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Electronic Supplementary Information

An Open Route to Asymmetric Substituted Al–Al Bonds using Al(I)- and Al(III)- Precursors

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Content:

S1. Experimental Section

All manipulations were carried out under a dry argon or nitrogen atmosphere using Schlenk line and glovebox techniques. Toluene and deuterated benzene was dried by refluxing with sodium/potassium under N_2 prior to use. The NMR (^1H, ^{13}C) spectra were recorded on Bruker Avance II 500 MHz spectrometer. Melting points of compounds were measured in a sealed glass tube using the Büchi-540 instrument. Elemental analysis were performed by the Analytisches Labor des Instituts für Anorganische Chemie der Universität Göttingen. Commercial reagents were purchased from Aldrich, Acros, or Alfa-Aesar Chemical Co. and used as received. Me_2-cAAC[1], AC→$AlCl_3$[2] and LAl:[3] were prepared according to the literatures.

cAAC→AlI_3 (1b): cAAC (0.221 g, 0.5 mmol) and AlI_3 (0.204 g, 0.5 mmol) were added into a flask. Toluene (30 mL) was added under stirring at room temperature. Since AlI3 is light sensitive, the reaction is undergoing without light. The mixture was stirred for 12h. After filtration, the filtrate was concentrated to 5 mL under vacuum and stored at −20 °C. After 12 h, colorless crystallize solid were obtained and collected by filtration (0.190 g, 55%). Suitable X-ray quality crystals were grown from C_6D_6. Mp: 224°C. ^1H NMR (500 MHz, C_6D_6, 298K, ppm): δ =0.78 (s, 6 H, CH_3),1.01 (d, $^3J_{HH}$ = 5 Hz, 6 H, CHMe_2), 1.31(s, 2 H, CH_2), 1.62 (d, $^3J_{HH}$ = 5 Hz, 6 H, CHMe_2), 1.83 (s, 6 H, CH_3), 2.58 (sept, $^3J_{HH}$ = 5 Hz, 2 H, CHMe$_2$), 6.98−7.15 (m, 3 H, C$_6H_3$).^{13}C NMR (125 MHz, C_6D_6, 298K, ppm): δ = 25.2, 27.9, 28.4, 29.1, 31.6, 51.2, 57.2, 81.9, 125.5, 131.2, 133.2, 145.6, 223.4. Anal. Calcd (%) for $C_{20}H_{31}NAlI_3$ (Mr = 693.16): C, 34.65; H, 4.51; N, 2.02. Found: C, 34.67; H, 5.01; N, 2.00.

LAl(Cl)-Al(Cl)$_2$cAAC (2a): LAl: (100 mg, 0.23 mmol) and CAAC-$AlCl_3$ (94 mg, 0.23 mmol) were added to a 100ml flask. Toluene was added to the mixture at room temperature. The solution was kept stirring overnight and the color changed from reddish to yellow. After filtration, the filtrate was dried under vacuum and light yellow powder was obtained (0.135 g, 70%). Colorless crystals were grown from *n*-hexane. Mp: 92 °C (dec.). ^1H NMR (298K, C_6D_6, 500MHz, ppm): δ = 6.89-7.23 (m,

9H, C_6H_3), 5.07 (s, 1H, γ-*H*), 3.84 (sept, $^3J_{HH}$ = 5 Hz, 2H), 3.60 (sept, $^3J_{HH}$ = 5 Hz, 2H), 2.61 (sept, $^3J_{HH}$ = 5 Hz, 2H) (C*H*Me$_2$), 1.68 (d, $^3J_{HH}$ = 5 Hz, 6H), 1.58 (d, $^3J_{HH}$ = 5 Hz, 6H), 1.27 (d, $^3J_{HH}$ = 5 Hz, 6H), 1.06 (d, $^3J_{HH}$ = 5 Hz, 6H), 1.02 (d, $^3J_{HH}$ = 5 Hz, 6H) (CH*Me*$_2$), 1.61 (s, 6H), 1.33 (s, 6H), 0.74 (s, 6H) (C*Me*, C*Me*$_2$), 1.24 (s, 2H, C*H*$_2$). ^{13}C NMR (298K, C_6D_6, 125 MHz, ppm): δ = 24.2, 24.4, 24.8, 25.0, 26.9, 27.5, 27.8, 29.1, 30.2, 30.7, 50.43, 55.6, 81.6 (*C*H*Me*$_2$, *CMe*$_2$, *C*H$_2$, C*Me*), 99.1(γ-*C*), 124.3,125.0, 125.1, 127.3, 129.8, 133.5, 142.5, 143.6, 145.2, 145.6 (*C*$_6$H$_3$), 169.6 (*C*N), 238.6 (carbene *carbon*). Anal. Calcd (%) for $C_{49}H_{72}N_3Al_2Cl_3$ (Mr = 863.44): C, 68.16; H, 8.40; N, 4.87. Found: C, 67.50; H, 8.62; N, 4.48.

LAl(I)-Al(I)$_2$cAAC (2b): LAl: (100 mg, 0.23 mmol) and CAAC-AlI$_3$ (157 mg, 0.23 mmol) were added to a 100ml flask. Toluene was added to the mixture at -70 ^{o}C. The solution was slowly warmed to room temperature and kept stirring overnight. The color changed from orange to yellow. After filtration, the filtrate was concentrated to 2 mL and kept at room temperature. Light yellow crystals were obtained 2 days later (0.140 g, 55%). Mp: 97 ^{o}C (dec.). ^{1}H NMR (298K, C_6D_6, 500MHz, ppm): δ = 6.98-7.28 (m, 9H, C_6H_3) 5.23 (s, 1H, γ-H), 4.12 (br, 1H), 4.01 (br, 1H), 3.70 (br, 1H), 3.50 (br, 1H), 3.08 (br, 1H), 2.37 (br, 1H), 1.74 (d, 3H) 1.71 (d, 3H), 1.70 (d, 3H), 1.67 (d, 3H), 1.58-1.62 (m, 14H), 1.32 (d, 3H), 1.27 (s, 3H), 1.26 (s, 3H), 1.23 (s, 3H), 0.99-1.02 (m, 15H), 0.60 (s, 3H) (C*Me*, C*Me*$_2$, CH*Me*$_2$, C*H*$_2$). ^{13}C NMR (298K, C_6D_6, 125 MHz, ppm): δ = 24.4, 24.6 24.7, 24.9, 25.5, 25.6, 25.9, 26.2, 26.6, 28.5, 28.6, 28.9, 29.3, 30.2, 30.3, 33.4, 33.6, 51.3, 56.9, 82.1 (*C*H*Me*$_2$, *CMe*$_2$, *C*H$_2$, C*Me*) 100.9 (γ-*C*), 124.6, 124.8, 125.2, 125.4, 130.2, 131.1, 133.2, 134.5, 143.1, 143.9, 144.7, 145.6, 146.2 (*C*$_6$H$_3$), 171.5 (*C*N), 230.8 (carbene *carbon*). Anal. Calcd (%) for $C_{49}H_{72}N_3Al_2I_3$ (Mr = 1137.79): C, 51.73; H, 6.38; N, 3.69. Found: C, 51.27; H, 5.81; N, 3.98.

S2. X-Ray Crystallographic Analysis

The crystals were selected under cooling, using a X-Temp2 device.[4] The data were collected from shock-cooled crystals at 100(2) K, on a BRUKER D8 three circle diffractometer equipped with an INCOATEC Mo Microsource and Ag Microsource with mirror optics (MoK_α radiation, λ = 0.71073 Å, AgK_α radiation, λ = 0.56086 Å) The data were integrated with SAINT.[5] A multi-scan absorption correction was applied using SADABS.[6] The structures were solved by SHELXT[7] and refined on F^2 using SHELXL[8] in the graphical user interface SHELXLE.[9]

Table S1. Crystal data and structure refinement of **1b**, **2a** and **2b**.

