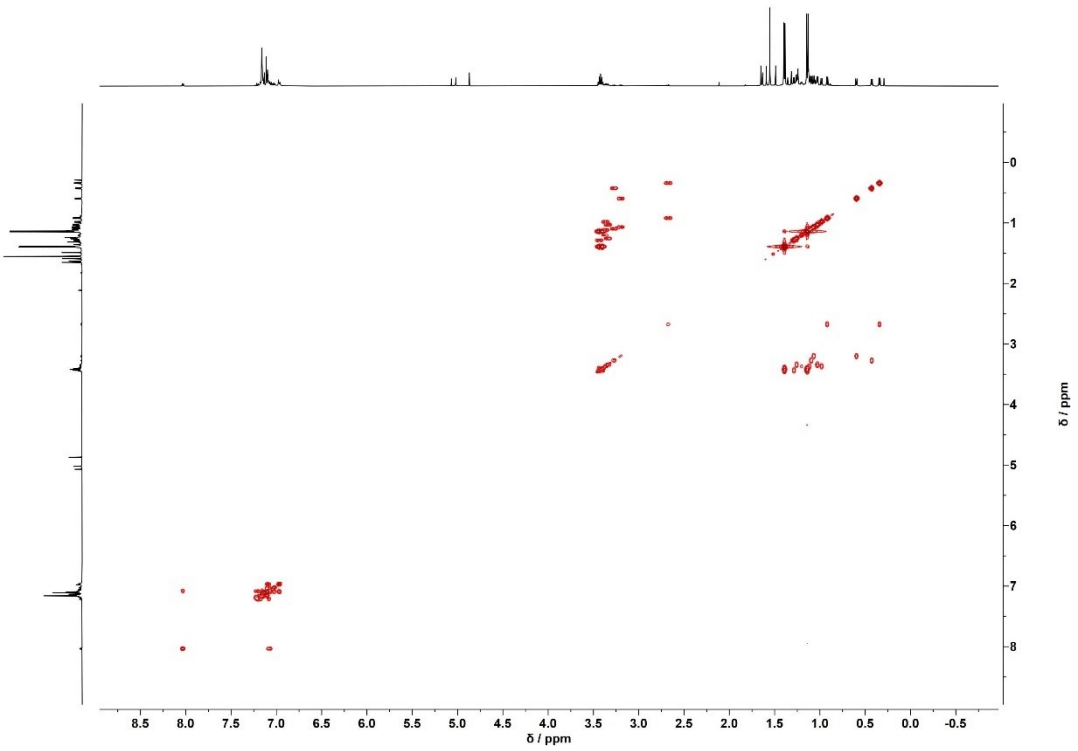


Figure S15: ^{1}H, ^{1}H COSY spectrum of **3** and **4** in C_6D_6.

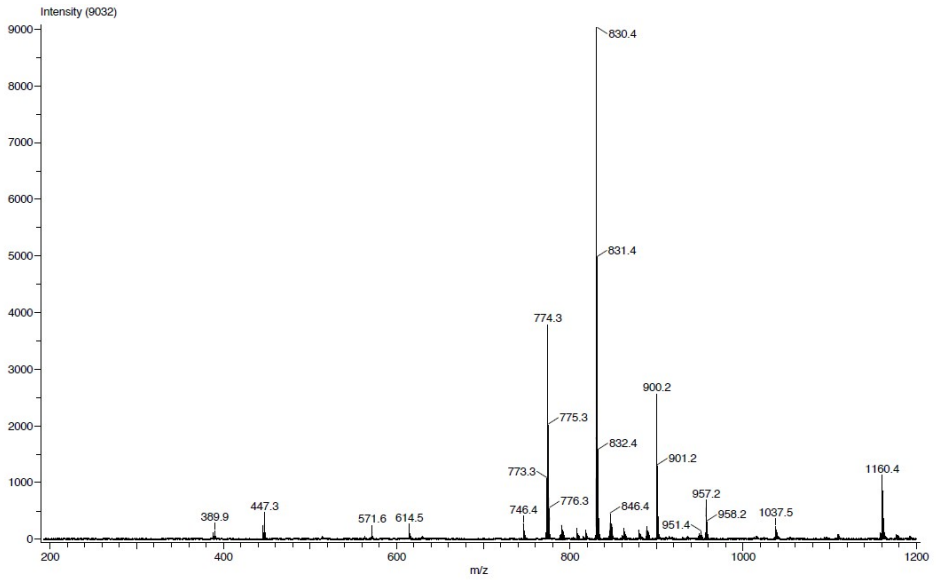
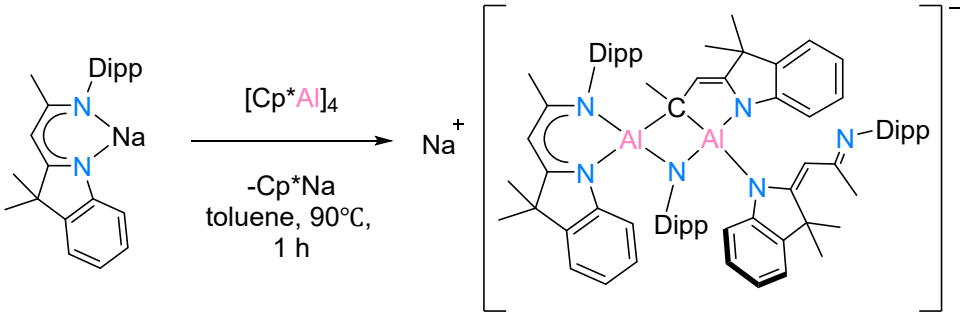


Figure S16: Mass spectrum of **3** and **4**.

Compound 5



5, 21.3%

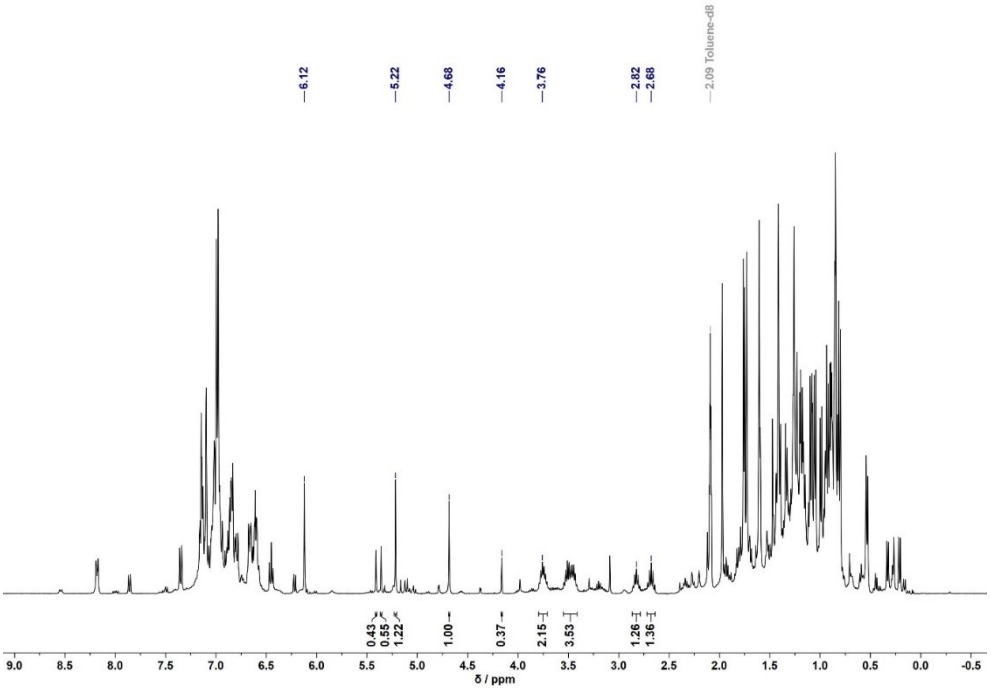


Figure S17: ^{1}H NMR spectrum of **5** in tol-d_8.

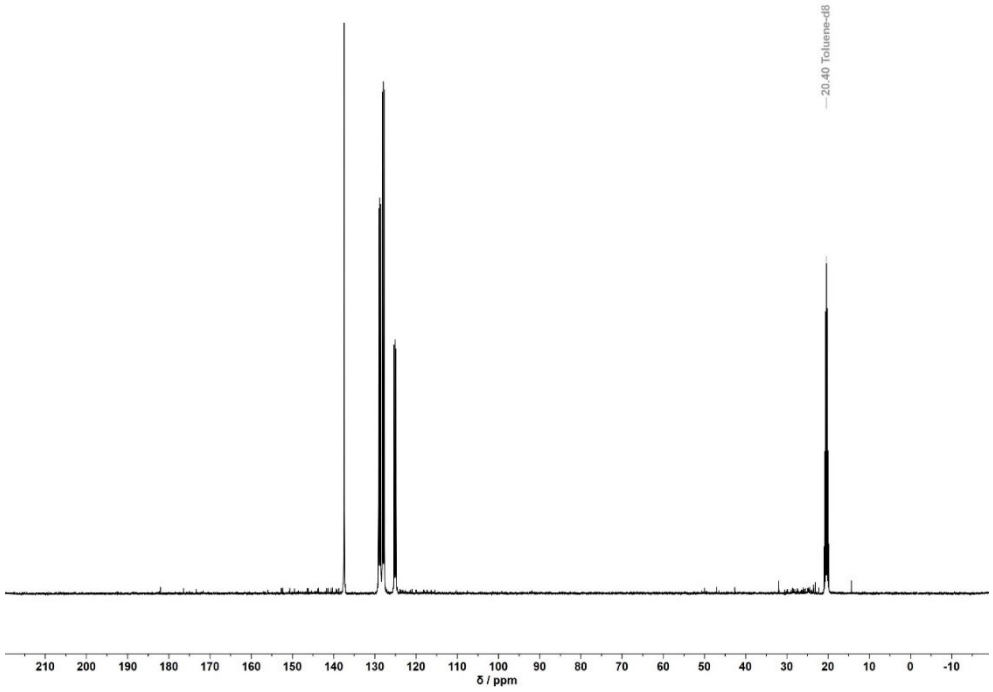


Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum of **5** in tol-d_8.

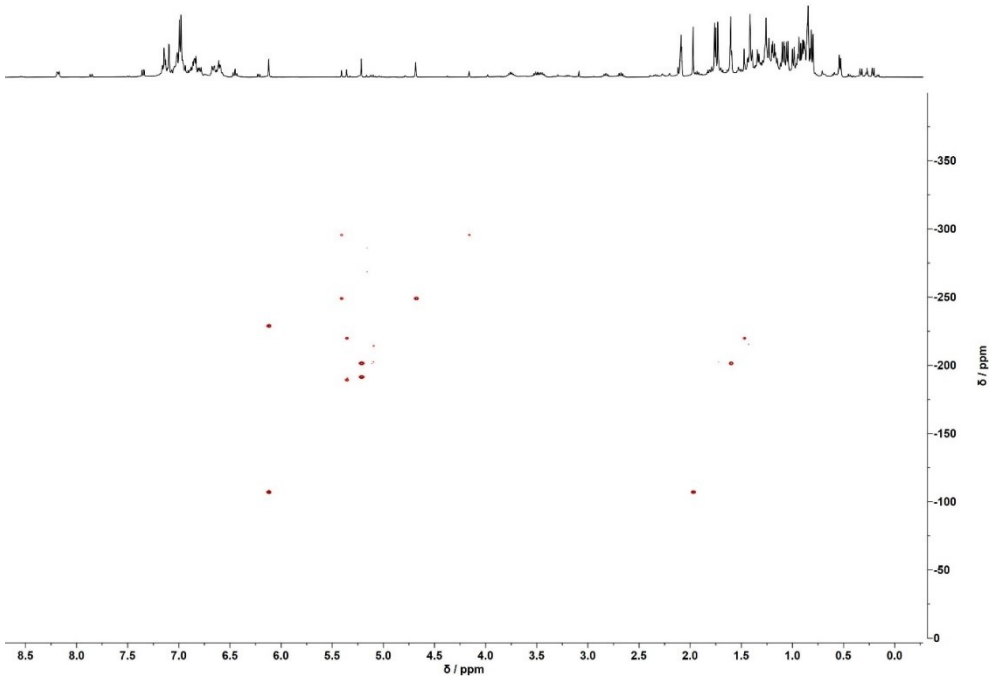


Figure S19: ^{1}H, ^{15}N HMBC spectrum of **5** in tol-d_8.

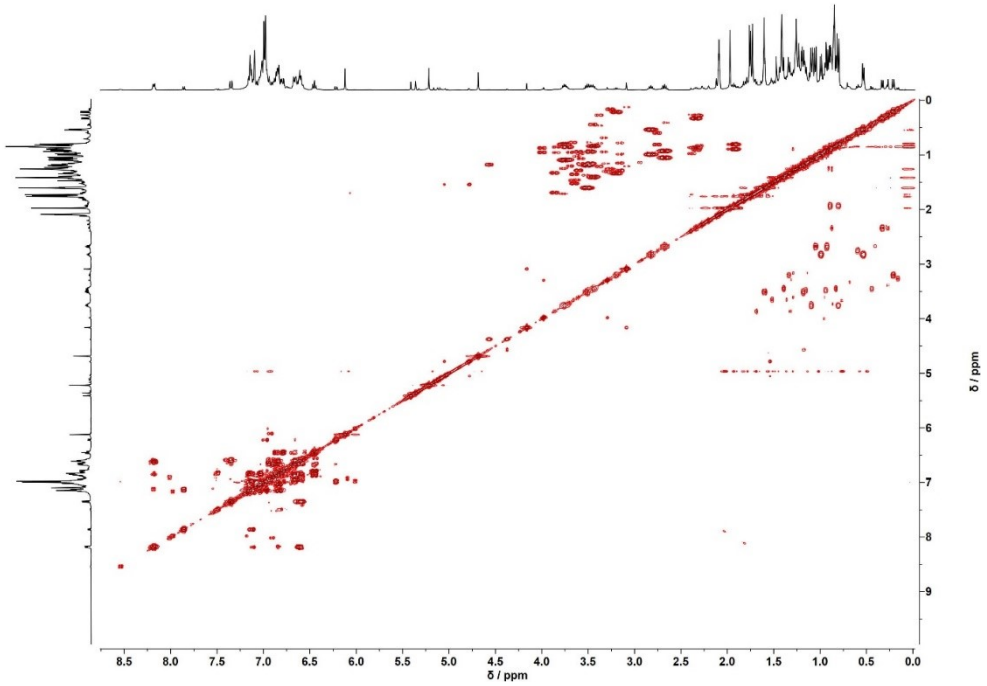


Figure S20: ^{1}H, ^{1}H COSY spectrum of **5** in tol-d_8.

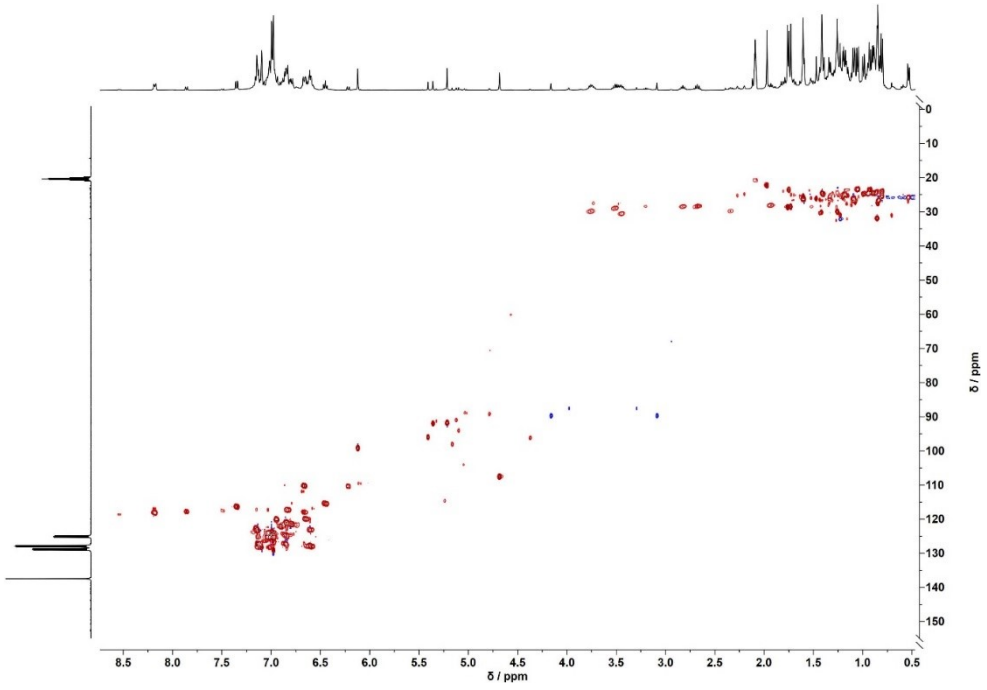


Figure S21: ^{1}H, ^{13}C HSQC spectrum of **5** in tol-d_8.

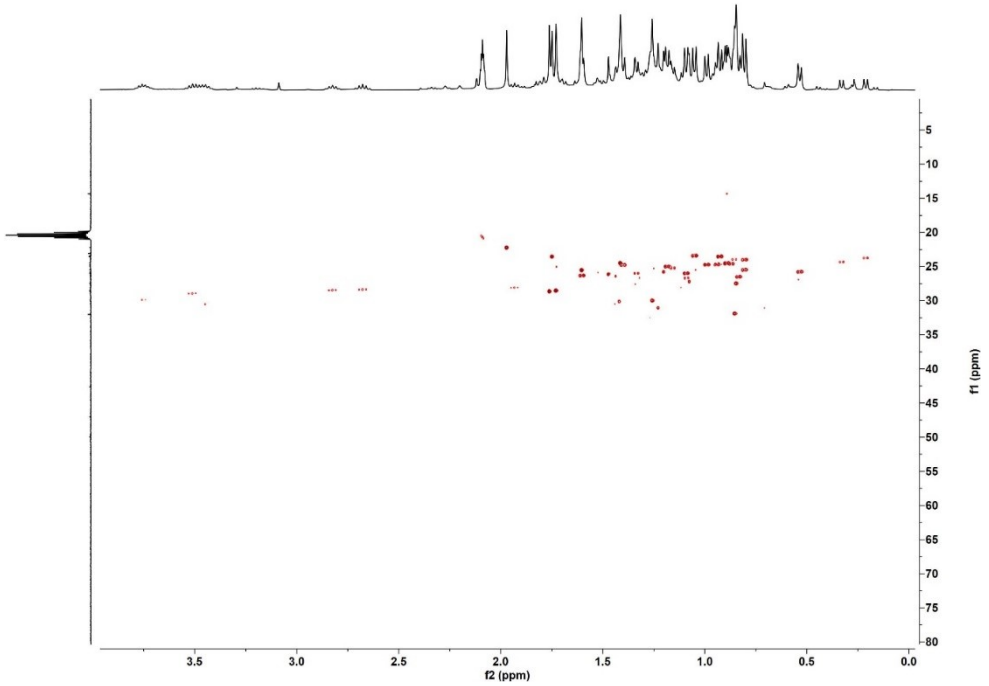


Figure S22: Detailed ^{1}H, ^{13}C HSQC spectrum of **5** in tol-d_8.

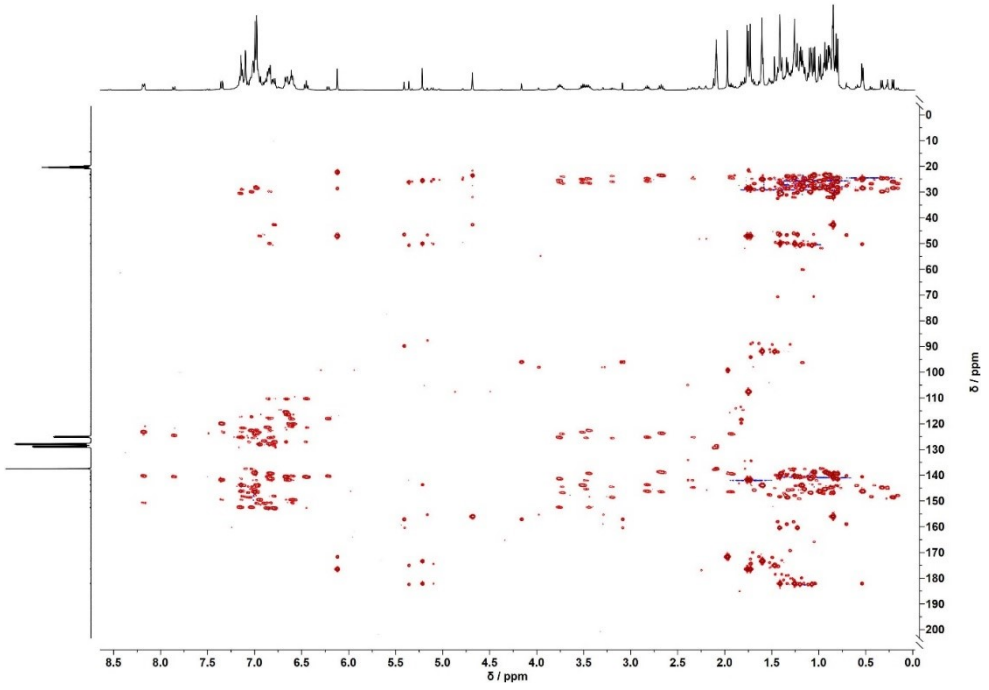


Figure S23: ^{1}H, ^{13}C HMBC spectrum of **5** in tol-d_8.

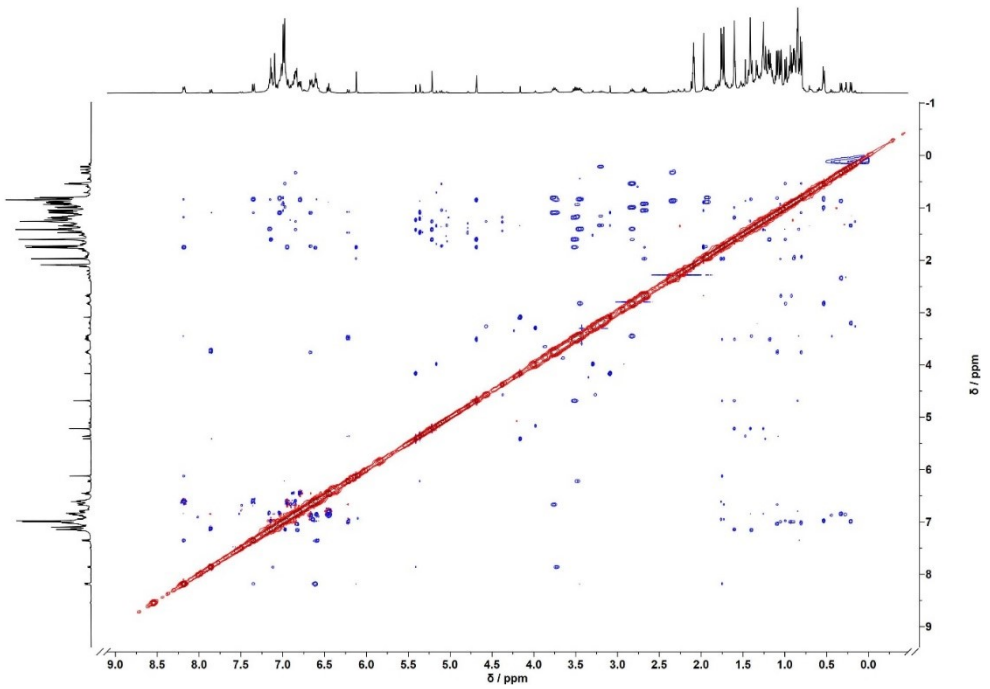


Figure S24: ^{1}H, ^{1}H NOESY spectrum of **5** in tol-d_8.

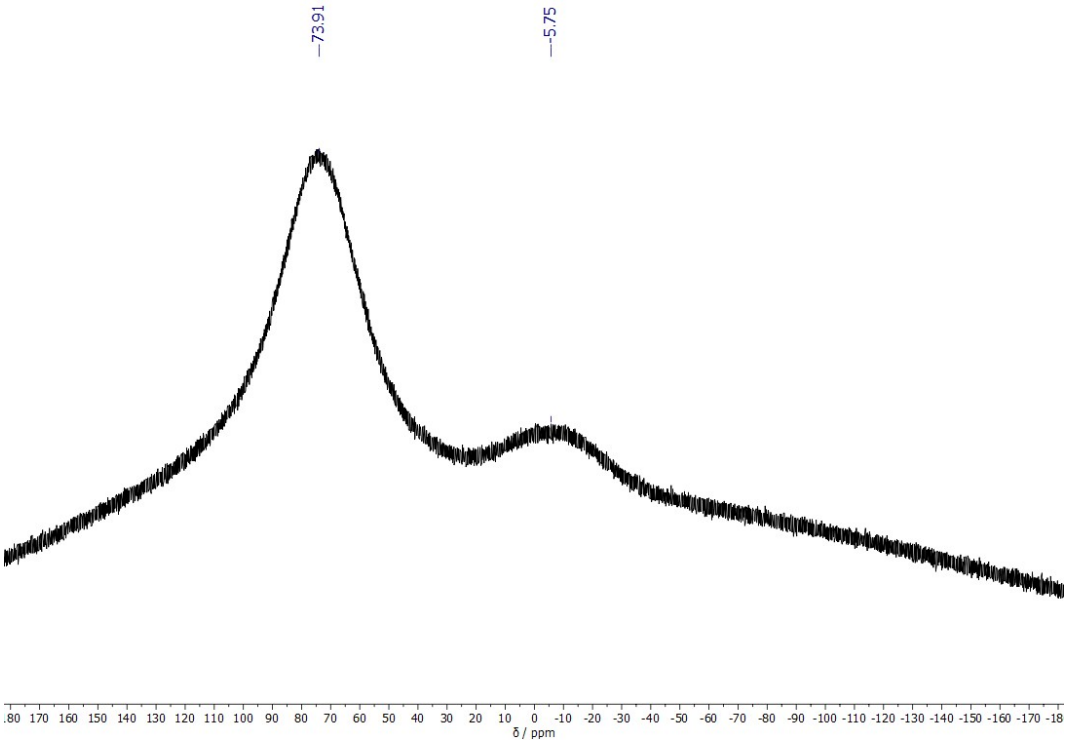


Figure S25: ^{27}Al spectrum of **5** in tol-d_8.

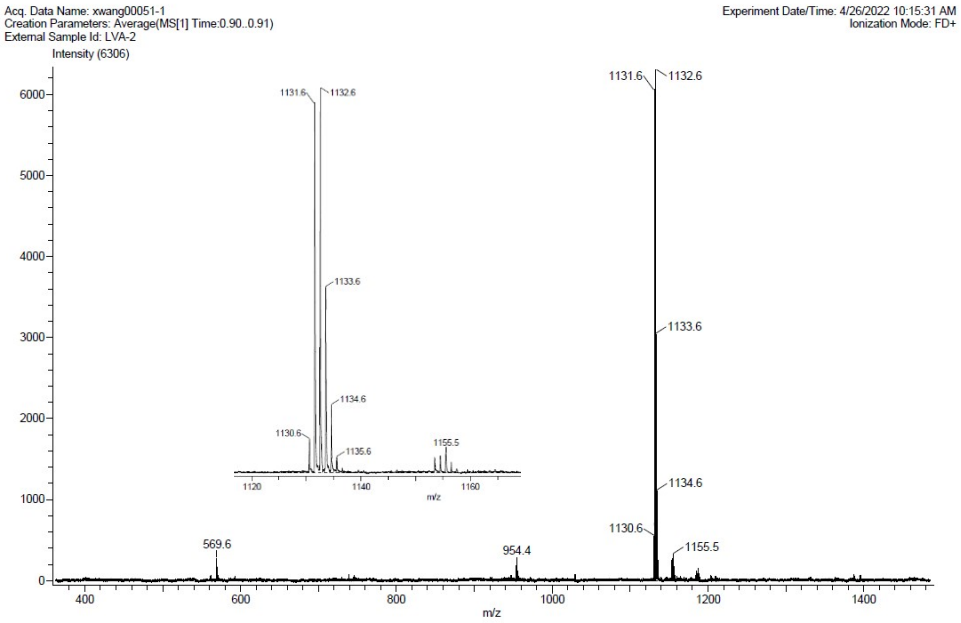
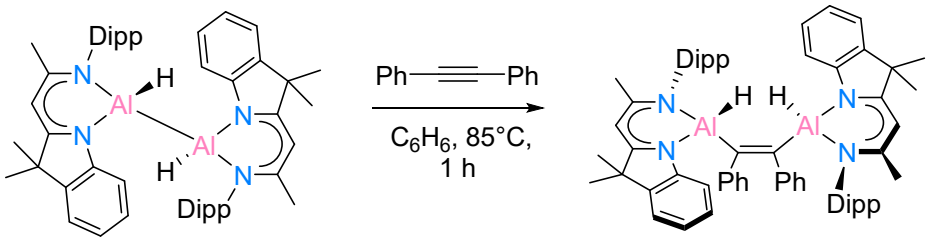


Figure S26: Mass spectrum of **5**.

