Electronic supplementary information

One Silicon Atom of Bis(silylene) Functions as a Selective Lewis Base under Adduct Formation with a Lewis Acid

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NMR Spectra

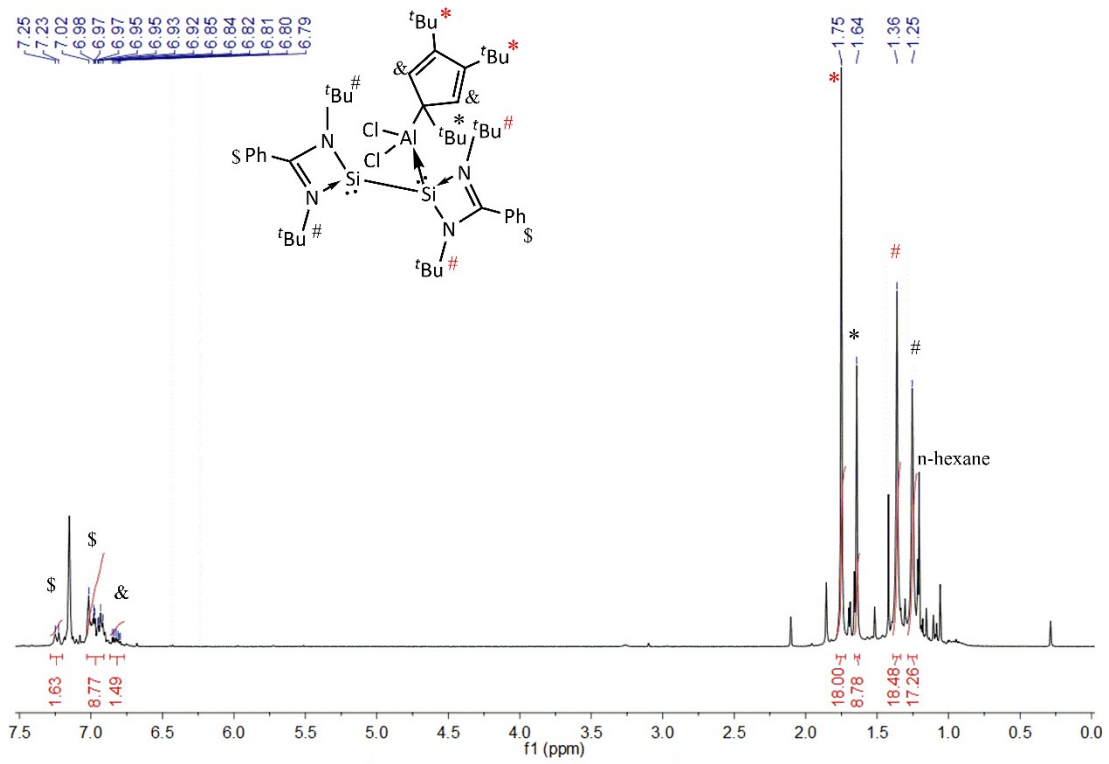

Figure S1.1 ^{1}H NMR of compound **1**.

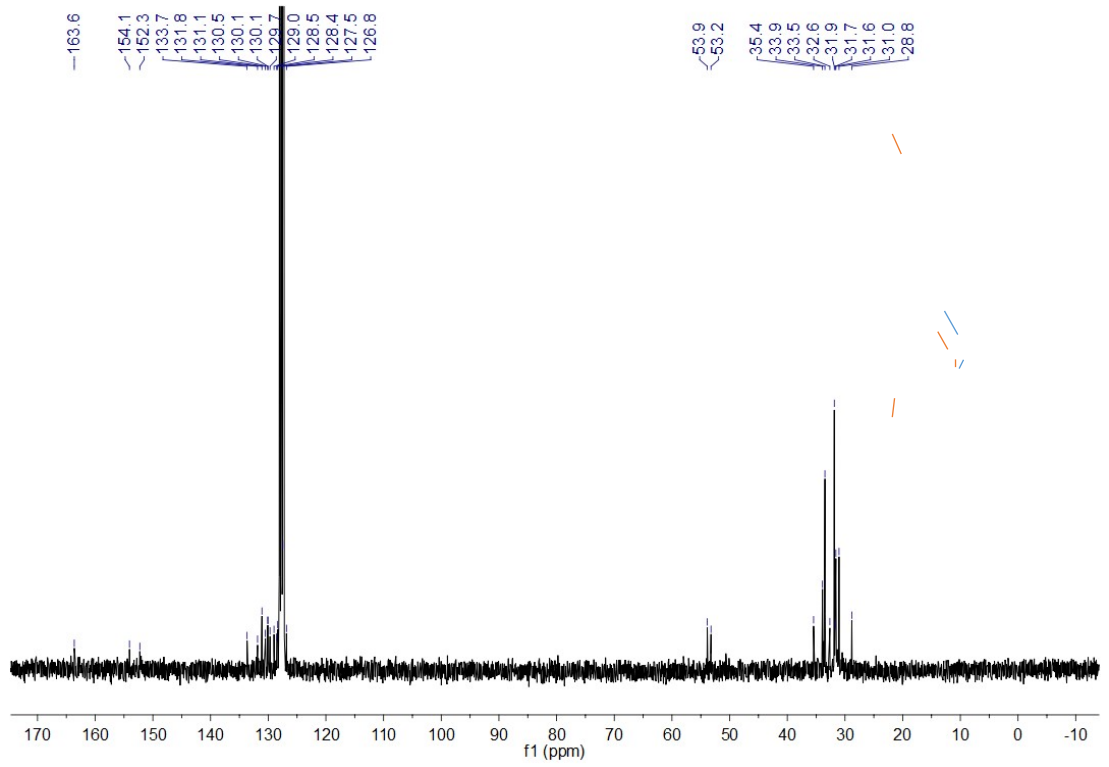

Figure S1.2 ^{13}C NMR of compound **1**.

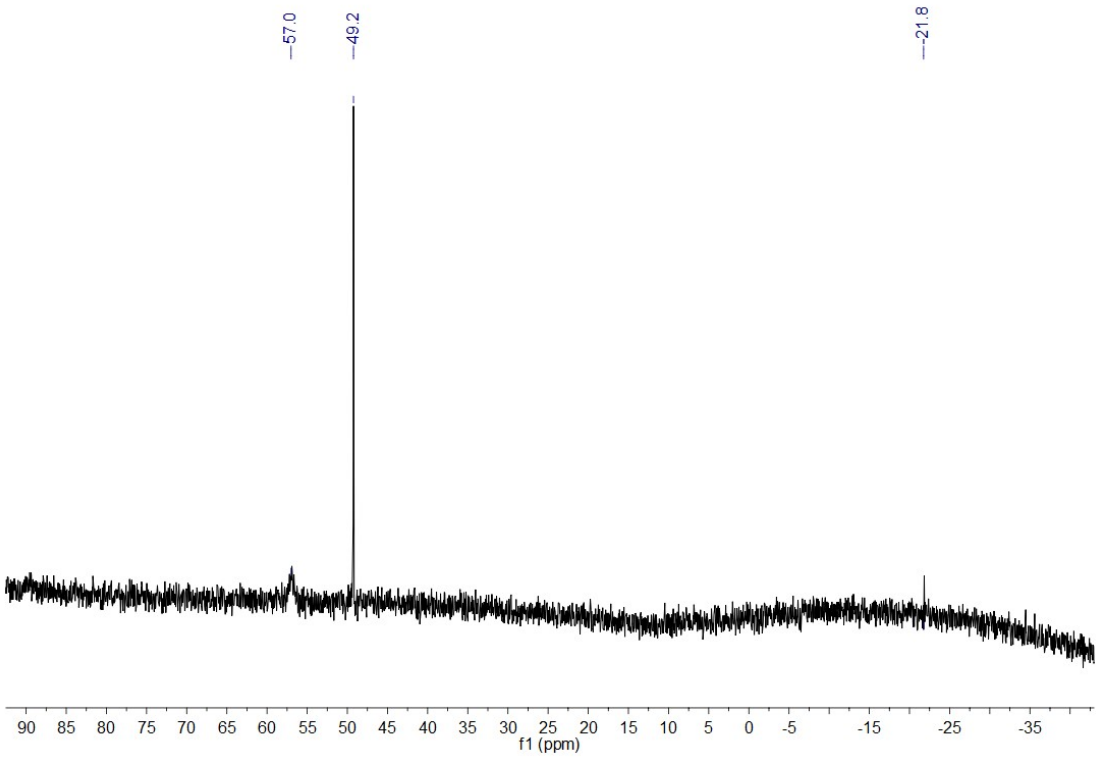

Figure S1.3 ^{29}Si NMR of compound **1** (grease peak at -21.8 ppm).