Compound	**1b**	**2a**	**2b**
Empirical formula	C20 H31 Al I3 N	C55 H86 Al2 Cl3 N3	C59.50 H84 Al2 I3 N3
CCDC number	1516682	1516005	1516006
Formula weight	693.14	949.57	1275.95
Temperature [K]	100(2)	100(2) K	100(2)
Wavelength [Å]	0.56086	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a [Å]	a = 9.092(2) Å	13.873(2)	10.457(2)
b [Å]	b = 17.918(3) Å	17.388(3)	19.397(2)
c [Å]	c = 15.271(2) Å	22.812(4)	29.510(3)
α [°]	90	90	90
β [°]	94.99(2)	91.73(2)	97.95(2)
γ [°]	90	90	90
V [Å^3]	2478.4(8)	5500.3(16)	5928.1(15)
Z	4	4	4
ρ [Mgm^{-3}]	1.858	1.147	1.430
μ [mm^{-1}]	2.028	0.235	1.649
F (000)	1320	2056	2588
Crystal size [mm]	0.2 x 0.2 x 0.3	0.3 x 0.2 x 0.2	0.1 x 0.2 x 0.2
θ-area [°]	1.386 to 21.375	1.473 to 25.739	1.260 to 26.463
Index ranges	-11<=h<=11, -23<=k<=23, -19<=l<=19	-16<=h<=16, -21<=k<=21, -27<=l<=27	-13<=h<=13, -24<=k<=24, -36<=l<=36
Total number reflect.	72237	113490	157393
Unique reflections	5700	10489	12214
R_{int}	0.0363	0.0639	0.0553
Data / restraints /	5700 / 0 / 234	10489 / 1565 / 741	12214 / 918 / 750

parameters			
Goodness-of-fit on F^2	1.042	1.238	1.073
$R1$ [$I>2\sigma(I)$]	R1 = 0.0157	0.0696	0.0285
$wR2$ [$I>2\sigma(I)$]	wR2 = 0.0295	0.1545	0.0648
$R1$ [all data]	R1 = 0.0208	0.0773	0.0353
$wR2$ [all data]	wR2 = 0.0311	0.1572	0.0685
Largest diff. peak and hole	0.877 and -0.738	0.672 and -0.619	1.101 and -0.428
max. / min. [e·Å $^{-3}$]			

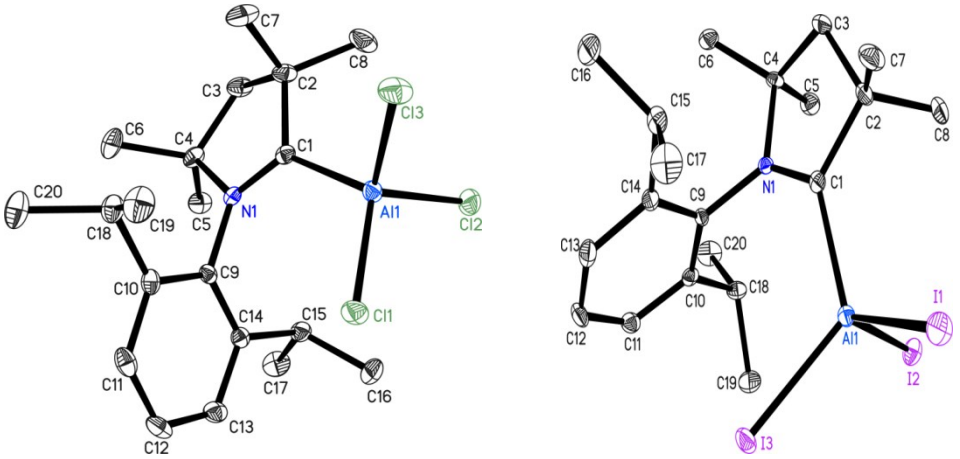


Figure S1. Molecular structure of **1a** (left) and **1b** (right) with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity.

In the structure of **1b**, close to I1 residual electron density peak with a height of about 0.88 eÅ^{-3} was found. It could be modelled as a disorder but the two positions refined very close to each other and the occupancy of the second position was under 10 %. Therefore we stayed with the model without disorder.

Table S2. Bond lengths [Å] and angles [°] for **1b**.

Al(1)-C(1)	2.0494(19)	C(2)-C(8)	1.538(3)
Al(1)-I(3)	2.5197(6)	C(2)-C(7)	1.543(3)
Al(1)-I(1)	2.5347(7)	C(2)-C(3)	1.546(3)
Al(1)-I(2)	2.5443(8)	C(3)-C(4)	1.526(3)
C(1)-N(1)	1.304(2)	C(4)-C(6)	1.517(2)
C(1)-C(2)	1.531(2)	C(4)-C(5)	1.536(3)

C(4)-N(1)	1.544(2)
N(1)-C(9)	1.466(2)
C(9)-C(10)	1.402(2)
C(9)-C(14)	1.412(2)
C(10)-C(11)	1.394(3)
C(10)-C(18)	1.514(3)
C(11)-C(12)	1.381(3)
C(12)-C(13)	1.386(3)
C(13)-C(14)	1.393(3)
C(14)-C(15)	1.525(2)
C(15)-C(17)	1.532(3)
C(15)-C(16)	1.537(3)
C(18)-C(19)	1.535(2)
C(18)-C(20)	1.539(3)

C(1)-Al(1)-I(3)	118.91(6)
C(1)-Al(1)-I(1)	113.76(6)
I(3)-Al(1)-I(1)	106.38(2)
C(1)-Al(1)-I(2)	98.07(5)
I(3)-Al(1)-I(2)	109.64(2)
I(1)-Al(1)-I(2)	109.65(2)
N(1)-C(1)-C(2)	109.60(15)
N(1)-C(1)-Al(1)	124.27(13)
C(2)-C(1)-Al(1)	124.85(13)
C(1)-C(2)-C(8)	112.96(15)
C(1)-C(2)-C(7)	108.93(15)
C(8)-C(2)-C(7)	108.29(16)
C(1)-C(2)-C(3)	103.14(14)
C(8)-C(2)-C(3)	113.82(16)
C(7)-C(2)-C(3)	109.54(15)
C(4)-C(3)-C(2)	106.59(14)
C(6)-C(4)-C(3)	115.51(15)
C(6)-C(4)-C(5)	109.95(15)
C(3)-C(4)-C(5)	110.98(15)
C(6)-C(4)-N(1)	111.27(14)
C(3)-C(4)-N(1)	99.33(14)
C(5)-C(4)-N(1)	109.29(14)
C(1)-N(1)-C(9)	122.65(15)
C(1)-N(1)-C(4)	113.91(14)
C(9)-N(1)-C(4)	122.64(14)
C(10)-C(9)-C(14)	122.41(16)
C(10)-C(9)-N(1)	122.24(15)
C(14)-C(9)-N(1)	115.34(15)
C(11)-C(10)-C(9)	117.16(17)
C(11)-C(10)-C(18)	118.66(16)
C(9)-C(10)-C(18)	124.18(16)
C(12)-C(11)-C(10)	121.86(17)
C(11)-C(12)-C(13)	119.80(18)
C(12)-C(13)-C(14)	121.29(17)
C(13)-C(14)-C(9)	117.37(16)
C(13)-C(14)-C(15)	118.40(16)
C(9)-C(14)-C(15)	124.22(16)
C(14)-C(15)-C(17)	111.52(16)
C(14)-C(15)-C(16)	111.14(15)
C(17)-C(15)-C(16)	110.52(16)
C(10)-C(18)-C(19)	112.00(15)
C(10)-C(18)-C(20)	109.93(15)
C(19)-C(18)-C(20)	109.36(15)

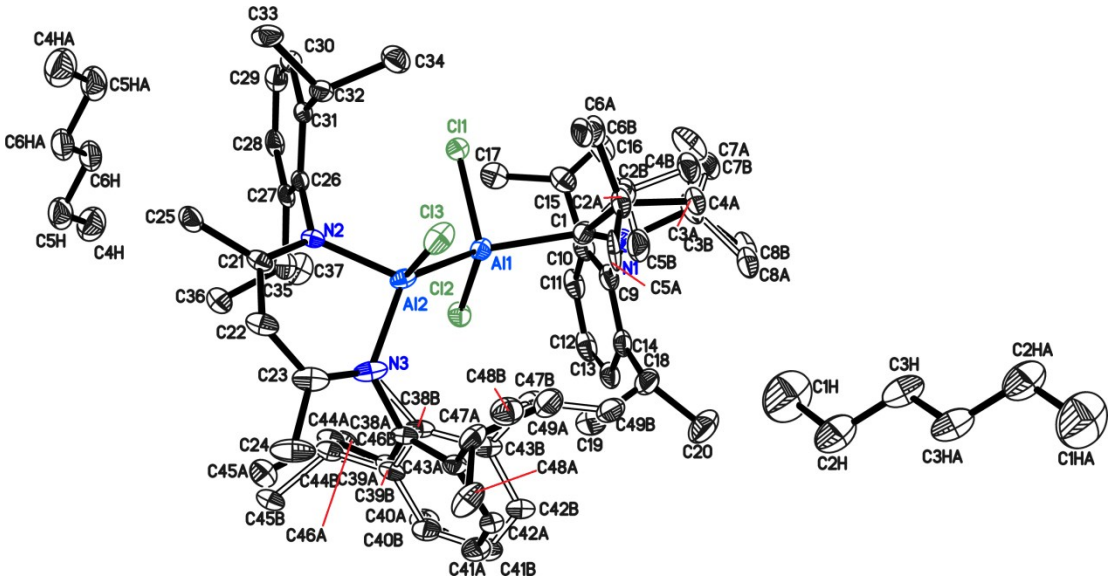


Figure S2. Molecular structure of **2a** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered ligands were refined on two positions. The occupancy of the main positions refined to 0.750(5) for C38-C46 and to 0.584(10) for C3-C6, respectively. For the disordered groups distance restraints and restraints for the anisotropic displacement parameters were used.[10]

Talble S3. Bond lengths [Å] and angles [°] for **2a**.

