Supporting Information: *Isolation of Reactive Intermediate in Deprotonation Reaction with Zinc Alkyls*

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Experimental Details

General remarks

Chloro(chloromethyl)dimethylsilane was received by Wacker Chemie AG. All manipulations were conducted under an atmosphere of dry argon using standard Schlenk techniques. THF and n-pentane were purified by distillation from sodium/benzophenone and stored under an atmosphere of argon. NMR spectra were recorded on the Bruker DPX 300. ^{1}H NMR spectra are referenced to internal the internal standards C_6D_5H at 7.16 ppm or $CHCl_3$ at 7.27 ppm, ^{13}C NMR spectra are referenced to C_6D_5H at 128.39 ppm or $CHCl_3$ at 77.00 ppm (external standard: TMS). The ^{29}Si NMR spectra are referenced to the external standard TMS (δ = 0.0). The GC-MS spectra were measured with the gas chromatography column HP 6890 [*J. & W. Scientific*; 25 m length, ID 0.2 mm, helium gas, 2.06 bar; temperature progam: 50 °C (1 min) - 40 °C/min - 300 °C (5 min)] and a HP Mass Selective Detector 5973 (EI(+)-MS, 70 eV). The elemental analysis was conducted on a *Leco CHNS–932/O VTF-900 analyzer.*

Synthesis of (*tert*-butylamino)(piperidinomethyl)dimethylsilane (1)

(*tert*-butylamino)(piperidinomethyl)dimethylsilane (**1**) was synthesised according to literature procedure.[1]

^{1}H-NMR (300.1 MHz, C_6D_6): δ = 0.20 [s, 6H; Si(CH_3)$_2$], 0.96 [br, 1H; SiNHC(CH$_3$)$_3$], 1.16 [s, 9H; SiNHC(CH_3)$_3$], 1.28-1.36 [m, 2H; NCCCH_2], 1.51-1.58 [m, 4H; NCCH_2C], 1.84 [s, 2H; SiCH_2N], 2.36 [br, 4H; NCH_2CC].

^{13}C{^{1}H}-NMR (75.5 MHz, C_6D_6): δ = 2.7 [2C, Si(CH$_3$)$_2$], 24.8 [1C, NCCCH$_2$], 27.3 [2C, NCCH$_2$C], 34.3 [3C, SiNC(CH$_3$)$_3$], 49.6 [1C, SiNC(CH$_3$)$_3$], 52.9 [1C, SiCH$_2$N], 59.1 [1C, NCH$_2$CC].

^{29}Si{^{1}H}-NMR (59.6 MHz, C_6D_6): δ = −6.0.

CHN

calculated:	C 63.09	H 12.35	N 12.26
measured:	C 62.0	H 12.1	N 12.0

Synthesis of [Zn(Et)$_2$\{(*tert*-butylamino)(piperidinomethyl)dimethylsilane\}] (2)

0.5 ml Et_2Zn (1 M in hexane) were added to 117 mg (0.51 mmol) of **1** frozen with liquid nitrogen. The reaction was allowed to warm to −80 °C. After storage for 20 h at −78 °C colourless crystals (170 mg, 0.48 mmol, 97%)* of **2** were obtained.

*Isolation and determination of yield was performed at low temperatures.

^{1}H-NMR (300.1 MHz, C_6D_6): δ = 0.18 [s, 6H; Si(CH_3)$_2$], 0.23-0.35 [br, 4H; ZnCH_2CH$_3$], 1.16 [s, 9H; NC(CH_3)$_3$], 0.80-0.97 [m, 2H; NCHCH$_2$CH_2], 1.23-1.58 [m, 4H; NCHCH_2CH$_2$], 1.51-1.58 [m, 6H; ZnCH$_2$CH_3], 1.81 [s, 2H; SiCH_2N], 2.35 [br, 4H; NCH_2CH$_2$CH$_2$], signal of N–H not clearly visible.