Compound 6



2 **6**, 76.7%

Compound **2** (30 mg, 0.038 mmol, 1.00 eq.) in C_6H_6 (1 mL) was added to diphenylacetylene (6.90 mg, 0.039 mmol, >99%, 1.03 eq.) and transferred to a J. Young NMR tube. The reaction was heated to 85°C for 1 h. The pale orange mixture was filtered and dried under reduced pressure. Suitable crystals for the SC-XRD experiment was obtained from the saturated C_6H_6 solution at ambient temperature after 1 d. Yield 28.3 mg, 0.030 mmol, 76.7%. ^{1}H NMR (298 K, tol-d_8, 400 MHz, solvent peak=2.09 ppm): 8.12 (d, 1H, 21-H, J = 7.7 Hz), 7.50 (d, 1H, 53-H, J = 7.7 Hz), 7.19-6.64 (Ar-H, solv-C_6H_6), 4.98 (s, 1H, 15-H), 4.96 (s, 1H, 47-H), 3.40 (sep, 2H, 7-H, 10-H), 3.17 (q, iPrCH), 3.05 (sep, 2H, 39-H, 42-H), 1.52 (s, 6H, 14-H, 46-H), 1.41 (d, 6H, 11-H, iPr, J = 6.7 Hz), 1.22 (d, 3H, iPr, J = 6.2 Hz), 1.18 (d, 6H, iPr, J = 6.8 Hz), 1.13 (s, 6H, 18-H, 19-H), 1.09 (s, 6H, 50-H, 51-H), 0.99 (d, 6H, iPr, J = 6.6 Hz). ^{13}C{^{1}H} NMR (298 K,tol-d_8, 101 MHz, solvent peak=20.40 ppm): 180.58 (16-C), 180.53 (48-C), 172.44 (13-C), 172.13 (45-C), 150.74 (25-H), 150.33 (57-H), 149.79 (Ph-C), 149.19 (Ph-C), 144.70 (Ph-C), 144.35 (31-C), 144.21 (32-C), 143.99 (2-C, 6-C), 142.46 (34-C, 38-C), 141.61 (20-C), 140.69 (52-C), 126.59 (35-C), 124.39 (26-C), 124.15 (58-C), 122.97 (22-C), 122.81 (54-C), 121.32 (21-C), 121.11 (53-C), 116.72 (24-C), 116.41 (11-C), 91.47 (15-C), 90.69 (47-C), 49.69 (17-H, 49-H), 28.50 (42-C, iPrCH), 28.43 (10-C, iPrCH), 27.16 (7-C, iPrCH), 26.86 (39-C, iPrCH), 26.52 (18-C), 26.36 (50-C), 25.89 (11-C, iPrCH), 25.04 (19-C), 24.80 (5-C, iPrCH), 24.73 (14-C), 24.57 (8-C, iPr), 24.43 (12-C, iPr), 24.39 (46-C), 24.20 (40-C, iPr), 24.07 (41-C, iPr). Elemental analysis: $C_{64}H_{74}Al_2N_4$ calculated C 80.64, H 7.82, N 5.88, found C 82.98, H 7.78, N 4.67. Due to the co-crystallized solvent molecules (C_6H_6), the results deviate from theoretical value. LIFDI-MS ([+], toluene): 790.3 (1) [**2a**+H]$^+$, 952.4 (100) [**6**]$^+$.

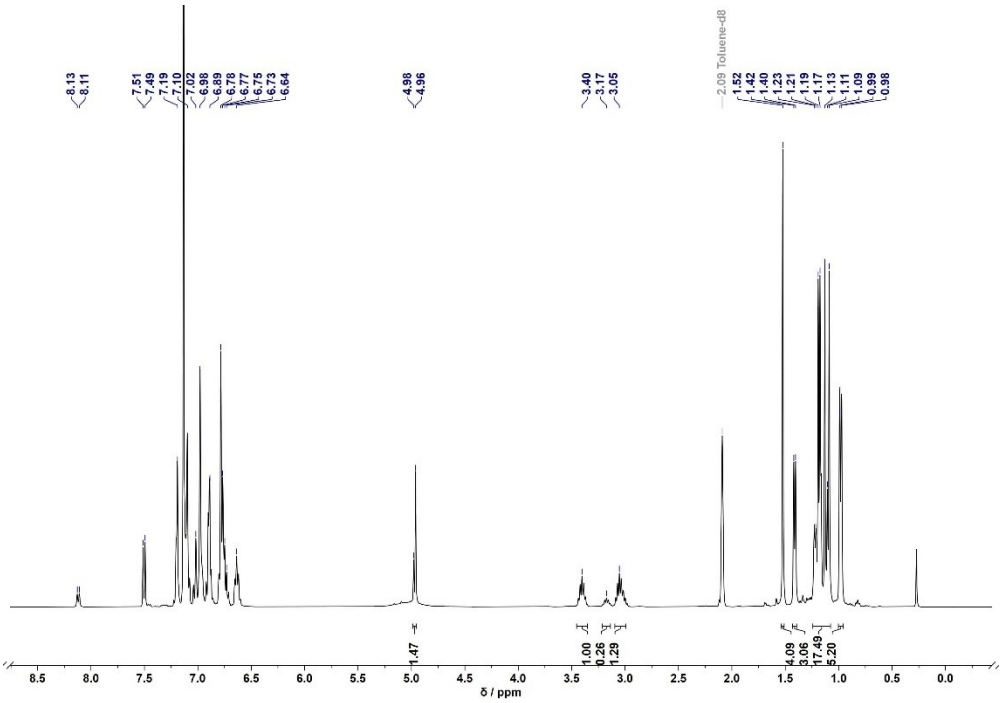


Figure S 27: ^{1}H NMR spectrum of **6** in tol-d_8.

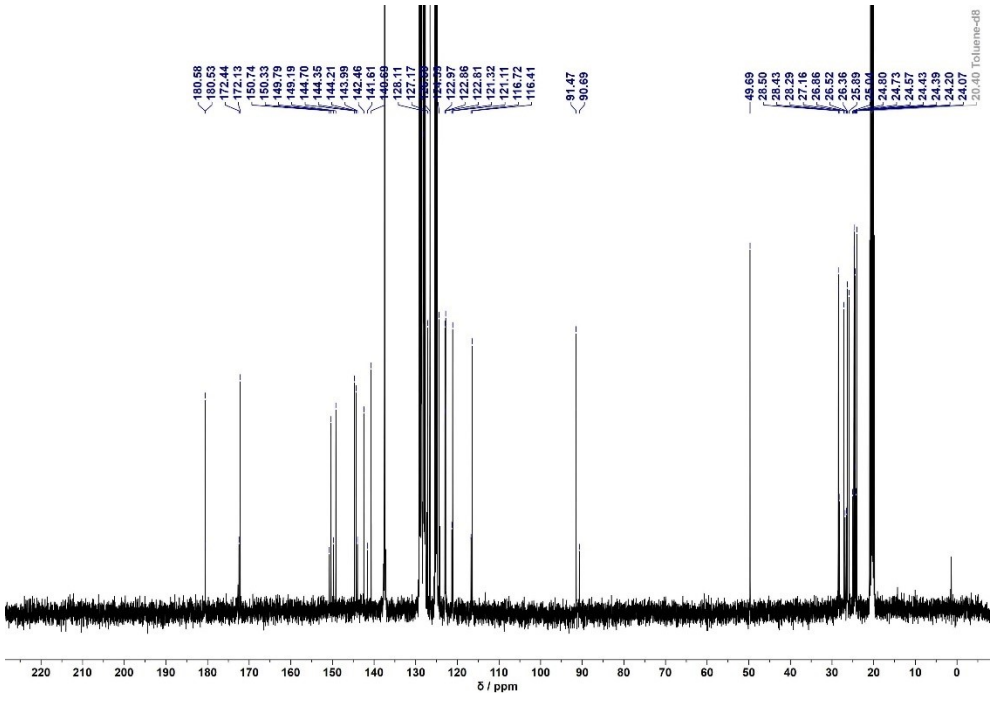


Figure S28: $^{13}C\{^{1}H\}$ NMR spectrum of **6** in tol-d_8.

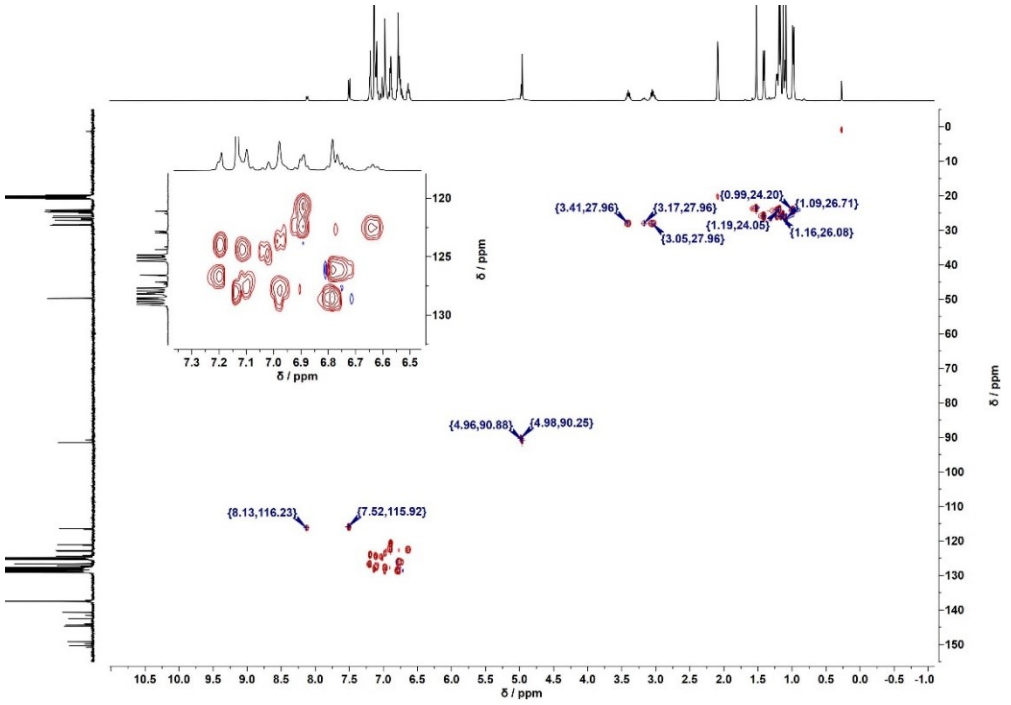


Figure S29: ^{1}H, ^{13}C HSQC spectrum of **6** in tol-d_8.

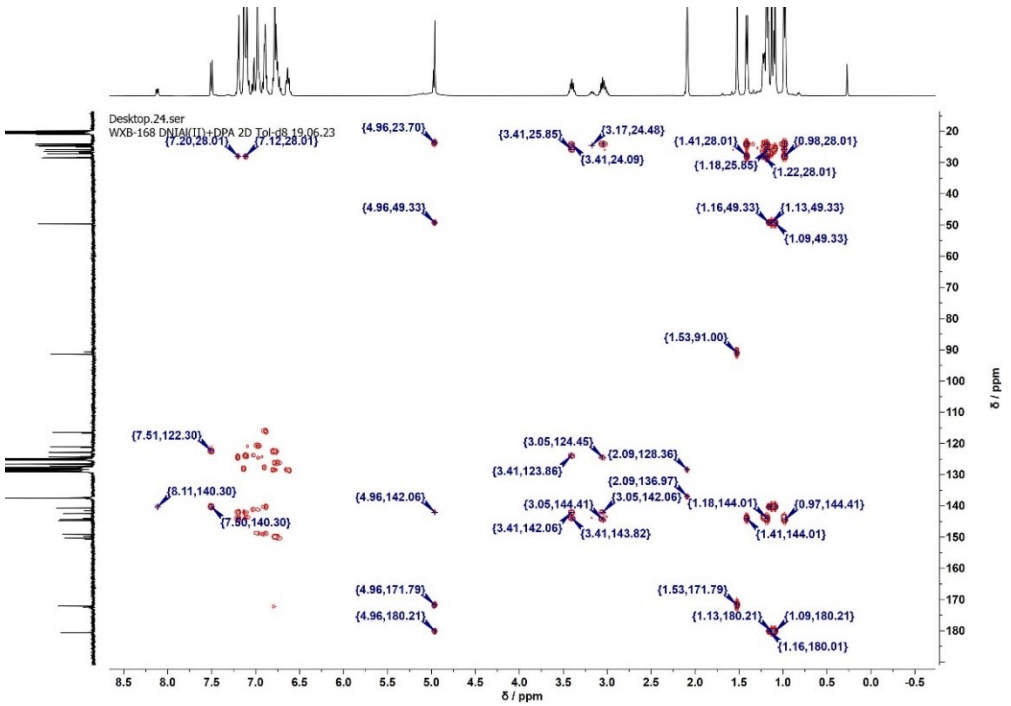


Figure S30: ^{1}H, ^{13}C HMBC spectrum of **6** in tol-d_8.

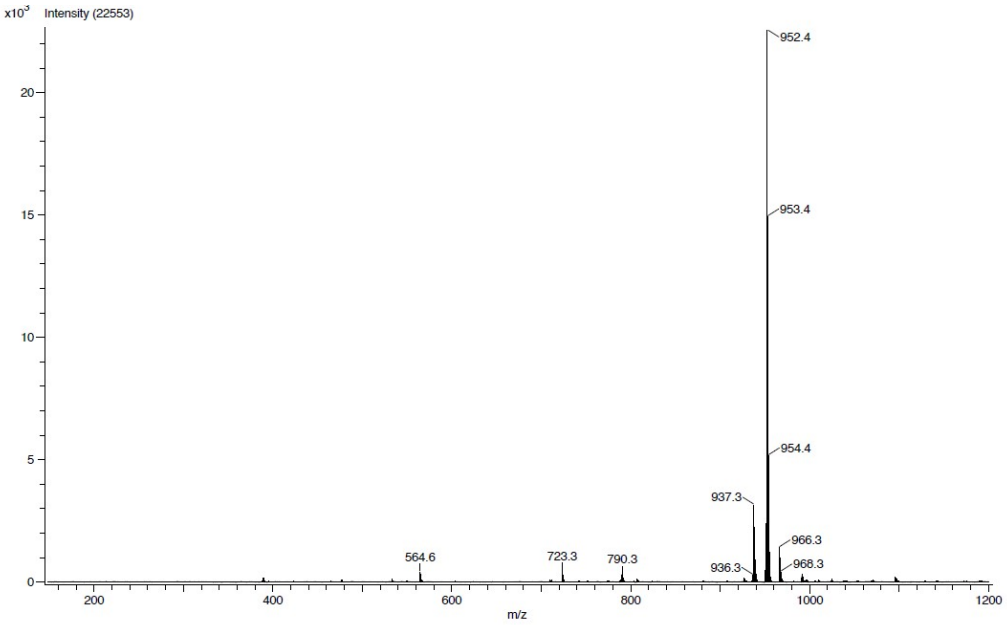
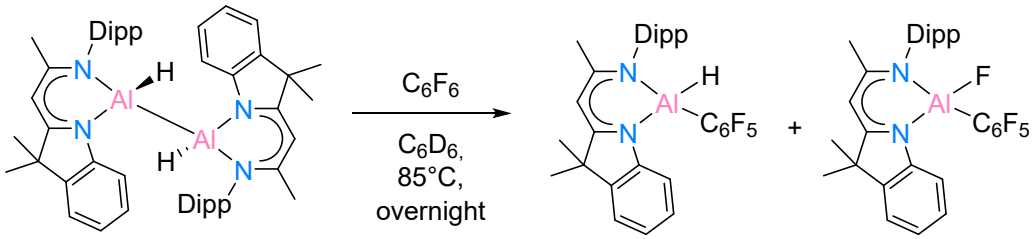


Figure S31: Mass spectrum of **6**.

Compound 7



2 **7a** **7b**

Compound **2** (20.1 mg, 0.026 mmol) was dissolved in C_6D_6 (0.6 mL) in J. Young NMR tube. Hexafluorobenzene (4.83 mg, 1.61 g/mL, 3.0 mmL, 0.026 mmol) was added to that solution and the mixture was heated to 85°C overnight. The yellow orange mixture has been used for NMR spectroscopy analyses without purification. ^{1}H NMR (298 K, C_6D_6, 600 MHz, solvent peak = 7.16 ppm): 7.57 (d, 1H, 5A-H, *J* = 7.81 Hz), 7.55 (d, 1H, 5B-H, *J* = 7.79 Hz), 7.38 (d, 1H, 5C-H, *J* = 7.85 Hz), 7.30 (d, 1H, 5D-H, *J* = 7.84 Hz), 6.82-7.22 (m, 24H), 5.84 (m, 1H, C_6F_5H-H), 5.19 (s, 1H, 11C-H), 5.17 (s, 1H, 11D-H), 5.10 (s, 2H, 11A/B-H), 3.11-3.39 (m, 6H, *i*Pr-H), 2.89 (hept, 1H, D*i*Pr-H, *J* = 6.72 Hz), 2.79 (hept, 1H, C*i*Pr-H, *J* = 6.73 Hz), 1.63 (s, 3H, 13A/B-H), 1.61 (s, 3H, 13C-H), 1.61 (s, 3H, 13A/B-H), 1.61 (s, 3H, 13D-H), 1.54 (d, 3H, Dipp-Me-C-H, *J* = 6.66 Hz), 1.49 (d, 3H, Dipp-Me-A/B-H, *J* = 6.65 Hz), 1.45 (d, 3H, Dipp-Me-D-H, J = 6.73 Hz), 1.41 (d, 3H, Dipp-Me-D-H, *J* = 6.77 Hz), 1.34 (d, 3H, Dipp-Me-A/B-H, *J* = 6.72 Hz), 1.24 (s, 3H, 8D/9D-H), 1.20 (s, 3H, 8C/9C-H), 1.01-1.11 (m, 33H), 1.00 (s, 6H, 8A/B/9A/B-H), 0.93 (d, 3H, Dipp-Me-D-H, *J* = 6.76 Hz), 0.87 (d, 3H, Dipp-Me-C-H, *J* = 6.72 Hz), 0.51 (d, 3H, Dipp-Me-D-H, *J* = 6.76 Hz), 0.46 (d, 3H, Dipp-Me-C-H, *J* = 6.75 Hz). ^{13}C NMR (298 K, C_6D_6, 125 MHz, solvent peak = 128.06 ppm): 182.68 (1C, 10A/B-C), 182.21 (1C, 10C-C), 181.80 (1C, 10D-C), 181.54 (1C, 10A/B-C), 174.26 (1C, 12A/B-C), 174.09 (1C, 12C-C), 173.46 (1C, 12D-C), 172.78 (1C, 12A/B-C), 148.96 (1C, Ar-C), 148.65 (1C, Ar-C), 148.16 (1C, Ar-C), 148.12 (1C, Ar-C), 145.77 (1C, Ar-C), 145.61 (1C, Ar-C), 144.97 (1C, Ar-C), 144.55 (1C, Ar-C), 144.48 (1C, Ar-C), 143.97 (1C, Ar-C), 143.85 (1C, Ar-C), 140.81 (1C, Ar-C), 150.50 (1C, Ar-C), 140.48 (1C, Ar-C), 140.45 (1C, Ar-C), 140.1 (1C, Ar-C), 136.73-139.10 (m, 6C, C_6F_6-C, ^1J(C-F) = 255 Hz), 138.70 (1C, Ar-C), 138.58 (1C, Ar-C), 137.32 (1C, Ar-C), 137.29 (1C, Ar-C), 127.63-128.72 (Ar-C), 125.45 (1C, Ar-C), 125.38 (1C, Ar-C), 125.18 (1C, Ar-C), 125.06 (1C, Ar-C), 124.87 (1C, Ar-C), 124.65 (1C, Ar-C), 124.33 (1C, Ar-C), 124.13 (1C, Ar-C), 123.90 (1C, Ar-C), 123.81 (1C, Ar-C), 122.32 (1C, Ar-C), 122.28 (1C, Ar-C), 122.09 (1C, Ar-C), 122.06 (1C, Ar-C), 115.30 (1C, 5A/B-C), 114.56 (2C, 5A/B/C-C), 113.71 (1C, 5D-C), 100.58 (td, 1C, C_6F_5H-C-H, ^2J(C-F) = 23.12 Hz, ^3J(C-F) = 3.46 Hz), 90.71 (1C, 11C-C), 90.56 (1C, 11D-C), 90.04 (2C, 11A/B-C), 50.74 (1C, 7A/B-C), 50.70 (1C, 7C-C), 50.42 (1C, 7D-C), 50.38 (1C, 7A/B-C), 28.83 (1C, *i*Pr-D-C), 28.78 (1C, *i*Pr-A/B-

C), 28.74 (1C, *i*Pr-C-C), 28.64 (1C, *i*Pr-A/B-C), 28.60 (1C, *i*Pr-A/B-C), 28.45 (1C, *i*Pr-A/B-C), 28.22 (1C, *i*Pr-C-C), 27.94 (1C, *i*Pr-D-C), 27.20 (1C, 8/9D-C), 27.16 (1C, 8/9C-C), 26.62 (1C, Me-C), 26.48 (1C, 8/9A/B-C), 26.44 (1C, 8/9A/B-C), 25.77 (1C, 8/9D-C), 25.72 (1C, 8/9C-C), 25.17 (1C, Dipp-Me-C), 24.97 (1C, Dipp-Me-C), 24.94 (1C, Dipp-Me-C), 24.88 (1C, Dipp-Me-C), 24.78 (1C, Dipp-Me-C), 24.74 (1C, Dipp-Me-C), 24.72 (1C, Dipp-Me-C), 24.66 (1C, Dipp-Me-C), 24.48 (1C, Dipp-Me-C), 24.45 (1C, Dipp-Me-C), 24.42 (1C, Dipp-Me-C), 23.88 (1C, Dipp-Me-C), 23.59 (1C, Dipp-Me-C), 23.52 (1C, Dipp-Me-C), 23.28 (1C, Dipp-Me-C). ^{19}F NMR (298 K, C_6D_6, 377 MHz, relative to $CFCl_3$): -121.55 (m, 2F, *m*-C_6F_5-R), -122.69 (m, 2F, *m*-C_6F_5-R), -139.16 (m, 2F, *m*-C_6F_5H), -152.63 (t, 1F, *p*-C_6F_5-R, *J* = 19.66 Hz), -153.51 (t, 1F, *p*-C_6F_5-R, *J* = 19.98 Hz), -154.18 (t, 1F, *p*-C_6F_5H, *J* = 20.76 Hz), -161.66 (ddd, 2F, *o*-C_6F_5-R, *J* = 27.50, 19.58, 12.57 Hz), -161.96 (ddd, 2F, *o*-C_6F_5-R, *J* = 26.34, 17.44, 9.56 Hz), -162.43 (m, 2F, *o*-C_6F_5H), -162.92 (s, C_6F_6). ^{15}N NMR (298 K, C_6D_6, 51 MHz, relative to CH_3NO_2): -209.63 (1N, NacNac-D-N), -208.81 (1N, NacNac-A/B-N), -208.65 (1N, Indole-D-N), -208.17 (1N, NacNac-C-N), -207.19 (1N, Indole-A/B-N), -204.26 (1N, Indole-C-N), -202.30 (1N, Indole-A/B-N), -201.32 (1N, NacNac-A/B-N). LIFDI ([+], toluene): m/z 389.9 (2) $[DNIAlH_2+H]^+$, 407.7 (22) $[DNIAlHF+H]^+$, 425.4 (20) $[DNIAlF_2+H]^+$, 536.6 (5) $[DNIAlC_6F_4H_2]^+$, 554 (90) $[DNIAlC_6F_5H]^+$, 572.4 (100) $[DNIAlC_6F_6]$. The remaining peaks cannot be reliably assigned and may possibly represent dimeric species.

Note: In the ^{1}H NMR spectrum, we see at least three ligand-containing products (visible through three backbone signals at 5.19 ppm, 5.17 ppm and 5.10 ppm, respectively). The carbon spectrum, however, shows four signals each for the carbon atoms C10 (180-183 ppm) and C12 (172-175 ppm), suggesting that in total, four products form in reasonable yield. In addition to that, C_6F_5H could be identified via ^{1}H and ^{19}F NMR spectroscopy, another proof for the successful C-F activation in C_6F_6. In the ^{19}F COSY NMR, apart from residual C_6F_6 and C_6F_5H, two further spin systems containing three fluorine sites are visible, indicating two species containing C_6F_5 groups. Both species show very similar diffusion coefficients in the ^{19}F DOSY NMR with a molecular mass of about 560 g/mol, which would suit both suggested products **7a** and **7b** shown equally well. As the molecular mass difference between these species is only ~3%, they cannot be unambiguously distinguished this way. The same applies to the two more downfield shifted ^{1}H backbone signals, so it is very likely they belong to **7a** and **7b**. The third ^{1}H backbone NMR signal at 5.10 ppm shows a somewhat larger diffusion coefficient in the ^{1}H DOSY NMR spectrum, indicating a species with lower molecular weight (~430 g/mol). A possible species here could be [DNIAlHF] or $[DNIAlF_2]$. Fluorine atoms directly bound to Al are expected to give broadened ^{19}F NMR signals which are also visible in the spectrum of the reaction mixture and could belong to [DNIAlHF], $[DNIAlF_2]$ or also **7b**. However, due to the broadening, no ^{19}F DOSY NMR signal could be obtained from these resonances.

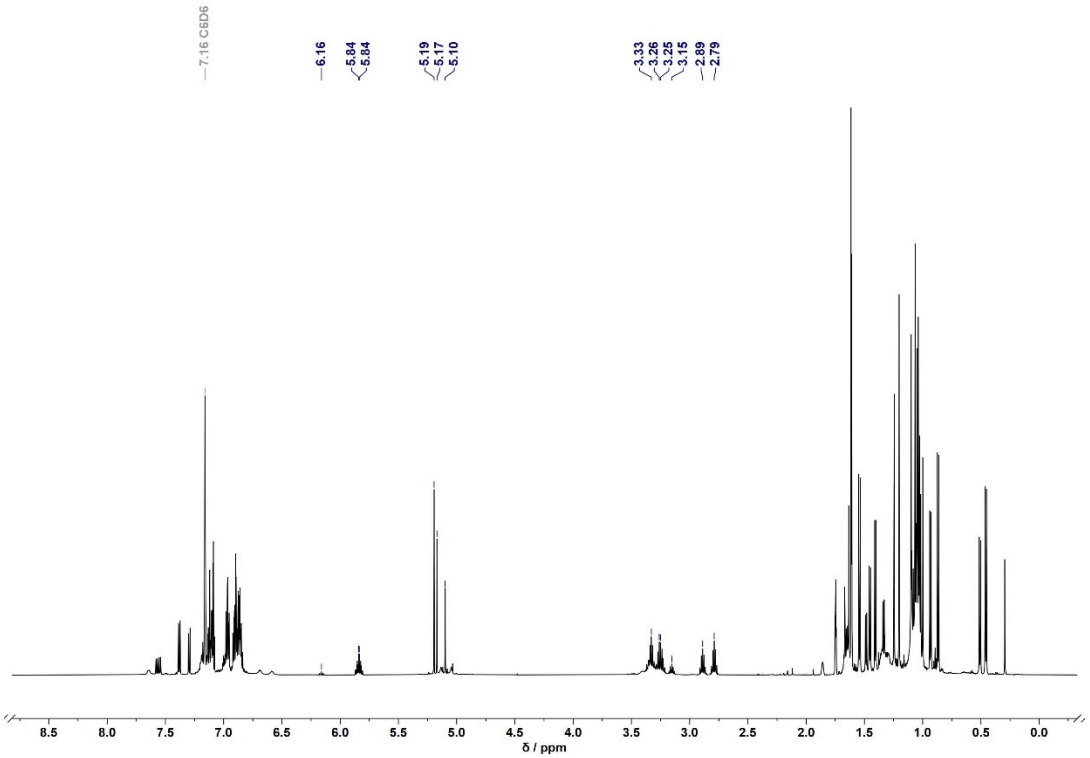


Figure S32: ^{1}H NMR spectrum of **7** in C_6D_6.

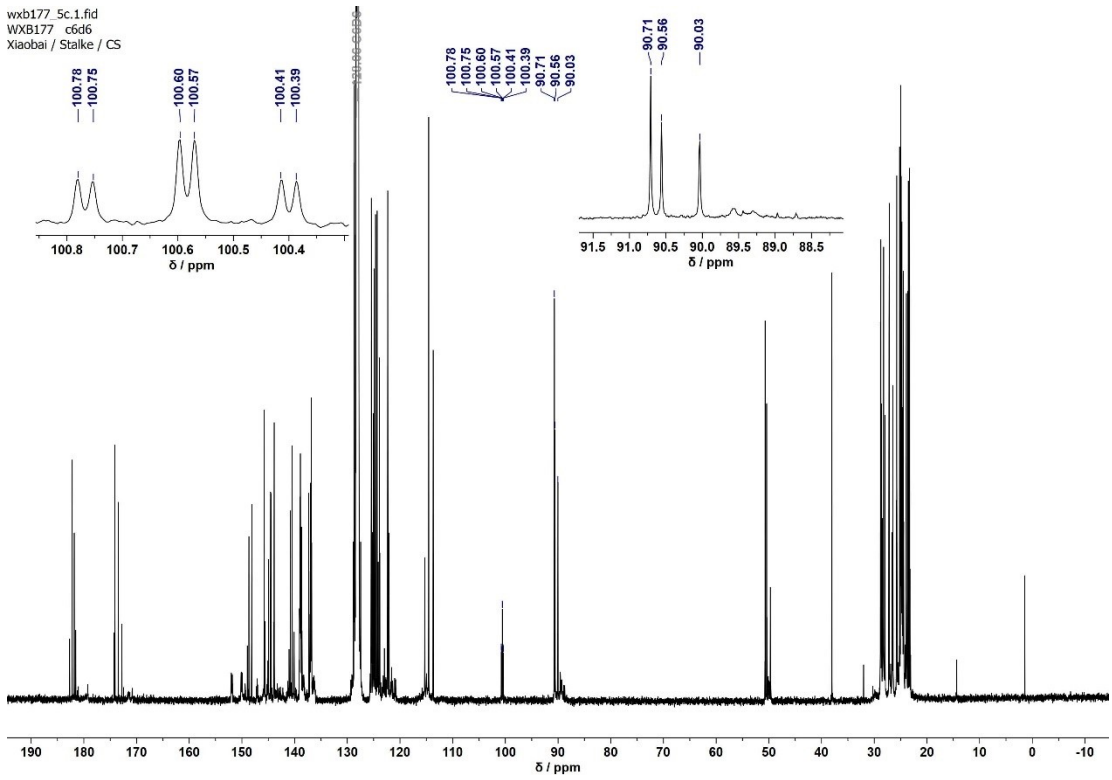


Figure S33: $^{13}C\{^{1}H\}$ NMR spectrum of **7** in C_6D_6.