Cl(1)-Al(1)	2.1854(14)	C(9)-N(1)	1.477(5)
Cl(3)-Al(2)	2.1978(14)	C(10)-C(11)	1.402(5)
Al(1)-C(1)	2.098(4)	C(10)-C(15)	1.519(6)
Al(1)-Cl(2)	2.1669(14)	C(11)-C(12)	1.375(6)
Al(1)-Al(2)	2.5953(16)	C(12)-C(13)	1.381(6)
Al(2)-N(2)	1.917(3)	C(13)-C(14)	1.392(5)
Al(2)-N(3)	1.923(3)	C(14)-C(18)	1.525(6)
N(2)-C(21)	1.340(4)	C(15)-C(17)	1.532(6)
N(2)-C(26)	1.455(4)	C(15)-C(16)	1.536(6)
C(4H)-C(5H)	1.512(7)	C(18)-C(19)	1.534(6)
C(5H)-C(6H)	1.523(7)	C(18)-C(20)	1.537(5)
C(6H)-C(6H)#1	1.519(9)	C(21)-C(22)	1.395(5)
C(9)-C(10)	1.403(6)	C(21)-C(25)	1.507(5)
C(9)-C(14)	1.403(5)	C(22)-C(23)	1.384(5)

C(24)-C(23)	1.505(5)	C(39A)-C(40A)	1.391(7)
C(26)-C(31)	1.405(4)	C(39A)-C(44A)	1.519(6)
C(26)-C(27)	1.408(5)	C(40A)-C(41A)	1.391(8)
C(27)-C(28)	1.397(5)	C(41A)-C(42A)	1.379(8)
C(27)-C(35)	1.522(5)	C(42A)-C(43A)	1.397(6)
C(28)-C(29)	1.375(5)	C(43A)-C(47A)	1.519(6)
C(29)-C(30)	1.385(5)	C(47A)-C(49A)	1.524(7)
C(30)-C(31)	1.399(4)	C(47A)-C(48A)	1.532(6)
C(31)-C(32)	1.518(5)	C(44A)-C(46A)	1.534(7)
C(32)-C(34)	1.520(5)	C(44A)-C(45A)	1.538(7)
C(32)-C(33)	1.532(5)	C(38B)-C(39B)	1.422(12)
C(35)-C(37)	1.529(5)	C(38B)-C(43B)	1.433(12)
C(35)-C(36)	1.531(5)	C(39B)-C(40B)	1.403(13)
C(1H)-C(2H)	1.499(8)	C(39B)-C(44B)	1.520(13)
C(2H)-C(3H)	1.519(8)	C(40B)-C(41B)	1.379(13)
C(3H)-C(3H)#2	1.502(9)	C(41B)-C(42B)	1.374(13)
C(1)-N(1)	1.299(5)	C(42B)-C(43B)	1.412(12)
C(1)-C(2A)	1.535(8)	C(43B)-C(47B)	1.522(12)
C(1)-C(2B)	1.548(11)	C(47B)-C(49B)	1.520(12)
N(1)-C(3A)	1.546(9)	C(47B)-C(48B)	1.524(12)
N(1)-C(3B)	1.552(11)	C(44B)-C(46B)	1.521(13)
C(3A)-C(7A)	1.513(10)	C(44B)-C(45B)	1.522(13)
C(3A)-C(8A)	1.515(10)		
C(3A)-C(4A)	1.526(10)	C(1)-Al(1)-Cl(2)	107.50(11)
C(4A)-C(2A)	1.541(9)	C(1)-Al(1)-Cl(1)	93.80(11)
C(2A)-C(5A)	1.529(9)	Cl(2)-Al(1)-Cl(1)	108.32(6)
C(2A)-C(6A)	1.538(10)	C(1)-Al(1)-Al(2)	127.35(12)
C(3B)-C(7B)	1.529(12)	Cl(2)-Al(1)-Al(2)	109.89(6)
C(3B)-C(8B)	1.534(12)	Cl(1)-Al(1)-Al(2)	107.80(5)
C(3B)-C(4B)	1.534(13)	N(2)-Al(2)-N(3)	95.23(14)
C(4B)-C(2B)	1.542(12)	N(2)-Al(2)-Cl(3)	102.58(10)
C(2B)-C(5B)	1.516(12)	N(3)-Al(2)-Cl(3)	102.63(10)
C(2B)-C(6B)	1.530(12)	N(2)-Al(2)-Al(1)	112.68(9)
C(23)-N(3)	1.346(5)	N(3)-Al(2)-Al(1)	124.87(10)
N(3)-C(38A)	1.443(6)	Cl(3)-Al(2)-Al(1)	115.19(6)
N(3)-C(38B)	1.514(11)	C(21)-N(2)-C(26)	118.0(3)
C(38A)-C(43A)	1.397(7)	C(21)-N(2)-Al(2)	118.5(2)
C(38A)-C(39A)	1.399(6)	C(26)-N(2)-Al(2)	123.1(2)

C(4H)-C(5H)-C(6H)	113.2(4)	C(34)-C(32)-C(33)	109.2(3)
C(6H)#1-C(6H)-C(5H)	114.4(4)	C(27)-C(35)-C(37)	113.4(3)
C(10)-C(9)-C(14)	123.2(3)	C(27)-C(35)-C(36)	111.5(3)
C(10)-C(9)-N(1)	120.4(3)	C(37)-C(35)-C(36)	110.0(3)
C(14)-C(9)-N(1)	116.4(3)	C(1H)-C(2H)-C(3H)	113.5(5)
C(11)-C(10)-C(9)	116.5(4)	C(3H)#2-C(3H)-C(2H)	114.6(5)
C(11)-C(10)-C(15)	117.4(4)	N(1)-C(1)-C(2A)	110.8(4)
C(9)-C(10)-C(15)	126.0(3)	N(1)-C(1)-C(2B)	105.2(5)
C(12)-C(11)-C(10)	121.9(4)	N(1)-C(1)-Al(1)	129.7(3)
C(11)-C(12)-C(13)	119.7(4)	C(2A)-C(1)-Al(1)	119.4(4)
C(12)-C(13)-C(14)	121.9(4)	C(2B)-C(1)-Al(1)	123.8(5)
C(13)-C(14)-C(9)	116.8(4)	C(1)-N(1)-C(9)	124.6(3)
C(13)-C(14)-C(18)	118.5(4)	C(1)-N(1)-C(3A)	113.2(4)
C(9)-C(14)-C(18)	124.6(3)	C(9)-N(1)-C(3A)	122.1(4)
C(10)-C(15)-C(17)	111.3(3)	C(1)-N(1)-C(3B)	119.0(5)
C(10)-C(15)-C(16)	111.6(4)	C(9)-N(1)-C(3B)	116.4(5)
C(17)-C(15)-C(16)	108.1(3)	C(7A)-C(3A)-C(8A)	110.8(8)
C(14)-C(18)-C(19)	111.0(3)	C(7A)-C(3A)-C(4A)	112.4(7)
C(14)-C(18)-C(20)	111.5(4)	C(8A)-C(3A)-C(4A)	114.2(8)
C(19)-C(18)-C(20)	110.1(4)	C(7A)-C(3A)-N(1)	106.3(7)
N(2)-C(21)-C(22)	122.9(3)	C(8A)-C(3A)-N(1)	111.4(8)
N(2)-C(21)-C(25)	120.6(3)	C(4A)-C(3A)-N(1)	101.0(5)
C(22)-C(21)-C(25)	116.5(3)	C(3A)-C(4A)-C(2A)	107.0(6)
C(23)-C(22)-C(21)	127.9(3)	C(5A)-C(2A)-C(1)	111.0(7)
C(31)-C(26)-C(27)	121.5(3)	C(5A)-C(2A)-C(6A)	108.1(10)
C(31)-C(26)-N(2)	120.3(3)	C(1)-C(2A)-C(6A)	112.1(10)
C(27)-C(26)-N(2)	118.2(3)	C(5A)-C(2A)-C(4A)	110.1(7)
C(28)-C(27)-C(26)	118.0(3)	C(1)-C(2A)-C(4A)	103.3(5)
C(28)-C(27)-C(35)	120.2(3)	C(6A)-C(2A)-C(4A)	112.2(9)
C(26)-C(27)-C(35)	121.8(3)	C(7B)-C(3B)-C(8B)	106.8(9)
C(29)-C(28)-C(27)	121.3(3)	C(7B)-C(3B)-C(4B)	110.1(10)
C(28)-C(29)-C(30)	119.9(3)	C(8B)-C(3B)-C(4B)	113.1(11)
C(29)-C(30)-C(31)	121.4(3)	C(7B)-C(3B)-N(1)	115.2(9)
C(30)-C(31)-C(26)	117.7(3)	C(8B)-C(3B)-N(1)	111.7(11)
C(30)-C(31)-C(32)	119.0(3)	C(4B)-C(3B)-N(1)	100.1(7)
C(26)-C(31)-C(32)	123.2(3)	C(3B)-C(4B)-C(2B)	106.4(8)
C(31)-C(32)-C(34)	110.2(3)	C(5B)-C(2B)-C(6B)	109.9(13)
C(31)-C(32)-C(33)	112.0(3)	C(5B)-C(2B)-C(4B)	113.0(10)