^{13}C{^{1}H}-NMR (75.5 MHz, C_6D_6): δ = 6.0 [2C, Si(CH$_3$)$_2$], 6.2 [br, 2C, ZnCH$_2$CH$_3$], 12.2 [br, 2C, ZnCH$_2$$CH_3$], 23.4 [1C, NCHCH$_2$$CH_2$], 27.0 [2C, NCH$CH_2CH_2$], 32.3 [1C, NCH$CH_2CH_2$], 34.4 [3C, NC($CH_3$)$_3$], 40.0 [1C, Si$CH_2$N], 42.4 [2C, N($CH_3$)$_2$], 48.8 [1C, N($CH_3$)], 50.2 [1C, N$C$(CH$_3$)$_3$], 63.5 [1C, N$C_2CH_2CH_2$], 67.0 [1C, N$CHCH_2CH_2$].

^{29}Si{^{1}H}-NMR (59.6 MHz, C_6D_6): δ = −5.35.

Synthesis of ethylzincsilylamide (3)

The solvent of **2** obtained via the procedure described above (543 mg, 2.38 mmol of **1**) was removed with a sringe at −70 °C. The residue was stored for 24 h at 0 °C leading to liquefaction followed by the formation of colourless crystals of **3** (437 mg, 1.36 mmol, 57%).

^{1}H-NMR (300.1 MHz, C_6D_6): $\delta = 0.27$ [s, 6H; Si(CH_3)$_2$], 0.60 [q, 2H, $^{3}J_{HH} = 8.2$ Hz; ZnCH_2CH$_3$], 0.72-0.89 [m, 1H; NCH$_2$CH$_2$CH_2], 1.16-1.24 [m, 2H; NCH$_2$CH_2CH$_2$], 1.29-1.42 [m, 2H; NCH$_2$CH_2CH_2], 1.47 [s, 9H; NC(CH_3)$_3$], 1.52 [s, 2H; SiCH_2N], 1.49-1.54 [m, 2H; NCH_2CH_2CH$_2$], 1.58-1.63 [m, 1H; NCH_2CH$_2$CH$_2$], 1.61 [t, 3H, $^{3}J_{HH} = 8.2$ Hz; ZnCH$_2$CH_3], 2.77-2.82 [m, 2H; NCH_2CH$_2$CH$_2$].

^{13}C{^{1}H}-NMR (75.5 MHz, C_6D_6): $\delta = 5.1$ [1C, ZnCH_2CH$_3$], 6.0 [2C, Si(CH_3)$_2$], 13.2 [1C, ZnCH$_2$CH_3], 23.6 [1C, NCH$_2$CH$_2$CH_2], 25.0 [2C, NCH$_2$CH_2CH$_2$], 38.3 [3C, NC(CH_3)$_3$], 52.4 [1C, NC(CH$_3$)$_3$], 54.4 [1C, SiCH_2N], 58.9 [2C, NCH_2CH$_2$CH$_2$].

^{29}Si{^{1}H}-NMR (59.6 MHz, C_6D_6): $\delta = -12.3$.