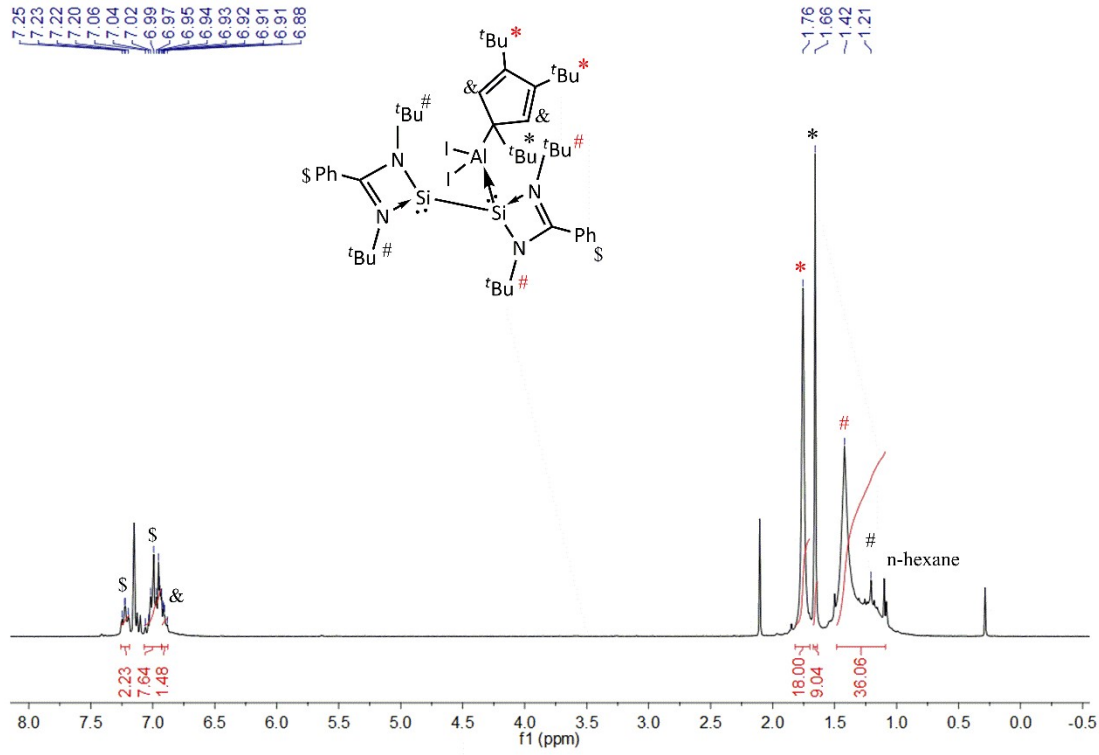

Figure S2.1 ^{1}H NMR of compound **2**.

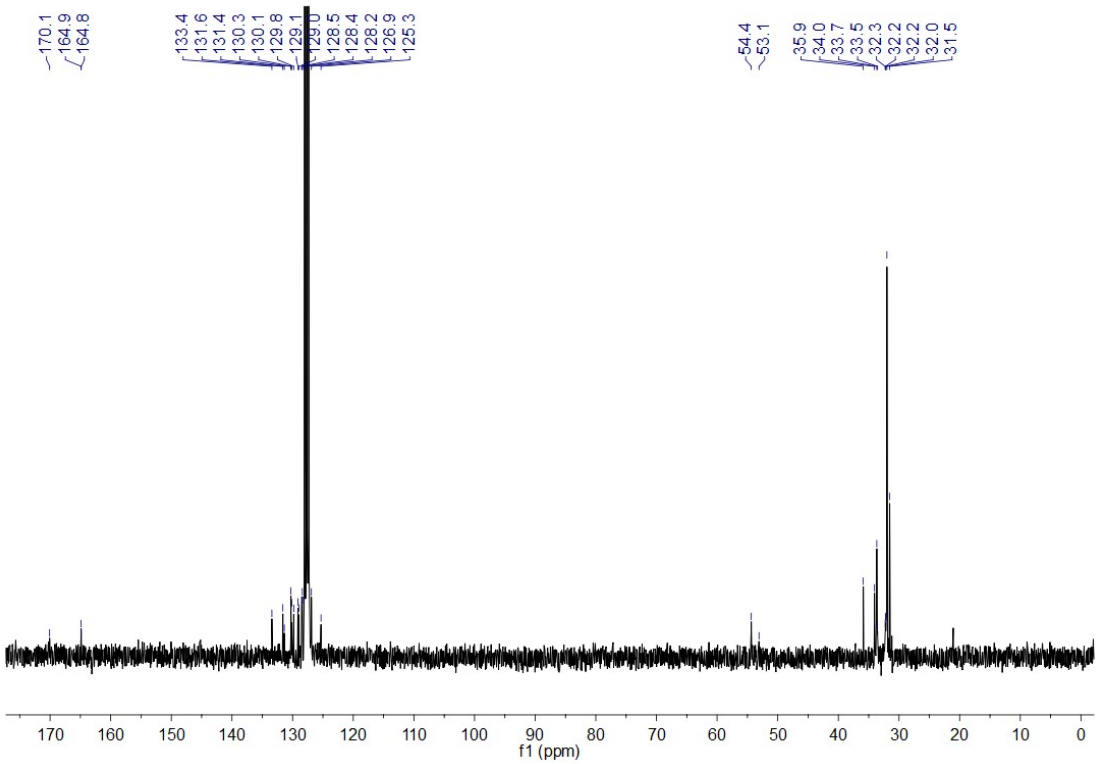

Figure S2.2 ^{13}C NMR of compound **2**.

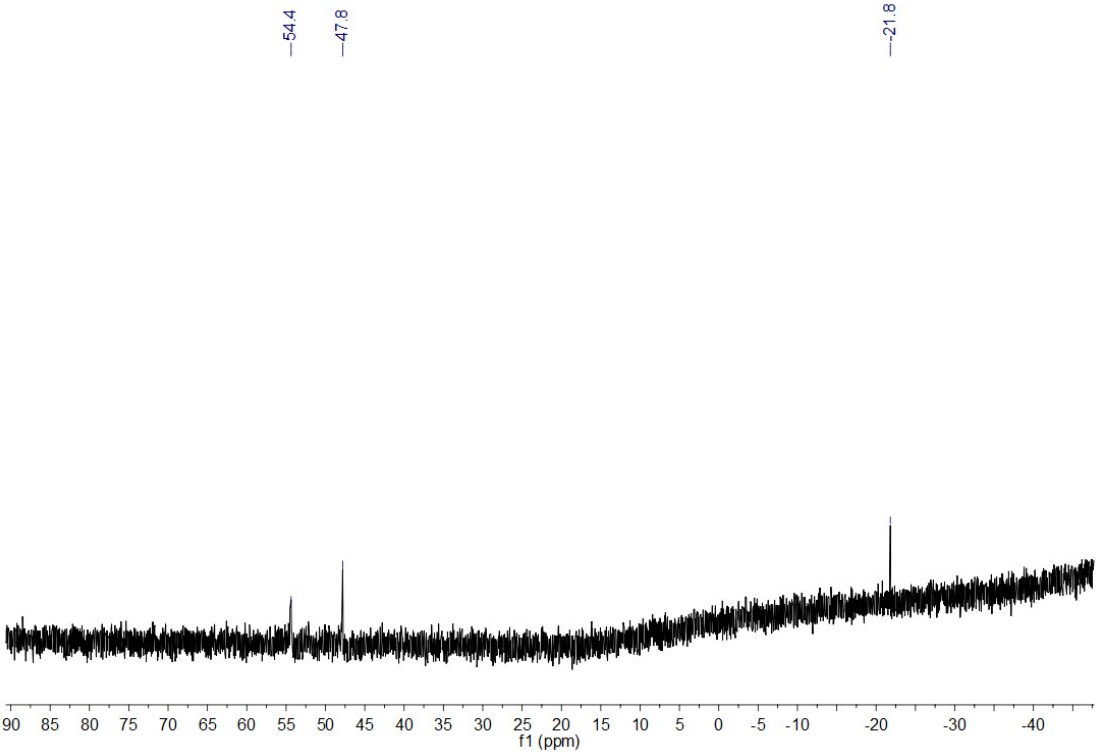

Figure S2.3 ^{29}Si NMR of compound **2** (grease peak at -21.8 ppm).

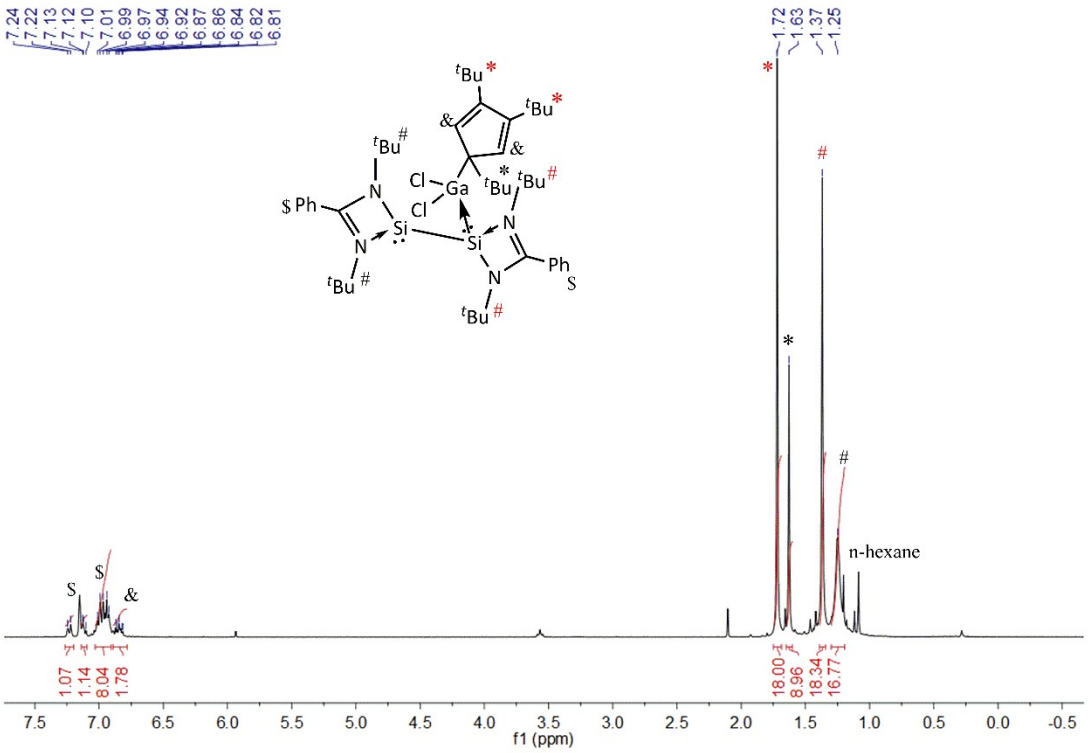

Figure S3.1 ^{1}H NMR of compound **3**.