C(6B)-C(2B)-C(4B)	112.8(12)	C(43A)-C(47A)-C(49A)	111.7(5)
C(5B)-C(2B)-C(1)	101.9(9)	C(43A)-C(47A)-C(48A)	111.7(4)
C(6B)-C(2B)-C(1)	111.7(13)	C(49A)-C(47A)-C(48A)	109.7(4)
C(4B)-C(2B)-C(1)	107.0(7)	C(39A)-C(44A)-C(46A)	113.0(6)
N(3)-C(23)-C(22)	122.5(3)	C(39A)-C(44A)-C(45A)	111.2(5)
N(3)-C(23)-C(24)	121.0(4)	C(46A)-C(44A)-C(45A)	108.8(6)
C(22)-C(23)-C(24)	116.6(4)	C(39B)-C(38B)-C(43B)	116.6(11)
C(23)-N(3)-C(38A)	114.9(4)	C(39B)-C(38B)-N(3)	113.4(10)
C(23)-N(3)-C(38B)	126.1(8)	C(43B)-C(38B)-N(3)	129.9(10)
C(23)-N(3)-Al(2)	118.2(2)	C(40B)-C(39B)-C(38B)	119.6(13)
C(38A)-N(3)-Al(2)	126.6(3)	C(40B)-C(39B)-C(44B)	118.5(13)
C(38B)-N(3)-Al(2)	114.8(8)	C(38B)-C(39B)-C(44B)	121.6(13)
C(43A)-C(38A)-C(39A)	122.3(5)	C(41B)-C(40B)-C(39B)	122.6(16)
C(43A)-C(38A)-N(3)	118.2(4)	C(42B)-C(41B)-C(40B)	119.5(17)
C(39A)-C(38A)-N(3)	119.4(5)	C(41B)-C(42B)-C(43B)	120.0(13)
C(40A)-C(39A)-C(38A)	118.0(5)	C(42B)-C(43B)-C(38B)	121.5(10)
C(40A)-C(39A)-C(44A)	119.6(5)	C(42B)-C(43B)-C(47B)	115.5(10)
C(38A)-C(39A)-C(44A)	122.0(5)	C(38B)-C(43B)-C(47B)	123.0(10)
C(39A)-C(40A)-C(41A)	120.8(6)	C(49B)-C(47B)-C(43B)	114.8(10)
C(42A)-C(41A)-C(40A)	120.0(6)	C(49B)-C(47B)-C(48B)	110.1(12)
C(41A)-C(42A)-C(43A)	121.2(5)	C(43B)-C(47B)-C(48B)	112.2(11)
C(38A)-C(43A)-C(42A)	117.7(4)	C(39B)-C(44B)-C(46B)	112.8(16)
C(38A)-C(43A)-C(47A)	124.4(4)	C(39B)-C(44B)-C(45B)	112.0(14)
C(42A)-C(43A)-C(47A)	117.9(4)	C(46B)-C(44B)-C(45B)	111.3(17)

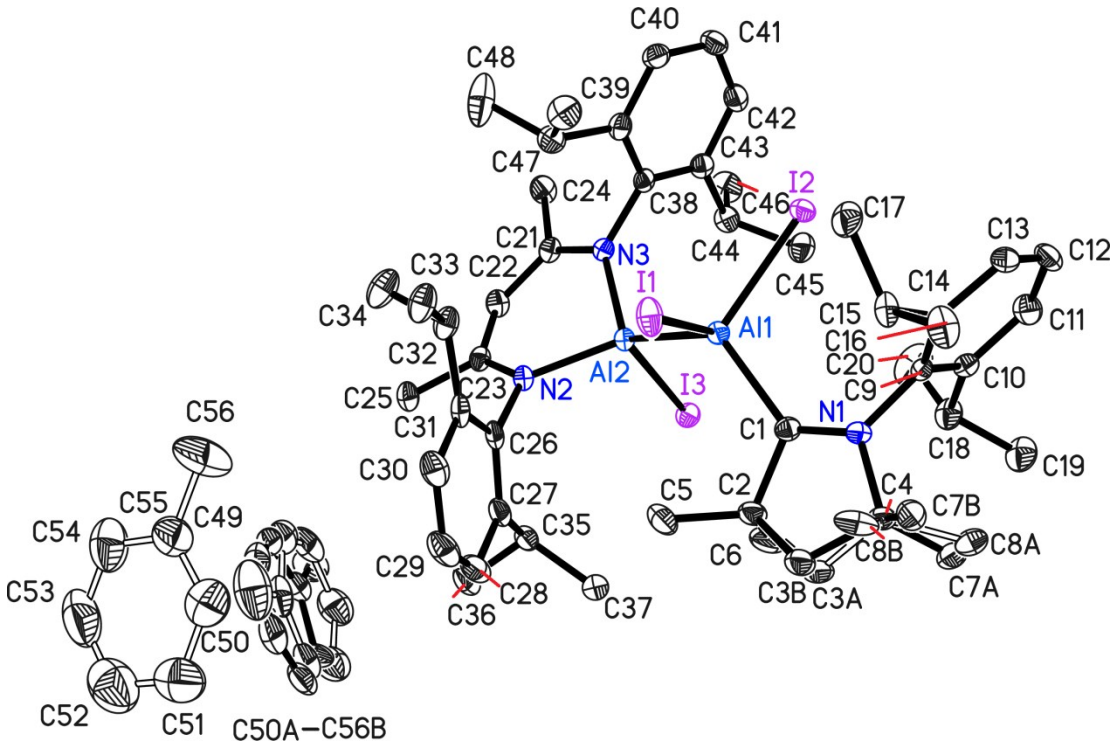


Figure S3. Molecular structure of **2b** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered toluene was refined on two positions. The occupancy of the main position refined to 0.557(6). The disordered ligand was refined on two positions. The occupancy of the main positions refined to 0.877(8). For the disordered groups distance restraints and restraints for the anisotropic displacement parameters were used.[10]

Talble S4. Bond lengths [Å] and angles [°] for **2b**.