CHN

calculated:	C 52.24	H 10.02	N 8.70
measured:	C 50.9	H 10.5	N 8.6

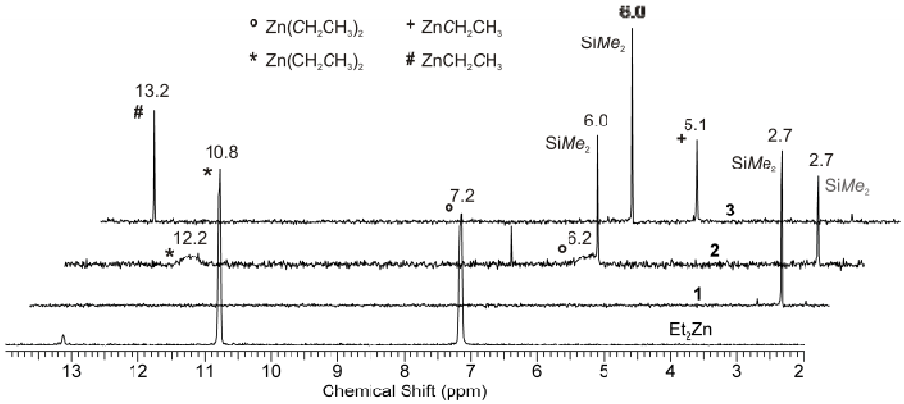

Fig. 1 Excerpt of the ^{13}C NMR spectra showing signals of the silicon bonded methyl groups and the zinc bonded ethyl groups of pure Et_2Zn and compounds **1** to **3** (the additional SiMe_2 signal in compound **2**, labelled in grey, results from some non-coordinated reagent **1**).

Synthesis of (*tert*-butylamino)(*N*,*N'*,*N'*-trimethylcyclohexyl-1*R*,2*R*-diamino-*N*-methyl)-dimethylsilane

(*tert*-butylamino)(*N*,*N'*,*N'*-trimethylcyclohexyl-1*R*,2*R*-diamino-*N*-methyl)dimethylsilane was synthesised according to literature procedure.[2]

^{1}H-NMR (300.1 MHz, C_6D_6): δ = 0.27 [s, 3H], 0.31 [s, 3H; Si(CH_3)$_2$], 0.97-1.06 [m, 4H; NCHCH$_2$CH_2], 1.24 [s, 9H; SiNHC(CH_3)$_3$], 1.59-1.84 [m, 5H; NCHCH_2CH$_2$, SiNHC(CH$_3$)$_3$], 1.78 + 2.10 [AB-system, 2H, $^{2}J_{HH}$ = 14.2 Hz; SiCH_2N], 2.23-2.31 [m, 2H; NCHCH$_2$CH$_2$], 2.28 [s, 6H; N(CH_3)$_2$], 2.33 [s, 3H; NCH_3].

^{13}C{^{1}H}-NMR (75.5 MHz, C_6D_6): δ = 3.1 + 3.4 [2C, Si(CH$_3$)$_2$], 24.4 [1C, NCHCH$_2$$CH_2$], 24.6 [1C, NCHCH$_2$$CH_2$], 26.5 [2C, NCH$CH_2CH_2$], 34.4 [3C, SiNHC($CH_3$)$_3$], 40.8 [2C, N($CH_3$)$_2$], 41.2 [1C, N$CH_3$], 44.4 [1C, SiCH$_2$N], 49.4 [1C, SiNH$C$(CH$_3$)$_3$], 64.7 [1C, N$CHCH_2CH_2$], 67.6 [1C, N$CHCH_2CH_2$].

^{29}Si{^{1}H}-NMR (59.6 MHz, C_6D_6): δ = −6.0.

Synthesis of (R_{C1},R_{C2},R_N)-[Zn(Et)$_2${(*tert*-butylamino)(*N*,*N'*,*N'*-trimethylcyclohexyl-1,2-diamino-*N*-methyl)-dimethylsilane}] (4)

0.7 ml Et$_2$Zn (1 M in hexane) were added to 193 mg (0.64 mmol) of (*tert*-butylamino)(*N*,*N'*,*N'*-trimethylcyclohexyl-1*R*,2*R*-diamino-*N*-methyl)dimethylsilane frozen with liquid nitrogen. The reaction was allowed to warm to −80 °C. After storage for 20 h at −78 °C colourless crystals (243 mg, 0.57 mmol, 89%) of **4** were obtained.

