Lewis Acid/Base Reactions of the Bis(amidinato)silylene [*i*PrNC(Ph)N*i*Pr]$_2$Si and Bis(guanidinato)silylene [*i*PrNC(N*i*Pr$_2$)N*i*Pr]$_2$Si with ElPh$_3$ (El = B, Al)

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Supporting Information

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Table S1. Crystal Data and Experimental Parameters for the Crystal Structure Analyses of 5, 6·0.5$C_6H_5CH_3$, and 7

	5	**6**·0.5$C_6H_5CH_3$	**7**
empirical formula	$C_{44}H_{53}AlN_4Si$	$C_{47.5}H_{75}BN_6Si$	$C_{44}H_{71}AlN_6Si$
formula mass, g mol^{-1}	692.97	769.03	739.13
collection *T*, K	100(2)	100(2)	100(2)
λ(Mo Kα), Å	0.71073	0.71073	0.71073
crystal system	orthorhombic	monoclinic	monoclinic
space group (no.)	$Pca2_1$ (29)	$P2_1/c$ (14)	$P2_1/n$ (14)
a, Å	17.7123(9)	10.762(5)	11.635(8)
b, Å	12.5593(7)	20.006(9)	23.239(15)
c, Å	17.9008(9)	22.148(10)	16.351(11)
β, deg	90	98.408(15)	90.39(2)
V, Å^3	3982.1(4)	4717(4)	4421(5)
Z	4	4	4
ρ(calcd), g cm^{-3}	1.156	1.083	1.111
μ, mm^{-1}	0.116	0.087	0.109
F(000)	1488	1684	1616
crystal dimensions, mm	0.10 x 0.09 x 0.09	0.14 x 0.14 x 0.12	0.65 x 0.30 x 0.15
2*θ* range, deg	3.242–52.042	2.756–52.042	3.046–52.042
index ranges	$-14 \le h \le 21$, $-15 \le k \le 10$, $-21 \le l \le 22$	$-13 \le h \le 13$, $-24 \le k \le 24$, $-27 \le l \le 27$	$-14 \le h \le 12$, $-28 \le k \le 28$, $-20 \le l \le 20$
number of collected reflections	18566	64867	61497
number of independent reflections	7807	9290	8711
R_{int}	0.0453	0.0396	0.0341
number of parameters	459	536	497
number of restraints	1	39	3
S^a	1.020	1.037	1.024
weight parameters a/b^b	0.0396/1.1026	0.0630/1.3374	0.0411/2.2050
$R1^c$ [$I > 2\sigma(I)$]	0.0466	0.0429	0.0362
$wR_2{}^d$ (all data)	0.1030	0.1251	0.0949
absolute structure parameter	–0.05(8)		
max./min. residual electronic density, e Å^{-3}	+0.707/–0.390	+0.533/–0.238	+0.352/–0.296

^{a} $S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{0.5}$; n = number of reflections; p = number of parameters.
^{b} $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$, with $P = [\max(F_o^2,0) + 2F_c^2] / 3$. ^{c} $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.
^{d} $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{0.5}$.