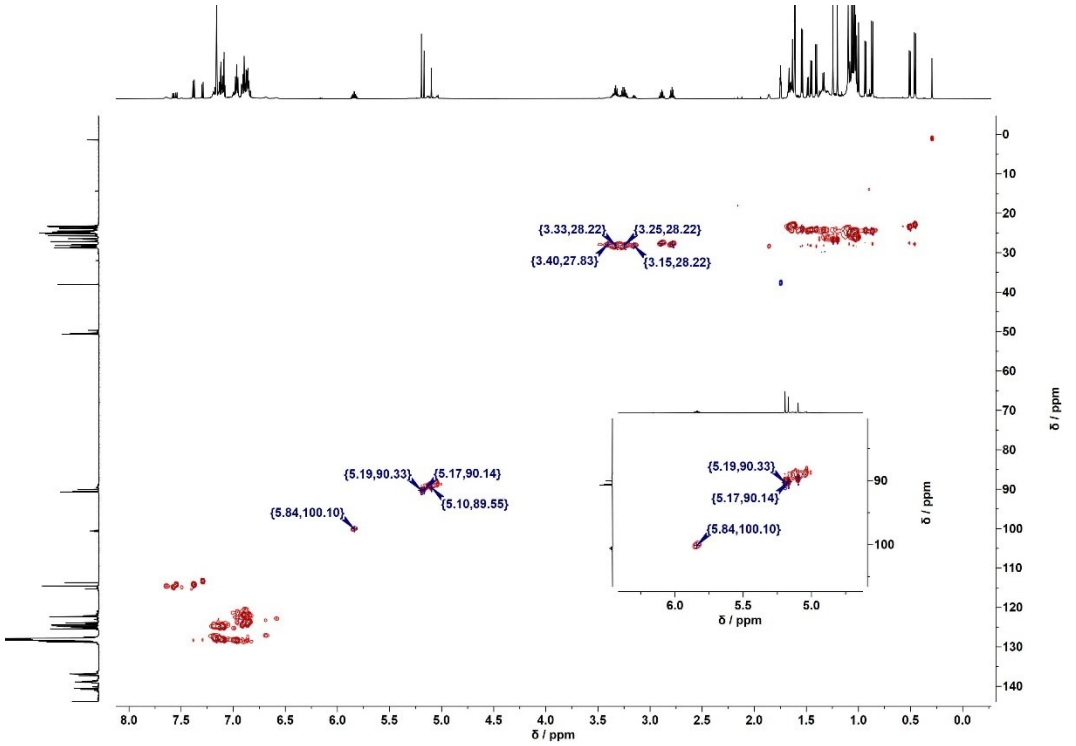


Figure S34: ^{1}H, ^{13}C HSQC spectrum of **7** in C_6D_6.

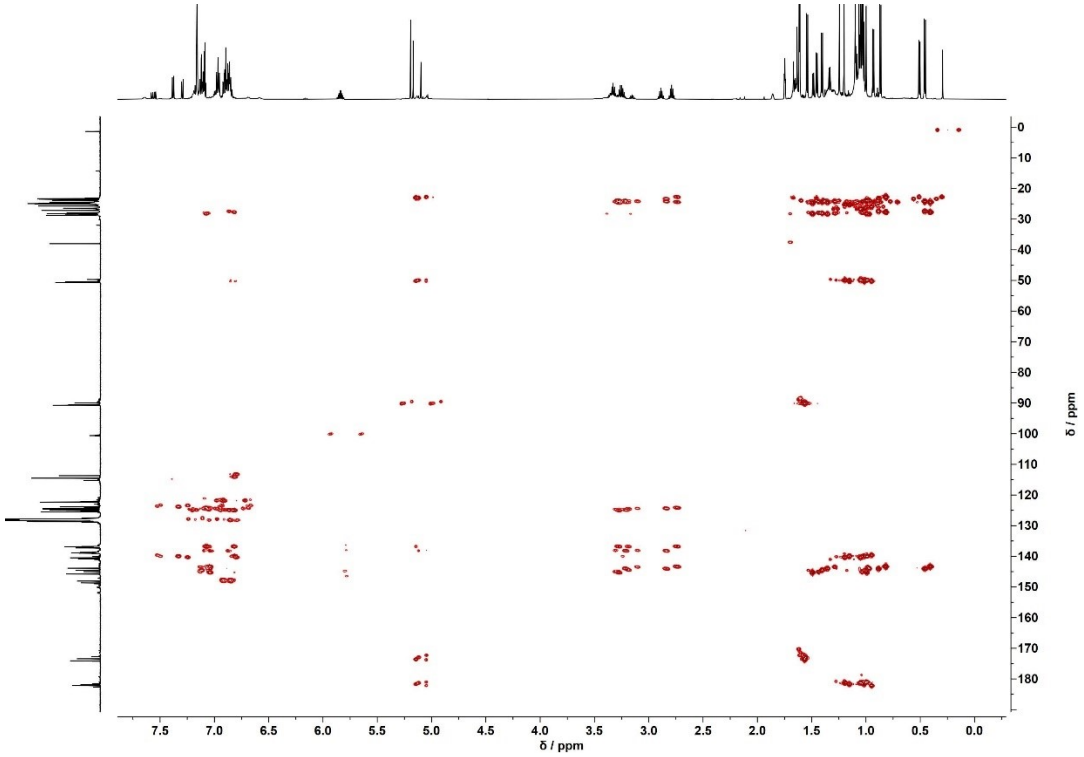


Figure S35: ^{1}H, ^{13}C HMBC spectrum of **7** in C_6D_6.

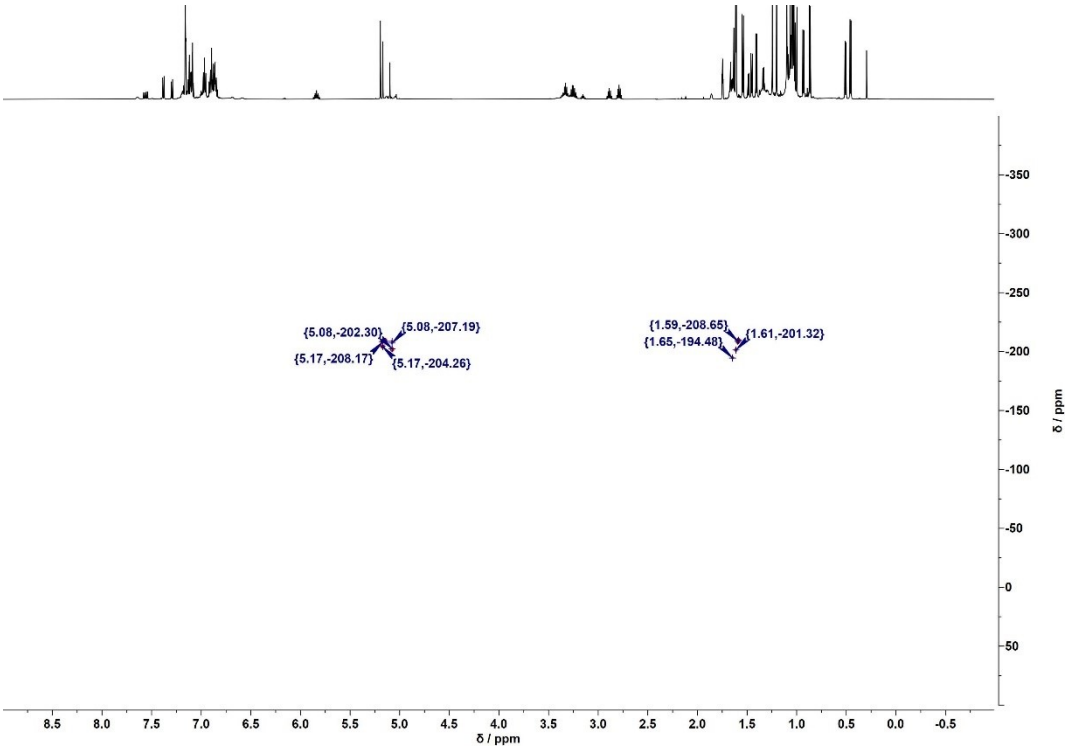


Figure S36: $^{1}H,^{15}N$ HMBC spectrum of **7** in C_6D_6.

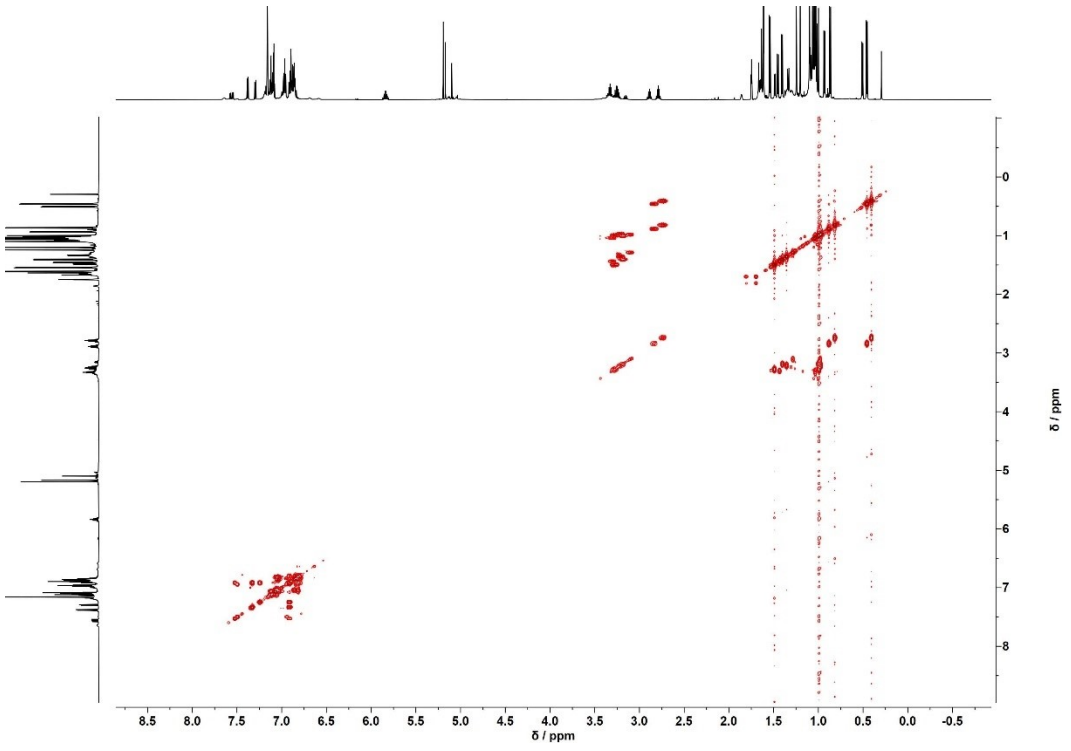


Figure S37: ^{1}H, ^{1}H COSY spectrum of **7** in C_6D_6.

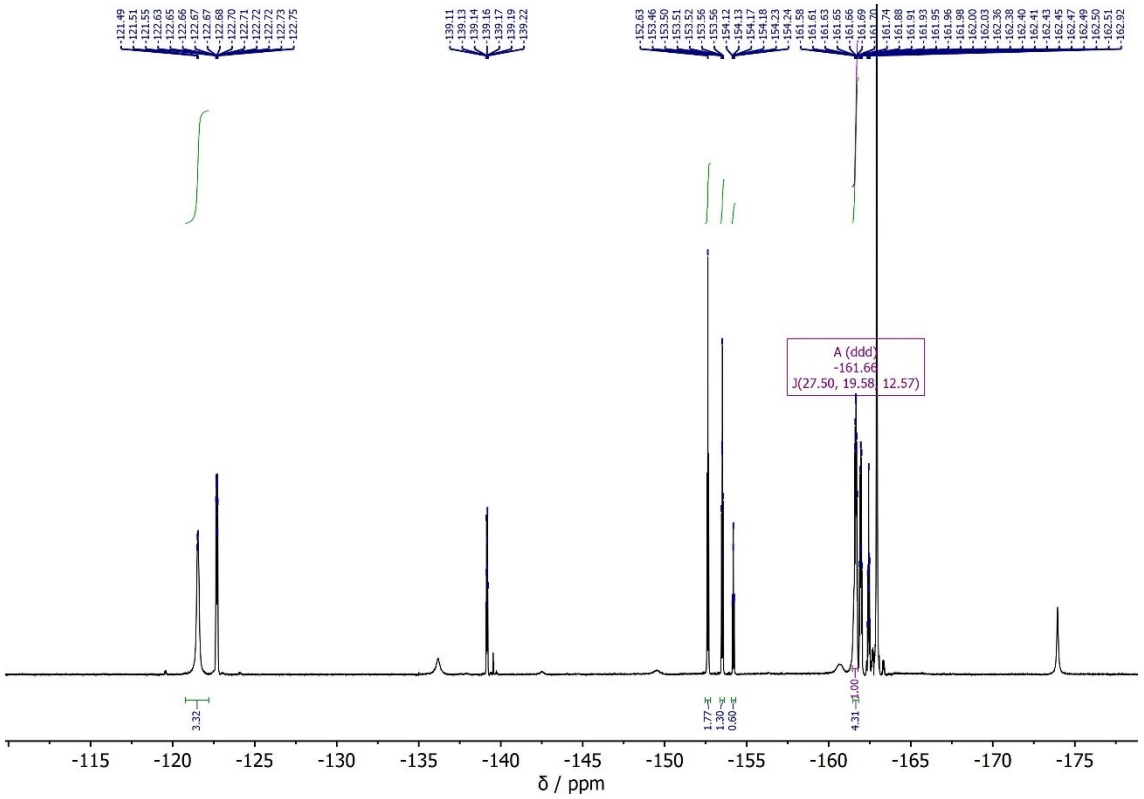


Figure S38: ^{19}F NMR spectrum of **7** in C_6D_6.

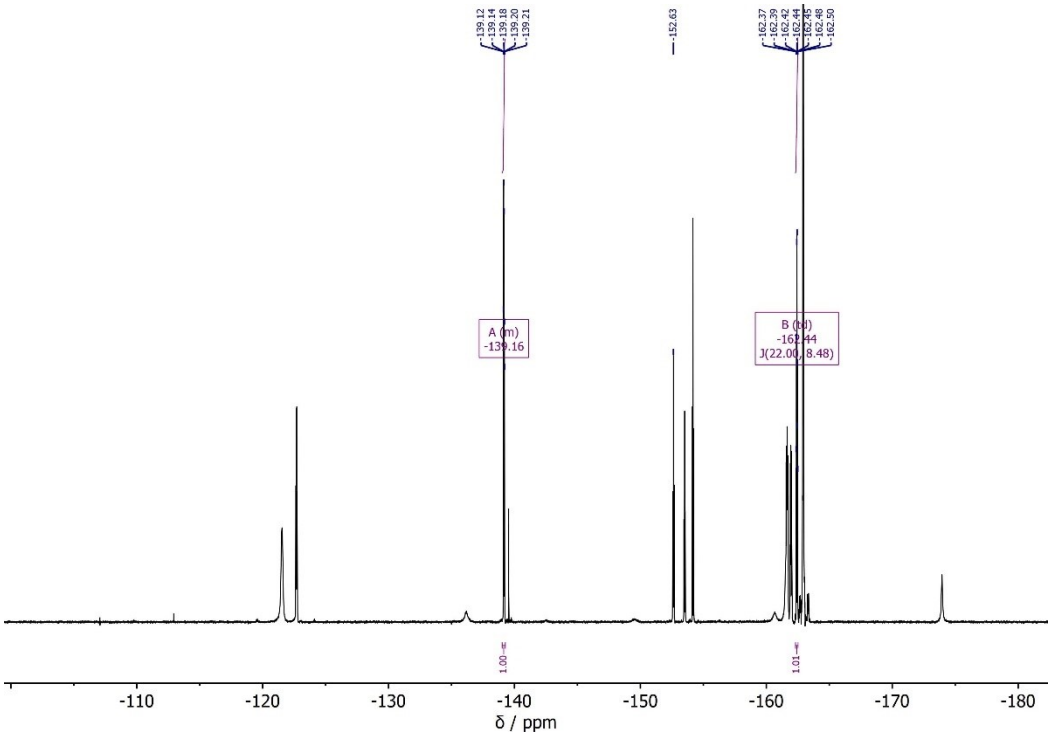


Figure S39: $^{19}F\{^1H\}$ NMR spectrum of **7** in C_6D_6.

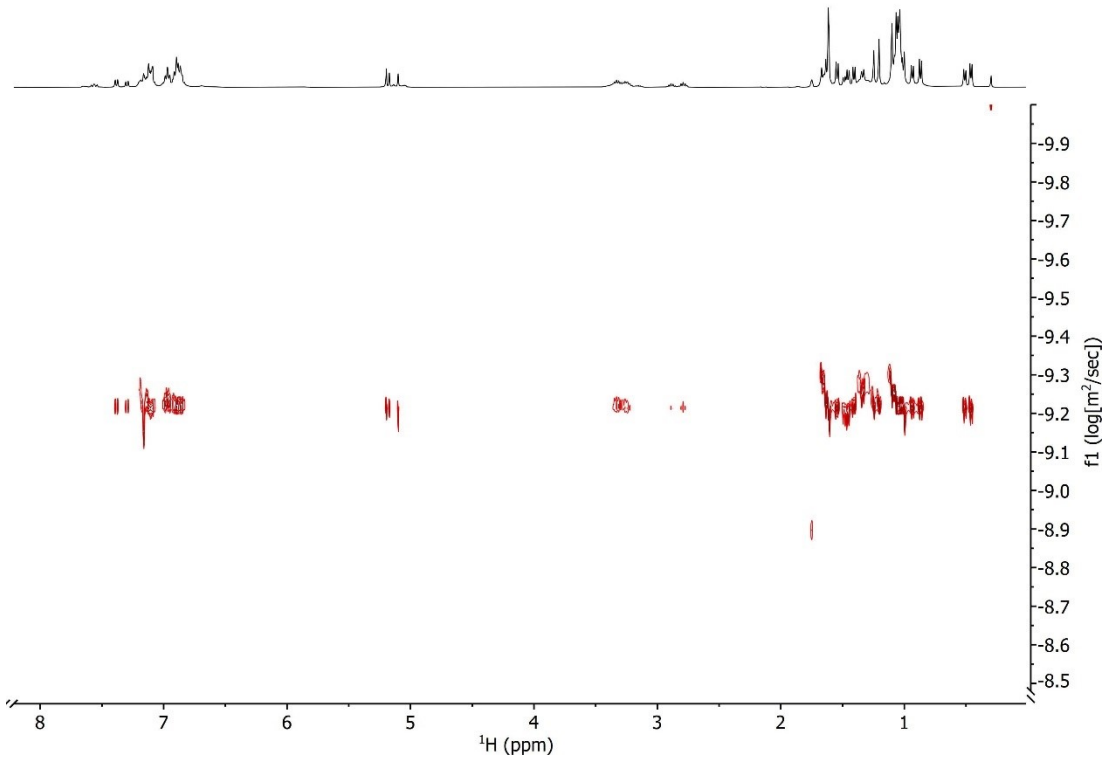


Figure S40: ^{1}H DOSY spectrum of **7** in C_6D_6.

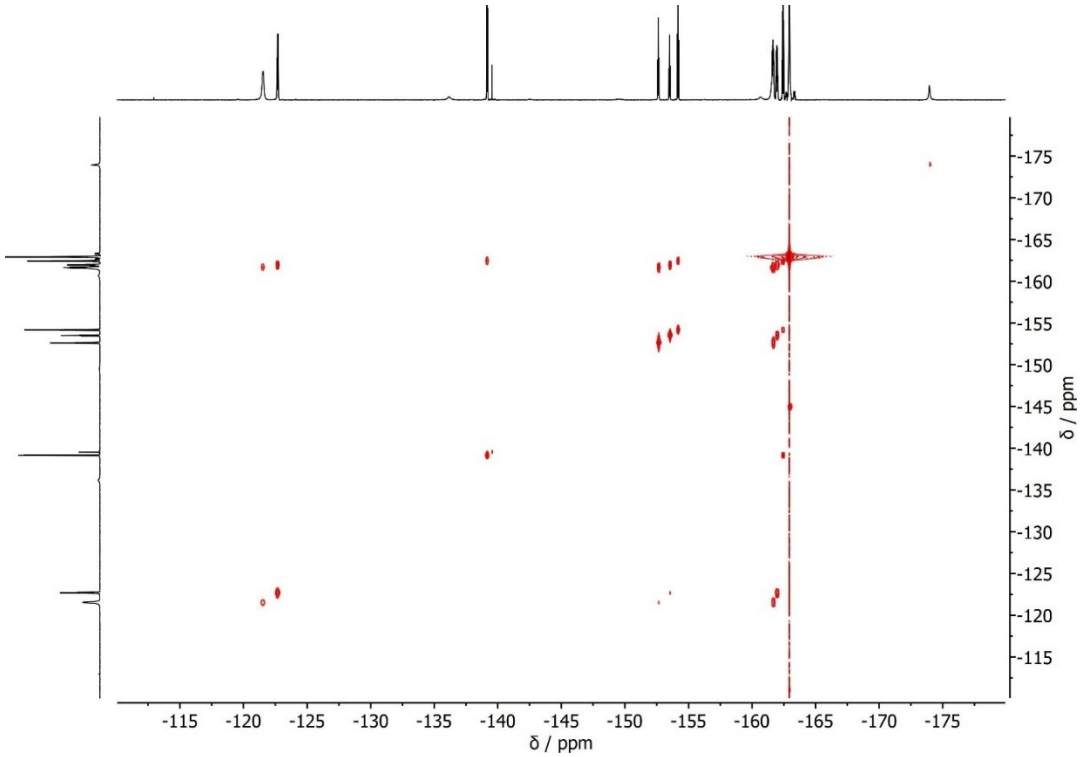


Figure S41: ^{19}F, ^{19}F COSY spectrum of **7** in C_6D_6.

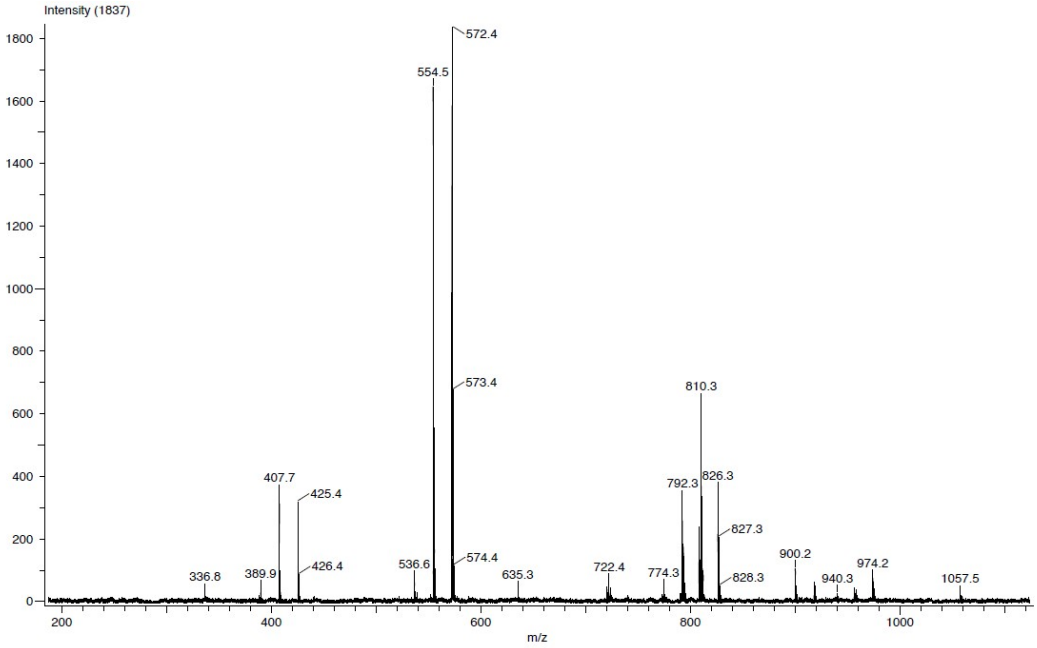


Figure S42: Mass spectrum of **7**.

UV Spectra and molecular orbitals calculations

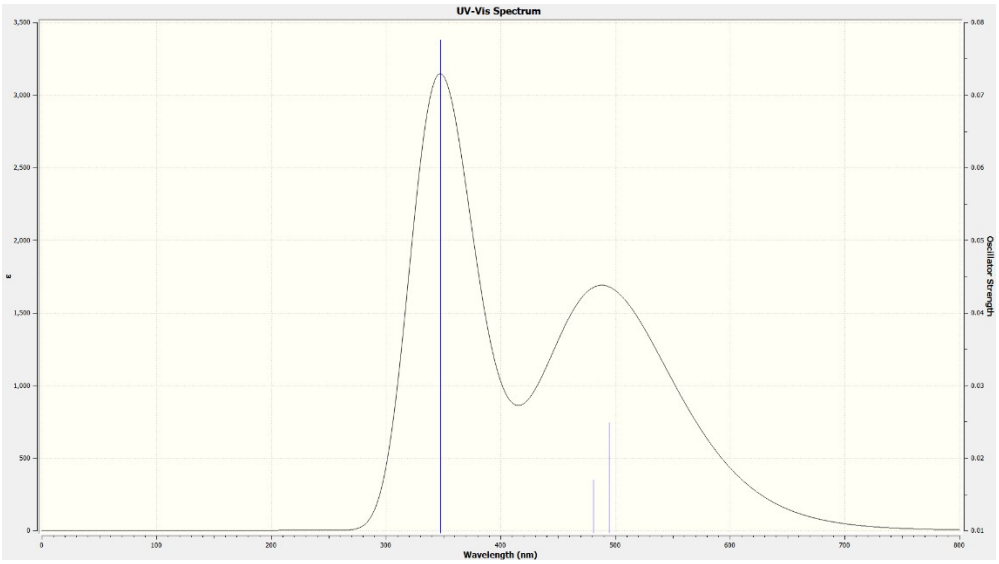
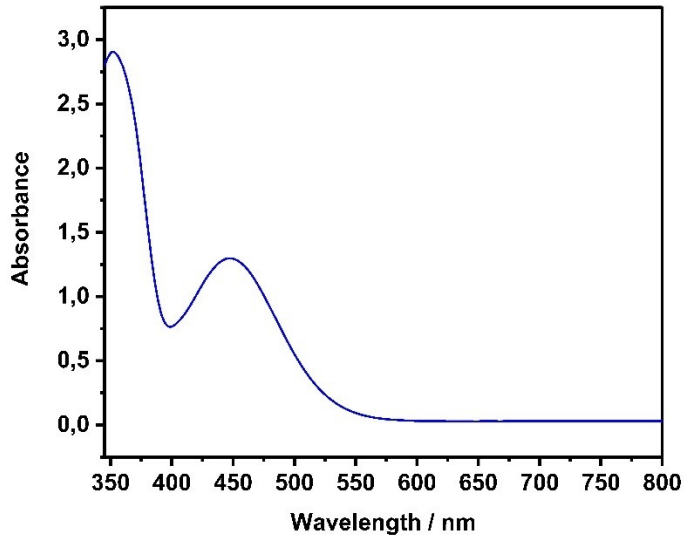


Figure S43: calculated UV spectra of **2** in gas phase.

UV-vis was measured by using 1 cm x 1 cm quarz cell with a *Agilent Technologies Cary 8454*. *Origin 2020* was used for plotting the data.



c

Figure S44: Measured UV-vis spectra of **2** c = 4.3 x10^{-5} M in toluene.

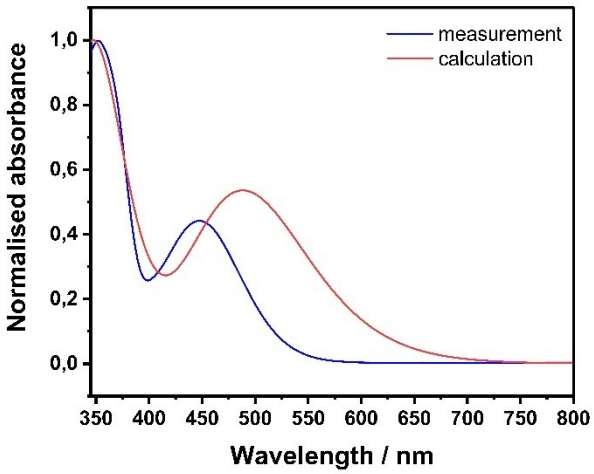


Figure S45: Normalized measured UV-vis spectra (blue, in toluene) and Normalized calculated UV-vis spectra (red, in gas phase).

Crystallographic data

General Data Acquisition and Processing

The diffraction data were collected using Mo Kα radiation and a Bruker Photon II detector. The data were integrated with SAINT.[2] A multi-scan absorption correction was applied using SADABS.[3] The structures were solved by SHELXT[4] and refined on F^2 using SHELXL[5] in the graphical user interface ShelXle.[6] All hydrogen atoms were placed according to geometrical criteria and refined with a riding model except those mentioned below. An overview of the crystallographic data for **2**,**3**, and **5** can be found in **Table S1** and **6** in **Table S2**, while individual bond lengths and angles are listed in **Table S3-S6**, respectively.

Table S1: Crystal data and structure refinement for compound **2**, **3**, **5** at 100(2)K.

Compound	**2**	**3**	**5**
CCDC	2313962	2313964	2313966
Empirical Formula	$C_{50}H_{64}Al_2N_4$	$C_{54}H_{72}Al_2N_4O_{0.06}$	$C_{75}H_{93}Al_2N_6Na$ $2(C_6H_{14})$
Formula weight	775.01	831.99	1327.84
T [K]	100(2)	100(2)	100(2)
λ [Å]	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	$P2_1/c$	$P\bar{1}$
a [Å]	14.229(2)	11.397(2)	13.176(2)
b [Å]	11.786(2)	19.267(3)	22.183(2)
c [Å]	27.277(3)	23.219(2)	28.270(3)
α [°]	-	-	87.90(2)
β [°]	93.07(2)	102.80(2)	77.90(2)
γ [°]	-	-	78.68(3)
V [Å^3]	4567.9(11)	4971.9(13)	7922.0(19)
Z	4	4	4
μ [mm^{-1}]	0.101	0.097	0.089
F(000)	1672	1802	2888
Crystal size [mm]	0.292x0.232x0.16	0.436x0.392x0.31	0.22x0.19x0.15
Θ max [°]	1.495 to 28.773	1.388 to 26.408	0.737 to 25.391

Reflections collected	113485	211152	142190
Independent reflections	11820	10165	29029
R_{int}	0.0532	0.0430	0.0783
Data/restraints/parameters	11820/0/533	10165/581/577	29029/2790/2070
GooF	1.111	1.034	1.014
$R1$ [$I > 2\sigma(I)$]	0.0408	0.0349	0.0546
$wR2$ [all data]	0.1079	0.0830	0.1359
Extinction coefficient	-	0.0022(3)	0.00144(13)
ρ_{max}/ρ_{min} [e A^{-3}]	0.289/-0.249	0.521/-0.401	0.439/-0.500
Shape and color	red block	red block	red block

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma(F_o^2)^2]^{1/2}$

Table S2: Crystal data and structure refinement for compound **6**, at 100(2)K.