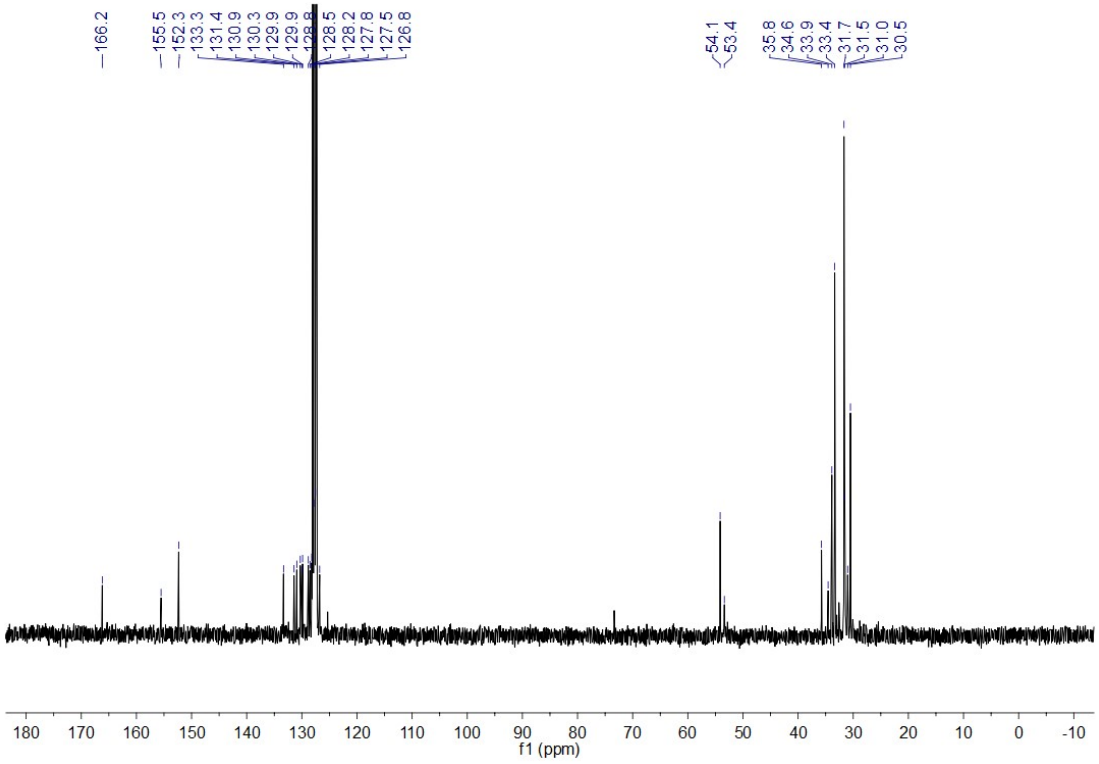

Figure S3.2 ^{13}C NMR of compound **3**.

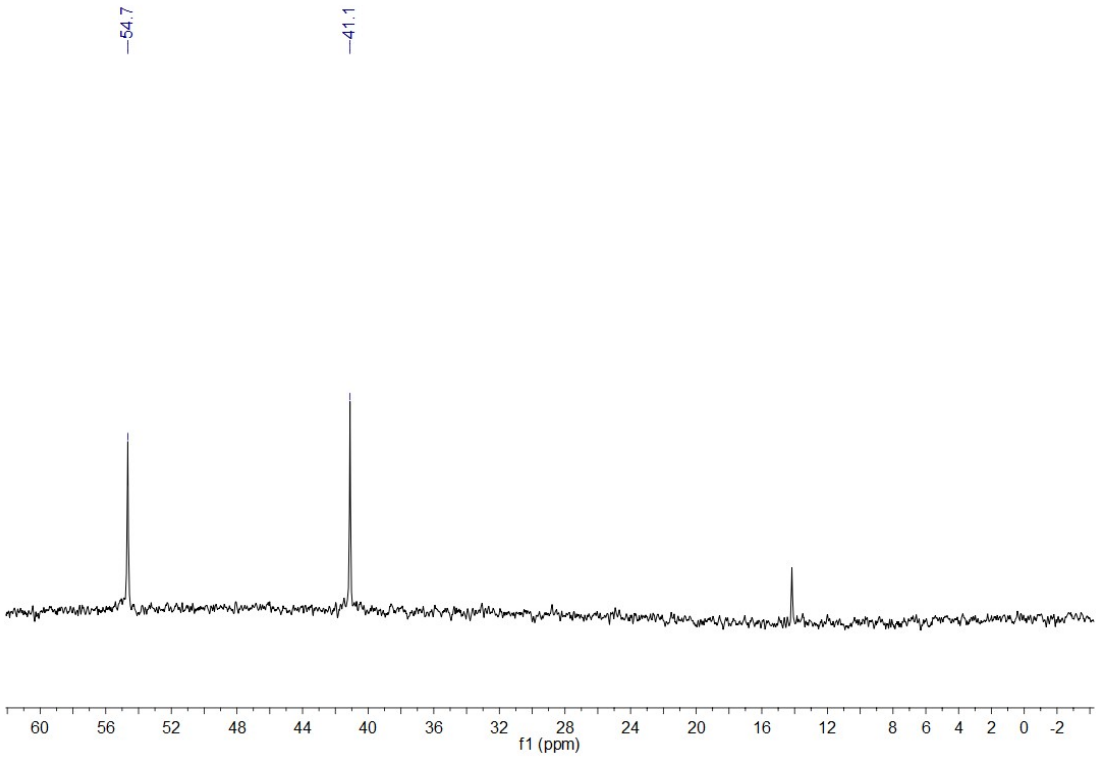

Figure S3.3 ^{29}Si NMR of compound **3** (unreacted LSiCl peak at 14.0 ppm).

Single Crystal X-Ray Data

All crystals were selected under cooling, using a X-Temp2 device.[1] The diffraction data were collected using an Incoatec Mo Microsource[2] and a Bruker Apex II detector. The data were integrated with SAINT.[3] A multi-scan absorption correction was applied using SADABS,[4] which was also used to apply a 3λ correction[5] for **1** and **3**. The structures were solved by SHELXT[6] and refined on F^2 using SHELXL[7] in the graphical user interface ShelXle.[8]

Table S1. Crystal data and structure refinement for compounds **1-3**.

Compound	**1**	**2**	**3**
CCDC	2248551	2248552	2248553
Empirical formula	$C_{54}H_{83}AlCl_2N_4Si_2$	$C_{61}H_{91}AlI_2N_4Si_2$	$C_{61}H_{91}Cl_2GaN_4Si_2$
Formula weight	942.30	1217.33	1077.17
Temperature (K)	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	13.685(2)	12.844(2)	15.547(2)
b (Å)	14.216(2)	14.573(2)	16.319(2)
c (Å)	16.579(3)	18.054(3)	26.239(3)
α (°)	81.82(3)	74.93(2)	79.42(2)
β (°)	68.84(2)	88.59(3)	88.48(3)
γ (°)	64.63(2)	72.68(2)	69.93(2)
V (Å^3)	2717.5(9)	3110.0(9)	6141.8(15)
Z	2	2	4
μ/mm^{-1}	0.218	1.103	0.613
Crystal size(mm)	0.372 · 0.236 · 0.138	0.240 · 0.109 · 0.106	0.459 · 0.325 · 0.118
Θ max (°)	27.528	29.184	27.509
Reflections collected	90699	143545	206173
Independent reflections (R_{int})	12528 (0.0400)	16776 (0.0494)	28165 (0.0422)
Data/restraints/parameters	12528 / 518 / 685	16776 / 87 / 654	28165 / 2780 / 1447
$R1^a$ ($I > 2\sigma(I)$)	0.0312	0.0265	0.0367
$wR2^b$(all data)	0.0776	0.0590	0.0942
$\Delta\rho_{max}/\Delta\rho_{min}$(e Å^{-3})	0.411 / -0.276	0.482 / -0.511	1.107 / -0.419

$^aR1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $^bwR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma(F_o^2)^2]^{1/2}$

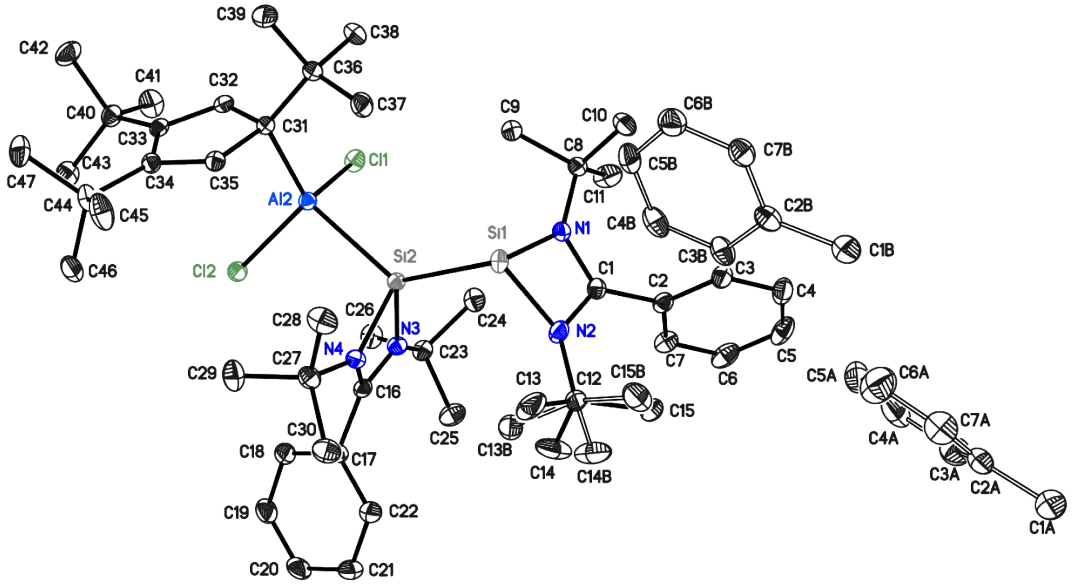

Figure S4: Asymmetric unit of **1**. Hydrogen atoms are omitted for clarity. ADPs are depicted at 50% probability level. Within the disordered *tert*-butyl group as well as the toluene molecules on special positions, equivalent bond lengths and angles were restrained to be similar. Additionally, ADPs of nearby atoms were restrained to be similar and ADPs were restrained to follow a rigid-bond model. All hydrogen atoms were placed using a riding model. Within the disordered *tert*-butyl group non-filled bonds depict the major position present at 54.9(7) %. Solid bonds depict the minor position, which occupies with a fraction of 45.1(7) %.