I(1)-Al(1)	2.6077(9)	N(3)-C(38)	1.458(3)
Al(1)-C(1)	2.094(3)	N(1)-C(1)	1.304(3)
Al(1)-I(2)	2.5537(8)	N(1)-C(9)	1.470(3)
Al(1)-Al(2)	2.6327(11)	N(1)-C(4)	1.549(3)
Al(2)-N(3)	1.919(2)	C(1)-C(2)	1.535(4)
Al(2)-N(2)	1.931(2)	C(2)-C(5)	1.527(4)
Al(2)-I(3)	2.6258(9)	C(2)-C(6)	1.534(4)
N(2)-C(23)	1.341(3)	C(2)-C(3A)	1.534(4)
N(2)-C(26)	1.457(3)	C(2)-C(3B)	1.543(14)
N(3)-C(21)	1.335(3)	C(3A)-C(4)	1.522(4)

C(4)-C(7B)	1.500(12)	C(41)-C(42)	1.378(4)
C(4)-C(8A)	1.510(4)	C(42)-C(43)	1.392(4)
C(4)-C(3B)	1.522(14)	C(43)-C(44)	1.515(4)
C(4)-C(7A)	1.528(4)	C(44)-C(45)	1.528(4)
C(4)-C(8B)	1.540(13)	C(44)-C(46)	1.535(4)
C(9)-C(14)	1.405(4)	C(47)-C(49)	1.519(4)
C(9)-C(10)	1.409(3)	C(47)-C(48)	1.532(4)
C(10)-C(11)	1.391(4)	C(50)-C(51)	1.361(11)
C(10)-C(18)	1.521(4)	C(50)-C(55)	1.373(11)
C(11)-C(12)	1.372(4)	C(50)-C(56)	1.482(13)
C(12)-C(13)	1.385(4)	C(51)-C(52)	1.383(11)
C(13)-C(14)	1.395(4)	C(52)-C(53)	1.376(12)
C(14)-C(15)	1.520(3)	C(53)-C(54)	1.380(12)
C(15)-C(17)	1.532(4)	C(54)-C(55)	1.360(11)
C(15)-C(16)	1.543(4)	C(50A)-C(51A)	1.380(9)
C(18)-C(20)	1.524(4)	C(50A)-C(55A)	1.397(8)
C(18)-C(19)	1.535(4)	C(50A)-C(56A)	1.485(9)
C(21)-C(22)	1.393(4)	C(51A)-C(53A)	1.370(9)
C(21)-C(24)	1.505(4)	C(53A)-C(52A)	1.388(9)
C(22)-C(23)	1.393(4)	C(52A)-C(54A)	1.355(9)
C(23)-C(25)	1.511(3)	C(54A)-C(55A)	1.385(8)
C(26)-C(27)	1.402(4)	C(50B)-C(51B)	1.373(10)
C(26)-C(31)	1.411(4)	C(50B)-C(55B)	1.388(11)
C(27)-C(28)	1.404(4)	C(50B)-C(56B)	1.497(11)
C(27)-C(35)	1.522(4)	C(51B)-C(52B)	1.350(10)
C(28)-C(29)	1.374(4)	C(52B)-C(53B)	1.364(10)
C(29)-C(30)	1.378(5)	C(53B)-C(54B)	1.383(10)
C(30)-C(31)	1.389(4)	C(54B)-C(55B)	1.371(11)
C(31)-C(32)	1.526(4)		
C(32)-C(33)	1.528(4)	C(1)-Al(1)-I(2)	110.61(8)
C(32)-C(34)	1.539(4)	C(1)-Al(1)-I(1)	91.24(8)
C(35)-C(36)	1.530(4)	I(2)-Al(1)-I(1)	105.25(3)
C(35)-C(37)	1.533(4)	C(1)-Al(1)-Al(2)	124.44(8)
C(38)-C(39)	1.402(4)	I(2)-Al(1)-Al(2)	107.50(3)
C(38)-C(43)	1.407(4)	I(1)-Al(1)-Al(2)	115.78(3)
C(39)-C(40)	1.393(4)	N(3)-Al(2)-N(2)	96.30(9)
C(39)-C(47)	1.515(4)	N(3)-Al(2)-I(3)	101.17(7)
C(40)-C(41)	1.376(4)	N(2)-Al(2)-I(3)	102.48(7)

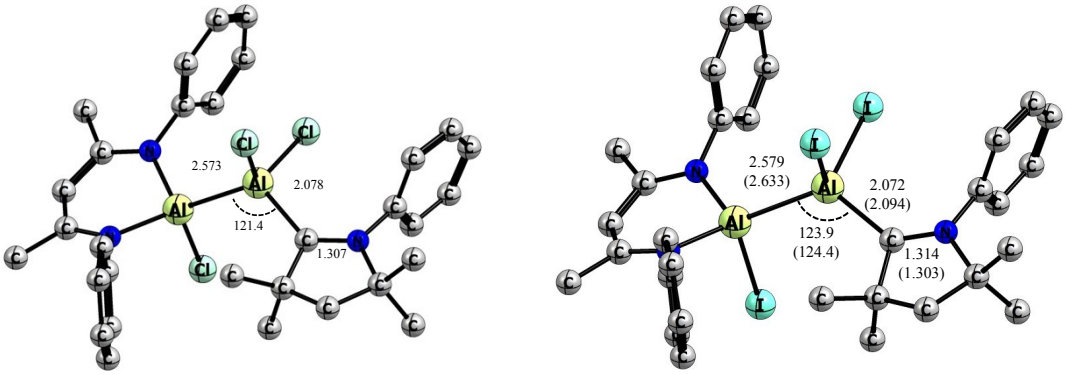
N(3)-Al(2)-Al(1)	118.30(7)	C(14)-C(9)-C(10)	121.8(2)
N(2)-Al(2)-Al(1)	126.24(7)	C(14)-C(9)-N(1)	121.2(2)
I(3)-Al(2)-Al(1)	108.77(3)	C(10)-C(9)-N(1)	117.0(2)
C(23)-N(2)-C(26)	117.8(2)	C(11)-C(10)-C(9)	117.7(2)
C(23)-N(2)-Al(2)	120.02(17)	C(11)-C(10)-C(18)	117.5(2)
C(26)-N(2)-Al(2)	121.96(16)	C(9)-C(10)-C(18)	124.8(2)
C(21)-N(3)-C(38)	115.7(2)	C(12)-C(11)-C(10)	121.8(3)
C(21)-N(3)-Al(2)	119.41(18)	C(11)-C(12)-C(13)	119.6(2)
C(38)-N(3)-Al(2)	124.86(16)	C(12)-C(13)-C(14)	121.6(2)
C(1)-N(1)-C(9)	126.2(2)	C(13)-C(14)-C(9)	117.4(2)
C(1)-N(1)-C(4)	115.1(2)	C(13)-C(14)-C(15)	116.8(2)
C(9)-N(1)-C(4)	118.14(19)	C(9)-C(14)-C(15)	125.6(2)
N(1)-C(1)-C(2)	108.6(2)	C(14)-C(15)-C(17)	110.6(2)
N(1)-C(1)-Al(1)	131.54(19)	C(14)-C(15)-C(16)	112.1(2)
C(2)-C(1)-Al(1)	119.34(18)	C(17)-C(15)-C(16)	108.0(2)
C(5)-C(2)-C(6)	108.9(3)	C(10)-C(18)-C(20)	111.0(2)
C(5)-C(2)-C(3A)	109.6(3)	C(10)-C(18)-C(19)	112.4(2)
C(6)-C(2)-C(3A)	114.2(3)	C(20)-C(18)-C(19)	109.9(2)
C(5)-C(2)-C(1)	115.2(2)	N(3)-C(21)-C(22)	124.0(2)
C(6)-C(2)-C(1)	106.0(2)	N(3)-C(21)-C(24)	120.3(2)
C(3A)-C(2)-C(1)	103.0(2)	C(22)-C(21)-C(24)	115.7(2)
C(5)-C(2)-C(3B)	123.3(11)	C(23)-C(22)-C(21)	127.7(2)
C(6)-C(2)-C(3B)	94.3(12)	N(2)-C(23)-C(22)	122.9(2)
C(1)-C(2)-C(3B)	106.1(6)	N(2)-C(23)-C(25)	121.2(2)
C(4)-C(3A)-C(2)	107.0(3)	C(22)-C(23)-C(25)	115.9(2)
C(8A)-C(4)-C(3A)	112.1(3)	C(27)-C(26)-C(31)	121.6(2)
C(7B)-C(4)-C(3B)	116.2(14)	C(27)-C(26)-N(2)	120.0(2)
C(8A)-C(4)-C(7A)	107.7(3)	C(31)-C(26)-N(2)	118.3(2)
C(3A)-C(4)-C(7A)	114.3(3)	C(26)-C(27)-C(28)	117.7(3)
C(7B)-C(4)-C(8B)	110.8(14)	C(26)-C(27)-C(35)	124.1(2)
C(3B)-C(4)-C(8B)	102.9(14)	C(28)-C(27)-C(35)	118.2(3)
C(7B)-C(4)-N(1)	114.6(10)	C(29)-C(28)-C(27)	121.2(3)
C(8A)-C(4)-N(1)	111.7(2)	C(28)-C(29)-C(30)	120.1(3)
C(3A)-C(4)-N(1)	100.2(2)	C(29)-C(30)-C(31)	121.6(3)
C(3B)-C(4)-N(1)	102.3(6)	C(30)-C(31)-C(26)	117.6(3)
C(7A)-C(4)-N(1)	110.9(3)	C(30)-C(31)-C(32)	120.3(2)
C(8B)-C(4)-N(1)	109.2(10)	C(26)-C(31)-C(32)	122.0(2)
C(4)-C(3B)-C(2)	106.5(9)	C(31)-C(32)-C(33)	113.7(2)