Compound	**6**
CCDC	2313965
Empirical Formula	$C_{64}H_{74}AlN_4$, 0.058($C_{14}H_{10}$), 2.383(C_6H_6)
Formula weight	1149.78
T [K]	100(2)
λ [Å]	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$
a [Å]	13.678(2)
b [Å]	24.176(3)
c [Å]	41.390(4)
α [°]	87.42(2)
β [°]	81.81(3)
γ [°]	83.70(2)
V [Å^3]	13459(3)
Z	8
μ [mm^{-1}]	0.089
F(000)	4941
Crystal size [mm]	0.27x0.22x0.21
Θ max [°]	0.848 to 26.402
Reflections collected	637374
Independent reflections	54987
R_{int}	0.0991
Data/restraints/parameters	54987/4854/3524
GooF	1.043
*R*1 [$I > 2\sigma(I)$]	0.0602

$wR2$ [all data]	0.1693
Extinction coefficient	-
ρ_{max}/ρ_{min} [e A^{-3}]	0.559/-0.387
Shape and color	yellow block

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma(F_o^2)^2]^{1/2}$

Crystal structure of 2

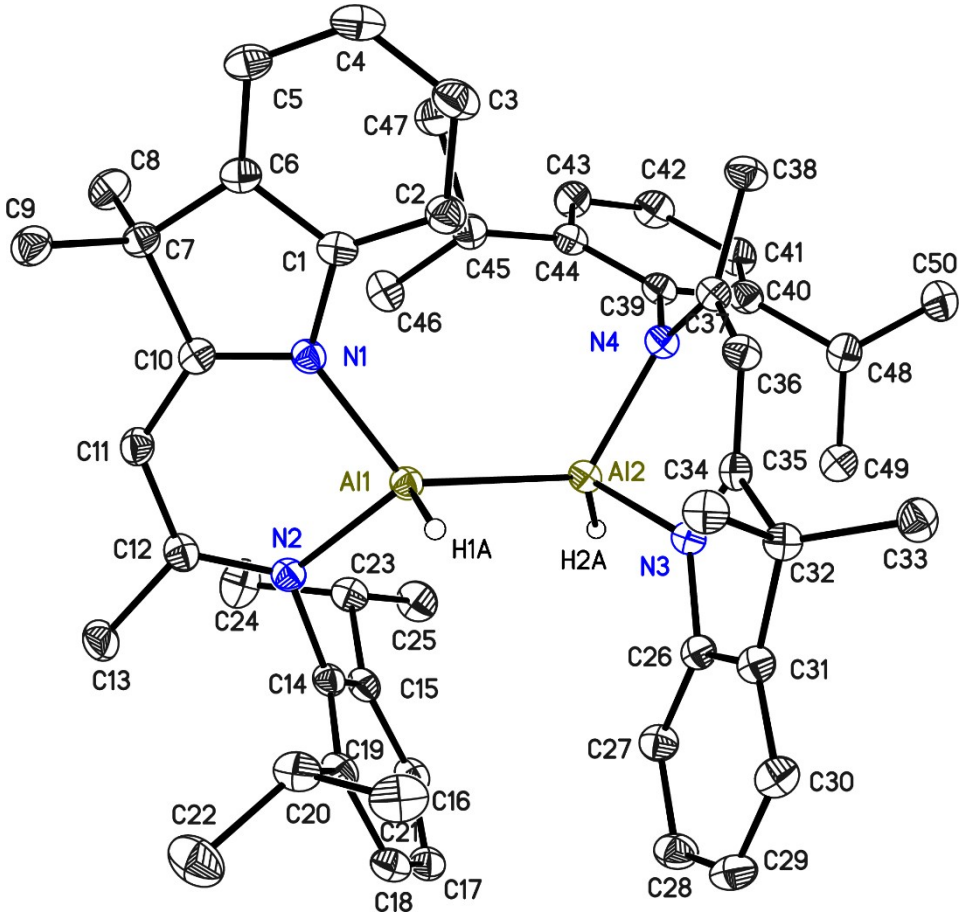


Figure S46: Asymmetric unit of **2** with thermal ellipsoids shown at 50% probability level. All ligand based hydrogen atoms are omitted for clarity. The data were collected on a split crystal. They were integrated with two orientation matrices. For the final model detwinned data were used with a fractional contribution of 0.1645 for the minor component. The hydrogen atoms bond to Al1, Al2 and C11 and C36 were refined freely.

Table S3: Bond lengths [Å] and angles [°] for **2**.

C(1)-C(2)	1.3862(18)	N(4)-C(37)	1.3417(15)
C(1)-C(6)	1.3973(17)	N(4)-C(39)	1.4455(15)
C(1)-N(1)	1.4215(15)	N(4)-Al(2)	1.9391(11)
Al(1)-H(1A)	1.519(12)	C(4)-C(5)	1.396(2)
Al(1)-N(1)	1.9235(11)	C(5)-C(6)	1.3811(17)
Al(1)-N(2)	1.9407(11)	C(6)-C(7)	1.5127(17)
Al(1)-Al(2)	2.6007(6)	C(7)-C(9)	1.5339(17)
N(1)-C(10)	1.3476(16)	C(7)-C(10)	1.5351(16)
C(2)-C(3)	1.3985(17)	C(7)-C(8)	1.5418(17)
C(3)-C(4)	1.390(2)	C(10)-C(11)	1.3841(17)

C(17)-C(18)	1.3847(18)	C(45)-C(47)	1.5325(18)
C(17)-C(16)	1.3857(18)	C(45)-C(46)	1.5338(18)
C(11)-C(12)	1.4156(17)	C(48)-C(50)	1.5274(19)
C(12)-N(2)	1.3251(16)	C(48)-C(49)	1.5317(19)
C(12)-C(13)	1.5058(17)	C(29)-C(28)	1.3875(19)
C(15)-C(16)	1.3926(17)	C(24)-C(23)	1.538(2)
C(15)-C(14)	1.4154(16)	C(25)-C(23)	1.5233(18)
C(15)-C(23)	1.5242(18)	Al(2)-H(2A)	1.528(13)
C(18)-C(19)	1.3968(17)	C(28)-C(27)	1.3960(18)
C(20)-C(19)	1.5234(17)	C(27)-C(26)	1.3880(16)
C(20)-C(21)	1.531(2)		
C(20)-C(22)	1.535(2)	C(2)-C(1)-C(6)	121.84(11)
C(14)-C(19)	1.4014(17)	C(2)-C(1)-N(1)	127.00(11)
C(14)-N(2)	1.4543(15)	C(6)-C(1)-N(1)	111.12(11)
N(3)-C(35)	1.3422(15)	H(1A)-Al(1)-N(1)	104.9(5)
N(3)-C(26)	1.4187(15)	H(1A)-Al(1)-N(2)	106.3(6)
N(3)-Al(2)	1.9257(11)	N(1)-Al(1)-N(2)	93.27(5)
C(30)-C(31)	1.3812(18)	H(1A)-Al(1)-Al(2)	107.6(6)
C(30)-C(29)	1.4008(18)	N(1)-Al(1)-Al(2)	124.92(4)
C(31)-C(26)	1.3941(17)	N(2)-Al(1)-Al(2)	117.79(3)
C(31)-C(32)	1.5120(17)	C(10)-N(1)-C(1)	108.04(10)
C(32)-C(35)	1.5291(17)	C(10)-N(1)-Al(1)	125.25(8)
C(32)-C(33)	1.5309(18)	C(1)-N(1)-Al(1)	126.29(8)
C(32)-C(34)	1.5445(17)	C(1)-C(2)-C(3)	117.29(12)
C(35)-C(36)	1.3975(17)	C(4)-C(3)-C(2)	121.41(13)
C(36)-C(37)	1.3985(17)	C(37)-N(4)-C(39)	119.42(10)
C(37)-C(38)	1.5100(17)	C(37)-N(4)-Al(2)	121.40(8)
C(39)-C(44)	1.4028(18)	C(39)-N(4)-Al(2)	119.07(7)
C(39)-C(40)	1.4148(18)	C(3)-C(4)-C(5)	120.34(12)
C(40)-C(41)	1.3933(18)	C(6)-C(5)-C(4)	118.88(12)
C(40)-C(48)	1.5247(18)	C(5)-C(6)-C(1)	120.23(12)
C(41)-C(42)	1.3833(19)	C(5)-C(6)-C(7)	131.41(12)
C(42)-C(43)	1.3842(19)	C(1)-C(6)-C(7)	108.33(10)
C(43)-C(44)	1.3958(17)	C(6)-C(7)-C(9)	112.50(10)
C(44)-C(45)	1.5229(17)	C(6)-C(7)-C(10)	100.50(10)

C(9)-C(7)-C(10)	112.10(10)	C(33)-C(32)-C(34)	110.27(10)
C(6)-C(7)-C(8)	111.66(10)	N(3)-C(35)-C(36)	124.52(11)
C(9)-C(7)-C(8)	110.02(11)	N(3)-C(35)-C(32)	111.81(10)
C(10)-C(7)-C(8)	109.75(10)	C(36)-C(35)-C(32)	123.66(10)
N(1)-C(10)-C(11)	125.41(11)	C(35)-C(36)-C(37)	125.58(11)
N(1)-C(10)-C(7)	111.68(10)	N(4)-C(37)-C(36)	122.33(11)
C(11)-C(10)-C(7)	122.88(11)	N(4)-C(37)-C(38)	119.51(11)
C(18)-C(17)-C(16)	120.01(12)	C(36)-C(37)-C(38)	118.17(10)
C(10)-C(11)-C(12)	125.64(12)	C(44)-C(39)-C(40)	120.83(11)
N(2)-C(12)-C(11)	122.39(11)	C(44)-C(39)-N(4)	120.56(11)
N(2)-C(12)-C(13)	120.42(11)	C(40)-C(39)-N(4)	118.48(11)
C(11)-C(12)-C(13)	117.16(11)	C(41)-C(40)-C(39)	118.06(12)
C(16)-C(15)-C(14)	117.54(11)	C(41)-C(40)-C(48)	119.89(11)
C(16)-C(15)-C(23)	121.20(11)	C(39)-C(40)-C(48)	122.00(11)
C(14)-C(15)-C(23)	121.26(11)	C(42)-C(41)-C(40)	121.70(12)
C(17)-C(18)-C(19)	121.08(12)	C(41)-C(42)-C(43)	119.48(12)
C(19)-C(20)-C(21)	111.45(11)	C(42)-C(43)-C(44)	121.26(12)
C(19)-C(20)-C(22)	111.58(11)	C(43)-C(44)-C(39)	118.63(12)
C(21)-C(20)-C(22)	109.78(12)	C(43)-C(44)-C(45)	118.94(11)
C(17)-C(16)-C(15)	121.44(11)	C(39)-C(44)-C(45)	122.41(11)
C(19)-C(14)-C(15)	121.84(11)	C(44)-C(45)-C(47)	112.14(11)
C(19)-C(14)-N(2)	120.22(10)	C(44)-C(45)-C(46)	110.46(10)
C(15)-C(14)-N(2)	117.70(11)	C(47)-C(45)-C(46)	110.80(11)
C(35)-N(3)-C(26)	108.38(10)	C(40)-C(48)-C(50)	112.85(11)
C(35)-N(3)-Al(2)	119.17(8)	C(40)-C(48)-C(49)	110.62(11)
C(26)-N(3)-Al(2)	127.98(8)	C(50)-C(48)-C(49)	110.04(11)
C(31)-C(30)-C(29)	118.40(12)	C(28)-C(29)-C(30)	120.68(12)
C(30)-C(31)-C(26)	120.27(11)	C(18)-C(19)-C(14)	118.03(11)
C(30)-C(31)-C(32)	131.18(11)	C(18)-C(19)-C(20)	119.17(11)
C(26)-C(31)-C(32)	108.47(10)	C(14)-C(19)-C(20)	122.79(11)
C(31)-C(32)-C(35)	100.43(9)	H(2A)-Al(2)-N(3)	111.3(6)
C(31)-C(32)-C(33)	113.57(10)	H(2A)-Al(2)-N(4)	107.1(6)
C(35)-C(32)-C(33)	113.22(10)	N(3)-Al(2)-N(4)	92.60(5)
C(31)-C(32)-C(34)	110.35(10)	H(2A)-Al(2)-Al(1)	125.0(6)
C(35)-C(32)-C(34)	108.57(10)	N(3)-Al(2)-Al(1)	97.89(4)

N(4)-Al(2)-Al(1)	117.33(4)	C(15)-C(23)-C(24)	113.00(11)
C(12)-N(2)-C(14)	120.52(10)	C(29)-C(28)-C(27)	121.42(12)
C(12)-N(2)-Al(1)	127.36(8)	C(26)-C(27)-C(28)	117.03(12)
C(14)-N(2)-Al(1)	111.81(8)	C(27)-C(26)-C(31)	122.18(11)
C(25)-C(23)-C(15)	113.40(11)	C(27)-C(26)-N(3)	127.01(11)
C(25)-C(23)-C(24)	108.43(11)	C(31)-C(26)-N(3)	110.79(10)

Crystal structure of 3

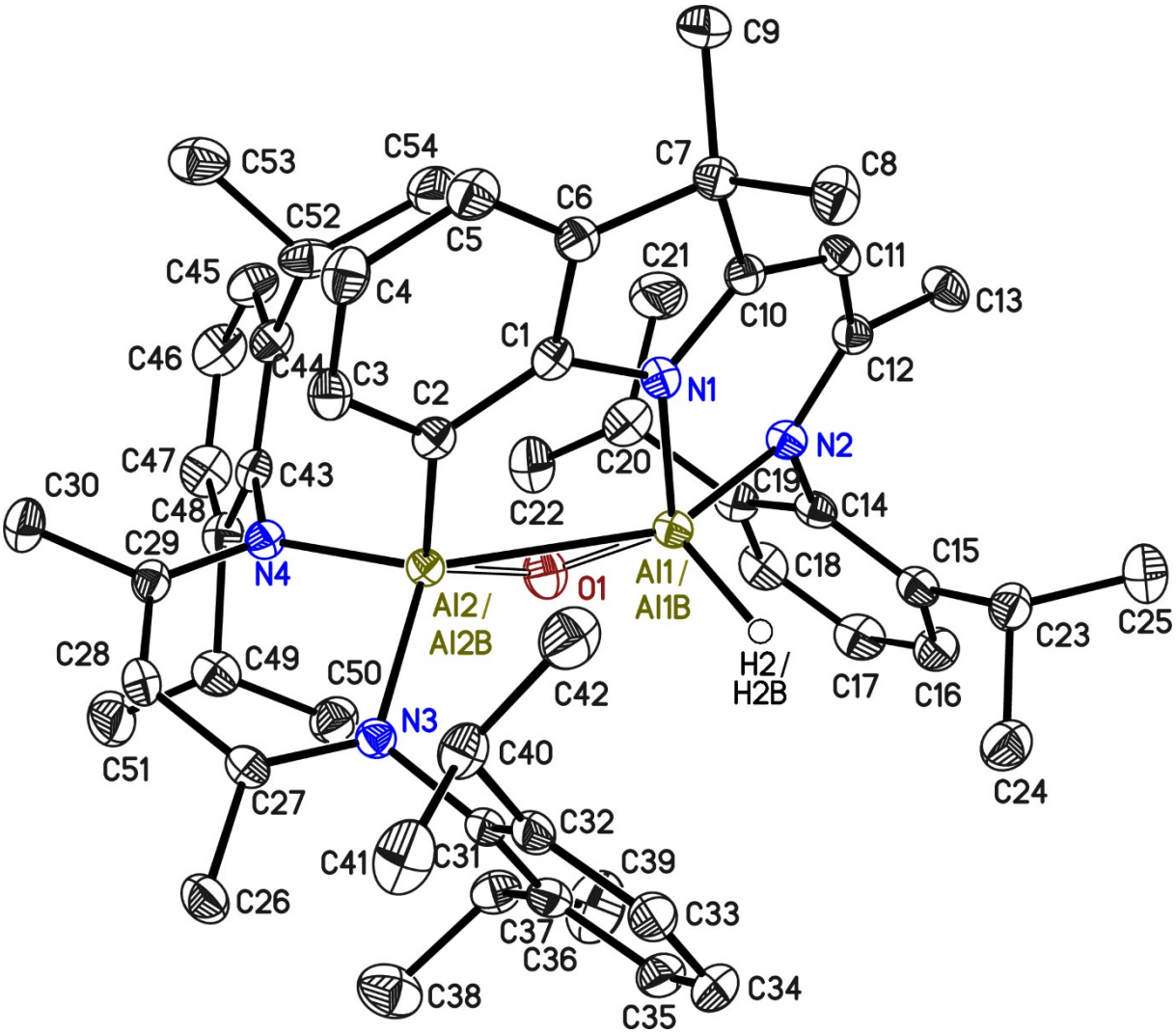


Figure S47: Asymmetric unit of **3** with thermal ellipsoids shown at 50% probability level. All ligand based hydrogen atoms are omitted for clarity. The occupancy of the oxygen atom refined to 0.055(3). The oxygen atom is refined with distance restraints and restraints for the anisotropic displacement parameters.

Table S4: Bond lengths [Å] and angles [°] for **3**.

Al(1)-O(1)	1.500(17)	Al(2)-N(3)	1.9303(11)
Al(1)-H(2)	1.538(15)	Al(2)-C(2)	2.0172(12)
Al(1)-N(1)	1.9046(10)	N(2)-C(12)	1.3390(16)
Al(1)-N(2)	1.9422(11)	N(2)-C(14)	1.4514(14)
Al(1)-Al(2)	2.6044(6)	C(2)-C(1)	1.3947(17)
Al(2)-O(1)	1.594(15)	C(2)-C(3)	1.4103(17)
Al(2)-N(4)	1.9149(11)	C(1)-C(6)	1.3965(16)

C(1)-N(1)	1.4220(15)	C(34)-C(35)	1.383(2)
N(1)-C(10)	1.3312(15)	C(35)-C(36)	1.3927(18)
N(3)-C(27)	1.3227(16)	C(36)-C(37)	1.5197(18)
N(3)-C(31)	1.4486(15)	C(37)-C(39)	1.5226(19)
N(4)-C(29)	1.3509(16)	C(37)-C(38)	1.535(2)
N(4)-C(43)	1.4489(15)	C(40)-C(42)	1.5331(19)
C(3)-C(4)	1.3940(18)	C(40)-C(41)	1.5379(19)
C(4)-C(5)	1.3993(19)	C(43)-C(44)	1.4049(17)
C(5)-C(6)	1.3829(17)	C(43)-C(48)	1.4112(17)
C(6)-C(7)	1.5180(17)	C(44)-C(45)	1.3976(17)
C(7)-C(9)	1.5303(17)	C(44)-C(52)	1.5161(17)
C(7)-C(10)	1.5399(15)	C(45)-C(46)	1.3780(19)
C(7)-C(8)	1.5418(17)	C(46)-C(47)	1.386(2)
C(10)-C(11)	1.3912(17)	C(47)-C(48)	1.3940(18)
C(11)-C(12)	1.4094(17)	C(48)-C(49)	1.5265(18)
C(12)-C(13)	1.5130(17)	C(49)-C(50)	1.5269(19)
C(14)-C(15)	1.4054(18)	C(49)-C(51)	1.531(2)
C(14)-C(19)	1.4111(18)	C(52)-C(54)	1.530(2)
C(15)-C(16)	1.3982(17)	C(52)-C(53)	1.5321(19)
C(15)-C(23)	1.5205(18)		
C(16)-C(17)	1.380(2)	O(1)-Al(1)-H(2)	116.7(8)
C(17)-C(18)	1.386(2)	O(1)-Al(1)-N(1)	113.5(6)
C(18)-C(19)	1.3959(17)	H(2)-Al(1)-N(1)	110.1(5)
C(19)-C(20)	1.5196(19)	O(1)-Al(1)-N(2)	119.8(6)
C(20)-C(21)	1.515(2)	H(2)-Al(1)-N(2)	102.3(5)
C(20)-C(22)	1.524(2)	N(1)-Al(1)-N(2)	91.31(5)
C(23)-C(24)	1.5343(19)	O(1)-Al(1)-Al(2)	33.8(6)
C(23)-C(25)	1.538(2)	H(2)-Al(1)-Al(2)	112.6(6)
C(26)-C(27)	1.5081(17)	N(1)-Al(1)-Al(2)	86.09(3)
C(27)-C(28)	1.4097(18)	N(2)-Al(1)-Al(2)	143.75(4)
C(28)-C(29)	1.3949(17)	O(1)-Al(2)-N(4)	113.7(6)
C(29)-C(30)	1.5092(17)	O(1)-Al(2)-N(3)	114.3(6)
C(31)-C(32)	1.4059(17)	N(4)-Al(2)-N(3)	95.58(5)
C(31)-C(36)	1.4092(17)	O(1)-Al(2)-C(2)	118.1(6)
C(32)-C(33)	1.3960(18)	N(4)-Al(2)-C(2)	107.84(5)
C(32)-C(40)	1.5216(17)	N(3)-Al(2)-C(2)	104.66(5)
C(33)-C(34)	1.3820(19)	O(1)-Al(2)-Al(1)	31.6(6)

N(4)-Al(2)-Al(1)	139.47(4)	C(10)-C(11)-C(12)	124.77(11)
N(3)-Al(2)-Al(1)	116.20(4)	N(2)-C(12)-C(11)	123.93(11)
C(2)-Al(2)-Al(1)	88.65(4)	N(2)-C(12)-C(13)	120.35(11)
Al(1)-O(1)-Al(2)	114.6(10)	C(11)-C(12)-C(13)	115.72(11)
C(12)-N(2)-C(14)	118.95(10)	C(15)-C(14)-C(19)	121.63(11)
C(12)-N(2)-Al(1)	125.70(8)	C(15)-C(14)-N(2)	119.82(11)
C(14)-N(2)-Al(1)	114.22(7)	C(19)-C(14)-N(2)	118.44(11)
C(1)-C(2)-C(3)	112.77(11)	C(16)-C(15)-C(14)	117.91(12)
C(1)-C(2)-Al(2)	115.52(8)	C(16)-C(15)-C(23)	118.76(12)
C(3)-C(2)-Al(2)	130.93(9)	C(14)-C(15)-C(23)	123.31(11)
C(2)-C(1)-C(6)	126.40(11)	C(17)-C(16)-C(15)	121.30(13)
C(2)-C(1)-N(1)	123.60(10)	C(16)-C(17)-C(18)	120.07(12)
C(6)-C(1)-N(1)	109.81(10)	C(17)-C(18)-C(19)	121.21(12)
C(10)-N(1)-C(1)	109.56(10)	C(18)-C(19)-C(14)	117.85(12)
C(10)-N(1)-Al(1)	128.12(8)	C(18)-C(19)-C(20)	121.03(12)
C(1)-N(1)-Al(1)	122.31(8)	C(14)-C(19)-C(20)	121.12(11)
C(27)-N(3)-C(31)	121.42(10)	C(21)-C(20)-C(19)	112.06(13)
C(27)-N(3)-Al(2)	120.73(8)	C(21)-C(20)-C(22)	109.70(12)
C(31)-N(3)-Al(2)	116.84(8)	C(19)-C(20)-C(22)	113.73(12)
C(29)-N(4)-C(43)	116.15(10)	C(15)-C(23)-C(24)	110.93(11)
C(29)-N(4)-Al(2)	118.27(8)	C(15)-C(23)-C(25)	111.87(11)
C(43)-N(4)-Al(2)	125.35(8)	C(24)-C(23)-C(25)	109.76(12)
C(4)-C(3)-C(2)	123.00(12)	N(3)-C(27)-C(28)	122.64(11)
C(3)-C(4)-C(5)	121.02(11)	N(3)-C(27)-C(26)	121.21(11)
C(6)-C(5)-C(4)	118.39(11)	C(28)-C(27)-C(26)	116.15(11)
C(5)-C(6)-C(1)	118.38(11)	C(29)-C(28)-C(27)	127.27(11)
C(5)-C(6)-C(7)	132.95(11)	N(4)-C(29)-C(28)	123.44(11)
C(1)-C(6)-C(7)	108.62(10)	N(4)-C(29)-C(30)	119.90(11)
C(6)-C(7)-C(9)	112.94(10)	C(28)-C(29)-C(30)	116.64(11)
C(6)-C(7)-C(10)	100.22(9)	C(32)-C(31)-C(36)	121.41(11)
C(9)-C(7)-C(10)	113.18(10)	C(32)-C(31)-N(3)	120.30(11)
C(6)-C(7)-C(8)	111.41(10)	C(36)-C(31)-N(3)	118.11(11)
C(9)-C(7)-C(8)	110.32(10)	C(33)-C(32)-C(31)	117.79(12)
C(10)-C(7)-C(8)	108.35(10)	C(33)-C(32)-C(40)	118.59(11)
N(1)-C(10)-C(11)	122.72(11)	C(31)-C(32)-C(40)	123.61(11)
N(1)-C(10)-C(7)	110.74(10)	C(34)-C(33)-C(32)	121.62(12)
C(11)-C(10)-C(7)	126.52(11)	C(33)-C(34)-C(35)	119.71(12)

C(34)-C(35)-C(36)	121.31(12)	C(45)-C(44)-C(52)	118.84(11)
C(35)-C(36)-C(31)	118.15(12)	C(43)-C(44)-C(52)	122.65(11)
C(35)-C(36)-C(37)	121.12(12)	C(46)-C(45)-C(44)	121.24(13)
C(31)-C(36)-C(37)	120.69(11)	C(45)-C(46)-C(47)	119.82(12)
C(36)-C(37)-C(39)	113.58(12)	C(46)-C(47)-C(48)	121.26(12)
C(36)-C(37)-C(38)	110.44(11)	C(47)-C(48)-C(43)	118.29(12)
C(39)-C(37)-C(38)	110.70(13)	C(47)-C(48)-C(49)	119.76(12)
C(32)-C(40)-C(42)	111.50(11)	C(43)-C(48)-C(49)	121.87(11)
C(32)-C(40)-C(41)	111.60(11)	C(48)-C(49)-C(50)	109.09(11)
C(42)-C(40)-C(41)	109.07(11)	C(48)-C(49)-C(51)	113.79(12)
C(44)-C(43)-C(48)	120.83(11)	C(50)-C(49)-C(51)	109.87(11)
C(44)-C(43)-N(4)	120.63(10)	C(44)-C(52)-C(54)	111.75(11)
C(48)-C(43)-N(4)	118.52(11)	C(44)-C(52)-C(53)	111.48(11)
C(45)-C(44)-C(43)	118.48(11)	C(54)-C(52)-C(53)	110.79(11)

Crystal structure of 5

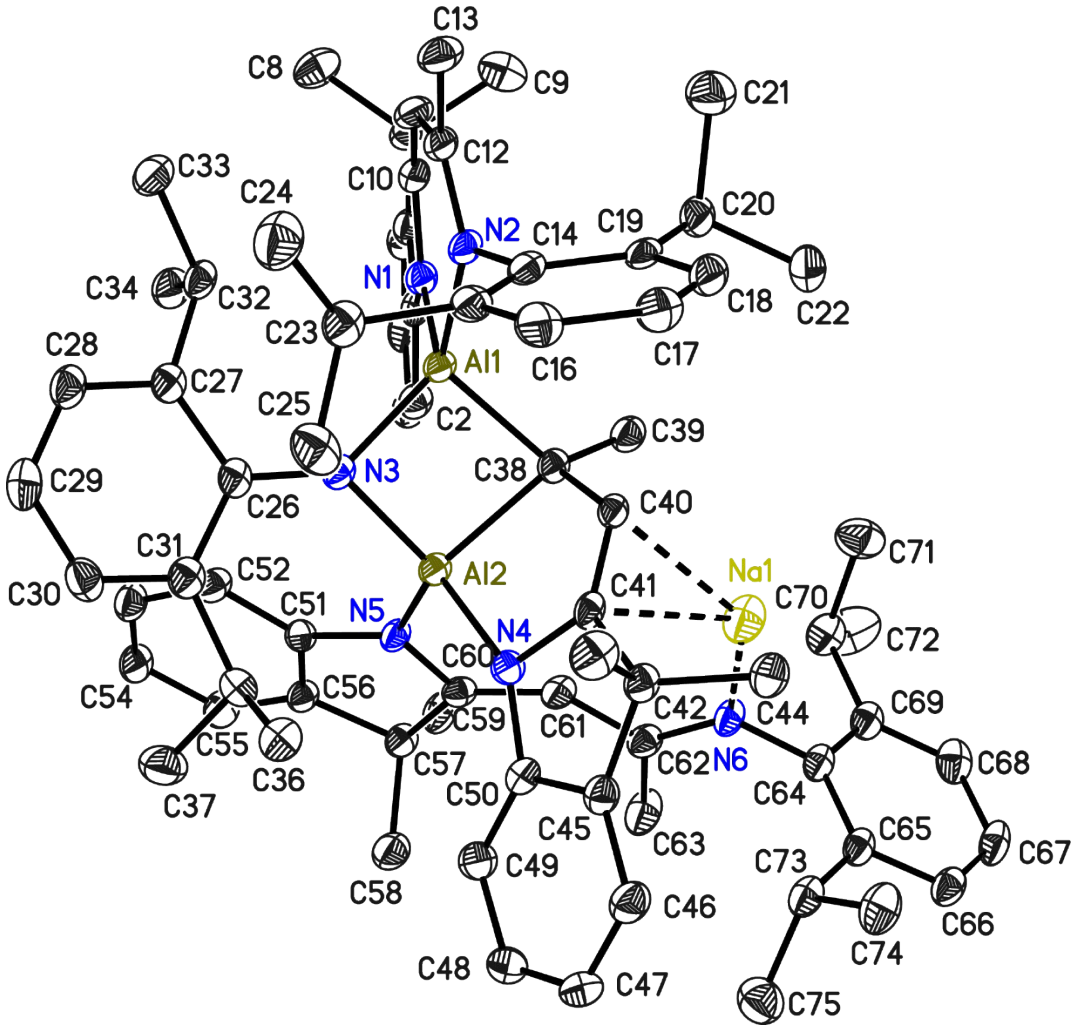


Figure S48: Molecule 1 of **5** with thermal ellipsoids shown at 50% probability level. All ligand based hydrogen atoms omitted for clarity.