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

Cl1-Al2	2.2005(7)	C3-C4	1.3942(18)
Cl2-Al2	2.1745(7)	C4-C5	1.382(2)
Si1-N1	1.8667(12)	C5-C6	1.384(2)
Si1-N2	1.8691(11)	C6-C7	1.3902(19)
Si1-C1	2.3379(14)	N1-C8	1.4799(15)
Si1-Si2	2.4245(10)	C8-C9	1.5259(17)
Si2-N3	1.8295(11)	C8-C11	1.5274(18)
Si2-N4	1.8522(11)	C8-C10	1.5327(18)
Si2-C16	2.3026(13)	N2-C12	1.4799(16)
Si2-Al2	2.5413(9)	C12-C14	1.476(4)
Al2-C31	2.0613(13)	C12-C15B	1.513(4)
C1-N1	1.3367(15)	C12-C15	1.518(4)
C1-N2	1.3456(16)	C12-C13B	1.523(3)
C1-C2	1.4922(17)	C12-C13	1.542(4)
C2-C3	1.3906(18)	C12-C14B	1.563(3)
C2-C7	1.3943(18)	C16-N3	1.3348(16)

C16-N4	1.3474(16)	C5A-C6A	1.373(9)
C16-C17	1.4902(16)	C6A-C7A	1.393(7)
C17-C22	1.3936(18)	C1B-C2B	1.506(7)
C17-C18	1.3936(18)	C2B-C3B	1.385(7)
C18-C19	1.3918(18)	C2B-C7B	1.387(5)
C19-C20	1.389(2)	C3B-C4B	1.383(7)
C20-C21	1.385(2)	C4B-C5B	1.382(5)
C21-C22	1.3855(18)	C5B-C6B	1.386(7)
N3-C23	1.4830(16)	C6B-C7B	1.389(7)
C23-C25	1.5259(17)		
C23-C24	1.5271(18)	N1-Si1-N2	69.50(5)
C23-C26	1.5300(18)	N1-Si1-C1	34.84(5)
N4-C27	1.4851(16)	N2-Si1-C1	35.12(4)
C27-C29	1.5251(18)	N1-Si1-Si2	106.11(4)
C27-C28	1.5272(18)	N2-Si1-Si2	106.24(4)
C27-C30	1.5310(18)	C1-Si1-Si2	114.11(4)
C31-C35	1.4643(17)	N3-Si2-N4	71.08(5)
C31-C32	1.4670(17)	N3-Si2-C16	35.40(5)
C31-C36	1.5547(16)	N4-Si2-C16	35.81(4)
C32-C33	1.3701(17)	N3-Si2-Si1	118.96(4)
C33-C34	1.4806(17)	N4-Si2-Si1	106.45(4)
C33-C40	1.5363(17)	C16-Si2-Si1	120.49(4)
C34-C35	1.3708(17)	N3-Si2-Al2	104.57(4)
C34-C44	1.5385(17)	N4-Si2-Al2	109.87(4)
C36-C38	1.5320(18)	C16-Si2-Al2	108.93(4)
C36-C37	1.5329(18)	Si1-Si2-Al2	130.15(3)
C36-C39	1.5408(18)	C31-Al2-Cl2	114.51(4)
C40-C43	1.5327(18)	C31-Al2-Cl1	111.10(4)
C40-C42	1.5352(18)	Cl2-Al2-Cl1	105.70(3)
C40-C41	1.5403(19)	C31-Al2-Si2	121.55(4)
C44-C47	1.5397(18)	Cl2-Al2-Si2	99.49(3)
C44-C46	1.5424(19)	Cl1-Al2-Si2	102.66(3)
C44-C45	1.5425(19)	N1-C1-N2	105.09(10)
C1A-C2A	1.494(8)	N1-C1-C2	128.44(11)
C2A-C3A	1.371(7)	N2-C1-C2	126.42(11)
C2A-C7A	1.391(6)	N1-C1-Si1	52.93(6)
C3A-C4A	1.378(7)	N2-C1-Si1	53.04(6)
C4A-C5A	1.394(8)	C2-C1-Si1	169.87(9)

C3-C2-C7	119.64(12)	C22-C17-C18	119.99(12)
C3-C2-C1	120.82(11)	C22-C17-C16	120.60(11)
C7-C2-C1	119.52(11)	C18-C17-C16	119.16(11)
C2-C3-C4	119.97(13)	C19-C18-C17	119.75(12)
C5-C4-C3	120.06(13)	C20-C19-C18	119.95(13)
C4-C5-C6	120.23(13)	C21-C20-C19	120.21(12)
C5-C6-C7	120.10(13)	C20-C21-C22	120.21(13)
C6-C7-C2	119.99(13)	C21-C22-C17	119.88(13)
C1-N1-C8	131.28(10)	C16-N3-C23	132.48(10)
C1-N1-Si1	92.23(8)	C16-N3-Si2	92.03(8)
C8-N1-Si1	134.67(8)	C23-N3-Si2	135.48(8)
N1-C8-C9	105.55(10)	N3-C23-C25	111.80(11)
N1-C8-C11	111.90(10)	N3-C23-C24	104.61(10)
C9-C8-C11	109.68(11)	C25-C23-C24	108.68(10)
N1-C8-C10	110.43(10)	N3-C23-C26	111.19(10)
C9-C8-C10	108.86(11)	C25-C23-C26	110.38(11)
C11-C8-C10	110.28(11)	C24-C23-C26	110.01(11)
C1-N2-C12	130.46(10)	C16-N4-C27	130.25(10)
C1-N2-Si1	91.84(8)	C16-N4-Si2	90.64(8)
C12-N2-Si1	133.25(9)	C27-N4-Si2	135.96(8)
C14-C12-N2	106.09(18)	N4-C27-C29	110.47(11)
N2-C12-C15B	110.90(18)	N4-C27-C28	105.29(10)
C14-C12-C15	112.5(3)	C29-C27-C28	109.79(11)
N2-C12-C15	114.32(19)	N4-C27-C30	112.10(10)
N2-C12-C13B	106.65(14)	C29-C27-C30	109.73(11)
C15B-C12-C13B	110.2(2)	C28-C27-C30	109.36(11)
C14-C12-C13	112.0(3)	C35-C31-C32	101.90(10)
N2-C12-C13	103.55(16)	C35-C31-C36	116.62(10)
C15-C12-C13	108.1(2)	C32-C31-C36	118.54(10)
N2-C12-C14B	113.73(17)	C35-C31-Al2	103.59(8)
C15B-C12-C14B	108.6(2)	C32-C31-Al2	91.84(8)
C13B-C12-C14B	106.7(2)	C36-C31-Al2	120.24(8)
N3-C16-N4	105.86(10)	C33-C32-C31	111.79(11)
N3-C16-C17	125.14(11)	C32-C33-C34	107.19(11)
N4-C16-C17	129.00(11)	C32-C33-C40	120.25(11)
N3-C16-Si2	52.57(6)	C34-C33-C40	132.56(11)
N4-C16-Si2	53.55(6)	C35-C34-C33	106.52(11)
C17-C16-Si2	174.63(9)	C35-C34-C44	121.07(11)

C33-C34-C44	132.39(11)	C47-C44-C45	105.50(12)
C34-C35-C31	112.36(11)	C46-C44-C45	106.41(11)
C38-C36-C37	109.33(10)	C3A-C2A-C7A	118.1(5)
C38-C36-C39	108.24(11)	C3A-C2A-C1A	121.6(5)
C37-C36-C39	108.56(11)	C7A-C2A-C1A	120.3(5)
C38-C36-C31	111.73(11)	C2A-C3A-C4A	122.5(5)
C37-C36-C31	111.14(10)	C3A-C4A-C5A	119.3(5)
C39-C36-C31	107.74(10)	C6A-C5A-C4A	118.9(6)
C43-C40-C42	109.96(11)	C5A-C6A-C7A	121.2(5)
C43-C40-C33	113.83(10)	C2A-C7A-C6A	119.9(5)
C42-C40-C33	109.42(10)	C3B-C2B-C7B	117.5(5)
C43-C40-C41	105.73(11)	C3B-C2B-C1B	121.3(4)
C42-C40-C41	107.48(11)	C7B-C2B-C1B	121.1(5)
C33-C40-C41	110.19(10)	C4B-C3B-C2B	121.6(5)
C34-C44-C47	112.62(11)	C5B-C4B-C3B	120.4(5)
C34-C44-C46	112.49(11)	C4B-C5B-C6B	118.9(5)
C47-C44-C46	109.81(11)	C5B-C6B-C7B	120.2(4)
C34-C44-C45	109.59(10)	C2B-C7B-C6B	121.4(5)