^{1}H-NMR (300.1 MHz, C_6D_6): δ = 0.25 [s, 3H; Si(CH_3)$_2$], 0.30 [s, 3H; Si(CH_3)$_2$], 0.33-0.43 [m, 4H; ZnCH_2CH$_3$], 0.61-0.78 [m, 4H; NCHCH$_2$CH_2], 1.27 [s, 9H; NC(CH_3)$_3$], 1.34-1.52 [m, 4H; NCHCH_2CH$_2$], 1.62 [br, 1H; NH], 1.84 [t, 6H, $^{3}J_{HH}$ = 8.2 Hz; ZnCH$_2$CH_3], 1.98 + 2.13 [AB-system, 2H, $^{2}J_{HH}$ = 13.9 Hz; SiCH_2N], 1.98-2.04 [m, 2H; NCHCH$_2$CH$_2$], 2.04 [s, 6H; N(CH_3)$_2$], 2.12 [s, 3H; N(CH_3)].

^{13}C{^{1}H}-NMR (75.5 MHz, C_6D_6): δ = 3.3 [1C, Si(CH$_3$)$_2$], 3.8 [2C, ZnCH$_2$CH$_3$], 4.2 [1C, Si(CH$_3$)$_2$], 15.5 [2C, ZnCH$_2$$CH_3$], 22.3 [1C, NCHCH$_2$$CH_2$], 22.6 [1C, NCHCH$_2$$CH_2$], 25.4 [1C, NCH$CH_2CH_2$], 25.6 [1C, NCH$CH_2CH_2$], 34.4 [3C, NC($CH_3$)$_3$], 40.0 [1C, Si$CH_2$N], 42.4 [2C, N($CH_3$)$_2$], 48.8 [1C, N($CH_3$)], 50.2 [1C, N$C$(CH$_3$)$_3$], 63.5 [1C, N$C$$_2CH_2CH_2$], 67.0 [1C, N$CHCH_2CH_2$].

^{29}Si{^{1}H}-NMR (59.6 MHz, C_6D_6): δ = −5.6.

Crystal Structure Determination

The crystals of both compounds were mounted in an inert oil (perfluoropolyalkylether) at –80 °C (N_2 stream), using the X-TEMP 2 device[3]. The crystal structure determination of **2** was accomplished on a Bruker Apex CCD diffractometer; programs used for data collection, cell determination and -refinement: Smart V. 5622 (Bruker AXS, 2001), integration: SaintPlus V. 6.02 (Bruker AXS, 1999), empirical absorption correction: Sadabs V. 2.01 (Bruker AXS, 1999). The crystal structure determination of **3** and (R_{C1},R_{C2},R_N)-**4** was accomplished on a Oxford Diffraction Xcalibur S, programs used for data collection, cell determination and -refinement: CrysAlis (Oxford, 2008); CrysAlis RED (Oxford, 2008), empirical absorption correction: Scale3 Abspack (Oxford, 2008). The structures were solved applying direct and Fourier methods, using SHELXS-90 (G. M. Sheldrick, University of Göttingen 1990) and SHELXL-97 (G. M. Sheldrick, SHELXL97, University of Göttingen 1997). The non-hydrogen atoms were refined anisotropically. All of the H-atoms – with the exception of the hydrogen bonded to the nitrogen in compounds **2** and (R_{C1},R_{C2},R_N)-**4** – were placed in geometrically calculated positions and each was assigned a fixed isotropic displacement parameter based on a riding-model. The hydrogen atoms H1N of compounds **2** and (R_{C1},R_{C2},R_N)-**4** were found and could be freely refined via Difference-Fourier-Synthesis. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 869490 [compound **2**], CCDC 869491 [compound **3**] and CCDC 869492 [compound (R_{C1},R_{C2},R_N)-**4**]. This data can be obtained free of charge on application to Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; [fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table 1 Crystal Data and Structural Refinement Details for compounds **2**,**3** and (R_{C1},R_{C2},R_N)-**4**.