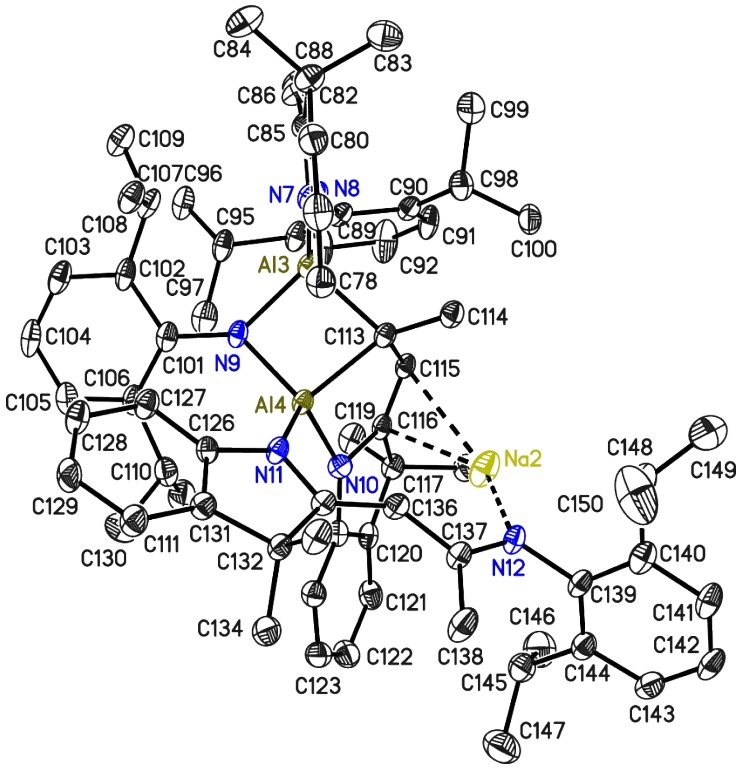


Figure S49: Molecule 2 of **5** with thermal ellipsoids shown at 50% probability level. All ligand based hydrogen atoms are omitted for clarity.

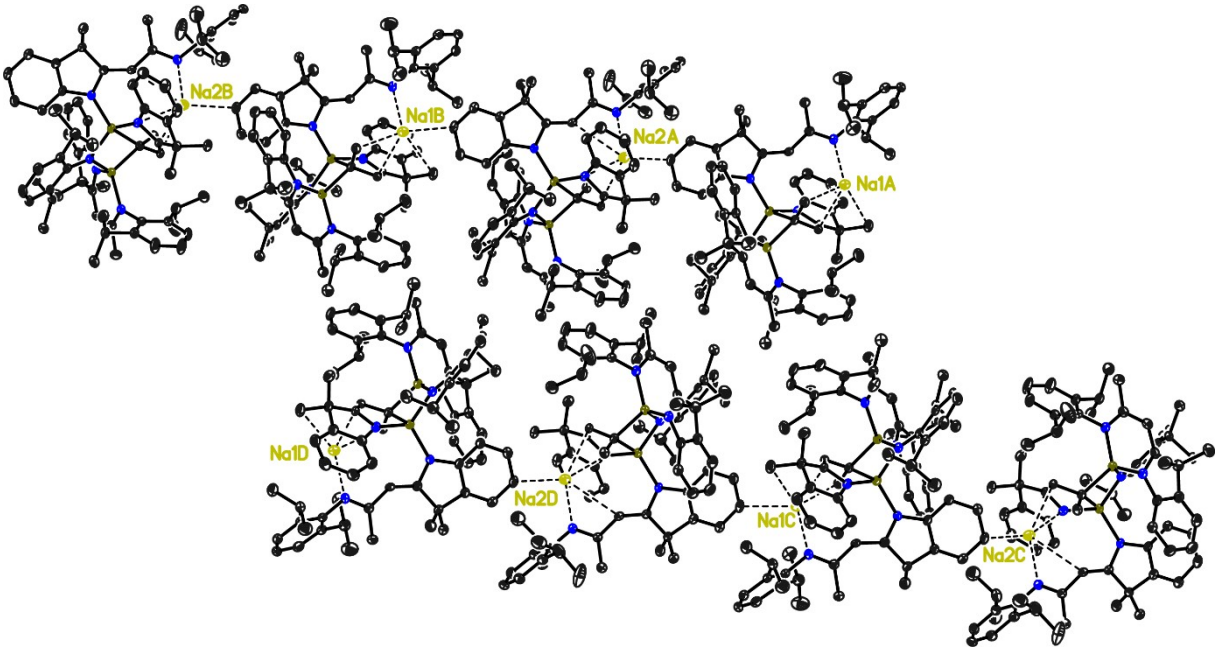


Figure S50: Polymeric structure of **5** with thermal ellipsoids shown at 50% probability level. All ligand based hydrogen atoms are omitted for clarity.

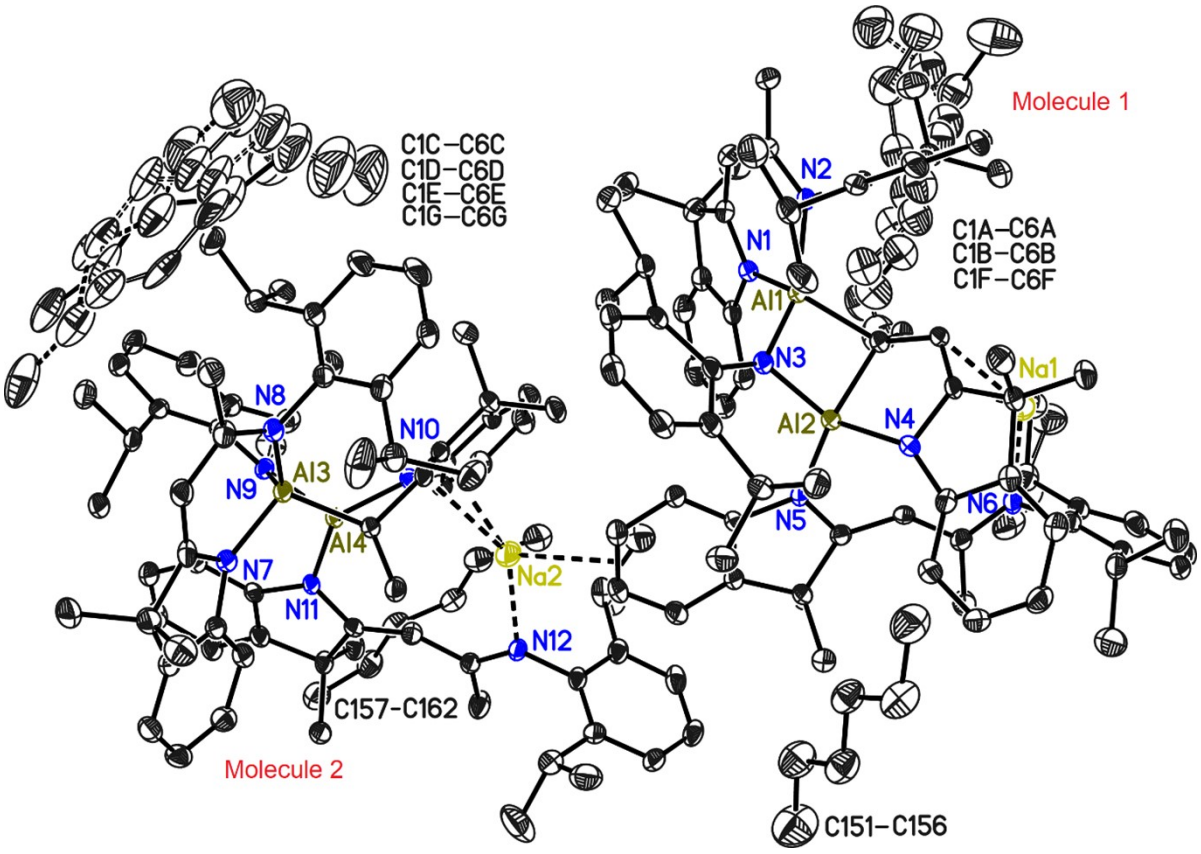


Figure S51: Asymmetric unit of **5** with thermal ellipsoids shown at 50% probability level. Hydrogen atoms are omitted for clarity. One hexane molecule is disordered over four positions (C1A-C6B, C1F-C6F) and one hexane molecule is disordered over three position (C1D-C6E, C1G-C6G). One iPr-group (C70-C72) is disordered over two positions. The occupancies of the minor positions refined to 0.237(2), 0.178(2), 0.171(3), 0.255(2), 2.84(3), and 0.262(18) respectively. All disordered molecules and groups were refined with distance restraints and restraints for anisotropic displacement parameters.

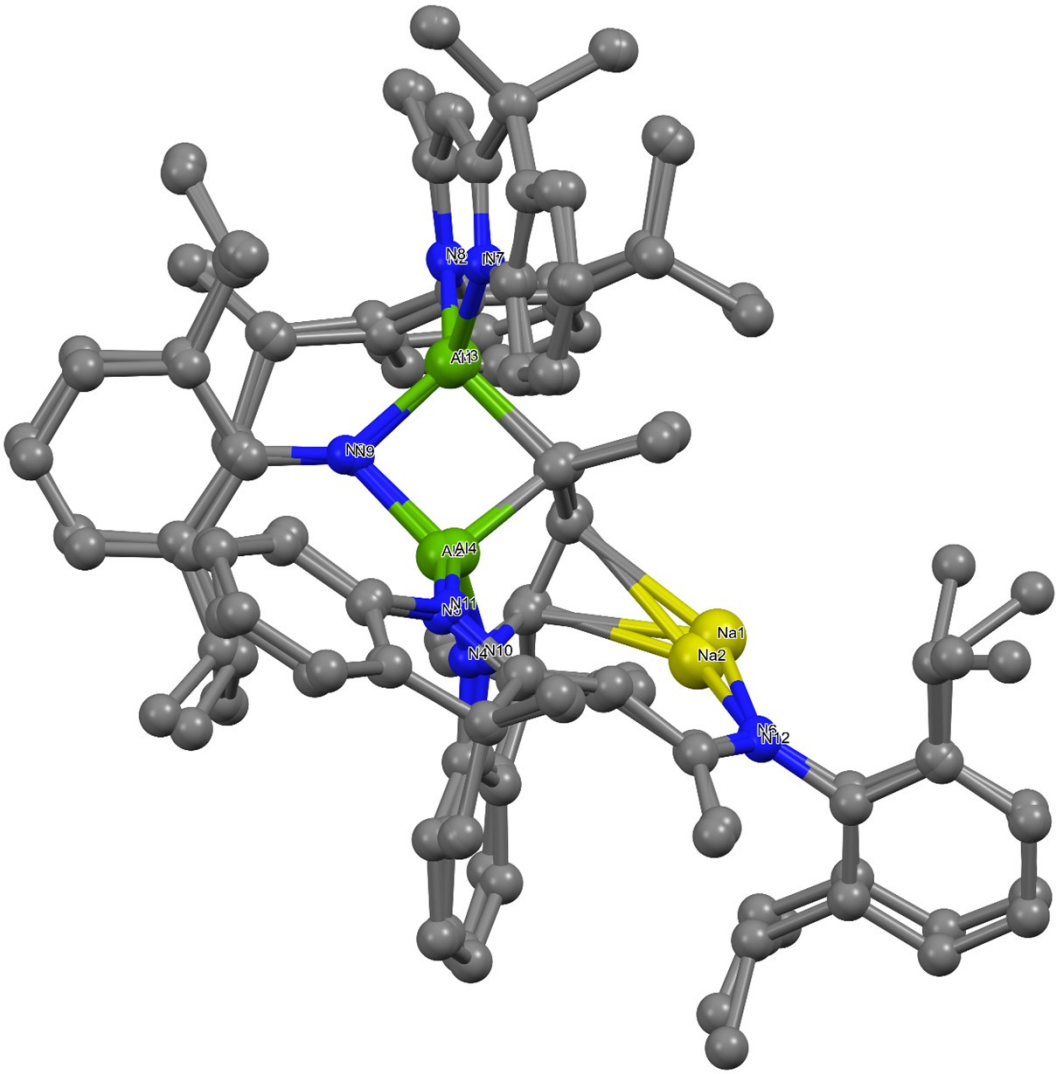


Figure S52: Overlap model of two molecules from asymmetric unit of **5** drawn using Mercury.

Table S5: Bond lengths [Å] and angles [°] for **5**.

N(1)-C(10)	1.347(3)	C(53)-C(52)	1.397(3)
N(1)-C(1)	1.429(3)	C(52)-C(51)	1.386(3)
N(1)-Al(1)	1.941(2)	C(10)-C(11)	1.389(3)
C(1)-C(2)	1.379(3)	Al(1)-C(38)	1.968(2)
C(1)-C(6)	1.395(3)	Na(1)-N(6)	2.343(2)
N(2)-C(12)	1.346(3)	Na(1)-C(40)	2.588(3)
N(2)-C(14)	1.459(3)	Na(1)-C(41)	2.718(3)
N(2)-Al(1)	1.927(2)	Na(1)-C(39)	2.985(3)
C(2)-C(3)	1.392(3)	Na(1)-C(129)#1	3.028(3)
N(3)-C(26)	1.413(3)	Na(1)-C(44)	3.075(3)
N(3)-Al(2)	1.871(2)	C(11)-C(12)	1.391(3)
N(3)-Al(1)	1.871(2)	C(19)-C(18)	1.395(3)
C(3)-C(4)	1.387(4)	C(19)-C(14)	1.416(3)
C(4)-C(5)	1.388(4)	C(19)-C(20)	1.520(4)
C(7)-C(6)	1.507(3)	C(40)-C(41)	1.351(3)
C(7)-C(10)	1.531(3)	C(40)-C(38)	1.521(3)
C(7)-C(8)	1.538(3)	Al(2)-N(4)	1.876(2)
C(7)-C(9)	1.547(4)	Al(2)-N(5)	1.917(2)
N(8)-C(87)	1.344(3)	Al(2)-C(38)	2.026(3)
N(8)-C(89)	1.458(3)	Na(2)-N(12)	2.366(2)
N(8)-Al(3)	1.937(2)	Na(2)-C(116)	2.559(2)
N(9)-C(101)	1.420(3)	Na(2)-C(115)	2.688(3)
N(9)-Al(4)	1.866(2)	Na(2)-C(136)	3.118(3)
N(9)-Al(3)	1.870(2)	C(27)-C(28)	1.388(3)
N(10)-C(125)	1.393(3)	C(27)-C(26)	1.443(3)
N(10)-C(116)	1.430(3)	C(27)-C(32)	1.517(3)
N(10)-Al(4)	1.873(2)	C(28)-C(29)	1.374(4)
N(10)-Na(2)	2.814(2)	C(15)-C(14)	1.393(4)
C(54)-C(53)	1.383(3)	C(15)-C(16)	1.400(3)
C(54)-C(55)	1.388(3)	C(15)-C(23)	1.513(3)
C(54)-Na(2)	2.943(3)	C(29)-C(30)	1.375(4)

C(12)-C(13)	1.505(3)	C(42)-C(44)	1.534(3)
C(32)-C(34)	1.528(3)	C(46)-C(45)	1.378(3)
C(32)-C(33)	1.535(3)	C(46)-C(47)	1.400(3)
C(36)-C(35)	1.534(3)	C(45)-C(50)	1.410(3)
N(4)-C(50)	1.392(3)	C(49)-C(50)	1.388(3)
N(4)-C(41)	1.414(3)	C(49)-C(48)	1.392(3)
C(16)-C(17)	1.381(4)	C(48)-C(47)	1.387(4)
C(17)-C(18)	1.376(4)	N(5)-C(51)	1.418(3)
C(20)-C(21)	1.533(4)	C(5)-C(6)	1.381(3)
C(20)-C(22)	1.536(3)	C(65)-C(66)	1.395(3)
C(58)-C(57)	1.541(3)	C(65)-C(64)	1.410(3)
C(57)-C(56)	1.507(3)	C(65)-C(73)	1.515(4)
C(57)-C(59)	1.529(3)	C(64)-C(69)	1.404(4)
C(57)-C(60)	1.542(3)	C(68)-C(67)	1.388(4)
C(56)-C(55)	1.385(3)	C(68)-C(69)	1.395(3)
C(56)-C(51)	1.397(3)	C(67)-C(66)	1.376(4)
C(25)-C(23)	1.522(4)	Al(3)-N(7)	1.938(2)
C(23)-C(24)	1.537(4)	Al(3)-C(113)	1.970(2)
N(6)-C(62)	1.310(3)	C(69)-C(70)	1.522(4)
N(6)-C(64)	1.436(3)	N(7)-C(85)	1.347(3)
C(62)-C(61)	1.440(3)	N(7)-C(76)	1.433(3)
C(62)-C(63)	1.508(3)	C(70)-C(71A)	1.478(12)
C(61)-C(60)	1.369(3)	C(70)-C(72)	1.531(6)
C(60)-N(5)	1.392(3)	C(70)-C(72A)	1.541(12)
C(31)-C(30)	1.395(3)	C(70)-C(71)	1.553(5)
C(31)-C(26)	1.431(3)	C(74)-C(73)	1.529(3)
C(31)-C(35)	1.520(3)	C(73)-C(75)	1.533(4)
C(39)-C(38)	1.541(3)	C(76)-C(77)	1.381(3)
C(35)-C(37)	1.538(3)	C(76)-C(81)	1.392(3)
C(43)-C(42)	1.540(3)	C(77)-C(78)	1.392(3)
C(42)-C(45)	1.526(3)	C(78)-C(79)	1.379(4)
C(42)-C(41)	1.531(3)	C(79)-C(80)	1.391(4)

C(80)-C(81)	1.379(3)	C(106)-C(110)	1.520(4)
C(81)-C(82)	1.510(3)	C(107)-C(108)	1.538(3)
C(82)-C(85)	1.533(3)	C(107)-C(109)	1.538(3)
C(82)-C(84)	1.535(4)	Al(4)-C(113)	2.030(2)
C(82)-C(83)	1.536(4)	C(110)-C(112)	1.530(4)
C(85)-C(86)	1.386(3)	C(110)-C(111)	1.535(4)
C(86)-C(87)	1.398(3)	C(113)-C(115)	1.518(3)
C(87)-C(88)	1.509(3)	C(113)-C(114)	1.541(3)
C(89)-C(94)	1.394(3)	C(115)-C(116)	1.344(3)
C(89)-C(90)	1.417(3)	C(116)-C(117)	1.537(3)
C(90)-C(91)	1.389(3)	C(117)-C(120)	1.524(3)
C(90)-C(98)	1.521(4)	C(117)-C(118)	1.537(3)
C(91)-C(92)	1.375(4)	C(117)-C(119)	1.541(3)
C(92)-C(93)	1.379(4)	C(120)-C(121)	1.375(3)
C(93)-C(94)	1.390(3)	C(120)-C(125)	1.408(3)
C(94)-C(95)	1.524(3)	C(121)-C(122)	1.391(4)
C(95)-C(97)	1.522(4)	C(122)-C(123)	1.393(4)
C(95)-C(96)	1.534(3)	C(123)-C(124)	1.384(3)
C(98)-C(99)	1.523(4)	C(124)-C(125)	1.389(3)
C(98)-C(100)	1.531(3)	C(126)-C(127)	1.387(3)
N(12)-C(137)	1.307(3)	C(126)-C(131)	1.389(3)
N(12)-C(139)	1.435(3)	C(127)-C(128)	1.396(3)
N(11)-C(135)	1.396(3)	C(128)-C(129)	1.385(4)
N(11)-C(126)	1.418(3)	C(129)-C(130)	1.397(3)
N(11)-Al(4)	1.930(2)	C(130)-C(131)	1.385(3)
C(101)-C(106)	1.427(4)	C(131)-C(132)	1.512(3)
C(101)-C(102)	1.439(3)	C(132)-C(134)	1.537(3)
C(102)-C(103)	1.395(3)	C(132)-C(135)	1.537(3)
C(102)-C(107)	1.511(4)	C(132)-C(133)	1.542(3)
C(103)-C(104)	1.369(4)	C(135)-C(136)	1.374(3)
C(104)-C(105)	1.380(4)	C(136)-C(137)	1.436(3)
C(105)-C(106)	1.405(3)	C(137)-C(138)	1.507(3)

C(139)-C(144)	1.399(4)	C(1F)-C(2F)	1.507(14)
C(139)-C(140)	1.406(3)	C(2F)-C(3F)	1.499(13)
C(140)-C(141)	1.400(3)	C(3F)-C(4F)	1.506(13)
C(140)-C(148)	1.517(4)	C(4F)-C(5F)	1.455(13)
C(141)-C(142)	1.373(4)	C(5F)-C(6F)	1.498(13)
C(142)-C(143)	1.376(4)	C(1C)-C(2C)	1.579(13)
C(143)-C(144)	1.403(3)	C(2C)-C(3C)	1.505(13)
C(144)-C(145)	1.517(4)	C(3C)-C(4C)	1.469(12)
C(145)-C(147)	1.528(4)	C(4C)-C(5C)	1.454(13)
C(145)-C(146)	1.531(4)	C(5C)-C(6C)	1.545(13)
C(148)-C(149)	1.522(4)	C(1D)-C(2D)	1.535(13)
C(148)-C(150)	1.533(4)	C(2D)-C(3D)	1.521(12)
C(151)-C(152)	1.506(4)	C(3D)-C(4D)	1.404(11)
C(152)-C(153)	1.509(4)	C(4D)-C(5D)	1.421(10)
C(153)-C(154)	1.515(4)	C(5D)-C(6D)	1.536(12)
C(154)-C(155)	1.509(4)	C(1E)-C(2E)	1.599(12)
C(155)-C(156)	1.518(4)	C(2E)-C(3E)	1.544(12)
C(157)-C(158)	1.522(4)	C(3E)-C(4E)	1.422(13)
C(158)-C(159)	1.520(4)	C(4E)-C(5E)	1.522(12)
C(159)-C(160)	1.517(4)	C(5E)-C(6E)	1.551(13)
C(160)-C(161)	1.521(4)	C(1G)-C(2G)	1.500(13)
C(161)-C(162)	1.522(4)	C(2G)-C(3G)	1.364(12)
C(1A)-C(2A)	1.533(8)	C(3G)-C(4G)	1.506(12)
C(2A)-C(3A)	1.541(7)	C(4G)-C(5G)	1.588(12)
C(3A)-C(4A)	1.501(8)	C(5G)-C(6G)	1.551(12)
C(4A)-C(5A)	1.437(8)		
C(5A)-C(6A)	1.588(8)	C(10)-N(1)-C(1)	107.61(19)
C(1B)-C(2B)	1.526(12)	C(10)-N(1)-Al(1)	124.11(16)
C(2B)-C(3B)	1.531(13)	C(1)-N(1)-Al(1)	128.27(16)
C(3B)-C(4B)	1.489(12)	C(2)-C(1)-C(6)	121.4(2)
C(4B)-C(5B)	1.464(11)	C(2)-C(1)-N(1)	127.6(2)
C(5B)-C(6B)	1.489(12)	C(6)-C(1)-N(1)	111.0(2)

C(12)-N(2)-C(14)	116.71(19)	N(1)-C(10)-C(11)	124.9(2)
C(12)-N(2)-Al(1)	125.90(16)	N(1)-C(10)-C(7)	112.1(2)
C(14)-N(2)-Al(1)	117.22(15)	C(11)-C(10)-C(7)	123.0(2)
C(1)-C(2)-C(3)	117.7(2)	N(3)-Al(1)-N(2)	124.46(9)
C(26)-N(3)-Al(2)	134.68(16)	N(3)-Al(1)-N(1)	117.46(9)
C(26)-N(3)-Al(1)	135.17(16)	N(2)-Al(1)-N(1)	93.45(9)
Al(2)-N(3)-Al(1)	89.59(9)	N(3)-Al(1)-C(38)	93.84(10)
C(4)-C(3)-C(2)	121.4(2)	N(2)-Al(1)-C(38)	118.20(9)
C(3)-C(4)-C(5)	120.2(2)	N(1)-Al(1)-C(38)	110.60(10)
C(6)-C(7)-C(10)	100.63(19)	N(6)-Na(1)-C(40)	135.30(8)
C(6)-C(7)-C(8)	113.2(2)	N(6)-Na(1)-C(41)	123.12(8)
C(10)-C(7)-C(8)	113.1(2)	C(40)-Na(1)-C(41)	29.36(7)
C(6)-C(7)-C(9)	111.4(2)	N(6)-Na(1)-C(39)	101.36(8)
C(10)-C(7)-C(9)	109.0(2)	C(40)-Na(1)-C(39)	53.36(7)
C(8)-C(7)-C(9)	109.3(2)	C(41)-Na(1)-C(39)	78.36(7)
C(87)-N(8)-C(89)	115.6(2)	N(6)-Na(1)-C(129)#1	101.81(8)
C(87)-N(8)-Al(3)	125.39(16)	C(40)-Na(1)-C(129)#1	120.59(8)
C(89)-N(8)-Al(3)	118.97(16)	C(41)-Na(1)-C(129)#1	132.31(8)
C(101)-N(9)-Al(4)	133.98(17)	C(39)-Na(1)-C(129)#1	109.90(8)
C(101)-N(9)-Al(3)	136.04(17)	N(6)-Na(1)-C(44)	133.02(8)
Al(4)-N(9)-Al(3)	89.82(9)	C(40)-Na(1)-C(44)	67.68(8)
C(125)-N(10)-C(116)	107.38(19)	C(41)-Na(1)-C(44)	52.20(7)
C(125)-N(10)-Al(4)	146.37(16)	C(39)-Na(1)-C(44)	119.24(8)
C(116)-N(10)-Al(4)	105.87(15)	C(129)#1-Na(1)-C(44)	86.50(7)
C(125)-N(10)-Na(2)	94.65(14)	C(10)-C(11)-C(12)	126.1(2)
C(116)-N(10)-Na(2)	64.91(12)	C(18)-C(19)-C(14)	116.9(2)
Al(4)-N(10)-Na(2)	103.86(9)	C(18)-C(19)-C(20)	120.5(2)
C(53)-C(54)-C(55)	120.4(2)	C(14)-C(19)-C(20)	122.6(2)
C(53)-C(54)-Na(2)	95.31(16)	C(41)-C(40)-C(38)	121.0(2)
C(55)-C(54)-Na(2)	121.91(18)	C(41)-C(40)-Na(1)	80.65(14)
C(54)-C(53)-C(52)	121.4(2)	C(38)-C(40)-Na(1)	96.95(14)
C(51)-C(52)-C(53)	117.9(2)	N(3)-Al(2)-N(4)	122.38(9)

N(3)-Al(2)-N(5)	116.15(9)	C(27)-C(32)-C(33)	115.0(2)
N(4)-Al(2)-N(5)	108.51(9)	C(34)-C(32)-C(33)	110.8(2)
N(3)-Al(2)-C(38)	91.98(9)	C(50)-N(4)-C(41)	107.35(18)
N(4)-Al(2)-C(38)	91.81(9)	C(50)-N(4)-Al(2)	145.54(16)
N(5)-Al(2)-C(38)	123.91(10)	C(41)-N(4)-Al(2)	106.69(15)
N(12)-Na(2)-C(116)	140.98(8)	C(17)-C(16)-C(15)	121.0(3)
N(12)-Na(2)-C(115)	144.20(8)	C(15)-C(14)-C(19)	122.5(2)
C(116)-Na(2)-C(115)	29.56(7)	C(15)-C(14)-N(2)	120.5(2)
N(12)-Na(2)-N(10)	110.60(7)	C(19)-C(14)-N(2)	117.0(2)
C(116)-Na(2)-N(10)	30.41(6)	C(18)-C(17)-C(16)	120.3(2)
C(115)-Na(2)-N(10)	51.05(7)	C(19)-C(20)-C(21)	112.7(2)
N(12)-Na(2)-C(54)	91.70(8)	C(19)-C(20)-C(22)	113.2(2)
C(116)-Na(2)-C(54)	127.31(8)	C(21)-C(20)-C(22)	108.4(2)
C(115)-Na(2)-C(54)	110.21(8)	C(17)-C(18)-C(19)	121.6(2)
N(10)-Na(2)-C(54)	157.70(7)	C(56)-C(57)-C(59)	109.2(2)
N(12)-Na(2)-C(136)	47.60(7)	C(56)-C(57)-C(58)	107.8(2)
C(116)-Na(2)-C(136)	95.95(8)	C(59)-C(57)-C(58)	112.9(2)
C(115)-Na(2)-C(136)	98.78(7)	C(56)-C(57)-C(60)	100.90(18)
N(10)-Na(2)-C(136)	67.78(6)	C(59)-C(57)-C(60)	112.5(2)
C(54)-Na(2)-C(136)	132.80(7)	C(58)-C(57)-C(60)	112.6(2)
C(28)-C(27)-C(26)	120.8(2)	C(55)-C(56)-C(51)	120.7(2)
C(28)-C(27)-C(32)	118.1(2)	C(55)-C(56)-C(57)	129.6(2)
C(26)-C(27)-C(32)	120.9(2)	C(51)-C(56)-C(57)	109.7(2)
C(29)-C(28)-C(27)	122.1(2)	C(15)-C(23)-C(25)	111.3(2)
C(14)-C(15)-C(16)	117.7(2)	C(15)-C(23)-C(24)	112.1(2)
C(14)-C(15)-C(23)	123.7(2)	C(25)-C(23)-C(24)	110.1(2)
C(16)-C(15)-C(23)	118.6(2)	C(62)-N(6)-C(64)	119.9(2)
C(28)-C(29)-C(30)	118.2(2)	C(62)-N(6)-Na(1)	123.56(16)
N(2)-C(12)-C(11)	122.7(2)	C(64)-N(6)-Na(1)	115.78(14)
N(2)-C(12)-C(13)	120.4(2)	N(6)-C(62)-C(61)	115.1(2)
C(11)-C(12)-C(13)	116.9(2)	N(6)-C(62)-C(63)	120.1(2)
C(27)-C(32)-C(34)	109.28(19)	C(61)-C(62)-C(63)	124.9(2)