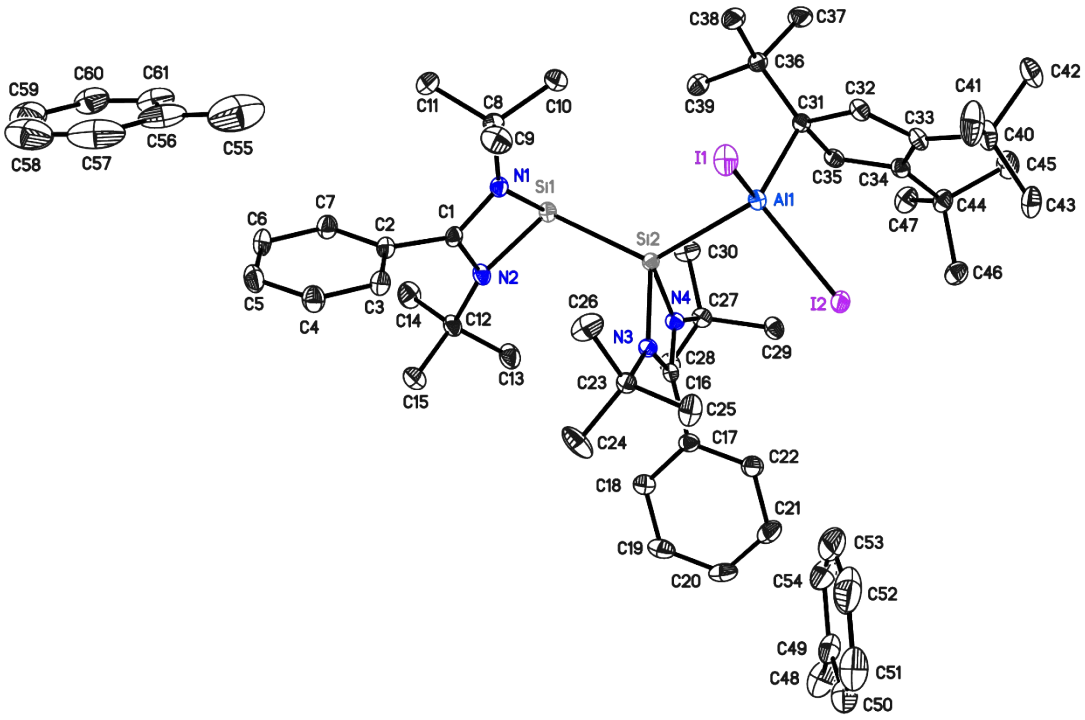

Figure S5: Asymmetric unit of **2**. Hydrogen atoms are omitted for clarity. ADPs are depicted at 50% probability level. All hydrogen atoms were placed using a riding model. The anisotropic displacement parameters of one toluene molecule (C55 to C61) were restrained by similarity and rigid bond restraints.

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

I1-Al1	2.6040(8)	C1-C2	1.488(2)
I2-Al1	2.5740(7)	C2-C3	1.391(2)
Si1-N1	1.8659(15)	C2-C7	1.395(2)
Si1-N2	1.8669(15)	C3-C4	1.387(2)
Si1-C1	2.3343(18)	C4-C5	1.388(3)
Si1-Si2	2.4399(8)	C5-C6	1.386(3)
Si2-N3	1.8396(14)	C6-C7	1.389(2)
Si2-N4	1.8492(15)	C8-C9	1.524(3)
Si2-C16	2.3130(18)	C8-C10	1.527(2)
Si2-Al1	2.5505(9)	C8-C11	1.534(2)
Al1-C31	2.0725(17)	C12-C13	1.525(2)
N1-C1	1.340(2)	C12-C15	1.526(2)
N1-C8	1.481(2)	C12-C14	1.527(2)
N2-C1	1.346(2)	N3-C16	1.341(2)
N2-C12	1.479(2)	N3-C23	1.488(2)

N4-C16	1.342(2)	C53-C54	1.391(4)
N4-C27	1.484(2)	C55-C56	1.500(4)
C16-C17	1.496(2)	C56-C61	1.389(3)
C17-C22	1.387(2)	C56-C57	1.404(4)
C17-C18	1.397(2)	C57-C58	1.388(4)
C18-C19	1.391(2)	C58-C59	1.370(4)
C19-C20	1.385(3)	C59-C60	1.377(3)
C20-C21	1.381(3)	C60-C61	1.368(3)
C21-C22	1.398(2)		
C23-C26	1.521(2)	N1-Si1-N2	69.73(7)
C23-C25	1.521(2)	N1-Si1-C1	35.02(6)
C23-C24	1.524(2)	N2-Si1-C1	35.19(6)
C27-C30	1.527(2)	N1-Si1-Si2	104.43(5)
C27-C29	1.528(2)	N2-Si1-Si2	105.07(5)
C27-C28	1.530(2)	C1-Si1-Si2	112.45(5)
C31-C32	1.471(2)	N3-Si2-N4	70.77(7)
C31-C35	1.471(2)	N3-Si2-C16	35.41(6)
C31-C36	1.560(2)	N4-Si2-C16	35.45(6)
C32-C33	1.366(2)	N3-Si2-Si1	118.37(5)
C33-C34	1.487(2)	N4-Si2-Si1	106.53(5)
C33-C40	1.543(2)	C16-Si2-Si1	119.56(5)
C34-C35	1.368(2)	N3-Si2-Al1	109.26(5)
C34-C44	1.538(2)	N4-Si2-Al1	109.03(6)
C36-C39	1.527(2)	C16-Si2-Al1	111.90(5)
C36-C38	1.534(2)	Si1-Si2-Al1	127.44(3)
C36-C37	1.541(2)	C31-Al1-Si2	123.74(5)
C40-C43	1.536(3)	C31-Al1-I2	111.97(5)
C40-C41	1.539(3)	Si2-Al1-I2	101.05(3)
C40-C42	1.544(3)	C31-Al1-I1	111.96(6)
C44-C45	1.536(2)	Si2-Al1-I1	102.49(3)
C44-C47	1.542(3)	I2-Al1-I1	103.28(2)
C44-C46	1.544(2)	C1-N1-C8	129.75(14)
C48-C49	1.505(3)	C1-N1-Si1	91.96(11)
C49-C54	1.385(3)	C8-N1-Si1	135.38(11)
C49-C50	1.387(3)	C1-N2-C12	130.27(14)
C50-C51	1.381(3)	C1-N2-Si1	91.73(11)
C51-C52	1.380(4)	C12-N2-Si1	133.06(12)
C52-C53	1.375(4)	N1-C1-N2	105.20(14)

N1-C1-C2	128.47(15)	C22-C17-C16	119.46(15)
N2-C1-C2	126.33(15)	C18-C17-C16	121.17(15)
N1-C1-Si1	53.02(8)	C19-C18-C17	120.18(17)
N2-C1-Si1	53.07(8)	C20-C19-C18	120.06(17)
C2-C1-Si1	171.17(12)	C21-C20-C19	120.15(17)
C3-C2-C7	119.67(16)	C20-C21-C22	120.03(18)
C3-C2-C1	119.34(15)	C17-C22-C21	120.19(17)
C7-C2-C1	120.93(15)	N3-C23-C26	105.50(13)
C4-C3-C2	120.21(16)	N3-C23-C25	111.14(14)
C3-C4-C5	119.93(17)	C26-C23-C25	109.99(16)
C6-C5-C4	120.17(17)	N3-C23-C24	110.68(14)
C5-C6-C7	120.10(17)	C26-C23-C24	109.36(16)
C6-C7-C2	119.88(17)	C25-C23-C24	110.06(16)
N1-C8-C9	110.65(14)	N4-C27-C30	105.73(13)
N1-C8-C10	105.23(14)	N4-C27-C29	110.47(14)
C9-C8-C10	109.78(15)	C30-C27-C29	109.66(14)
N1-C8-C11	111.12(14)	N4-C27-C28	111.52(13)
C9-C8-C11	110.67(16)	C30-C27-C28	108.76(14)
C10-C8-C11	109.23(15)	C29-C27-C28	110.58(14)
N2-C12-C13	104.67(13)	C32-C31-C35	101.33(14)
N2-C12-C15	112.52(14)	C32-C31-C36	117.66(14)
C13-C12-C15	109.68(15)	C35-C31-C36	116.24(14)
N2-C12-C14	110.56(14)	C32-C31-Al1	95.40(11)
C13-C12-C14	108.76(16)	C35-C31-Al1	104.41(11)
C15-C12-C14	110.46(15)	C36-C31-Al1	118.51(11)
C16-N3-C23	130.98(14)	C33-C32-C31	112.36(15)
C16-N3-Si2	91.95(10)	C32-C33-C34	106.98(15)
C23-N3-Si2	137.05(11)	C32-C33-C40	120.11(16)
C16-N4-C27	130.20(14)	C34-C33-C40	132.90(16)
C16-N4-Si2	91.50(10)	C35-C34-C33	106.51(15)
C27-N4-Si2	137.00(11)	C35-C34-C44	121.93(15)
N3-C16-N4	105.55(14)	C33-C34-C44	131.56(15)
N3-C16-C17	126.91(15)	C34-C35-C31	112.63(15)
N4-C16-C17	127.52(15)	C39-C36-C38	108.83(15)
N3-C16-Si2	52.65(8)	C39-C36-C37	108.12(15)
N4-C16-Si2	53.06(8)	C38-C36-C37	107.30(14)
C17-C16-Si2	175.45(12)	C39-C36-C31	111.73(14)
C22-C17-C18	119.36(16)	C38-C36-C31	112.32(14)