Figure S1. ^{1}H NMR spectrum of compound 4

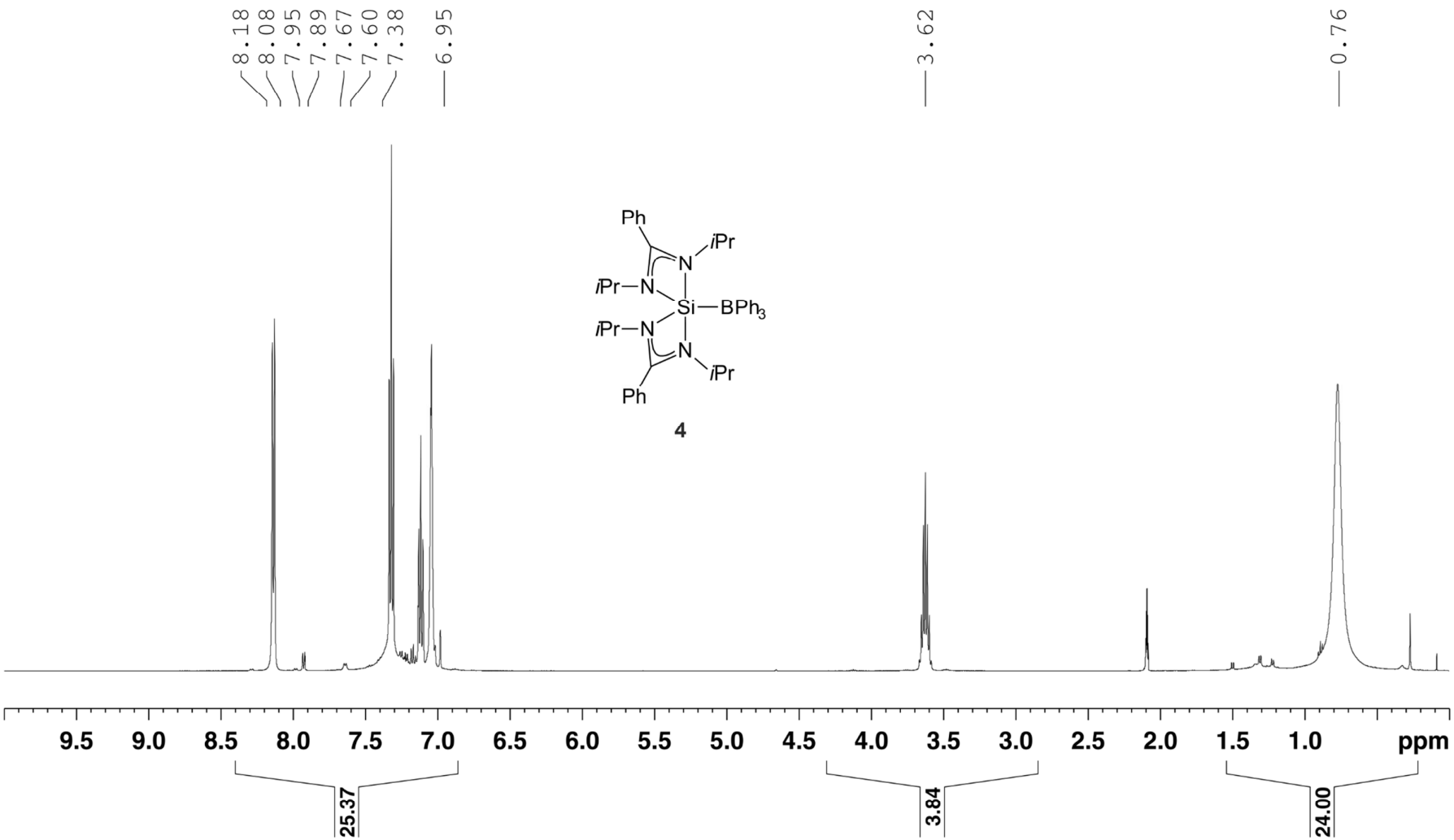

Figure S2. ^{13}C NMR spectrum of compound 4