compound	**2**	**3**	(R_{C1},R_{C2},R_N)-**4**
empirical formula	$C_{16}H_{38}N_2SiZn$	$C_{14}H_{32}N_2SiZn$	$C_{20}H_{47}N_3SiZn$
molecular mass [g·mol^{-1}]	351.94	321.88	423.07
temperature [K]	173(2)	173(2)	173(2)
wave length [Å]	0.71073	0.71073	0.71073
crystal system	monoclinc	triclinic	monoclinc
space group	$P2_1/c$	$P1;^{-}$	$C2$
***a* [Å]**	12.126(5)	8.3337(2)	14.7303(5)
***b* [Å]**	10.691(5)	9.9823(2)	10.1126(3)

***c* [Å]**	16.231(7)	11.3766(2)	17.4314(6)
***α* [°]**	90	100.862(18)	90
***β* [°]**	106.918(7)	91.5344(17)	107.870(4)
***γ* [°]**	90	109.845(2)	90
cell volume V [Å^3]	2013.3(15)	870.03(3)	2471.35(13)
Z	4	2	4
calculated density *ρ* [g·cm^{-3}]	1.161	1.229	1.137
absorption coefficient *μ* [mm^{-1}]	1.275	1.469	1.050
***F*(000)**	768	348	928
crystal size [mm^3]	0.60 x 0.20 x 0.20	0.40 x 0.20 x 0.20	0.30 x 0.30 x 0.30
range for data collection 2*θ* [°]	2.31 – 26.99°	2.22 – 27.00°	2.46 – 26.00°
index ranges	−15 < h < 15	−10 < h < 10	−18 < h < 18
	−13 < k < 13	−12 < k < 12	−12 < k < 12
	−20 < l < 20	−14 < l < 14	−21 < l < 21
reflections collected	43766	46205	22745
independent reflections	4390 [R_{int} = 0.0417]	3799 [R_{int} = 0.0296]	4845 [R_{int} = 0.0312]
refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
data / restraints / parameter	4390 / 0 / 192	3799 / 0 / 169	4390 / 0 / 192
goodness-of-fit on F^2	1.048	1.093	1.037
final R-values [I > 2σ(I)]	*R1* = 0.0271	*R1* = 0.0192	*R1* = 0.0238
	wR2 = 0.0684	*wR2* = 0.0552	*wR2* = 0.0542
R-values (all data)	*R1* = 0.0323	*R1* = 0.0220	*R1* = 0.0266
	wR2 = 0.0715	*wR2* = 0.0556	*wR2* = 0.0546
Flack-X-parameter[4]			0.010(7)
largest diff. peak and hole [e·Å^{-3}]	0.487 and −0.163	0.295 and −0.246	0.364 and −0.184

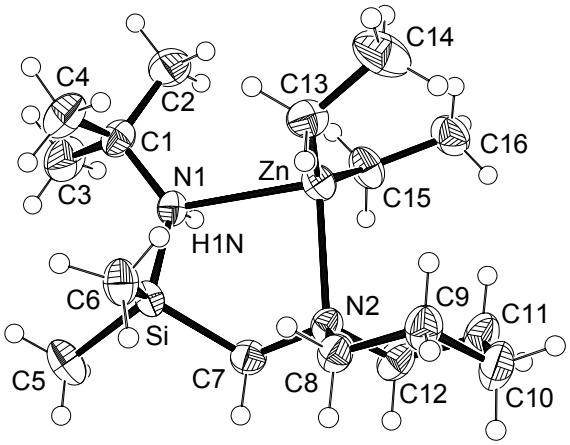

Fig. 2 ORTEP plot of **2** at 50 % probability level.