C(60)-C(61)-C(62)	137.7(2)	C(42)-C(41)-Na(1)	98.98(14)
C(61)-C(60)-N(5)	118.5(2)	C(45)-C(46)-C(47)	119.8(2)
C(61)-C(60)-C(57)	131.4(2)	C(46)-C(45)-C(50)	120.1(2)
N(5)-C(60)-C(57)	110.03(19)	C(46)-C(45)-C(42)	131.1(2)
C(30)-C(31)-C(26)	120.4(2)	C(50)-C(45)-C(42)	108.8(2)
C(30)-C(31)-C(35)	115.1(2)	C(42)-C(44)-Na(1)	85.28(14)
C(26)-C(31)-C(35)	124.5(2)	C(50)-C(49)-C(48)	118.8(2)
C(29)-C(30)-C(31)	122.6(2)	C(47)-C(48)-C(49)	121.3(2)
N(3)-C(26)-C(31)	122.9(2)	C(48)-C(47)-C(46)	119.7(2)
N(3)-C(26)-C(27)	121.7(2)	C(60)-N(5)-C(51)	108.40(18)
C(31)-C(26)-C(27)	115.4(2)	C(60)-N(5)-Al(2)	123.74(15)
C(38)-C(39)-Na(1)	81.80(13)	C(51)-N(5)-Al(2)	127.84(16)
C(40)-C(38)-C(39)	111.24(19)	C(6)-C(5)-C(4)	118.9(2)
C(40)-C(38)-Al(1)	116.05(16)	C(52)-C(51)-C(56)	120.8(2)
C(39)-C(38)-Al(1)	116.10(16)	C(52)-C(51)-N(5)	128.6(2)
C(40)-C(38)-Al(2)	97.71(15)	C(56)-C(51)-N(5)	110.6(2)
C(39)-C(38)-Al(2)	130.28(17)	C(49)-C(50)-N(4)	128.4(2)
Al(1)-C(38)-Al(2)	82.60(9)	C(49)-C(50)-C(45)	120.3(2)
C(31)-C(35)-C(36)	110.9(2)	N(4)-C(50)-C(45)	111.2(2)
C(31)-C(35)-C(37)	112.9(2)	C(56)-C(55)-C(54)	118.8(2)
C(36)-C(35)-C(37)	110.1(2)	C(5)-C(6)-C(1)	120.4(2)
C(45)-C(42)-C(41)	99.69(18)	C(5)-C(6)-C(7)	131.1(2)
C(45)-C(42)-C(44)	112.7(2)	C(1)-C(6)-C(7)	108.6(2)
C(41)-C(42)-C(44)	113.9(2)	C(66)-C(65)-C(64)	118.0(2)
C(45)-C(42)-C(43)	110.9(2)	C(66)-C(65)-C(73)	120.2(2)
C(41)-C(42)-C(43)	110.8(2)	C(64)-C(65)-C(73)	121.8(2)
C(44)-C(42)-C(43)	108.6(2)	C(69)-C(64)-C(65)	121.5(2)
C(40)-C(41)-N(4)	118.3(2)	C(69)-C(64)-N(6)	119.9(2)
C(40)-C(41)-C(42)	132.0(2)	C(65)-C(64)-N(6)	118.5(2)
N(4)-C(41)-C(42)	109.70(19)	C(67)-C(68)-C(69)	121.0(3)
C(40)-C(41)-Na(1)	69.98(14)	C(66)-C(67)-C(68)	120.2(2)
N(4)-C(41)-Na(1)	101.28(14)	C(67)-C(66)-C(65)	121.3(2)

N(9)-Al(3)-N(8)	124.17(9)	C(81)-C(82)-C(84)	113.7(2)
N(9)-Al(3)-N(7)	116.90(9)	C(85)-C(82)-C(84)	113.9(2)
N(8)-Al(3)-N(7)	93.75(9)	C(81)-C(82)-C(83)	110.6(2)
N(9)-Al(3)-C(113)	93.51(10)	C(85)-C(82)-C(83)	108.6(2)
N(8)-Al(3)-C(113)	119.65(9)	C(84)-C(82)-C(83)	109.5(2)
N(7)-Al(3)-C(113)	109.97(10)	N(7)-C(85)-C(86)	125.0(2)
C(68)-C(69)-C(64)	118.1(2)	N(7)-C(85)-C(82)	112.2(2)
C(68)-C(69)-C(70)	120.6(2)	C(86)-C(85)-C(82)	122.8(2)
C(64)-C(69)-C(70)	121.3(2)	C(85)-C(86)-C(87)	126.4(2)
C(85)-N(7)-C(76)	107.5(2)	N(8)-C(87)-C(86)	122.8(2)
C(85)-N(7)-Al(3)	124.12(16)	N(8)-C(87)-C(88)	120.4(2)
C(76)-N(7)-Al(3)	128.33(16)	C(86)-C(87)-C(88)	116.8(2)
C(71A)-C(70)-C(69)	110.3(8)	C(94)-C(89)-C(90)	121.6(2)
C(69)-C(70)-C(72)	115.6(3)	C(94)-C(89)-N(8)	121.0(2)
C(71A)-C(70)-C(72A)	111.8(10)	C(90)-C(89)-N(8)	117.4(2)
C(69)-C(70)-C(72A)	105.8(8)	C(91)-C(90)-C(89)	117.9(2)
C(69)-C(70)-C(71)	111.4(3)	C(91)-C(90)-C(98)	120.0(2)
C(72)-C(70)-C(71)	107.2(4)	C(89)-C(90)-C(98)	122.0(2)
C(65)-C(73)-C(74)	111.6(2)	C(92)-C(91)-C(90)	121.0(2)
C(65)-C(73)-C(75)	111.9(2)	C(91)-C(92)-C(93)	120.0(3)
C(74)-C(73)-C(75)	110.6(2)	C(92)-C(93)-C(94)	121.7(3)
C(77)-C(76)-C(81)	121.1(2)	C(93)-C(94)-C(89)	117.7(2)
C(77)-C(76)-N(7)	128.0(2)	C(93)-C(94)-C(95)	118.8(2)
C(81)-C(76)-N(7)	110.9(2)	C(89)-C(94)-C(95)	123.5(2)
C(76)-C(77)-C(78)	117.8(2)	C(97)-C(95)-C(94)	110.7(2)
C(79)-C(78)-C(77)	121.4(2)	C(97)-C(95)-C(96)	110.8(2)
C(78)-C(79)-C(80)	120.4(2)	C(94)-C(95)-C(96)	112.1(2)
C(81)-C(80)-C(79)	118.6(2)	C(90)-C(98)-C(99)	112.9(2)
C(80)-C(81)-C(76)	120.7(2)	C(90)-C(98)-C(100)	112.6(2)
C(80)-C(81)-C(82)	130.5(2)	C(99)-C(98)-C(100)	109.1(2)
C(76)-C(81)-C(82)	108.8(2)	C(137)-N(12)-C(139)	119.8(2)
C(81)-C(82)-C(85)	100.2(2)	C(137)-N(12)-Na(2)	115.71(16)

C(139)-N(12)-Na(2)	121.61(14)	C(114)-C(113)-Al(4)	131.39(17)
C(135)-N(11)-C(126)	107.96(18)	Al(3)-C(113)-Al(4)	82.48(9)
C(135)-N(11)-Al(4)	123.67(15)	C(116)-C(115)-C(113)	120.8(2)
C(126)-N(11)-Al(4)	127.89(15)	C(116)-C(115)-Na(2)	69.91(14)
N(9)-C(101)-C(106)	122.9(2)	C(113)-C(115)-Na(2)	94.24(14)
N(9)-C(101)-C(102)	121.0(2)	C(115)-C(116)-N(10)	117.6(2)
C(106)-C(101)-C(102)	116.1(2)	C(115)-C(116)-C(117)	132.6(2)
C(103)-C(102)-C(101)	120.3(2)	N(10)-C(116)-C(117)	109.7(2)
C(103)-C(102)-C(107)	117.6(2)	C(115)-C(116)-Na(2)	80.53(15)
C(101)-C(102)-C(107)	121.9(2)	N(10)-C(116)-Na(2)	84.68(13)
C(104)-C(103)-C(102)	122.7(3)	C(117)-C(116)-Na(2)	101.41(14)
C(103)-C(104)-C(105)	118.2(2)	C(120)-C(117)-C(116)	100.39(18)
C(104)-C(105)-C(106)	122.1(3)	C(120)-C(117)-C(118)	112.0(2)
C(105)-C(106)-C(101)	120.4(2)	C(116)-C(117)-C(118)	112.6(2)
C(105)-C(106)-C(110)	114.3(2)	C(120)-C(117)-C(119)	111.8(2)
C(101)-C(106)-C(110)	125.3(2)	C(116)-C(117)-C(119)	111.4(2)
C(102)-C(107)-C(108)	109.7(2)	C(118)-C(117)-C(119)	108.5(2)
C(102)-C(107)-C(109)	115.2(2)	C(121)-C(120)-C(125)	120.0(2)
C(108)-C(107)-C(109)	111.1(2)	C(121)-C(120)-C(117)	131.0(2)
N(9)-Al(4)-N(10)	121.65(9)	C(125)-C(120)-C(117)	109.1(2)
N(9)-Al(4)-N(11)	114.06(9)	C(120)-C(121)-C(122)	120.0(2)
N(10)-Al(4)-N(11)	110.04(9)	C(121)-C(122)-C(123)	119.6(2)
N(9)-Al(4)-C(113)	91.69(9)	C(124)-C(123)-C(122)	121.1(2)
N(10)-Al(4)-C(113)	90.92(9)	C(123)-C(124)-C(125)	118.9(2)
N(11)-Al(4)-C(113)	126.90(9)	C(124)-C(125)-N(10)	127.8(2)
C(106)-C(110)-C(112)	110.9(2)	C(124)-C(125)-C(120)	120.3(2)
C(106)-C(110)-C(111)	113.9(2)	N(10)-C(125)-C(120)	111.8(2)
C(112)-C(110)-C(111)	109.5(2)	C(127)-C(126)-C(131)	121.0(2)
C(115)-C(113)-C(114)	111.27(19)	C(127)-C(126)-N(11)	127.9(2)
C(115)-C(113)-Al(3)	113.03(16)	C(131)-C(126)-N(11)	111.1(2)
C(114)-C(113)-Al(3)	117.47(17)	C(126)-C(127)-C(128)	117.7(2)
C(115)-C(113)-Al(4)	97.70(15)	C(129)-C(128)-C(127)	121.4(2)

C(128)-C(129)-C(130)	120.3(2)	C(139)-C(144)-C(145)	121.7(2)
C(128)-C(129)-Na(1)#2	94.74(16)	C(143)-C(144)-C(145)	120.4(2)
C(130)-C(129)-Na(1)#2	123.68(18)	C(144)-C(145)-C(147)	113.4(2)
C(131)-C(130)-C(129)	118.4(2)	C(144)-C(145)-C(146)	110.0(2)
C(130)-C(131)-C(126)	121.0(2)	C(147)-C(145)-C(146)	110.4(2)
C(130)-C(131)-C(132)	129.4(2)	C(140)-C(148)-C(149)	113.0(2)
C(126)-C(131)-C(132)	109.6(2)	C(140)-C(148)-C(150)	111.2(3)
C(131)-C(132)-C(134)	108.3(2)	C(149)-C(148)-C(150)	110.5(2)
C(131)-C(132)-C(135)	100.87(18)	C(151)-C(152)-C(153)	113.9(3)
C(134)-C(132)-C(135)	113.0(2)	C(152)-C(153)-C(154)	114.8(2)
C(131)-C(132)-C(133)	109.0(2)	C(155)-C(154)-C(153)	115.3(2)
C(134)-C(132)-C(133)	113.1(2)	C(154)-C(155)-C(156)	113.9(3)
C(135)-C(132)-C(133)	111.7(2)	C(159)-C(158)-C(157)	112.8(2)
C(136)-C(135)-N(11)	118.2(2)	C(160)-C(159)-C(158)	114.9(2)
C(136)-C(135)-C(132)	131.4(2)	C(159)-C(160)-C(161)	113.1(2)
N(11)-C(135)-C(132)	110.30(19)	C(160)-C(161)-C(162)	113.7(2)
C(135)-C(136)-C(137)	137.2(2)	C(1A)-C(2A)-C(3A)	113.0(6)
C(135)-C(136)-Na(2)	139.81(17)	C(4A)-C(3A)-C(2A)	111.8(5)
C(137)-C(136)-Na(2)	78.44(13)	C(5A)-C(4A)-C(3A)	112.8(6)
N(12)-C(137)-C(136)	115.2(2)	C(4A)-C(5A)-C(6A)	113.2(6)
N(12)-C(137)-C(138)	119.9(2)	C(1B)-C(2B)-C(3B)	121.3(14)
C(136)-C(137)-C(138)	124.8(2)	C(4B)-C(3B)-C(2B)	117.9(13)
C(144)-C(139)-C(140)	121.8(2)	C(5B)-C(4B)-C(3B)	153.3(16)
C(144)-C(139)-N(12)	120.1(2)	C(4B)-C(5B)-C(6B)	126.1(14)
C(140)-C(139)-N(12)	118.0(2)	C(3F)-C(2F)-C(1F)	119.4(19)
C(141)-C(140)-C(139)	117.7(2)	C(2F)-C(3F)-C(4F)	115.6(15)
C(141)-C(140)-C(148)	120.5(2)	C(5F)-C(4F)-C(3F)	140(2)
C(139)-C(140)-C(148)	121.8(2)	C(4F)-C(5F)-C(6F)	129.7(19)
C(142)-C(141)-C(140)	121.2(3)	C(3C)-C(2C)-C(1C)	117.5(17)
C(141)-C(142)-C(143)	120.4(2)	C(4C)-C(3C)-C(2C)	145.2(17)
C(142)-C(143)-C(144)	121.1(3)	C(5C)-C(4C)-C(3C)	127.9(17)
C(139)-C(144)-C(143)	117.8(2)	C(4C)-C(5C)-C(6C)	124.7(18)

C(3D)-C(2D)-C(1D)	101.5(12)	C(4E)-C(5E)-C(6E)	106.0(12)
C(4D)-C(3D)-C(2D)	121.1(12)	C(3G)-C(2G)-C(1G)	125.4(13)
C(3D)-C(4D)-C(5D)	115.3(10)	C(2G)-C(3G)-C(4G)	112.3(11)
C(4D)-C(5D)-C(6D)	114.5(10)	C(3G)-C(4G)-C(5G)	103.6(11)
C(3E)-C(2E)-C(1E)	119.1(12)	C(6G)-C(5G)-C(4G)	117.0(13)
C(4E)-C(3E)-C(2E)	111.6(13)		
C(3E)-C(4E)-C(5E)	116.6(13)		

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 x,y+1,z

Crystal structure of 6

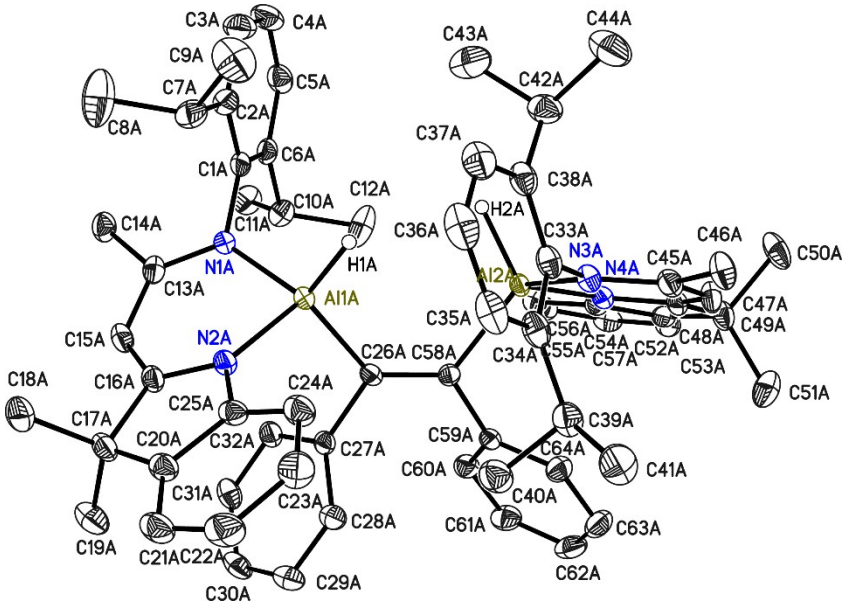


Figure S53: Molecule 1 of **6** with thermal ellipsoids shown at 50% probability level. All ligand based and solvent hydrogen atoms are omitted for clarity. The hydrogen atoms bond to aluminum atoms were refined freely. All Al-H distances were restrained to be similar.

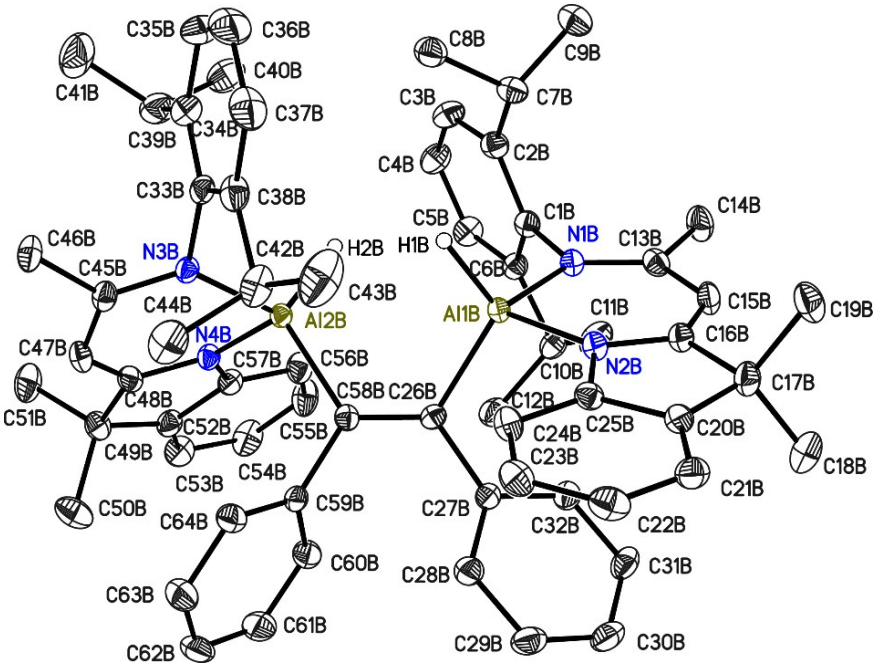


Figure S54: Molecule 2 of **6** with thermal ellipsoids shown at 50% probability level. All ligand based and solvent hydrogen atoms are omitted for clarity.

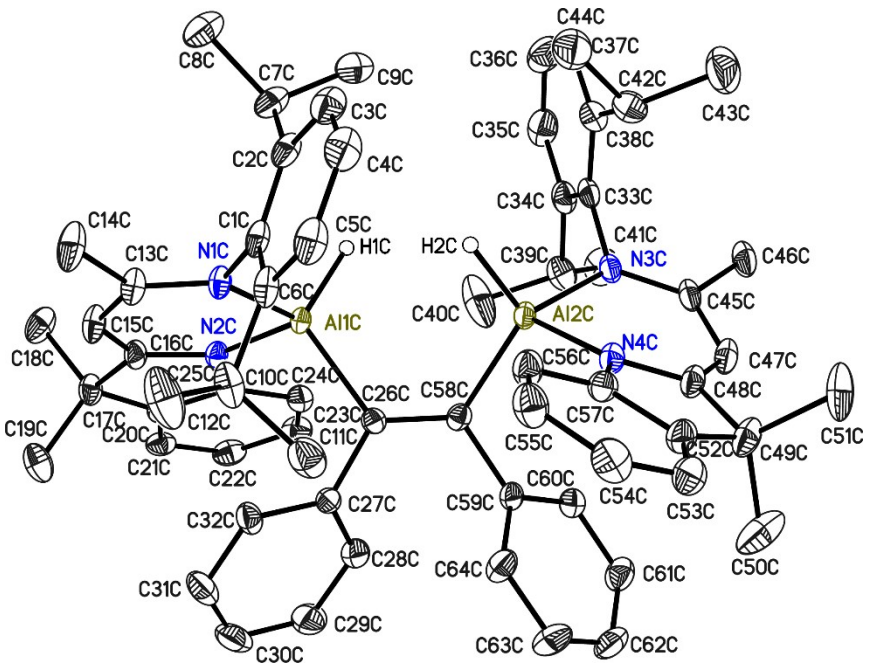


Figure S55: Molecule 3 of **6** with thermal ellipsoids shown at 50% probability level. All ligand based and solvent hydrogen atoms are omitted for clarity.

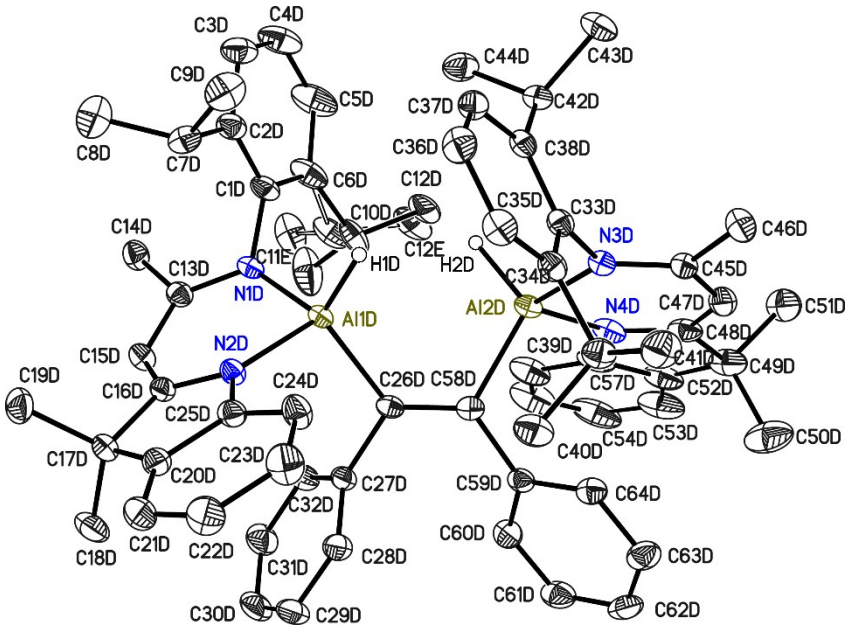


Figure S56: Molecule 4 of **6** with thermal ellipsoids shown at 50% probability level. All ligand based and solvent hydrogen atoms are omitted for clarity. One isopropyl group is disordered over two positions. The occupancy of the minor position refined to 0.323(14). The disordered part groups were refined with distance restraints and restraints for the anisotropic displacement parameters.

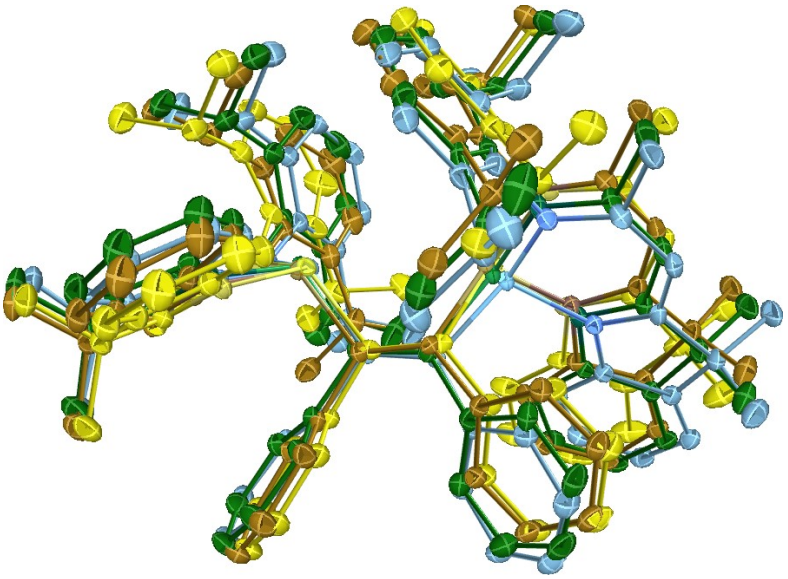


Figure S57: Overlay of all four molecules.

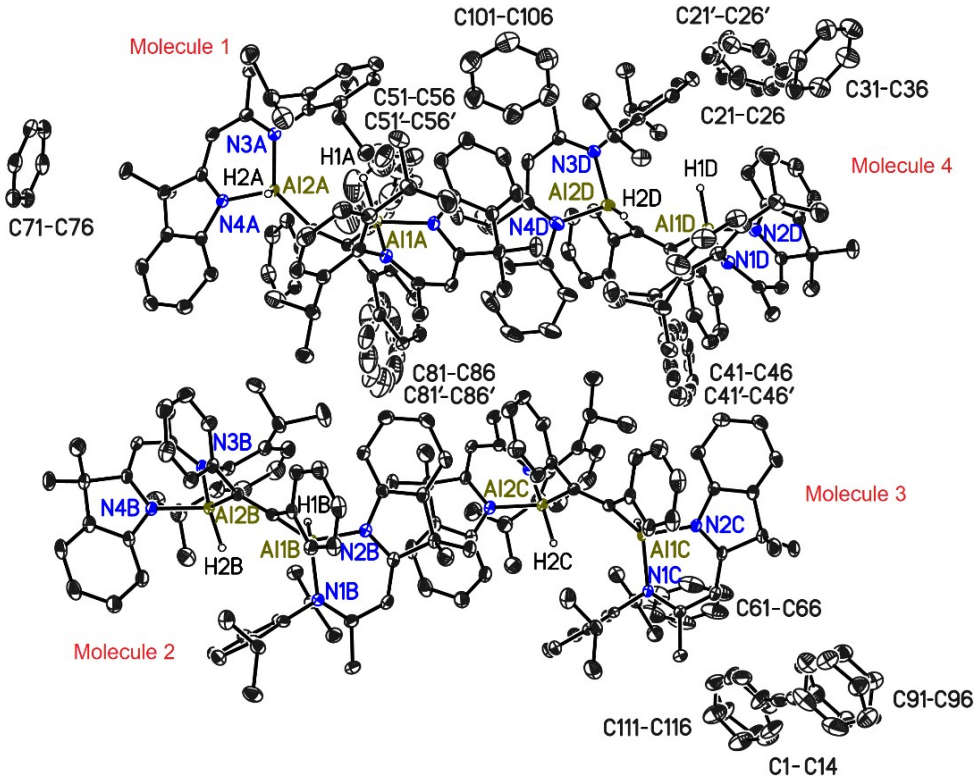


Figure S58: Solvent molecule of **6**. All hydrogen atoms are omitted for clarity.4 of the 10 benzene molecules are disordered about two positions. The occupancies of the minor positions refined to 0.341(16), 0.423(13), 0.365(13), and 0.381(11), respectively. Two further molecules are disordered with one diphenylacetylene molecule. The occupancy of the diphenylacetylene molecule refined to 0.233(6). All disordered part were refined with distance restraints and restraints for the anisotropic displacement parameters.

Table S6: Bond lengths [Å] and angles [°] for **6**.