C(31)-C(32)-C(34)	113.1(2)		
C(33)-C(32)-C(34)	107.1(2)	C(51)-C(50)-C(56)	120.8(9)
C(27)-C(35)-C(36)	111.6(2)	C(55)-C(50)-C(56)	120.4(10)
C(27)-C(35)-C(37)	112.3(2)	C(50)-C(51)-C(52)	122.4(10)
C(36)-C(35)-C(37)	108.4(2)	C(53)-C(52)-C(51)	117.4(11)
C(39)-C(38)-C(43)	121.5(2)	C(52)-C(53)-C(54)	120.8(12)
C(39)-C(38)-N(3)	117.6(2)	C(55)-C(54)-C(53)	120.0(11)
C(43)-C(38)-N(3)	120.8(2)	C(54)-C(55)-C(50)	120.4(11)
C(40)-C(39)-C(38)	118.3(2)	C(51A)-C(50A)-C(55A)	117.4(6)
C(40)-C(39)-C(47)	119.2(2)	C(51A)-C(50A)-C(56A)	122.5(6)
C(38)-C(39)-C(47)	122.4(2)	C(55A)-C(50A)-C(56A)	120.1(6)
C(41)-C(40)-C(39)	121.0(3)	C(53A)-C(51A)-C(50A)	121.9(8)
C(40)-C(41)-C(42)	119.9(3)	C(51A)-C(53A)-C(52A)	120.3(7)
C(41)-C(42)-C(43)	121.8(3)	C(54A)-C(52A)-C(53A)	118.5(7)
C(42)-C(43)-C(38)	117.5(2)	C(52A)-C(54A)-C(55A)	121.8(7)
C(42)-C(43)-C(44)	119.0(2)	C(54A)-C(55A)-C(50A)	120.1(7)
C(38)-C(43)-C(44)	123.5(2)	C(51B)-C(50B)-C(55B)	118.8(8)
C(43)-C(44)-C(45)	110.7(2)	C(51B)-C(50B)-C(56B)	120.2(10)
C(43)-C(44)-C(46)	112.4(2)	C(55B)-C(50B)-C(56B)	121.0(10)
C(45)-C(44)-C(46)	109.9(2)	C(52B)-C(51B)-C(50B)	120.5(9)
C(39)-C(47)-C(49)	112.9(2)	C(51B)-C(52B)-C(53B)	121.3(9)
C(39)-C(47)-C(48)	111.0(3)	C(52B)-C(53B)-C(54B)	119.2(8)
C(49)-C(47)-C(48)	110.1(2)	C(55B)-C(54B)-C(53B)	119.5(9)
C(51)-C(50)-C(55)	118.9(9)	C(54B)-C(55B)-C(50B)	120.5(10)

S3. Theoretical Calculations

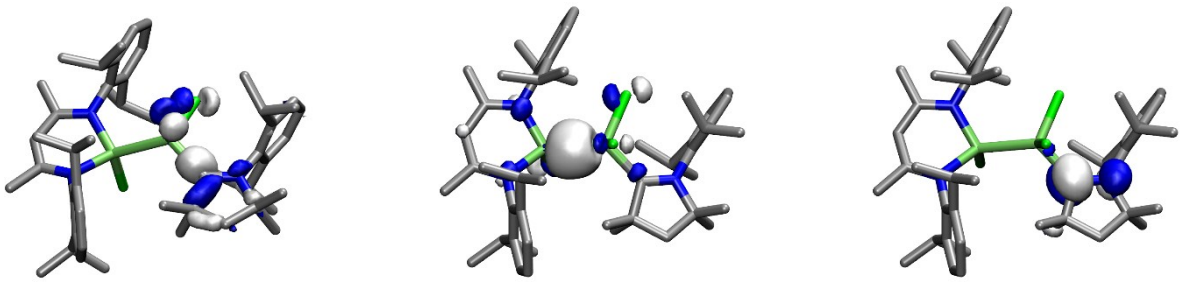
Geometry optimizations were performed using the Gaussian 09 optimizer[11] together with TurboMole V7.0.[12] energies and gradients. All geometry optimizations were computed using the functional BP86[13] functional in combination with the def2-TZVPP basis set.[14] In the case of BP86 the dispersion interactions were estimated using the D3 approximations of Grimme with Becke-Johnson (BJ) damping.[15] The stationary points were located with the Berny algorithm[16] using redundant internal coordinates. Analytical Hessians were computed to determine the nature of stationary points (one and zero imaginary frequencies for transition states and minima,

respectively)[17] and to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects using the standard statistical-mechanics relationships for an ideal gas.[18] The atomic partial charges have been estimated with the natural bond orbital (NBO)[19] method using NBO 5.9.[20]



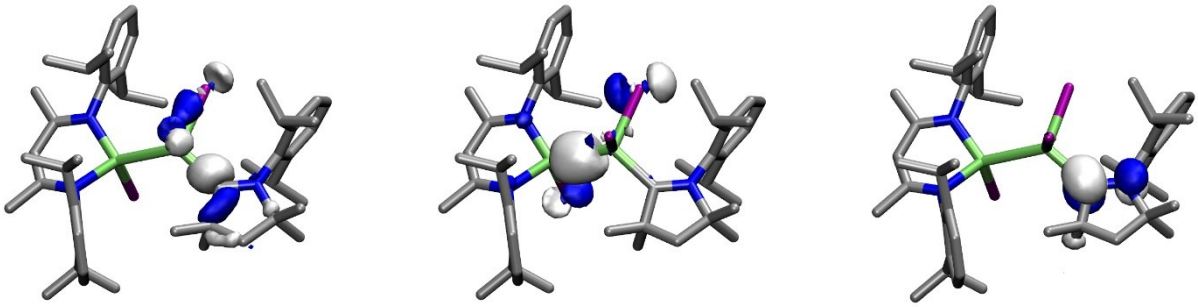
2a **2b**

Figure S4. X-ray structure (in parenthesis) and optimized geometry at the BP86+D3(BJ)/def2-TZVPP level of theory. Bond distances and angles are in Å and [°], respectively. Hydrogen atoms and isopropyl groups were omitted for clarity.



HOMO-15 (-7.34 eV) HOMO (-4.82 eV) LUMO (-2.54 eV)

2a



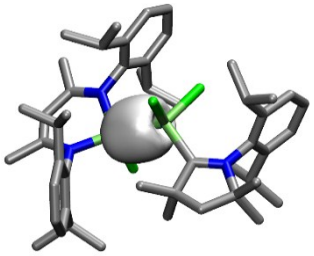
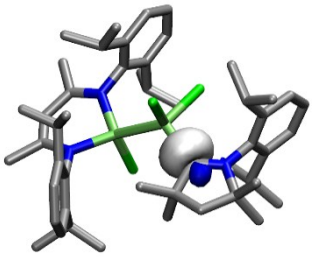
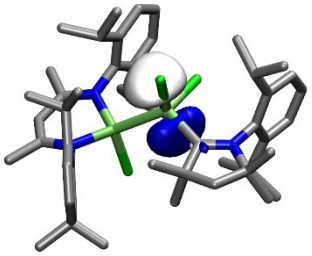
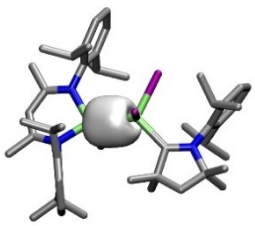
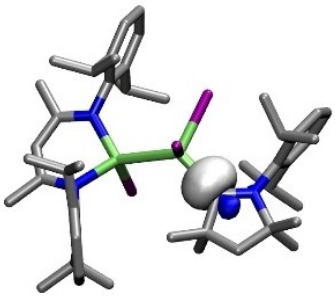
HOMO-15 (-6.97 eV) HOMO (-4.76 eV) LUMO (-2.66 eV)

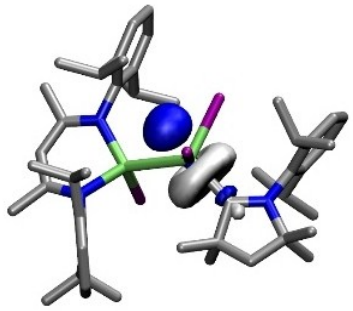
2b

Figure S5. Molecular orbital and energies at the BP86+D3(BJ)/def2-TZVPP level of theory.