C37-C36-C31	108.35(14)	C50-C49-C48	120.2(2)
C43-C40-C41	105.24(17)	C51-C50-C49	121.1(2)
C43-C40-C33	114.67(16)	C52-C51-C50	120.1(2)
C41-C40-C33	109.18(15)	C53-C52-C51	119.5(2)
C43-C40-C42	110.26(16)	C52-C53-C54	120.4(2)
C41-C40-C42	107.61(18)	C49-C54-C53	120.5(2)
C33-C40-C42	109.58(16)	C61-C56-C57	116.5(3)
C45-C44-C34	112.99(15)	C61-C56-C55	121.0(3)
C45-C44-C47	105.26(15)	C57-C56-C55	122.5(2)
C34-C44-C47	109.90(14)	C58-C57-C56	121.3(2)
C45-C44-C46	109.89(15)	C59-C58-C57	120.6(3)
C34-C44-C46	111.75(14)	C58-C59-C60	118.6(3)
C47-C44-C46	106.66(15)	C61-C60-C59	121.3(2)
C54-C49-C50	118.3(2)	C60-C61-C56	121.7(2)
C54-C49-C48	121.5(2)		

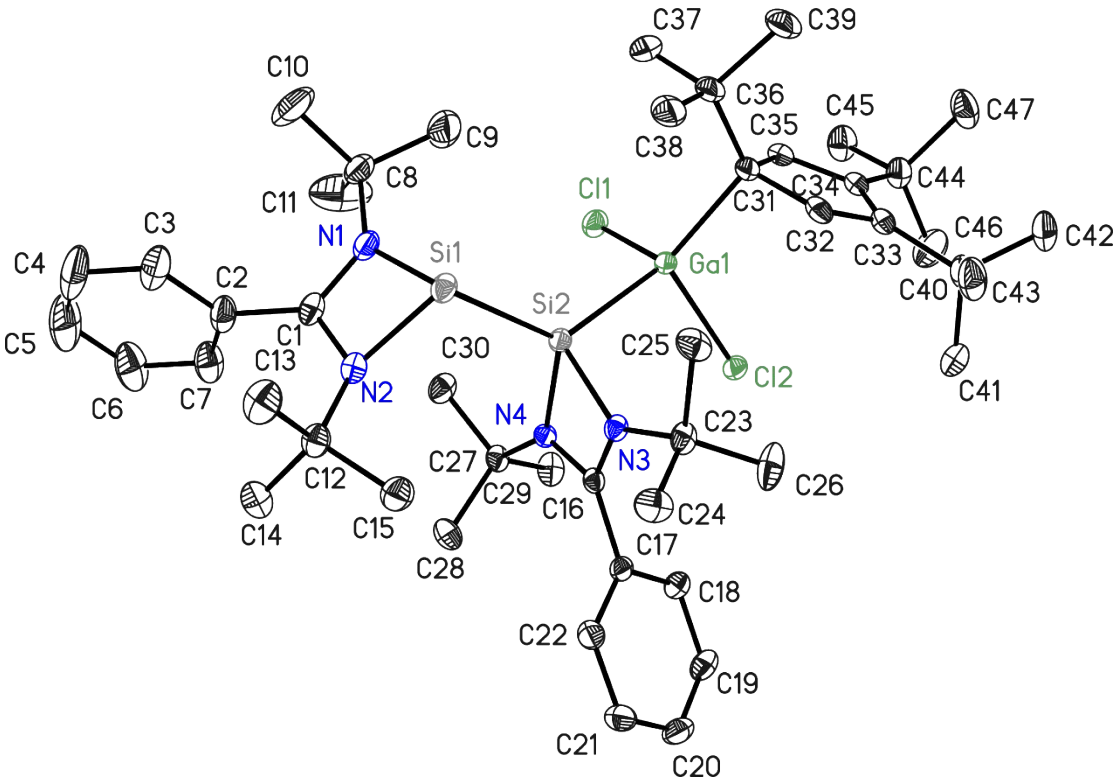

Figure S6: Structure of molecule 1 of **3**. Hydrogen atoms are omitted for clarity. ADPs are depicted at 50% probability level. All hydrogen atoms were placed using a riding model.

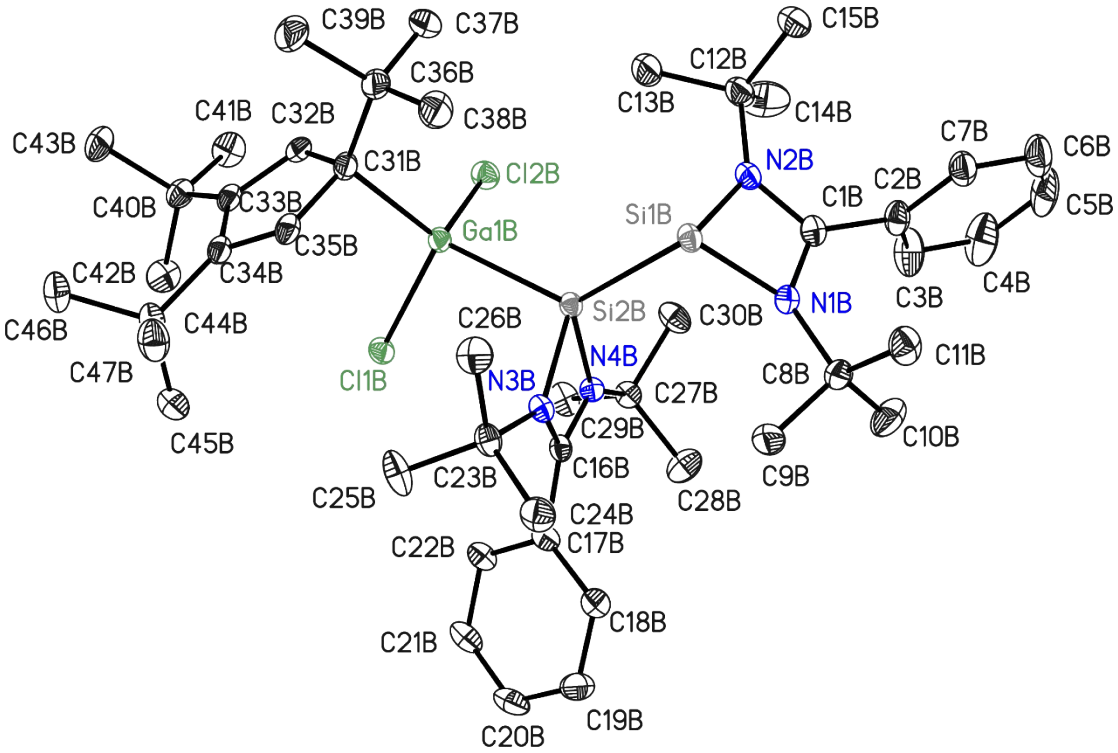

Figure S7: Structure of molecule 2 of **3**. Hydrogen atoms are omitted for clarity. ADPs are depicted at 50% probability level. All hydrogen atoms were placed using a riding model.

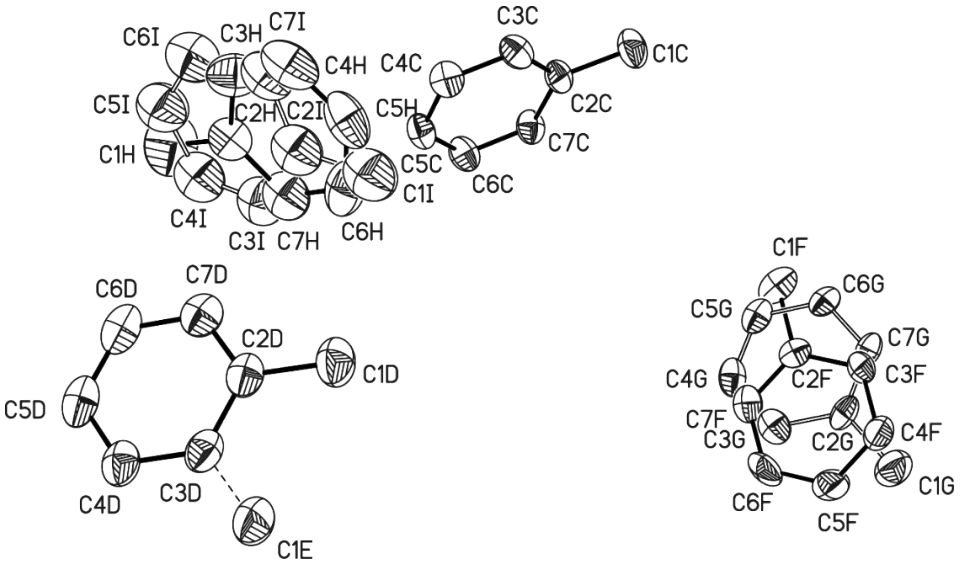

Figure S8: Structure of the solvent molecules of **3**. Hydrogen atoms are omitted for clarity. ADPs are depicted at 50% probability level. All hydrogen atoms were placed using a riding model. All toluene molecules were restrained to have similar bond lengths and angles between different molecules and for all bond lengths and angles within the benzene ring. Additionally, the individual molecules were restrained to lie in a plane. The atomic displacement parameters of disordered toluene molecules were restrained by similarity and rigid bond restraints. The positions and atomic displacement parameters of the benzene ring of one toluene molecule (C2D to C7D) were constrained to be identical to its counterpart (C2E to C7E). The occupancies of the minor positions refine to 0.350 (E), 0.415(4) (G), 0.185(4) (I).