Al(1A)-H(1A)	1.512(15)	C(24A)-C(25A)	1.373(3)
Al(1A)-N(2A)	1.9170(19)	C(26A)-C(58A)	1.360(3)
Al(1A)-N(1A)	1.9312(19)	C(26A)-C(27A)	1.507(3)
Al(1A)-C(26A)	2.003(2)	C(27A)-C(32A)	1.396(3)
N(1A)-C(13A)	1.339(3)	C(27A)-C(28A)	1.401(3)
N(1A)-C(1A)	1.452(3)	C(28A)-C(29A)	1.384(3)
N(2A)-C(16A)	1.343(3)	C(29A)-C(30A)	1.383(4)
N(2A)-C(25A)	1.418(3)	C(30A)-C(31A)	1.385(3)
C(1A)-C(6A)	1.403(3)	C(31A)-C(32A)	1.390(3)
C(1A)-C(2A)	1.404(3)	Al(2A)-H(2A)	1.531(15)
C(2A)-C(3A)	1.393(3)	Al(2A)-N(4A)	1.9236(19)
C(2A)-C(7A)	1.524(3)	Al(2A)-N(3A)	1.9343(19)
C(3A)-C(4A)	1.385(4)	Al(2A)-C(58A)	1.999(2)
C(4A)-C(5A)	1.376(4)	N(3A)-C(45A)	1.340(3)
C(5A)-C(6A)	1.395(3)	N(3A)-C(33A)	1.450(3)
C(6A)-C(10A)	1.520(3)	N(4A)-C(48A)	1.342(3)
C(7A)-C(9A)	1.520(4)	N(4A)-C(57A)	1.424(3)
C(7A)-C(8A)	1.520(4)	C(33A)-C(38A)	1.403(3)
C(10A)-C(12A)	1.520(3)	C(33A)-C(34A)	1.408(3)
C(10A)-C(11A)	1.527(3)	C(34A)-C(35A)	1.393(3)
C(13A)-C(15A)	1.398(3)	C(34A)-C(39A)	1.524(4)
C(13A)-C(14A)	1.509(3)	C(35A)-C(36A)	1.387(4)
C(15A)-C(16A)	1.391(3)	C(36A)-C(37A)	1.379(4)
C(16A)-C(17A)	1.532(3)	C(37A)-C(38A)	1.397(3)
C(17A)-C(20A)	1.503(3)	C(38A)-C(42A)	1.518(3)
C(17A)-C(18A)	1.528(3)	C(39A)-C(40A)	1.526(3)
C(17A)-C(19A)	1.531(3)	C(39A)-C(41A)	1.534(3)
C(20A)-C(21A)	1.389(3)	C(42A)-C(43A)	1.522(4)
C(20A)-C(25A)	1.391(3)	C(42A)-C(44A)	1.529(4)
C(21A)-C(22A)	1.389(4)	C(45A)-C(47A)	1.395(3)
C(22A)-C(23A)	1.387(4)	C(45A)-C(46A)	1.510(3)
C(23A)-C(24A)	1.397(3)	C(47A)-C(48A)	1.387(3)

C(48A)-C(49A)	1.524(3)	C(6B)-C(10B)	1.519(3)
C(49A)-C(52A)	1.501(3)	C(7B)-C(8B)	1.530(3)
C(49A)-C(51A)	1.528(3)	C(7B)-C(9B)	1.532(3)
C(49A)-C(50A)	1.539(3)	C(10B)-C(12B)	1.526(3)
C(52A)-C(53A)	1.383(3)	C(10B)-C(11B)	1.534(3)
C(52A)-C(57A)	1.391(3)	C(13B)-C(15B)	1.402(3)
C(53A)-C(54A)	1.391(3)	C(13B)-C(14B)	1.508(3)
C(54A)-C(55A)	1.386(3)	C(15B)-C(16B)	1.386(3)
C(55A)-C(56A)	1.398(3)	C(16B)-C(17B)	1.535(3)
C(56A)-C(57A)	1.379(3)	C(17B)-C(20B)	1.507(3)
C(58A)-C(59A)	1.508(3)	C(17B)-C(18B)	1.534(3)
C(59A)-C(64A)	1.399(3)	C(17B)-C(19B)	1.542(3)
C(59A)-C(60A)	1.400(3)	C(20B)-C(21B)	1.379(3)
C(60A)-C(61A)	1.384(3)	C(20B)-C(25B)	1.395(3)
C(61A)-C(62A)	1.385(4)	C(21B)-C(22B)	1.388(3)
C(62A)-C(63A)	1.381(4)	C(22B)-C(23B)	1.391(3)
C(63A)-C(64A)	1.390(3)	C(23B)-C(24B)	1.388(3)
Al(1B)-H(1B)	1.525(15)	C(24B)-C(25B)	1.380(3)
Al(1B)-N(2B)	1.9153(19)	C(26B)-C(58B)	1.357(3)
Al(1B)-N(1B)	1.9282(19)	C(26B)-C(27B)	1.503(3)
Al(1B)-C(26B)	1.990(2)	C(27B)-C(32B)	1.399(3)
N(1B)-C(13B)	1.333(3)	C(27B)-C(28B)	1.401(3)
N(1B)-C(1B)	1.455(3)	C(28B)-C(29B)	1.389(3)
N(2B)-C(16B)	1.338(3)	C(29B)-C(30B)	1.381(4)
N(2B)-C(25B)	1.416(3)	C(30B)-C(31B)	1.382(3)
C(1B)-C(2B)	1.404(3)	C(31B)-C(32B)	1.392(3)
C(1B)-C(6B)	1.410(3)	Al(2B)-H(2B)	1.518(16)
C(2B)-C(3B)	1.394(3)	Al(2B)-N(4B)	1.9145(18)
C(2B)-C(7B)	1.522(3)	Al(2B)-N(3B)	1.9284(19)
C(3B)-C(4B)	1.384(3)	Al(2B)-C(58B)	1.994(2)
C(4B)-C(5B)	1.383(3)	N(3B)-C(45B)	1.341(3)
C(5B)-C(6B)	1.399(3)	N(3B)-C(33B)	1.453(3)

N(4B)-C(48B)	1.343(3)	C(62B)-C(63B)	1.382(4)
N(4B)-C(57B)	1.417(3)	C(63B)-C(64B)	1.391(3)
C(33B)-C(34B)	1.396(3)	Al(1C)-H(1C)	1.525(16)
C(33B)-C(38B)	1.408(3)	Al(1C)-N(2C)	1.9154(19)
C(34B)-C(35B)	1.397(3)	Al(1C)-N(1C)	1.9294(19)
C(34B)-C(39B)	1.518(3)	Al(1C)-C(26C)	1.997(2)
C(35B)-C(36B)	1.376(4)	N(1C)-C(13C)	1.337(3)
C(36B)-C(37B)	1.377(4)	N(1C)-C(1C)	1.452(3)
C(37B)-C(38B)	1.393(3)	N(2C)-C(16C)	1.339(3)
C(38B)-C(42B)	1.526(3)	N(2C)-C(25C)	1.417(3)
C(39B)-C(40B)	1.530(4)	C(1C)-C(2C)	1.403(3)
C(39B)-C(41B)	1.532(4)	C(1C)-C(6C)	1.410(3)
C(42B)-C(43B)	1.523(3)	C(2C)-C(3C)	1.395(3)
C(42B)-C(44B)	1.528(4)	C(2C)-C(7C)	1.522(3)
C(45B)-C(47B)	1.403(3)	C(3C)-C(4C)	1.388(4)
C(45B)-C(46B)	1.506(3)	C(4C)-C(5C)	1.378(4)
C(47B)-C(48B)	1.386(3)	C(5C)-C(6C)	1.396(3)
C(48B)-C(49B)	1.535(3)	C(6C)-C(10C)	1.519(4)
C(49B)-C(52B)	1.506(3)	C(7C)-C(9C)	1.526(4)
C(49B)-C(51B)	1.532(3)	C(7C)-C(8C)	1.534(3)
C(49B)-C(50B)	1.536(3)	C(10C)-C(12C)	1.530(3)
C(52B)-C(53B)	1.382(3)	C(10C)-C(11C)	1.533(4)
C(52B)-C(57B)	1.392(3)	C(13C)-C(15C)	1.403(3)
C(53B)-C(54B)	1.394(4)	C(13C)-C(14C)	1.509(3)
C(54B)-C(55B)	1.384(4)	C(15C)-C(16C)	1.384(3)
C(55B)-C(56B)	1.397(3)	C(16C)-C(17C)	1.531(3)
C(56B)-C(57B)	1.378(3)	C(17C)-C(20C)	1.504(3)
C(58B)-C(59B)	1.499(3)	C(17C)-C(19C)	1.532(3)
C(59B)-C(64B)	1.392(3)	C(17C)-C(18C)	1.539(3)
C(59B)-C(60B)	1.400(3)	C(20C)-C(21C)	1.384(3)
C(60B)-C(61B)	1.386(3)	C(20C)-C(25C)	1.395(3)
C(61B)-C(62B)	1.386(4)	C(21C)-C(22C)	1.389(4)

C(22C)-C(23C)	1.391(4)	C(45C)-C(46C)	1.506(3)
C(23C)-C(24C)	1.390(3)	C(47C)-C(48C)	1.388(3)
C(24C)-C(25C)	1.381(3)	C(48C)-C(49C)	1.534(3)
C(26C)-C(58C)	1.364(3)	C(49C)-C(52C)	1.507(3)
C(26C)-C(27C)	1.505(3)	C(49C)-C(51C)	1.532(4)
C(27C)-C(32C)	1.397(3)	C(49C)-C(50C)	1.532(4)
C(27C)-C(28C)	1.398(3)	C(52C)-C(53C)	1.383(3)
C(28C)-C(29C)	1.390(3)	C(52C)-C(57C)	1.391(3)
C(29C)-C(30C)	1.379(4)	C(53C)-C(54C)	1.391(4)
C(30C)-C(31C)	1.378(4)	C(54C)-C(55C)	1.386(4)
C(31C)-C(32C)	1.397(3)	C(55C)-C(56C)	1.395(3)
Al(2C)-H(2C)	1.519(16)	C(56C)-C(57C)	1.378(3)
Al(2C)-N(4C)	1.9178(19)	C(58C)-C(59C)	1.503(3)
Al(2C)-N(3C)	1.932(2)	C(59C)-C(60C)	1.391(3)
Al(2C)-C(58C)	1.995(2)	C(59C)-C(64C)	1.398(3)
N(3C)-C(45C)	1.341(3)	C(60C)-C(61C)	1.392(3)
N(3C)-C(33C)	1.453(3)	C(61C)-C(62C)	1.383(4)
N(4C)-C(48C)	1.341(3)	C(62C)-C(63C)	1.383(4)
N(4C)-C(57C)	1.419(3)	C(63C)-C(64C)	1.386(3)
C(33C)-C(38C)	1.404(3)	Al(1D)-H(1D)	1.513(15)
C(33C)-C(34C)	1.406(3)	Al(1D)-N(2D)	1.9165(19)
C(34C)-C(35C)	1.397(4)	Al(1D)-N(1D)	1.923(2)
C(34C)-C(39C)	1.511(3)	Al(1D)-C(26D)	1.994(2)
C(35C)-C(36C)	1.377(4)	N(1D)-C(13D)	1.348(3)
C(36C)-C(37C)	1.383(4)	N(1D)-C(1D)	1.448(3)
C(37C)-C(38C)	1.394(4)	N(2D)-C(16D)	1.339(3)
C(38C)-C(42C)	1.522(4)	N(2D)-C(25D)	1.416(3)
C(39C)-C(40C)	1.520(4)	C(1D)-C(6D)	1.404(3)
C(39C)-C(41C)	1.530(3)	C(1D)-C(2D)	1.408(3)
C(42C)-C(44C)	1.525(4)	C(2D)-C(3D)	1.394(3)
C(42C)-C(43C)	1.528(4)	C(2D)-C(7D)	1.521(3)
C(45C)-C(47C)	1.399(3)	C(3D)-C(4D)	1.381(4)

C(4D)-C(5D)	1.376(4)	Al(2D)-C(58D)	1.980(2)
C(5D)-C(6D)	1.394(4)	N(3D)-C(45D)	1.337(3)
C(6D)-C(10E)	1.523(10)	N(3D)-C(33D)	1.452(3)
C(6D)-C(10D)	1.544(6)	N(4D)-C(48D)	1.333(3)
C(7D)-C(8D)	1.521(4)	N(4D)-C(57D)	1.419(3)
C(7D)-C(9D)	1.532(4)	C(33D)-C(38D)	1.406(3)
C(10D)-C(12D)	1.525(7)	C(33D)-C(34D)	1.408(3)
C(10D)-C(11D)	1.537(6)	C(34D)-C(35D)	1.391(3)
C(13D)-C(15D)	1.392(3)	C(34D)-C(39D)	1.519(3)
C(13D)-C(14D)	1.507(3)	C(35D)-C(36D)	1.383(3)
C(15D)-C(16D)	1.390(3)	C(36D)-C(37D)	1.381(3)
C(16D)-C(17D)	1.533(3)	C(37D)-C(38D)	1.393(3)
C(17D)-C(20D)	1.503(3)	C(38D)-C(42D)	1.523(3)
C(17D)-C(18D)	1.532(3)	C(39D)-C(40D)	1.531(3)
C(17D)-C(19D)	1.532(3)	C(39D)-C(41D)	1.535(3)
C(20D)-C(21D)	1.384(3)	C(42D)-C(44D)	1.524(3)
C(20D)-C(25D)	1.390(3)	C(42D)-C(43D)	1.529(3)
C(21D)-C(22D)	1.392(4)	C(45D)-C(47D)	1.402(3)
C(22D)-C(23D)	1.390(4)	C(45D)-C(46D)	1.507(3)
C(23D)-C(24D)	1.395(3)	C(47D)-C(48D)	1.382(4)
C(24D)-C(25D)	1.384(3)	C(48D)-C(49D)	1.537(3)
C(26D)-C(58D)	1.360(3)	C(49D)-C(52D)	1.503(4)
C(26D)-C(27D)	1.500(3)	C(49D)-C(50D)	1.533(4)
C(27D)-C(32D)	1.394(3)	C(49D)-C(51D)	1.539(3)
C(27D)-C(28D)	1.398(3)	C(52D)-C(53D)	1.394(4)
C(28D)-C(29D)	1.386(3)	C(52D)-C(57D)	1.396(4)
C(29D)-C(30D)	1.383(4)	C(53D)-C(54D)	1.386(5)
C(30D)-C(31D)	1.379(4)	C(54D)-C(55D)	1.382(5)
C(31D)-C(32D)	1.389(3)	C(55D)-C(56D)	1.391(4)
Al(2D)-H(2D)	1.520(16)	C(56D)-C(57D)	1.379(4)
Al(2D)-N(4D)	1.906(2)	C(58D)-C(59D)	1.501(3)
Al(2D)-N(3D)	1.9222(19)	C(59D)-C(64D)	1.397(3)

C(59D)-C(60D)	1.397(3)	C(71)-C(72)	1.397(4)
C(60D)-C(61D)	1.387(3)	C(72)-C(73)	1.373(4)
C(61D)-C(62D)	1.382(4)	C(73)-C(74)	1.385(4)
C(62D)-C(63D)	1.382(4)	C(74)-C(75)	1.384(3)
C(63D)-C(64D)	1.388(3)	C(75)-C(76)	1.380(4)
C(10E)-C(11E)	1.525(11)	C(101)-C(102)	1.379(4)
C(10E)-C(12E)	1.548(12)	C(101)-C(106)	1.383(4)
C(21)-C(22)	1.385(7)	C(102)-C(103)	1.384(4)
C(21)-C(26)	1.386(7)	C(103)-C(104)	1.377(4)
C(22)-C(23)	1.399(8)	C(104)-C(105)	1.387(4)
C(23)-C(24)	1.406(8)	C(105)-C(106)	1.381(4)
C(24)-C(25)	1.358(8)	C(41)-C(42)	1.382(8)
C(25)-C(26)	1.386(8)	C(41)-C(46)	1.391(8)
C(21')-C(22')	1.382(12)	C(42)-C(43)	1.378(8)
C(21')-C(26')	1.384(12)	C(43)-C(44)	1.388(8)
C(22')-C(23')	1.396(12)	C(44)-C(45)	1.368(8)
C(23')-C(24')	1.393(11)	C(45)-C(46)	1.388(8)
C(24')-C(25')	1.370(12)	C(41')-C(42')	1.373(10)
C(25')-C(26')	1.376(13)	C(41')-C(46')	1.396(9)
C(31)-C(32)	1.373(4)	C(42')-C(43')	1.373(10)
C(31)-C(36)	1.385(4)	C(43')-C(44')	1.389(10)
C(32)-C(33)	1.385(4)	C(44')-C(45')	1.362(11)
C(33)-C(34)	1.384(4)	C(45')-C(46')	1.383(10)
C(34)-C(35)	1.383(4)	C(51)-C(56)	1.362(12)
C(35)-C(36)	1.383(4)	C(51)-C(52)	1.369(12)
C(61)-C(66)	1.376(5)	C(52)-C(53)	1.397(12)
C(61)-C(62)	1.390(4)	C(53)-C(54)	1.392(12)
C(62)-C(63)	1.375(5)	C(54)-C(55)	1.368(12)
C(63)-C(64)	1.383(5)	C(55)-C(56)	1.392(11)
C(64)-C(65)	1.390(4)	C(51')-C(56')	1.358(9)
C(65)-C(66)	1.370(5)	C(51')-C(52')	1.366(8)
C(71)-C(76)	1.380(4)	C(52')-C(53')	1.394(7)

C(53')-C(54')	1.393(7)	C(112)-C(113)	1.385(6)
C(54')-C(55')	1.390(8)	C(113)-C(114)	1.377(6)
C(55')-C(56')	1.404(10)	C(114)-C(115)	1.365(7)
C(81)-C(86)	1.357(9)	C(115)-C(116)	1.359(8)
C(81)-C(82)	1.398(8)	C(91)-C(92)	1.389(7)
C(82)-C(83)	1.392(8)	C(91)-C(96)	1.397(6)
C(83)-C(84)	1.388(8)	C(92)-C(93)	1.368(7)
C(84)-C(85)	1.396(9)	C(93)-C(94)	1.386(7)
C(85)-C(86)	1.385(9)	C(94)-C(95)	1.384(6)
C(81')-C(82')	1.356(12)	C(95)-C(96)	1.378(7)
C(81')-C(86')	1.395(11)		
C(82')-C(83')	1.402(12)	H(1A)-Al(1A)-N(2A)	111.1(10)
C(83')-C(84')	1.394(11)	H(1A)-Al(1A)-N(1A)	110.9(10)
C(84')-C(85')	1.374(11)	N(2A)-Al(1A)-N(1A)	92.05(8)
C(85')-C(86')	1.388(12)	H(1A)-Al(1A)-C(26A)	114.9(10)
C(1)-C(6)	1.382(12)	N(2A)-Al(1A)-C(26A)	104.96(8)
C(1)-C(2)	1.386(13)	N(1A)-Al(1A)-C(26A)	119.99(8)
C(1)-C(7)	1.392(15)	C(13A)-N(1A)-C(1A)	116.59(18)
C(2)-C(3)	1.364(13)	C(13A)-N(1A)-Al(1A)	125.20(15)
C(3)-C(4)	1.386(12)	C(1A)-N(1A)-Al(1A)	117.94(13)
C(4)-C(5)	1.370(13)	C(16A)-N(2A)-C(25A)	108.14(18)
C(5)-C(6)	1.374(13)	C(16A)-N(2A)-Al(1A)	122.90(15)
C(7)-C(8)	1.200(17)	C(25A)-N(2A)-Al(1A)	128.37(15)
C(8)-C(9)	1.375(18)	C(6A)-C(1A)-C(2A)	121.7(2)
C(9)-C(10)	1.385(12)	C(6A)-C(1A)-N(1A)	120.26(19)
C(9)-C(14)	1.392(13)	C(2A)-C(1A)-N(1A)	118.07(19)
C(10)-C(11)	1.365(13)	C(3A)-C(2A)-C(1A)	117.8(2)
C(11)-C(12)	1.372(13)	C(3A)-C(2A)-C(7A)	120.2(2)
C(12)-C(13)	1.390(12)	C(1A)-C(2A)-C(7A)	122.0(2)
C(13)-C(14)	1.365(13)	C(4A)-C(3A)-C(2A)	121.3(2)
C(111)-C(112)	1.386(6)	C(5A)-C(4A)-C(3A)	119.9(2)
C(111)-C(116)	1.388(7)	C(4A)-C(5A)-C(6A)	121.2(2)

C(5A)-C(6A)-C(1A)	118.1(2)	C(58A)-C(26A)-C(27A)	120.85(19)
C(5A)-C(6A)-C(10A)	119.8(2)	C(58A)-C(26A)-Al(1A)	127.18(16)
C(1A)-C(6A)-C(10A)	122.1(2)	C(27A)-C(26A)-Al(1A)	110.84(14)
C(9A)-C(7A)-C(8A)	110.1(2)	C(32A)-C(27A)-C(28A)	117.3(2)
C(9A)-C(7A)-C(2A)	112.7(2)	C(32A)-C(27A)-C(26A)	121.06(19)
C(8A)-C(7A)-C(2A)	111.2(2)	C(28A)-C(27A)-C(26A)	121.61(19)
C(6A)-C(10A)-C(12A)	110.5(2)	C(29A)-C(28A)-C(27A)	120.9(2)
C(6A)-C(10A)-C(11A)	113.39(19)	C(30A)-C(29A)-C(28A)	121.0(2)
C(12A)-C(10A)-C(11A)	110.5(2)	C(29A)-C(30A)-C(31A)	119.2(2)
N(1A)-C(13A)-C(15A)	122.6(2)	C(30A)-C(31A)-C(32A)	119.9(2)
N(1A)-C(13A)-C(14A)	120.6(2)	C(31A)-C(32A)-C(27A)	121.8(2)
C(15A)-C(13A)-C(14A)	116.8(2)	H(2A)-Al(2A)-N(4A)	108.3(9)
C(16A)-C(15A)-C(13A)	124.4(2)	H(2A)-Al(2A)-N(3A)	110.7(9)
N(2A)-C(16A)-C(15A)	125.0(2)	N(4A)-Al(2A)-N(3A)	93.55(8)
N(2A)-C(16A)-C(17A)	111.76(19)	H(2A)-Al(2A)-C(58A)	113.9(9)
C(15A)-C(16A)-C(17A)	123.1(2)	N(4A)-Al(2A)-C(58A)	107.36(8)
C(20A)-C(17A)-C(18A)	110.4(2)	N(3A)-Al(2A)-C(58A)	120.39(9)
C(20A)-C(17A)-C(19A)	113.2(2)	C(45A)-N(3A)-C(33A)	117.01(18)
C(18A)-C(17A)-C(19A)	111.4(2)	C(45A)-N(3A)-Al(2A)	127.01(15)
C(20A)-C(17A)-C(16A)	100.37(18)	C(33A)-N(3A)-Al(2A)	115.91(14)
C(18A)-C(17A)-C(16A)	110.19(19)	C(48A)-N(4A)-C(57A)	107.94(17)
C(19A)-C(17A)-C(16A)	110.82(19)	C(48A)-N(4A)-Al(2A)	125.04(15)
C(21A)-C(20A)-C(25A)	120.0(2)	C(57A)-N(4A)-Al(2A)	126.99(14)
C(21A)-C(20A)-C(17A)	131.1(2)	C(38A)-C(33A)-C(34A)	121.8(2)
C(25A)-C(20A)-C(17A)	108.8(2)	C(38A)-C(33A)-N(3A)	118.8(2)
C(22A)-C(21A)-C(20A)	118.4(2)	C(34A)-C(33A)-N(3A)	119.4(2)
C(23A)-C(22A)-C(21A)	120.8(2)	C(35A)-C(34A)-C(33A)	117.7(2)
C(22A)-C(23A)-C(24A)	121.0(2)	C(35A)-C(34A)-C(39A)	120.1(2)
C(25A)-C(24A)-C(23A)	117.5(2)	C(33A)-C(34A)-C(39A)	122.2(2)
C(24A)-C(25A)-C(20A)	122.2(2)	C(36A)-C(35A)-C(34A)	121.3(2)
C(24A)-C(25A)-N(2A)	127.0(2)	C(37A)-C(36A)-C(35A)	120.2(2)
C(20A)-C(25A)-N(2A)	110.8(2)	C(36A)-C(37A)-C(38A)	121.0(2)

C(37A)-C(38A)-C(33A)	118.0(2)	C(26A)-C(58A)-C(59A)	122.02(19)
C(37A)-C(38A)-C(42A)	119.6(2)	C(26A)-C(58A)-Al(2A)	125.50(16)
C(33A)-C(38A)-C(42A)	122.2(2)	C(59A)-C(58A)-Al(2A)	111.80(14)
C(34A)-C(39A)-C(40A)	112.2(2)	C(64A)-C(59A)-C(60A)	117.1(2)
C(34A)-C(39A)-C(41A)	112.2(2)	C(64A)-C(59A)-C(58A)	120.01(19)
C(40A)-C(39A)-C(41A)	109.7(2)	C(60A)-C(59A)-C(58A)	122.77(19)
C(38A)-C(42A)-C(43A)	112.9(2)	C(61A)-C(60A)-C(59A)	121.5(2)
C(38A)-C(42A)-C(44A)	110.4(2)	C(60A)-C(61A)-C(62A)	120.4(2)
C(43A)-C(42A)-C(44A)	110.6(2)	C(63A)-C(62A)-C(61A)	119.3(2)
N(3A)-C(45A)-C(47A)	122.9(2)	C(62A)-C(63A)-C(64A)	120.3(2)
N(3A)-C(45A)-C(46A)	120.0(2)	C(63A)-C(64A)-C(59A)	121.4(2)
C(47A)-C(45A)-C(46A)	117.1(2)	H(1B)-Al(1B)-N(2B)	108.3(10)
C(48A)-C(47A)-C(45A)	125.8(2)	H(1B)-Al(1B)-N(1B)	113.0(10)
N(4A)-C(48A)-C(47A)	125.5(2)	N(2B)-Al(1B)-N(1B)	94.12(8)
N(4A)-C(48A)-C(49A)	112.09(19)	H(1B)-Al(1B)-C(26B)	112.8(10)
C(47A)-C(48A)-C(49A)	122.4(2)	N(2B)-Al(1B)-C(26B)	105.18(8)
C(52A)-C(49A)-C(48A)	100.49(18)	N(1B)-Al(1B)-C(26B)	120.60(9)
C(52A)-C(49A)-C(51A)	112.50(19)	C(13B)-N(1B)-C(1B)	119.49(18)
C(48A)-C(49A)-C(51A)	111.1(2)	C(13B)-N(1B)-Al(1B)	126.62(15)
C(52A)-C(49A)-C(50A)	111.1(2)	C(1B)-N(1B)-Al(1B)	113.87(13)
C(48A)-C(49A)-C(50A)	110.53(19)	C(16B)-N(2B)-C(25B)	108.65(18)
C(51A)-C(49A)-C(50A)	110.8(2)	C(16B)-N(2B)-Al(1B)	125.08(15)
C(53A)-C(52A)-C(57A)	120.4(2)	C(25B)-N(2B)-Al(1B)	126.03(14)
C(53A)-C(52A)-C(49A)	130.6(2)	C(2B)-C(1B)-C(6B)	121.6(2)
C(57A)-C(52A)-C(49A)	108.94(19)	C(2B)-C(1B)-N(1B)	118.10(19)
C(52A)-C(53A)-C(54A)	118.5(2)	C(6B)-C(1B)-N(1B)	120.24(19)
C(55A)-C(54A)-C(53A)	120.7(2)	C(3B)-C(2B)-C(1B)	118.0(2)
C(54A)-C(55A)-C(56A)	121.1(2)	C(3B)-C(2B)-C(7B)	119.6(2)
C(57A)-C(56A)-C(55A)	117.4(2)	C(1B)-C(2B)-C(7B)	122.3(2)
C(56A)-C(57A)-C(52A)	121.8(2)	C(4B)-C(3B)-C(2B)	121.4(2)
C(56A)-C(57A)-N(4A)	127.7(2)	C(5B)-C(4B)-C(3B)	119.7(2)
C(52A)-C(57A)-N(4A)	110.52(19)	C(4B)-C(5B)-C(6B)	121.4(2)

C(5B)-C(6B)-C(1B)	117.7(2)	C(58B)-C(26B)-C(27B)	124.30(19)
C(5B)-C(6B)-C(10B)	119.3(2)	C(58B)-C(26B)-Al(1B)	122.08(15)
C(1B)-C(6B)-C(10B)	122.97(19)	C(27B)-C(26B)-Al(1B)	111.94(14)
C(2B)-C(7B)-C(8B)	112.76(19)	C(32B)-C(27B)-C(28B)	116.6(2)
C(2B)-C(7B)-C(9B)	110.02(19)	C(32B)-C(27B)-C(26B)	118.69(19)
C(8B)-C(7B)-C(9B)	111.17(19)	C(28B)-C(27B)-C(26B)	124.39(19)
C(6B)-C(10B)-C(12B)	112.86(19)	C(29B)-C(28B)-C(27B)	121.3(2)
C(6B)-C(10B)-C(11B)	110.75(19)	C(30B)-C(29B)-C(28B)	121.0(2)
C(12B)-C(10B)-C(11B)	109.9(2)	C(29B)-C(30B)-C(31B)	119.1(2)
N(1B)-C(13B)-C(15B)	122.8(2)	C(30B)-C(31B)-C(32B)	120.0(2)
N(1B)-C(13B)-C(14B)	120.6(2)	C(31B)-C(32B)-C(27B)	122.1(2)
C(15B)-C(13B)-C(14B)	116.6(2)	H(2B)-Al(2B)-N(4B)	110.9(10)
C(16B)-C(15B)-C(13B)	126.2(2)	H(2B)-Al(2B)-N(3B)	111.2(10)
N(2B)-C(16B)-C(15B)	125.1(2)	N(4B)-Al(2B)-N(3B)	92.95(8)
N(2B)-C(16B)-C(17B)	111.56(19)	H(2B)-Al(2B)-C(58B)	114.1(10)
C(15B)-C(16B)-C(17B)	123.4(2)	N(4B)-Al(2B)-C(58B)	104.44(8)
C(20B)-C(17B)-C(18B)	112.2(2)	N(3B)-Al(2B)-C(58B)	120.64(8)
C(20B)-C(17B)-C(16B)	100.41(17)	C(45B)-N(3B)-C(33B)	116.74(18)
C(18B)-C(17B)-C(16B)	111.16(19)	C(45B)-N(3B)-Al(2B)	124.71(15)
C(20B)-C(17B)-C(19B)	110.62(19)	C(33B)-N(3B)-Al(2B)	117.77(14)
C(18B)-C(17B)-C(19B)	111.4(2)	C(48B)-N(4B)-C(57B)	108.17(17)
C(16B)-C(17B)-C(19B)	110.63(19)	C(48B)-N(4B)-Al(2B)	122.93(15)
C(21B)-C(20B)-C(25B)	119.9(2)	C(57B)-N(4B)-Al(2B)	127.91(14)
C(21B)-C(20B)-C(17B)	131.4(2)	C(34B)-C(33B)-C(38B)	121.8(2)
C(25B)-C(20B)-C(17B)	108.61(19)	C(34B)-C(33B)-N(3B)	118.5(2)
C(20B)-C(21B)-C(22B)	119.0(2)	C(38B)-C(33B)-N(3B)	119.7(2)
C(21B)-C(22B)-C(23B)	120.4(2)	C(33B)-C(34B)-C(35B)	118.1(2)
C(24B)-C(23B)-C(22B)	121.1(2)	C(33B)-C(34B)-C(39B)	122.5(2)
C(25B)-C(24B)-C(23B)	117.8(2)	C(35B)-C(34B)-C(39B)	119.4(2)
C(24B)-C(25B)-C(20B)	121.8(2)	C(36B)-C(35B)-C(34B)	120.9(3)
C(24B)-C(25B)-N(2B)	127.5(2)	C(35B)-C(36B)-C(37B)	120.3(2)
C(20B)-C(25B)-N(2B)	110.69(19)	C(36B)-C(37B)-C(38B)	121.4(2)