2a **2b**

Figure S6. NBO charges at the BP86+D3(BJ)/def2-TZVPP of compound **2a** and **2b**.

Orbital	Occ.	Contribution from atoms to the orb	Atomic orbitals
		2a	
	1.94	Al (51.74 %) - Al (48.26%)	Al: s (53.96%) p (45.44%) d (0.59%) Al: s (58.47%) p (41.11%) d (0.41%)
	1.67	C	C: s (37.74%) p (62.18%) d (0.08%)
	0.28	Al	Al: s (0.02%) p (99.40%) d (0.55%)
		2b	
	1.93	Al (52.23 %) - Al (47.77%)	Al: s (40.05%) p (59.31%) d (0.63%) Al: s (59.11%) p (40.57%) d (0.32%)
	1.67	C	C: s (37.69%) p (62.22%) d (0.08%)



0.34	Al	Al: s (10.53%) p (89.14%) d (0.32%)

Figure S7. NBO results at the BP86/def2-TZVPP//BP86/def2-SVP of compound **2a** and **2b**.

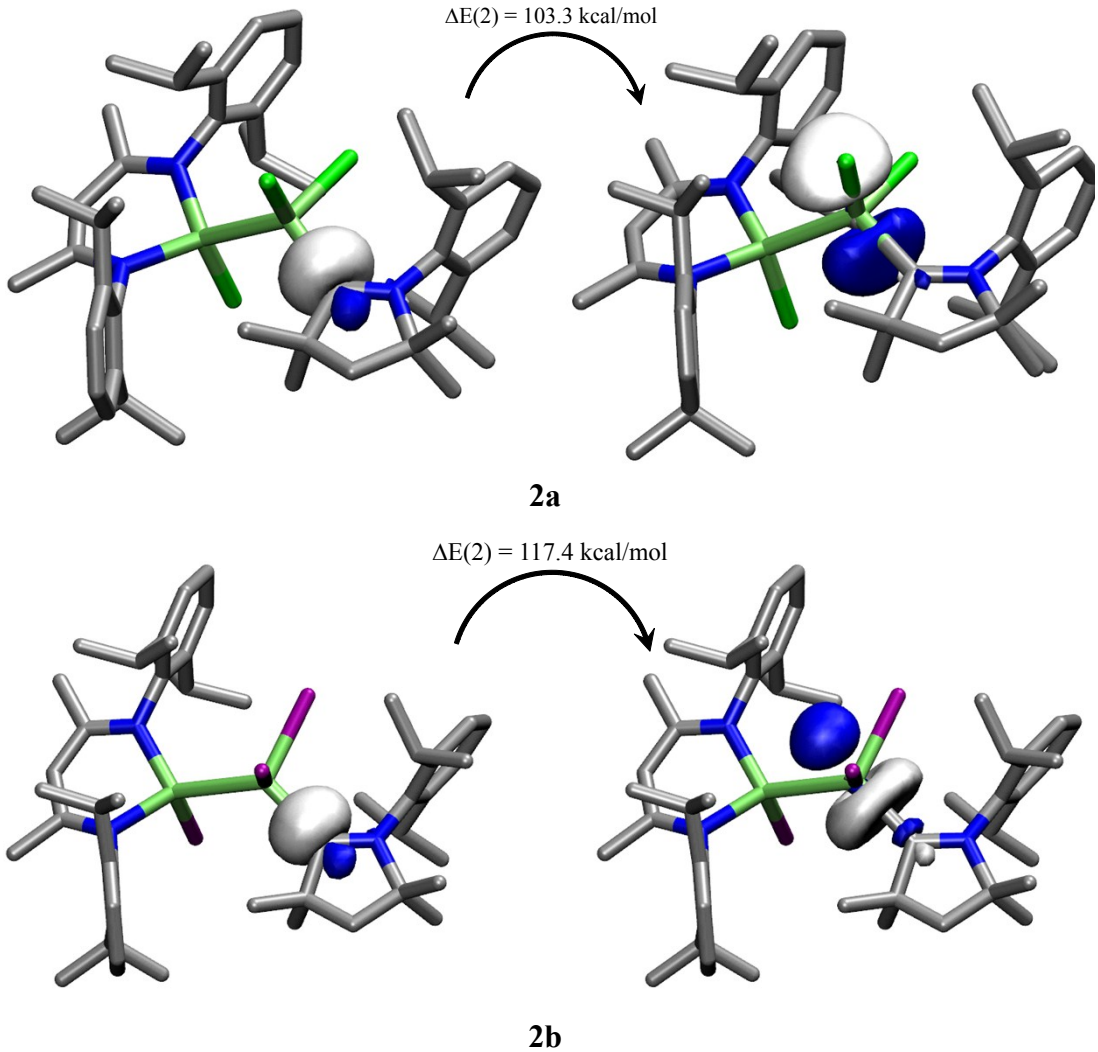


Figure S8. NBO perturbative energy in kcal/mol.

Cartesian coordinates and Electronic energies at the BP86+D3(BJ)/def2-TZVPP level of theory.

2a

E(BP86+D3(BJ)/def2-TZVPP) = -3942.0491520850

Cl	-0.238192	9.002971	24.277920
Al	1.721807	10.015681	24.339498
Cl	2.044437	10.815715	26.341760
Al	2.186258	11.970184	22.732616
N	1.627945	12.182226	20.887377
Cl	4.358990	12.310992	22.594806
N	1.447281	13.643628	23.350262
N	3.203449	7.417359	25.098616
C	2.736463	8.210475	24.170161
C	2.922087	7.555985	22.815802
C	1.730418	7.714479	21.873868
H	1.959003	7.237568	20.911945
H	1.525072	8.771938	21.671973
H	0.821725	7.269965	22.293865
C	4.139063	8.274871	22.187249
H	4.284793	7.905543	21.163699
H	5.062921	8.111183	22.755475
H	3.964523	9.357218	22.139710
C	3.207052	6.074388	23.143811
H	2.282421	5.494965	23.019759
H	3.963447	5.642383	22.477171
C	3.655249	6.025684	24.612226
C	5.163370	5.836611	24.781979
H	5.415427	4.808169	24.493171
H	5.462816	5.976121	25.827575
H	5.747352	6.515044	24.152092
C	2.931912	4.941036	25.401922
H	1.844710	5.045482	25.322811
H	3.218554	4.962039	26.460227
H	3.214156	3.962381	24.992184
C	3.414509	7.789833	26.489057
C	4.636399	8.420237	26.814495
C	4.875296	8.722861	28.158920
H	5.803667	9.223225	28.431867
C	3.942319	8.417831	29.144088
H	4.148598	8.660143	30.186595
C	2.730750	7.836792	28.790181
H	1.981934	7.646992	29.558437