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

Cl1-Ga1	2.2788(8)	C19-C20	1.386(3)
Ga1-C31	2.0688(17)	C20-C21	1.387(3)
Ga1-Cl2	2.2368(6)	C21-C22	1.392(2)
Ga1-Si2	2.4910(7)	C23-C25	1.526(2)
Si1-N1	1.8621(16)	C23-C26	1.528(2)
Si1-N2	1.8755(16)	C23-C24	1.534(3)
Si1-C1	2.3312(19)	C27-C30	1.526(2)
Si1-Si2	2.4339(7)	C27-C28	1.528(2)
N1-C1	1.330(2)	C27-C29	1.532(2)
N1-C8	1.482(2)	C31-C32	1.475(2)
C1-N2	1.350(2)	C31-C35	1.478(2)
C1-C2	1.491(3)	C31-C36	1.558(2)
Si2-N4	1.8271(14)	C32-C33	1.358(2)
Si2-N3	1.8427(15)	C33-C34	1.502(2)
Si2-C16	2.2999(17)	C33-C40	1.539(2)
N2-C12	1.487(2)	C34-C35	1.360(2)
C2-C3	1.391(3)	C34-C44	1.535(2)
C2-C7	1.397(3)	C36-C38	1.534(3)
N3-C16	1.346(2)	C36-C37	1.534(3)
N3-C23	1.486(2)	C36-C39	1.543(3)
C3-C4	1.403(3)	C40-C42	1.537(3)
N4-C16	1.340(2)	C40-C41	1.539(3)
N4-C27	1.483(2)	C40-C43	1.544(3)
C4-C5	1.382(4)	C44-C46	1.532(3)
C5-C6	1.377(4)	C44-C45	1.540(3)
C6-C7	1.384(3)	C44-C47	1.548(3)
C8-C9	1.508(3)	Cl1B-Ga1B	2.2375(6)
C8-C11	1.520(3)	Ga1B-C31B	2.0793(18)
C8-C10	1.522(3)	Ga1B-Cl2B	2.2777(8)
C12-C15	1.526(2)	Ga1B-Si2B	2.4788(7)
C12-C14	1.529(3)	Si1B-N2B	1.8589(16)
C12-C13	1.531(2)	Si1B-N1B	1.8641(15)
C16-C17	1.488(2)	Si1B-C1B	2.3264(19)
C17-C22	1.390(2)	Si1B-Si2B	2.4282(7)
C17-C18	1.397(2)	N1B-C1B	1.345(2)
C18-C19	1.392(2)	N1B-C8B	1.476(2)

C1B-N2B	1.335(2)	C32B-C33B	1.361(2)
C1B-C2B	1.489(2)	C33B-C34B	1.500(2)
Si2B-N4B	1.8320(14)	C33B-C40B	1.540(2)
Si2B-N3B	1.8427(15)	C34B-C35B	1.362(2)
Si2B-C16B	2.2996(17)	C34B-C44B	1.542(2)
N2B-C12B	1.478(2)	C36B-C37B	1.526(3)
C2B-C7B	1.391(3)	C36B-C38B	1.533(3)
C2B-C3B	1.396(3)	C36B-C39B	1.543(3)
N3B-C16B	1.345(2)	C40B-C42B	1.533(2)
N3B-C23B	1.488(2)	C40B-C41B	1.537(3)
C3B-C4B	1.383(3)	C40B-C43B	1.539(2)
N4B-C16B	1.337(2)	C44B-C46B	1.536(3)
N4B-C27B	1.483(2)	C44B-C45B	1.539(3)
C4B-C5B	1.380(4)	C44B-C47B	1.541(3)
C5B-C6B	1.378(3)	C1C-C2C	1.508(3)
C6B-C7B	1.395(3)	C2C-C7C	1.387(3)
C8B-C9B	1.526(3)	C2C-C3C	1.392(3)
C8B-C10B	1.530(3)	C3C-C4C	1.383(3)
C8B-C11B	1.531(2)	C4C-C5C	1.382(3)
C12B-C13B	1.517(3)	C5C-C6C	1.381(3)
C12B-C15B	1.528(3)	C6C-C7C	1.386(3)
C12B-C14B	1.537(3)	C1D-C2D	1.502(4)
C16B-C17B	1.488(2)	C2D-C7D	1.390(3)
C17B-C22B	1.394(2)	C2D-C3D	1.391(3)
C17B-C18B	1.395(2)	C3D-C4D	1.385(3)
C18B-C19B	1.392(2)	C4D-C5D	1.380(3)
C19B-C20B	1.384(3)	C5D-C6D	1.373(4)
C20B-C21B	1.381(3)	C6D-C7D	1.386(3)
C21B-C22B	1.393(2)	C1E-C2E	1.489(7)
C23B-C26B	1.523(2)	C2E-C7E	1.385(3)
C23B-C25B	1.528(2)	C2E-C3E	1.391(3)
C23B-C24B	1.531(2)	C3E-C4E	1.390(3)
C27B-C30B	1.528(2)	C4E-C5E	1.386(3)
C27B-C28B	1.528(2)	C5E-C6E	1.373(4)
C27B-C29B	1.529(2)	C6E-C7E	1.380(3)
C31B-C35B	1.474(2)	C1F-C2F	1.487(6)
C31B-C32B	1.475(2)	C2F-C7F	1.387(6)
C31B-C36B	1.559(2)	C2F-C3F	1.392(8)

C3F-C4F	1.373(7)	C1-N1-C8	131.35(15)
C4F-C5F	1.374(6)	C1-N1-Si1	92.30(11)
C5F-C6F	1.369(6)	C8-N1-Si1	135.86(13)
C6F-C7F	1.381(7)	N1-C1-N2	105.49(15)
C1G-C2G	1.506(8)	N1-C1-C2	126.96(16)
C2G-C7G	1.375(9)	N2-C1-C2	127.53(16)
C2G-C3G	1.406(8)	N1-C1-Si1	52.95(9)
C3G-C4G	1.374(8)	N2-C1-Si1	53.55(9)
C4G-C5G	1.363(9)	C2-C1-Si1	170.25(13)
C5G-C6G	1.390(8)	N4-Si2-N3	71.33(6)
C6G-C7G	1.379(9)	N4-Si2-C16	35.62(6)
C1H-C2H	1.490(5)	N3-Si2-C16	35.80(6)
C2H-C3H	1.383(5)	N4-Si2-Si1	118.91(5)
C2H-C7H	1.402(5)	N3-Si2-Si1	107.59(5)
C3H-C4H	1.350(6)	C16-Si2-Si1	120.78(5)
C4H-C5H	1.327(6)	N4-Si2-Ga1	105.53(5)
C5H-C6H	1.392(6)	N3-Si2-Ga1	106.97(5)
C6H-C7H	1.404(6)	C16-Si2-Ga1	108.27(4)
C1I-C2I	1.510(13)	Si1-Si2-Ga1	130.18(3)
C2I-C7I	1.367(12)	C1-N2-C12	128.26(15)
C2I-C3I	1.420(12)	C1-N2-Si1	91.06(11)
C3I-C4I	1.367(13)	C12-N2-Si1	130.34(11)
C4I-C5I	1.412(12)	C3-C2-C7	119.80(19)
C5I-C6I	1.356(12)	C3-C2-C1	120.32(19)
C6I-C7I	1.380(12)	C7-C2-C1	119.88(17)
		C16-N3-C23	130.48(14)
C31-Ga1-Cl2	108.80(5)	C16-N3-Si2	90.96(10)
C31-Ga1-Cl1	108.09(6)	C23-N3-Si2	136.63(11)
Cl2-Ga1-Cl1	103.75(2)	C2-C3-C4	118.9(2)
C31-Ga1-Si2	131.07(5)	C16-N4-C27	131.96(13)
Cl2-Ga1-Si2	98.87(2)	C16-N4-Si2	91.82(10)
Cl1-Ga1-Si2	103.20(3)	C27-N4-Si2	136.10(11)
N1-Si1-N2	69.60(7)	C5-C4-C3	120.5(2)
N1-Si1-C1	34.75(6)	C6-C5-C4	120.5(2)
N2-Si1-C1	35.39(6)	C5-C6-C7	119.6(2)
N1-Si1-Si2	104.78(5)	C6-C7-C2	120.6(2)
N2-Si1-Si2	104.90(5)	N1-C8-C9	105.19(16)
C1-Si1-Si2	112.79(5)	N1-C8-C11	110.88(17)