C(37B)-C(38B)-C(33B)	117.5(2)	C(26B)-C(58B)-C(59B)	122.53(19)
C(37B)-C(38B)-C(42B)	121.0(2)	C(26B)-C(58B)-Al(2B)	122.75(16)
C(33B)-C(38B)-C(42B)	121.5(2)	C(59B)-C(58B)-Al(2B)	113.52(14)
C(34B)-C(39B)-C(40B)	111.1(2)	C(64B)-C(59B)-C(60B)	117.9(2)
C(34B)-C(39B)-C(41B)	111.6(2)	C(64B)-C(59B)-C(58B)	119.60(19)
C(40B)-C(39B)-C(41B)	110.0(2)	C(60B)-C(59B)-C(58B)	122.5(2)
C(43B)-C(42B)-C(38B)	113.1(2)	C(61B)-C(60B)-C(59B)	120.6(2)
C(43B)-C(42B)-C(44B)	108.6(2)	C(60B)-C(61B)-C(62B)	120.8(2)
C(38B)-C(42B)-C(44B)	112.7(2)	C(63B)-C(62B)-C(61B)	119.2(2)
N(3B)-C(45B)-C(47B)	122.8(2)	C(62B)-C(63B)-C(64B)	120.1(2)
N(3B)-C(45B)-C(46B)	120.4(2)	C(63B)-C(64B)-C(59B)	121.3(2)
C(47B)-C(45B)-C(46B)	116.60(19)	H(1C)-Al(1C)-N(2C)	109.0(10)
C(48B)-C(47B)-C(45B)	124.8(2)	H(1C)-Al(1C)-N(1C)	111.2(10)
N(4B)-C(48B)-C(47B)	124.5(2)	N(2C)-Al(1C)-N(1C)	93.84(8)
N(4B)-C(48B)-C(49B)	111.68(19)	H(1C)-Al(1C)-C(26C)	113.3(10)
C(47B)-C(48B)-C(49B)	123.8(2)	N(2C)-Al(1C)-C(26C)	106.44(8)
C(52B)-C(49B)-C(51B)	111.19(19)	N(1C)-Al(1C)-C(26C)	120.53(9)
C(52B)-C(49B)-C(48B)	100.42(17)	C(13C)-N(1C)-C(1C)	117.63(18)
C(51B)-C(49B)-C(48B)	111.57(19)	C(13C)-N(1C)-Al(1C)	126.93(15)
C(52B)-C(49B)-C(50B)	112.1(2)	C(1C)-N(1C)-Al(1C)	115.37(14)
C(51B)-C(49B)-C(50B)	110.8(2)	C(16C)-N(2C)-C(25C)	108.28(17)
C(48B)-C(49B)-C(50B)	110.28(19)	C(16C)-N(2C)-Al(1C)	125.00(15)
C(53B)-C(52B)-C(57B)	120.5(2)	C(25C)-N(2C)-Al(1C)	126.49(14)
C(53B)-C(52B)-C(49B)	130.9(2)	C(2C)-C(1C)-C(6C)	121.9(2)
C(57B)-C(52B)-C(49B)	108.59(19)	C(2C)-C(1C)-N(1C)	118.6(2)
C(52B)-C(53B)-C(54B)	118.3(2)	C(6C)-C(1C)-N(1C)	119.6(2)
C(55B)-C(54B)-C(53B)	120.6(2)	C(3C)-C(2C)-C(1C)	117.9(2)
C(54B)-C(55B)-C(56B)	121.4(2)	C(3C)-C(2C)-C(7C)	119.8(2)
C(57B)-C(56B)-C(55B)	117.3(2)	C(1C)-C(2C)-C(7C)	122.3(2)
C(56B)-C(57B)-C(52B)	121.9(2)	C(4C)-C(3C)-C(2C)	121.3(2)
C(56B)-C(57B)-N(4B)	127.1(2)	C(5C)-C(4C)-C(3C)	119.7(2)
C(52B)-C(57B)-N(4B)	111.03(19)	C(4C)-C(5C)-C(6C)	121.7(2)

C(5C)-C(6C)-C(1C)	117.5(2)	C(58C)-C(26C)-C(27C)	122.98(19)
C(5C)-C(6C)-C(10C)	120.0(2)	C(58C)-C(26C)-Al(1C)	124.02(16)
C(1C)-C(6C)-C(10C)	122.5(2)	C(27C)-C(26C)-Al(1C)	112.07(14)
C(2C)-C(7C)-C(9C)	112.4(2)	C(32C)-C(27C)-C(28C)	117.1(2)
C(2C)-C(7C)-C(8C)	110.7(2)	C(32C)-C(27C)-C(26C)	119.1(2)
C(9C)-C(7C)-C(8C)	111.1(2)	C(28C)-C(27C)-C(26C)	123.6(2)
C(6C)-C(10C)-C(12C)	111.7(2)	C(29C)-C(28C)-C(27C)	121.3(2)
C(6C)-C(10C)-C(11C)	112.5(2)	C(30C)-C(29C)-C(28C)	120.8(3)
C(12C)-C(10C)-C(11C)	109.4(2)	C(31C)-C(30C)-C(29C)	119.0(2)
N(1C)-C(13C)-C(15C)	122.7(2)	C(30C)-C(31C)-C(32C)	120.5(2)
N(1C)-C(13C)-C(14C)	120.8(2)	C(27C)-C(32C)-C(31C)	121.4(2)
C(15C)-C(13C)-C(14C)	116.5(2)	H(2C)-Al(2C)-N(4C)	109.2(10)
C(16C)-C(15C)-C(13C)	125.8(2)	H(2C)-Al(2C)-N(3C)	111.7(10)
N(2C)-C(16C)-C(15C)	125.5(2)	N(4C)-Al(2C)-N(3C)	91.85(8)
N(2C)-C(16C)-C(17C)	111.90(19)	H(2C)-Al(2C)-C(58C)	114.3(10)
C(15C)-C(16C)-C(17C)	122.6(2)	N(4C)-Al(2C)-C(58C)	105.42(9)
C(20C)-C(17C)-C(16C)	100.38(17)	N(3C)-Al(2C)-C(58C)	121.05(9)
C(20C)-C(17C)-C(19C)	112.6(2)	C(45C)-N(3C)-C(33C)	117.58(19)
C(16C)-C(17C)-C(19C)	111.27(19)	C(45C)-N(3C)-Al(2C)	125.10(16)
C(20C)-C(17C)-C(18C)	110.85(19)	C(33C)-N(3C)-Al(2C)	116.64(14)
C(16C)-C(17C)-C(18C)	109.96(19)	C(48C)-N(4C)-C(57C)	108.20(18)
C(19C)-C(17C)-C(18C)	111.3(2)	C(48C)-N(4C)-Al(2C)	122.40(16)
C(21C)-C(20C)-C(25C)	120.2(2)	C(57C)-N(4C)-Al(2C)	128.69(15)
C(21C)-C(20C)-C(17C)	131.2(2)	C(38C)-C(33C)-C(34C)	121.8(2)
C(25C)-C(20C)-C(17C)	108.63(19)	C(38C)-C(33C)-N(3C)	117.7(2)
C(20C)-C(21C)-C(22C)	118.6(2)	C(34C)-C(33C)-N(3C)	120.5(2)
C(21C)-C(22C)-C(23C)	120.6(2)	C(35C)-C(34C)-C(33C)	117.7(2)
C(24C)-C(23C)-C(22C)	121.1(2)	C(35C)-C(34C)-C(39C)	120.0(2)
C(25C)-C(24C)-C(23C)	117.7(2)	C(33C)-C(34C)-C(39C)	122.3(2)
C(24C)-C(25C)-C(20C)	121.7(2)	C(36C)-C(35C)-C(34C)	121.3(3)
C(24C)-C(25C)-N(2C)	127.6(2)	C(35C)-C(36C)-C(37C)	120.1(3)
C(20C)-C(25C)-N(2C)	110.74(19)	C(36C)-C(37C)-C(38C)	121.3(3)

C(37C)-C(38C)-C(33C)	117.8(2)	C(26C)-C(58C)-C(59C)	120.55(19)
C(37C)-C(38C)-C(42C)	120.1(2)	C(26C)-C(58C)-Al(2C)	125.43(16)
C(33C)-C(38C)-C(42C)	121.9(2)	C(59C)-C(58C)-Al(2C)	112.89(14)
C(34C)-C(39C)-C(40C)	111.0(2)	C(60C)-C(59C)-C(64C)	117.5(2)
C(34C)-C(39C)-C(41C)	112.9(2)	C(60C)-C(59C)-C(58C)	120.5(2)
C(40C)-C(39C)-C(41C)	110.4(2)	C(64C)-C(59C)-C(58C)	122.0(2)
C(38C)-C(42C)-C(44C)	112.9(2)	C(59C)-C(60C)-C(61C)	121.7(2)
C(38C)-C(42C)-C(43C)	110.1(2)	C(62C)-C(61C)-C(60C)	119.9(2)
C(44C)-C(42C)-C(43C)	110.5(2)	C(61C)-C(62C)-C(63C)	119.3(2)
N(3C)-C(45C)-C(47C)	122.1(2)	C(62C)-C(63C)-C(64C)	120.8(2)
N(3C)-C(45C)-C(46C)	120.3(2)	C(63C)-C(64C)-C(59C)	120.8(2)
C(47C)-C(45C)-C(46C)	117.5(2)	H(1D)-Al(1D)-N(2D)	108.5(10)
C(48C)-C(47C)-C(45C)	124.4(2)	H(1D)-Al(1D)-N(1D)	111.8(10)
N(4C)-C(48C)-C(47C)	124.8(2)	N(2D)-Al(1D)-N(1D)	92.85(8)
N(4C)-C(48C)-C(49C)	111.5(2)	H(1D)-Al(1D)-C(26D)	115.6(10)
C(47C)-C(48C)-C(49C)	123.6(2)	N(2D)-Al(1D)-C(26D)	101.93(9)
C(52C)-C(49C)-C(51C)	110.8(2)	N(1D)-Al(1D)-C(26D)	121.87(9)
C(52C)-C(49C)-C(50C)	111.6(2)	C(13D)-N(1D)-C(1D)	114.74(19)
C(51C)-C(49C)-C(50C)	111.6(2)	C(13D)-N(1D)-Al(1D)	124.64(15)
C(52C)-C(49C)-C(48C)	100.58(18)	C(1D)-N(1D)-Al(1D)	118.44(14)
C(51C)-C(49C)-C(48C)	111.6(2)	C(16D)-N(2D)-C(25D)	108.40(18)
C(50C)-C(49C)-C(48C)	110.2(2)	C(16D)-N(2D)-Al(1D)	123.11(15)
C(53C)-C(52C)-C(57C)	120.3(2)	C(25D)-N(2D)-Al(1D)	127.93(15)
C(53C)-C(52C)-C(49C)	131.2(2)	C(6D)-C(1D)-C(2D)	121.6(2)
C(57C)-C(52C)-C(49C)	108.4(2)	C(6D)-C(1D)-N(1D)	120.9(2)
C(52C)-C(53C)-C(54C)	118.5(2)	C(2D)-C(1D)-N(1D)	117.5(2)
C(55C)-C(54C)-C(53C)	120.6(2)	C(3D)-C(2D)-C(1D)	118.3(2)
C(54C)-C(55C)-C(56C)	121.4(2)	C(3D)-C(2D)-C(7D)	119.5(2)
C(57C)-C(56C)-C(55C)	117.2(2)	C(1D)-C(2D)-C(7D)	122.2(2)
C(56C)-C(57C)-C(52C)	122.0(2)	C(4D)-C(3D)-C(2D)	120.4(3)
C(56C)-C(57C)-N(4C)	127.0(2)	C(5D)-C(4D)-C(3D)	120.3(3)
C(52C)-C(57C)-N(4C)	111.0(2)	C(4D)-C(5D)-C(6D)	121.8(3)

C(5D)-C(6D)-C(1D)	117.3(3)	C(24D)-C(25D)-N(2D)	127.0(2)
C(5D)-C(6D)-C(10E)	116.7(5)	C(20D)-C(25D)-N(2D)	110.9(2)
C(1D)-C(6D)-C(10E)	124.0(5)	C(58D)-C(26D)-C(27D)	122.7(2)
C(5D)-C(6D)-C(10D)	122.4(3)	C(58D)-C(26D)-Al(1D)	123.17(16)
C(1D)-C(6D)-C(10D)	119.9(3)	C(27D)-C(26D)-Al(1D)	112.51(15)
C(8D)-C(7D)-C(2D)	112.7(2)	C(32D)-C(27D)-C(28D)	118.0(2)
C(8D)-C(7D)-C(9D)	111.0(2)	C(32D)-C(27D)-C(26D)	119.7(2)
C(2D)-C(7D)-C(9D)	110.4(2)	C(28D)-C(27D)-C(26D)	122.2(2)
C(12D)-C(10D)-C(11D)	109.9(6)	C(29D)-C(28D)-C(27D)	120.4(2)
C(12D)-C(10D)-C(6D)	112.0(5)	C(30D)-C(29D)-C(28D)	120.7(2)
C(11D)-C(10D)-C(6D)	109.5(4)	C(31D)-C(30D)-C(29D)	119.7(2)
N(1D)-C(13D)-C(15D)	122.8(2)	C(30D)-C(31D)-C(32D)	119.9(3)
N(1D)-C(13D)-C(14D)	120.2(2)	C(31D)-C(32D)-C(27D)	121.3(2)
C(15D)-C(13D)-C(14D)	116.9(2)	H(2D)-Al(2D)-N(4D)	111.3(10)
C(16D)-C(15D)-C(13D)	124.7(2)	H(2D)-Al(2D)-N(3D)	111.0(10)
N(2D)-C(16D)-C(15D)	124.7(2)	N(4D)-Al(2D)-N(3D)	94.03(9)
N(2D)-C(16D)-C(17D)	111.54(19)	H(2D)-Al(2D)-C(58D)	111.3(10)
C(15D)-C(16D)-C(17D)	123.7(2)	N(4D)-Al(2D)-C(58D)	103.31(9)
C(20D)-C(17D)-C(18D)	112.4(2)	N(3D)-Al(2D)-C(58D)	123.79(9)
C(20D)-C(17D)-C(19D)	111.5(2)	C(45D)-N(3D)-C(33D)	120.30(18)
C(18D)-C(17D)-C(19D)	110.4(2)	C(45D)-N(3D)-Al(2D)	126.23(15)
C(20D)-C(17D)-C(16D)	100.54(18)	C(33D)-N(3D)-Al(2D)	113.47(14)
C(18D)-C(17D)-C(16D)	110.79(19)	C(48D)-N(4D)-C(57D)	109.2(2)
C(19D)-C(17D)-C(16D)	110.96(19)	C(48D)-N(4D)-Al(2D)	125.06(16)
C(21D)-C(20D)-C(25D)	120.5(2)	C(57D)-N(4D)-Al(2D)	125.27(17)
C(21D)-C(20D)-C(17D)	130.9(2)	C(38D)-C(33D)-C(34D)	121.1(2)
C(25D)-C(20D)-C(17D)	108.62(19)	C(38D)-C(33D)-N(3D)	118.87(19)
C(20D)-C(21D)-C(22D)	118.1(2)	C(34D)-C(33D)-N(3D)	119.85(19)
C(23D)-C(22D)-C(21D)	121.1(2)	C(35D)-C(34D)-C(33D)	118.1(2)
C(22D)-C(23D)-C(24D)	121.0(2)	C(35D)-C(34D)-C(39D)	119.1(2)
C(25D)-C(24D)-C(23D)	117.3(2)	C(33D)-C(34D)-C(39D)	122.7(2)
C(24D)-C(25D)-C(20D)	122.1(2)	C(36D)-C(35D)-C(34D)	121.4(2)

C(37D)-C(36D)-C(35D) 119.9(2)
C(36D)-C(37D)-C(38D) 121.2(2)
C(37D)-C(38D)-C(33D) 118.3(2)
C(37D)-C(38D)-C(42D) 119.2(2)
C(33D)-C(38D)-C(42D) 122.3(2)
C(34D)-C(39D)-C(40D) 112.1(2)
C(34D)-C(39D)-C(41D) 110.85(19)
C(40D)-C(39D)-C(41D) 109.9(2)
C(38D)-C(42D)-C(44D) 113.12(19)
C(38D)-C(42D)-C(43D) 109.42(19)
C(44D)-C(42D)-C(43D) 111.0(2)
N(3D)-C(45D)-C(47D) 122.7(2)
N(3D)-C(45D)-C(46D) 120.5(2)
C(47D)-C(45D)-C(46D) 116.7(2)
C(48D)-C(47D)-C(45D) 126.0(2)
N(4D)-C(48D)-C(47D) 124.9(2)
N(4D)-C(48D)-C(49D) 111.1(2)
C(47D)-C(48D)-C(49D) 124.0(2)
C(52D)-C(49D)-C(50D) 110.7(2)
C(52D)-C(49D)-C(48D) 100.7(2)
C(50D)-C(49D)-C(48D) 108.9(2)
C(52D)-C(49D)-C(51D) 113.4(2)
C(50D)-C(49D)-C(51D) 111.1(2)
C(48D)-C(49D)-C(51D) 111.4(2)
C(53D)-C(52D)-C(57D) 119.1(3)
C(53D)-C(52D)-C(49D) 132.2(3)
C(57D)-C(52D)-C(49D) 108.6(2)
C(54D)-C(53D)-C(52D) 119.0(3)
C(55D)-C(54D)-C(53D) 120.9(3)
C(54D)-C(55D)-C(56D) 121.0(3)
C(57D)-C(56D)-C(55D) 117.8(3)
C(56D)-C(57D)-C(52D) 122.2(2)
C(56D)-C(57D)-N(4D) 127.5(2)
C(52D)-C(57D)-N(4D) 110.3(2)
C(26D)-C(58D)-C(59D) 124.80(19)
C(26D)-C(58D)-Al(2D) 118.25(16)
C(59D)-C(58D)-Al(2D) 114.47(15)
C(64D)-C(59D)-C(60D) 116.7(2)
C(64D)-C(59D)-C(58D) 118.8(2)
C(60D)-C(59D)-C(58D) 124.3(2)
C(61D)-C(60D)-C(59D) 121.2(2)
C(62D)-C(61D)-C(60D) 120.9(2)
C(61D)-C(62D)-C(63D) 119.1(2)
C(62D)-C(63D)-C(64D) 119.8(2)
C(63D)-C(64D)-C(59D) 122.3(2)
C(6D)-C(10E)-C(11E) 118.0(9)
C(6D)-C(10E)-C(12E) 107.8(10)
C(11E)-C(10E)-C(12E) 108.7(12)
C(22)-C(21)-C(26) 119.6(6)
C(21)-C(22)-C(23) 120.9(6)
C(22)-C(23)-C(24) 118.7(6)
C(25)-C(24)-C(23) 119.4(6)
C(24)-C(25)-C(26) 122.2(7)
C(21)-C(26)-C(25) 119.2(7)
C(22')-C(21')-C(26') 117.6(12)
C(21')-C(22')-C(23') 119.5(11)
C(24')-C(23')-C(22') 122.6(12)
C(25')-C(24')-C(23') 116.5(12)
C(24')-C(25')-C(26') 121.5(14)
C(25')-C(26')-C(21') 122.0(15)
C(32)-C(31)-C(36) 119.8(3)
C(31)-C(32)-C(33) 120.9(3)
C(34)-C(33)-C(32) 119.4(3)
C(35)-C(34)-C(33) 119.7(3)

C(34)-C(35)-C(36)	120.5(3)	C(56)-C(51)-C(52)	122.2(14)
C(35)-C(36)-C(31)	119.6(3)	C(51)-C(52)-C(53)	119.9(14)
C(66)-C(61)-C(62)	119.2(4)	C(54)-C(53)-C(52)	117.9(13)
C(63)-C(62)-C(61)	120.3(3)	C(55)-C(54)-C(53)	121.3(12)
C(62)-C(63)-C(64)	120.6(3)	C(54)-C(55)-C(56)	120.3(12)
C(63)-C(64)-C(65)	118.7(4)	C(51)-C(56)-C(55)	118.4(12)
C(66)-C(65)-C(64)	120.6(3)	C(56')-C(51')-C(52')	120.8(8)
C(65)-C(66)-C(61)	120.6(3)	C(51')-C(52')-C(53')	119.9(7)
C(76)-C(71)-C(72)	119.9(3)	C(54')-C(53')-C(52')	119.4(6)
C(73)-C(72)-C(71)	119.6(3)	C(55')-C(54')-C(53')	120.8(6)
C(72)-C(73)-C(74)	120.5(2)	C(54')-C(55')-C(56')	117.6(7)
C(75)-C(74)-C(73)	119.9(2)	C(51')-C(56')-C(55')	121.5(7)
C(76)-C(75)-C(74)	119.9(2)	C(86)-C(81)-C(82)	120.6(7)
C(75)-C(76)-C(71)	120.3(2)	C(83)-C(82)-C(81)	118.7(7)
C(102)-C(101)-C(106)	120.7(3)	C(84)-C(83)-C(82)	120.7(7)
C(101)-C(102)-C(103)	119.6(3)	C(83)-C(84)-C(85)	119.5(7)
C(104)-C(103)-C(102)	119.9(3)	C(86)-C(85)-C(84)	119.4(7)
C(103)-C(104)-C(105)	120.5(3)	C(81)-C(86)-C(85)	121.1(7)
C(106)-C(105)-C(104)	119.7(3)	C(82')-C(81')-C(86')	122.1(12)
C(105)-C(106)-C(101)	119.7(3)	C(81')-C(82')-C(83')	119.0(11)
C(42)-C(41)-C(46)	119.9(6)	C(84')-C(83')-C(82')	120.2(12)
C(43)-C(42)-C(41)	120.7(6)	C(85')-C(84')-C(83')	119.1(12)
C(42)-C(43)-C(44)	118.7(7)	C(84')-C(85')-C(86')	121.4(12)
C(45)-C(44)-C(43)	121.4(7)	C(85')-C(86')-C(81')	118.1(12)
C(44)-C(45)-C(46)	119.8(8)	C(6)-C(1)-C(2)	120.0(12)
C(45)-C(46)-C(41)	119.5(7)	C(6)-C(1)-C(7)	120.1(12)
C(42')-C(41')-C(46')	120.0(9)	C(2)-C(1)-C(7)	119.9(12)
C(41')-C(42')-C(43')	120.0(10)	C(3)-C(2)-C(1)	117.8(14)
C(42')-C(43')-C(44')	120.1(11)	C(2)-C(3)-C(4)	121.7(13)
C(45')-C(44')-C(43')	120.2(11)	C(5)-C(4)-C(3)	120.8(13)
C(44')-C(45')-C(46')	120.2(10)	C(4)-C(5)-C(6)	117.4(14)
C(45')-C(46')-C(41')	119.5(9)	C(5)-C(6)-C(1)	122.2(14)

C(8)-C(7)-C(1)	176.5(12)	C(113)-C(112)-C(111)	118.7(6)
C(7)-C(8)-C(9)	174.7(14)	C(114)-C(113)-C(112)	120.7(5)
C(8)-C(9)-C(10)	129.5(16)	C(115)-C(114)-C(113)	120.2(5)
C(8)-C(9)-C(14)	109.3(15)	C(116)-C(115)-C(114)	119.9(6)
C(10)-C(9)-C(14)	121.1(14)	C(115)-C(116)-C(111)	121.0(6)
C(11)-C(10)-C(9)	120.2(15)	C(92)-C(91)-C(96)	118.7(6)
C(10)-C(11)-C(12)	119.6(16)	C(93)-C(92)-C(91)	120.9(5)
C(11)-C(12)-C(13)	119.3(15)	C(92)-C(93)-C(94)	120.3(6)
C(14)-C(13)-C(12)	122.4(15)	C(95)-C(94)-C(93)	119.7(6)
C(13)-C(14)-C(9)	117.0(15)	C(96)-C(95)-C(94)	120.1(6)
C(112)-C(111)-C(116)	119.6(5)	C(95)-C(96)-C(91)	120.4(6)

Computational Details

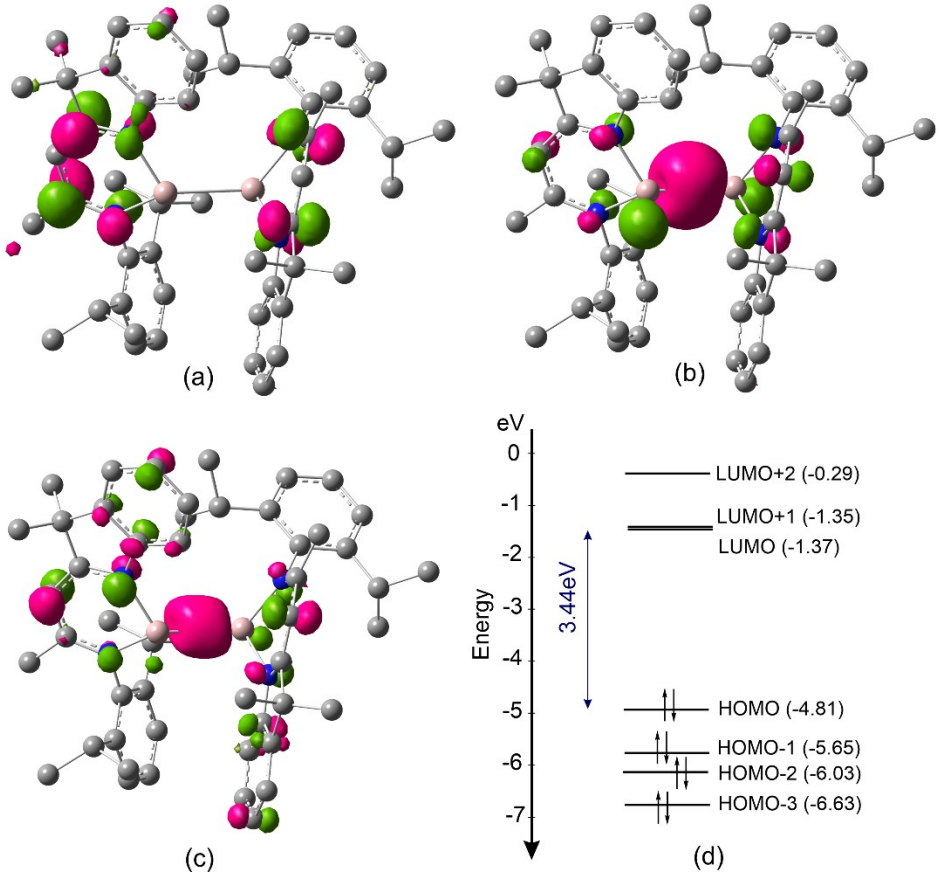


Figure S 59: Molecular orbitals in [{DNI(H)Al}$_2$] (**2**) in its singlet ground state: (**a**) LUMO; (**b**) HOMO; (**c**) HOMO-2; (**d**) energetic diagram of MOs with HOMO-LUMO gap given in blue. Surfaces are drawn at isovalue of 0.05 au.

Table S7: Topological properties of electron density in the region of Al−Al chemical bonding in compound **2** analysed with the use of QTAIM.[7]

	(Rank, σ)	$\rho(r)$	$\nabla^2\rho(r)$	λ_1	λ_2	λ_3
BCP1	(3,–1)	0.058	-0.049	0.058	-0.049	0.058
BCP2	(3,–1)	0.058	-0.042	0.058	-0.042	0.058
NNA	(3,–3)	0.059	-0.092	0.059	-0.092	0.059

(Rank, σ) denotes the number of non-zero curvatures of the electron density, and the sum of their signs; $\rho(r)$ refers to the electron density at a critical point (CP)(eBohr^{-3}); $\nabla^2\rho(r)$ is a Laplacian of the density (eBohr^{-5}) and λ_n are curvatures of the electron density (eBohr^{-5}).

Description of reaction mechanism

In the case of the first reaction (see paths A-B in Figure 6), a 1.3 kcal/mol gap is observed between products and reactants, indicating that both direct and indirect reactions had nearly the same energy barrier of 19 kcal/mol. The transition state involves the breakage of a bond in one of the Dipp-amide residues, leading to the formation of a Al−C bond and the shift of the Dipp-amide fragment to give a μ-bridge between both Al atoms. However, for the second step of the reaction (paths C-D), we encounter a larger gap of ΔG = -13.2 kcal/mol between the intermediate and the final product. Unfortunately, we were unable to estimate a reasonable reaction mode for this step. Nevertheless, the topological analysis of electron density of the intermediate molecule in the solvated medium, provided some valuable insights into potential reaction path, as depicted in Figure S60. Based on the analysis of the electron density and the Laplacian at the bond critical points (see Table S8), we propose that both lone pairs of the nitrogen atom N4 from the DNI-Na molecule will initiate the attack on the most positively charged aluminium atom (Al2, $q = +1.96$ au). This attack would lead to the breakage of the weak Al−Al bond, where the lowest electron density is observed. Consequently, the remaining aluminium atom (Al1, $q = +1.44$) would attack the C38 atom. Moreover, the bonds C40−C38 and C41−N4 predominantly exhibit double bond character. This is evident when comparing $\rho(r)$ and $\nabla^2\rho(r)$ at the BCPs, both having higher absolute values compared to the C40−C41 bond. Therefore, the attack would cause a shift in the position of the π-bonds, leading to the formation of a new π-bond between C40 and C41. As a result of these reactions, the final product would have a double bridge between the aluminium atoms, forming an Al_2CN four-membered ring. This mechanism and bonding rearrangement provide insights into the structural changes that occur during the reaction and the formation of the final product. A table containing a more detailed description regarding the electron density topology of the intermediate can be found in Table S8

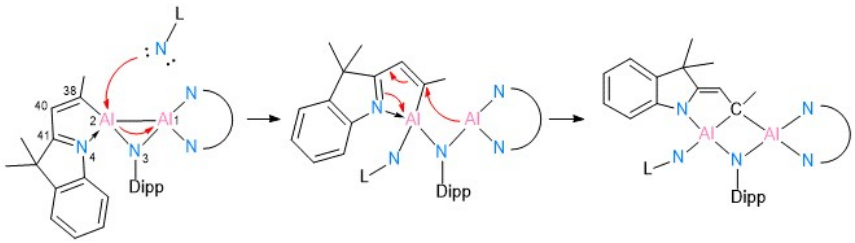


Figure S60 Possible mechanism involving intermediate and the compound **5**. (L = DNI ligand)

Table S8: Topological quantities[8] of the electron density of the intermediate molecule of the mechanism of **Figure 6** $\rho(\mathbf{r})$, $\nabla^2 \rho(\mathbf{r})$, ε, V, G, K, L are given in atomic units and refer to the electron density (e bohr^{-3}), Laplacian of the electron density (e bohr^{-5}), ellipticity (dimensionless), potential energy density (Hartree bohr^{-3}), Lagrangian form of kinetic energy density (Hartree bohr^{-3}), Hamiltonian form of kinetic energy density (Hartree bohr^{-3}), Lagrangian density (Hartree bohr^{-3}), respectively.

Bond	$\rho(\mathbf{r})$	$\nabla^2 \rho(\mathbf{r})$	ε	V	G	K	L
Al1–Al2	0.0487	-0.0302	0.2958	-0.0370	0.0147	0.0223	0.0076
Al2–N4	0.0557	0.2933	0.0790	-0.1295	0.1261	0.0034	-0.1227
N4–C41	0.3498	-0.9358	0.0957	-0.9370	0.3515	0.5855	0.2340
C41–C40	0.2944	-0.7904	0.1619	0.3695	0.0860	0.2836	0.1976
C40–C38	0.3261	-0.8948	0.1979	-0.4647	0.1205	0.3442	0.2237
C38–Al2	0.0710	0.2702	0.0678	-0.0996	0.0836	0.0160	-0.0676

For details please see: https://data.goettingen-research-online.de/privateurl.xhtml?token=c15c2a19-a359-4a71-84dd-5a99e3a7f017

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