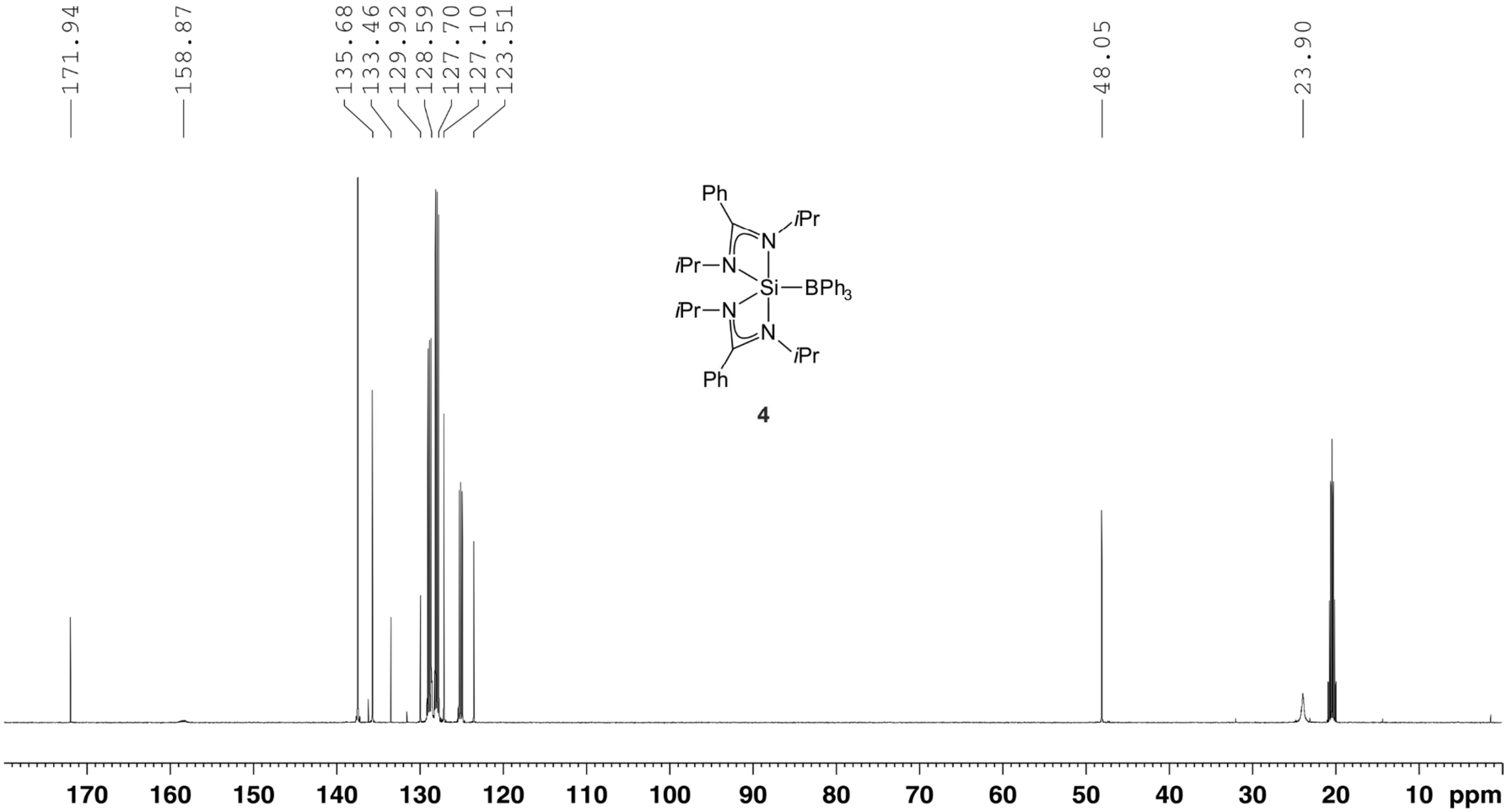

Figure S3. ^{1}H NMR spectrum of compound 5

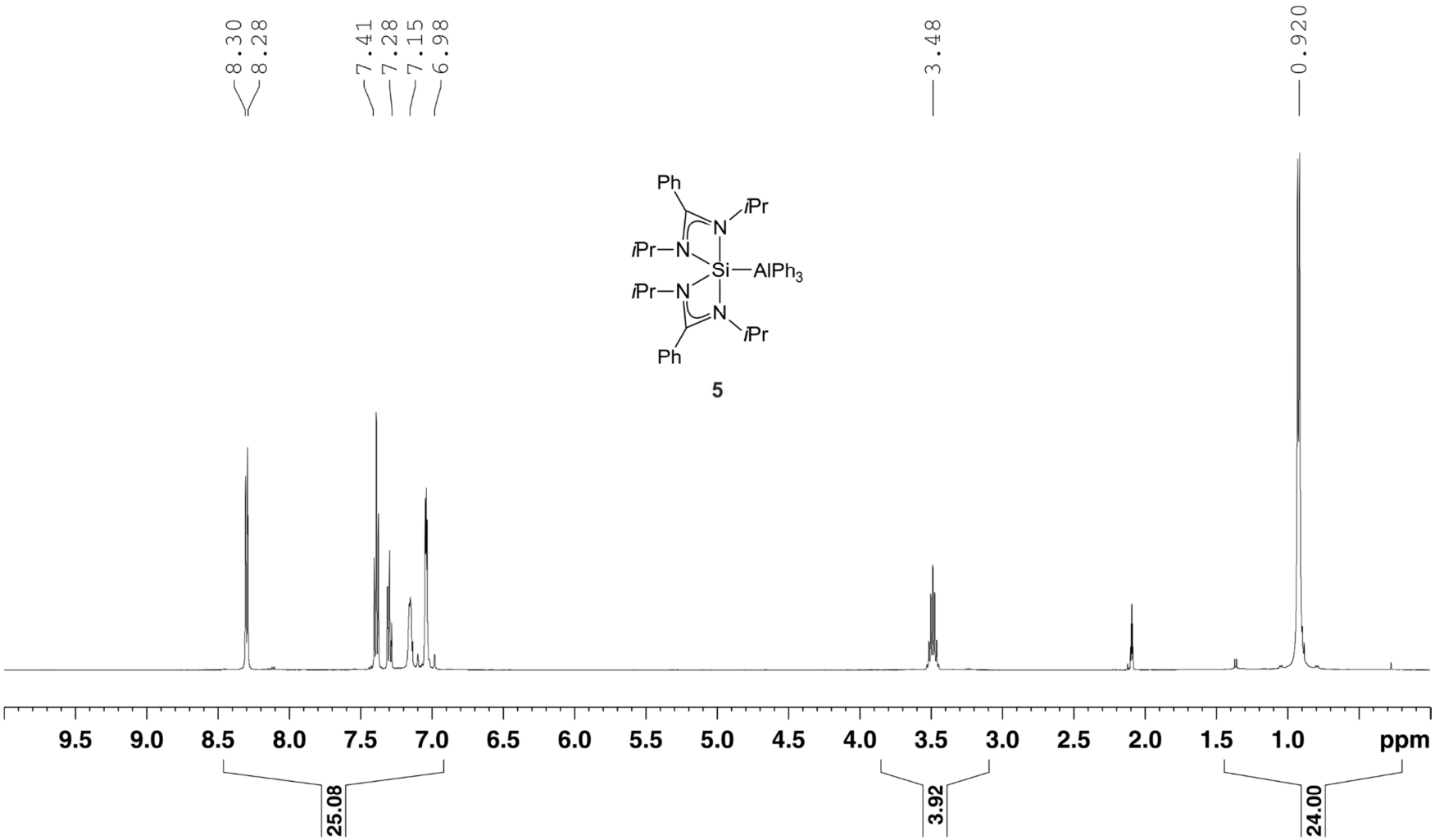

Figure S4. ^{13}C NMR spectrum of compound 5