C	2.425895	7.523268	27.459251
C	1.021093	7.026545	27.149055
H	0.928815	6.892472	26.062755
C	0.694473	5.698317	27.853418
H	-0.308737	5.356950	27.563150
H	0.693494	5.830345	28.944349
H	1.408741	4.901426	27.617844
C	-0.021191	8.082232	27.565110
H	0.210287	9.062955	27.140126
H	-0.056494	8.179417	28.659588
H	-1.017144	7.779878	27.216022
C	5.653492	8.869373	25.776059
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C	7.087701	8.443024	26.121982
H	7.167233	7.363655	26.305226
H	7.453089	8.961633	27.018561
H	7.765263	8.703153	25.297307
C	5.577171	10.388772	25.572559
H	6.283510	10.711881	24.796847
H	5.812861	10.921501	26.503993
H	4.573031	10.696916	25.265189
C	1.275230	14.684856	22.522963
C	1.356791	14.572454	21.125960
H	1.216097	15.494014	20.567000
C	1.429663	13.401108	20.358315
C	0.938267	16.040637	23.086424
H	0.597623	16.716116	22.295603
H	1.823083	16.481270	23.564924
H	0.166707	15.966717	23.862028
C	1.249892	13.565190	18.869563
H	0.826955	12.668939	18.404934
H	2.225428	13.752984	18.400270
H	0.605340	14.423902	18.654241
C	1.537618	11.022335	20.038979
C	2.633937	10.614505	19.245428
C	2.489567	9.455056	18.468860
H	3.327362	9.123428	17.854432
C	1.296863	8.741515	18.443968
H	1.203623	7.851250	17.821445
C	0.219389	9.167914	19.218399
H	-0.709594	8.600919	19.202076
C	0.319565	10.297302	20.037156
C	-0.860477	10.748362	20.884387
H	-0.448520	11.111856	21.839700

C	-1.844055	9.621658	21.212180
H	-2.409972	9.305686	20.323504
H	-2.570061	9.974843	21.955653
H	-1.334974	8.750321	21.639001
C	3.927034	11.410230	19.133065
H	3.840178	12.296033	19.775536
C	-1.612137	11.916794	20.221707
H	-1.941331	11.636117	19.210952
H	-0.994776	12.818256	20.145723
H	-2.503094	12.174745	20.809565
C	4.161871	11.868239	17.680674
H	4.399475	11.012083	17.033350
H	5.010678	12.564393	17.634948
H	3.283002	12.365926	17.252975
C	5.150174	10.618238	19.617551
H	5.259740	9.677013	19.059509
H	5.078045	10.392586	20.685029
H	6.063996	11.208947	19.465516
C	1.160031	13.827904	24.753640
C	-0.093386	13.390199	25.240674
C	-0.380228	13.582883	26.595266
H	-1.334925	13.244651	26.993203
C	0.544523	14.177795	27.450484
H	0.304778	14.311171	28.505485
C	1.781805	14.576260	26.959280
H	2.514280	15.015593	27.636965
C	2.117227	14.408922	25.609457
C	3.508304	14.800921	25.140957
H	3.555889	14.666515	24.052088
C	4.550117	13.857534	25.761756
H	4.294175	12.813498	25.560462
H	4.594087	13.990660	26.852543
H	5.547704	14.054605	25.346070
C	3.853676	16.262655	25.466598
H	4.833171	16.524429	25.043003
H	3.907524	16.426512	26.552129
H	3.110725	16.965978	25.066486
C	-1.105080	12.723644	24.321356
H	-0.533165	12.072219	23.638273
C	-1.861698	13.749611	23.459653
H	-1.200197	14.277969	22.763937
H	-2.357145	14.493941	24.099523
H	-2.636013	13.247162	22.864077
C	-2.103148	11.831762	25.064648

H	-2.682313	11.243461	24.341135
H	-2.816086	12.428061	25.652723
H	-1.594142	11.127719	25.732673

2b

E(BP86+D3(BJ)/def2-TZVPP) = -3454.8236882800

I	-0.365812	8.612620	24.006869
Al	1.839353	9.982129	24.306034
I	1.893268	10.930553	26.690833
Al	2.177162	11.984321	22.715406
N	1.582882	12.170060	20.874842
I	4.746323	12.412804	22.483380
N	1.496416	13.681813	23.338536
N	3.287011	7.378659	25.128041
C	2.915753	8.215375	24.185435
C	3.291863	7.630341	22.830977
C	2.289826	7.864076	21.702988
H	2.699503	7.465971	20.765992
H	2.098706	8.933227	21.545351
H	1.329256	7.381870	21.909235
C	4.621848	8.325176	22.447376
H	4.911893	7.993769	21.442185
H	5.437485	8.083056	23.136786
H	4.512882	9.418134	22.435859
C	3.488694	6.130242	23.122969
H	2.555197	5.598193	22.895051
H	4.285934	5.690370	22.511210
C	3.794509	6.012575	24.622202
C	5.278795	5.816210	24.939651
H	5.564214	4.801472	24.634258
H	5.462952	5.907879	26.016909
H	5.926574	6.520235	24.409503
C	3.009954	4.880837	25.273484
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H	3.213130	4.825916	26.348961
H	3.328870	3.932982	24.820152
C	3.400281	7.696061	26.545864
C	4.575400	8.364840	26.965302
C	4.727109	8.631401	28.329505
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C	3.762353	8.247023	29.252939
H	3.899661	8.464104	30.312127
C	2.608407	7.610978	28.814573
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C	2.385677	7.333261	27.459362
C	1.027391	6.759035	27.080564
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C	0.765092	5.384589	27.721511
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H	1.543397	4.647386	27.497304
C	-0.102017	7.715581	27.505447
H	0.054136	8.724901	27.112954
H	-0.164410	7.780610	28.600903
H	-1.064383	7.345003	27.128795
C	5.654913	8.863124	26.016166
H	5.467246	8.432931	25.029178
C	7.064123	8.431060	26.450826
H	7.131655	7.348547	26.618788
H	7.367905	8.932657	27.379486
H	7.794763	8.706909	25.678141
C	5.592766	10.387403	25.848437
H	6.379320	10.730733	25.163790
H	5.719424	10.897742	26.812945
H	4.629164	10.705947	25.437423
C	1.369816	14.710920	22.483568
C	1.490281	14.575774	21.092073
H	1.417697	15.498094	20.521679
C	1.486784	13.397011	20.333454
C	1.029381	16.081650	23.007025
H	0.799129	16.762532	22.182151
H	1.865664	16.495895	23.583652
H	0.172771	16.036343	23.691245
C	1.331016	13.571664	18.843886
H	2.315785	13.768815	18.398112
H	0.688978	14.431498	18.624892
H	0.916690	12.680293	18.364138
C	1.364162	11.006932	20.047769
C	2.381552	10.506906	19.202192
C	2.126763	9.328569	18.485338
H	2.904719	8.929620	17.833881
C	0.910216	8.666453	18.585333
H	0.738950	7.744103	18.029974
C	-0.099098	9.196933	19.386369
H	-1.059207	8.688505	19.441474
C	0.094743	10.375533	20.114025
C	-1.063743	11.002948	20.877202
H	-0.677664	11.330612	21.855387

C	-2.231692	10.045010	21.128214
H	-2.773006	9.822858	20.196741
H	-2.946365	10.513561	21.817721
H	-1.901502	9.103516	21.580412
C	3.713824	11.206393	18.975960
H	3.744576	12.105776	19.605559
C	-1.599809	12.242318	20.132391
H	-1.833178	11.986419	19.089114
H	-0.890759	13.075452	20.135010
H	-2.523636	12.596955	20.607494
C	3.875437	11.621269	17.500932
H	3.995282	10.737564	16.858327
H	4.772674	12.243789	17.379517
H	3.011857	12.182961	17.126086
C	4.903419	10.328129	19.384298
H	4.926207	9.395910	18.801338
H	4.859300	10.078358	20.446842
H	5.846948	10.862477	19.208833
C	1.180572	13.938541	24.727433
C	-0.089795	13.546840	25.205154
C	-0.437523	13.874556	26.518769
H	-1.410658	13.576479	26.904247
C	0.454677	14.542937	27.353107
H	0.170498	14.781877	28.377961
C	1.721177	14.871242	26.883816
H	2.432760	15.357551	27.551268
C	2.112196	14.578716	25.570701
C	3.534013	14.897676	25.141666
H	3.623888	14.697792	24.065311
C	4.512664	13.957570	25.863568
H	4.236228	12.909980	25.706206
H	4.504074	14.146958	26.946796
H	5.534979	14.103622	25.489466
C	3.927842	16.361042	25.394647
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H	3.950329	16.589753	26.469407
H	3.233798	17.070146	24.923275
C	-1.054272	12.773226	24.323617
H	-0.441139	12.108481	23.690021
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H	-2.395931	14.453073	23.984190
H	-2.576907	13.132614	22.808788
C	-2.006797	11.874218	25.116160

H	-2.544236	11.207360	24.429723
H	-2.756945	12.461725	25.664891
H	-1.459032	11.247492	25.830735

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