C9-C8-C11	109.0(2)	C35-C31-C36	115.42(15)
N1-C8-C10	111.60(17)	C32-C31-Ga1	104.74(11)
C9-C8-C10	109.5(2)	C35-C31-Ga1	100.77(11)
C11-C8-C10	110.5(2)	C36-C31-Ga1	115.84(11)
N2-C12-C15	104.90(14)	C33-C32-C31	112.65(16)
N2-C12-C14	112.52(15)	C32-C33-C34	106.67(15)
C15-C12-C14	109.73(15)	C32-C33-C40	120.96(16)
N2-C12-C13	109.88(15)	C34-C33-C40	132.26(15)
C15-C12-C13	109.64(15)	C35-C34-C33	106.86(15)
C14-C12-C13	110.03(16)	C35-C34-C44	120.92(16)
N4-C16-N3	105.64(13)	C33-C34-C44	132.14(15)
N4-C16-C17	128.05(14)	C34-C35-C31	112.34(16)
N3-C16-C17	126.30(14)	C38-C36-C37	109.72(16)
N4-C16-Si2	52.56(8)	C38-C36-C39	108.70(17)
N3-C16-Si2	53.23(8)	C37-C36-C39	107.79(16)
C17-C16-Si2	175.67(12)	C38-C36-C31	111.00(15)
C22-C17-C18	120.21(15)	C37-C36-C31	111.53(16)
C22-C17-C16	120.13(15)	C39-C36-C31	108.00(15)
C18-C17-C16	119.66(15)	C42-C40-C41	109.73(16)
C19-C18-C17	119.33(16)	C42-C40-C33	114.00(15)
C20-C19-C18	120.34(17)	C41-C40-C33	110.78(15)
C19-C20-C21	120.23(16)	C42-C40-C43	105.37(15)
C20-C21-C22	119.87(17)	C41-C40-C43	107.40(16)
C17-C22-C21	119.98(16)	C33-C40-C43	109.23(15)
N3-C23-C25	105.10(14)	C46-C44-C34	112.62(15)
N3-C23-C26	111.42(14)	C46-C44-C45	106.16(16)
C25-C23-C26	109.43(16)	C34-C44-C45	110.19(15)
N3-C23-C24	111.33(14)	C46-C44-C47	111.28(17)
C25-C23-C24	108.79(14)	C34-C44-C47	110.68(16)
C26-C23-C24	110.60(16)	C45-C44-C47	105.59(16)
N4-C27-C30	104.98(13)	C31B-Ga1B-Cl1B	108.92(5)
N4-C27-C28	110.45(14)	C31B-Ga1B-Cl2B	109.96(6)
C30-C27-C28	109.66(15)	Cl1B-Ga1B-Cl2B	102.21(2)
N4-C27-C29	110.99(13)	C31B-Ga1B-Si2B	129.85(5)
C30-C27-C29	109.41(15)	Cl1B-Ga1B-Si2B	99.71(2)
C28-C27-C29	111.15(14)	Cl2B-Ga1B-Si2B	102.76(3)
C32-C31-C35	101.41(14)	N2B-Si1B-N1B	69.71(7)
C32-C31-C36	116.46(15)	N2B-Si1B-C1B	35.00(6)

N1B-Si1B-C1B	35.30(6)	C5B-C6B-C7B	120.2(2)
N2B-Si1B-Si2B	105.67(5)	C2B-C7B-C6B	119.27(19)
N1B-Si1B-Si2B	104.33(5)	N1B-C8B-C9B	104.52(14)
C1B-Si1B-Si2B	113.21(5)	N1B-C8B-C10B	111.81(15)
C1B-N1B-C8B	129.80(14)	C9B-C8B-C10B	109.77(16)
C1B-N1B-Si1B	91.48(11)	N1B-C8B-C11B	110.55(14)
C8B-N1B-Si1B	132.41(12)	C9B-C8B-C11B	109.93(16)
N2B-C1B-N1B	105.12(14)	C10B-C8B-C11B	110.13(16)
N2B-C1B-C2B	127.25(16)	N2B-C12B-C13B	105.28(15)
N1B-C1B-C2B	127.55(15)	N2B-C12B-C15B	110.95(15)
N2B-C1B-Si1B	52.99(9)	C13B-C12B-C15B	109.67(17)
N1B-C1B-Si1B	53.23(8)	N2B-C12B-C14B	110.67(16)
C2B-C1B-Si1B	168.47(12)	C13B-C12B-C14B	109.90(19)
N4B-Si2B-N3B	71.23(6)	C15B-C12B-C14B	110.26(17)
N4B-Si2B-C16B	35.54(6)	N4B-C16B-N3B	105.82(14)
N3B-Si2B-C16B	35.79(6)	N4B-C16B-C17B	127.96(15)
N4B-Si2B-Si1B	120.54(5)	N3B-C16B-C17B	126.19(15)
N3B-Si2B-Si1B	108.35(5)	N4B-C16B-Si2B	52.78(8)
C16B-Si2B-Si1B	122.53(5)	N3B-C16B-Si2B	53.24(8)
N4B-Si2B-Ga1B	105.74(5)	C17B-C16B-Si2B	174.60(12)
N3B-Si2B-Ga1B	107.10(5)	C22B-C17B-C18B	120.05(15)
C16B-Si2B-Ga1B	108.21(4)	C22B-C17B-C16B	119.05(15)
Si1B-Si2B-Ga1B	128.36(3)	C18B-C17B-C16B	120.88(15)
C1B-N2B-C12B	130.59(15)	C19B-C18B-C17B	119.70(17)
C1B-N2B-Si1B	92.01(11)	C20B-C19B-C18B	119.97(18)
C12B-N2B-Si1B	136.01(12)	C21B-C20B-C19B	120.57(17)
C7B-C2B-C3B	119.97(18)	C20B-C21B-C22B	120.01(17)
C7B-C2B-C1B	120.19(16)	C21B-C22B-C17B	119.68(17)
C3B-C2B-C1B	119.83(17)	N3B-C23B-C26B	105.05(14)
C16B-N3B-C23B	130.33(14)	N3B-C23B-C25B	110.97(14)
C16B-N3B-Si2B	90.96(10)	C26B-C23B-C25B	109.12(16)
C23B-N3B-Si2B	136.18(11)	N3B-C23B-C24B	112.02(14)
C4B-C3B-C2B	120.1(2)	C26B-C23B-C24B	108.84(15)
C16B-N4B-C27B	132.06(13)	C25B-C23B-C24B	110.63(15)
C16B-N4B-Si2B	91.68(10)	N4B-C27B-C30B	104.83(13)
C27B-N4B-Si2B	136.23(11)	N4B-C27B-C28B	110.96(14)
C5B-C4B-C3B	119.8(2)	C30B-C27B-C28B	109.89(15)
C6B-C5B-C4B	120.59(19)	N4B-C27B-C29B	110.80(14)

C30B-C27B-C29B	109.56(15)	C5C-C4C-C3C	120.2(2)
C28B-C27B-C29B	110.64(15)	C6C-C5C-C4C	119.3(2)
C35B-C31B-C32B	101.73(14)	C5C-C6C-C7C	120.2(2)
C35B-C31B-C36B	117.07(15)	C6C-C7C-C2C	121.2(2)
C32B-C31B-C36B	116.92(15)	C7D-C2D-C3D	118.8(2)
C35B-C31B-Ga1B	104.67(11)	C7D-C2D-C1D	121.4(3)
C32B-C31B-Ga1B	97.05(11)	C3D-C2D-C1D	119.8(3)
C36B-C31B-Ga1B	116.50(11)	C4D-C3D-C2D	120.2(2)
C33B-C32B-C31B	112.06(16)	C5D-C4D-C3D	120.4(2)
C32B-C33B-C34B	107.02(15)	C6D-C5D-C4D	119.9(2)
C32B-C33B-C40B	120.30(16)	C5D-C6D-C7D	120.3(2)
C34B-C33B-C40B	132.67(15)	C6D-C7D-C2D	120.5(2)
C35B-C34B-C33B	106.59(15)	C7E-C2E-C3E	120.2(2)
C35B-C34B-C44B	121.40(15)	C7E-C2E-C1E	121.2(4)
C33B-C34B-C44B	131.97(15)	C3E-C2E-C1E	118.5(4)
C34B-C35B-C31B	112.40(15)	C4E-C3E-C2E	118.8(2)
C37B-C36B-C38B	109.35(16)	C5E-C4E-C3E	120.5(2)
C37B-C36B-C39B	108.62(16)	C6E-C5E-C4E	120.3(2)
C38B-C36B-C39B	107.93(17)	C5E-C6E-C7E	119.9(2)
C37B-C36B-C31B	111.14(16)	C6E-C7E-C2E	120.4(2)
C38B-C36B-C31B	111.43(15)	C7F-C2F-C3F	118.5(4)
C39B-C36B-C31B	108.27(15)	C7F-C2F-C1F	121.7(4)
C42B-C40B-C41B	106.05(15)	C3F-C2F-C1F	119.8(4)
C42B-C40B-C43B	110.77(16)	C4F-C3F-C2F	119.4(6)
C41B-C40B-C43B	105.90(15)	C3F-C4F-C5F	122.0(6)
C42B-C40B-C33B	112.79(14)	C6F-C5F-C4F	118.9(5)
C41B-C40B-C33B	109.85(15)	C5F-C6F-C7F	120.3(5)
C43B-C40B-C33B	111.13(14)	C6F-C7F-C2F	121.0(5)
C46B-C44B-C45B	109.91(15)	C7G-C2G-C3G	119.2(7)
C46B-C44B-C47B	105.68(15)	C7G-C2G-C1G	120.6(7)
C45B-C44B-C47B	106.81(15)	C3G-C2G-C1G	120.2(6)
C46B-C44B-C34B	113.07(15)	C4G-C3G-C2G	119.9(7)
C45B-C44B-C34B	111.51(15)	C5G-C4G-C3G	120.2(7)
C47B-C44B-C34B	109.51(14)	C4G-C5G-C6G	120.6(6)
C7C-C2C-C3C	117.80(19)	C7G-C6G-C5G	119.5(6)
C7C-C2C-C1C	120.8(2)	C2G-C7G-C6G	120.5(8)
C3C-C2C-C1C	121.35(19)	C3H-C2H-C7H	116.6(3)
C4C-C3C-C2C	121.2(2)	C3H-C2H-C1H	121.2(4)

C7H-C2H-C1H	122.2(4)	C7I-C2I-C1I	124.3(14)
C4H-C3H-C2H	123.8(4)	C3I-C2I-C1I	120.5(14)
C5H-C4H-C3H	119.1(4)	C4I-C3I-C2I	119.1(14)
C4H-C5H-C6H	122.0(4)	C3I-C4I-C5I	121.4(14)
C5H-C6H-C7H	118.3(4)	C6I-C5I-C4I	119.3(14)
C2H-C7H-C6H	120.0(4)	C5I-C6I-C7I	116.1(15)
C7I-C2I-C3I	114.7(13)	C2I-C7I-C6I	124.4(15)

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