list of bond lengths [Å] and angles [°] for 2			
C(1)-N(1)	1.501(2)	**C(1)-C(2)**	1.528(3)
C(1)-C(4)	1.528(2)	**C(1)-C(3)**	1.534(2)
C(7)-Si	1.8925(17)	**C(5)-Si**	1.8737(18)
C(8)-C(9)	1.521(2)	**C(6)-Si**	1.8726(18)
C(10)-C(11)	1.524(3)	**C(7)-N(2)**	1.491(2)
C(12)-N(2)	1.493(2)	**C(8)-N(2)**	1.489(2)
C(13)-Zn	2.0040(18)	**C(9)-C(10)**	1.528(2)
C(15)-C(16)	1.519(2)	**C(11)-C(12)**	1.517(3)
N(1)-Zn	2.5652(16)	**C(13)-C(14)**	1.528(3)
N(2)-Zn	2.3261(15)	**C(15)-Zn**	2.0087(18)
N(1)-Si	1.7508(16)	**N(1)-H(1N)**	0.810(18)
C(2)-C(1)-C(4)	109.52(15)	**N(1)-C(1)-C(2)**	108.85(13)
C(2)-C(1)-C(3)	108.77(15)	**N(1)-C(1)-C(4)**	109.75(14)
N(2)-C(7)-Si	117.33(10)	**N(1)-C(1)-C(3)**	110.44(14)
N(2)-C(8)-C(9)	112.73(13)	**C(4)-C(1)-C(3)**	109.50(16)
C(8)-C(9)-C(10)	110.51(15)	**C(1)-N(1)-Zn**	119.51(9)
C(11)-C(10)-C(9)	108.91(14)	**C(1)-N(1)-H(1N)**	107.2(13)
C(12)-C(11)-C(10)	111.01(15)	**Zn-N(1)-H(1N)**	84.6(12)
N(2)-C(12)-C(11)	112.23(14)	**C(8)-N(2)-C(12)**	109.16(12)
C(14)-C(13)-Zn	114.26(13)	**C(8)-N(2)-Zn**	113.09(9)
C(16)-C(15)-Zn	115.40(12)	**C(12)-N(2)-Zn**	111.54(10)
C(1)-N(1)-Si	128.12(11)	**N(1)-Si-C(5)**	116.27(8)
Si-N(1)-Zn	98.88(5)	**N(1)-Si-C(7)**	100.43(7)
Si-N(1)-H(1N)	110.2(13)	**C(5)-Si-C(7)**	105.97(9)
C(8)-N(2)-C(7)	109.20(12)	**C(13)-Zn-N(2)**	109.99(6)
C(7)-N(2)-C(12)	108.44(12)	**C(13)-Zn-N(1)**	104.09(6)
C(7)-N(2)-Zn	105.24(9)	**N(2)-Zn-N(1)**	86.35(4)
N(1)-Si-C(6)	112.93(7)	**C(6)-Si-C(5)**	107.25(9)
C(6)-Si-C(7)	113.87(8)	**C(13)-Zn-C(15)**	139.33(7)
C(15)-Zn-N(2)	104.74(7)	**C(15)-Zn-N(1)**	98.50(6)

Table 2 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for **2**.

	x	y	z	U(eq)	
C(1)	3283(1)	11256(2)	596(1)	37(1)	
C(2)	2986(2)	10762(2)	−326(1)	50(1)	
C(3)	2913(2)	12631(2)	571(2)	58(1)	
C(4)	4582(2)	11157(2)	1019(1)	53(1)	
C(5)	2869(2)	11807(2)	2816(1)	51(1)	
C(6)	4408(1)	9625(2)	2728(1)	40(1)	
C(7)	1708(1)	9330(1)	2277(1)	35(1)	
C(8)	2451(1)	7218(2)	2592(1)	34(1)	
C(9)	2375(2)	5848(2)	2328(1)	42(1)	
C(10)	1144(2)	5366(2)	2159(1)	51(1)	
C(11)	333(2)	6200(2)	1488(1)	51(1)	
C(12)	451(1)	7558(2)	1771(1)	42(1)	
C(13)	3708(1)	7393(2)	815(1)	39(1)	
C(14)	3687(2)	6303(2)	201(1)	64(1)	
C(15)	675(2)	8471(2)	−254(1)	42(1)	
C(16)	195(2)	7334(2)	−804(1)	49(1)	
N(2)	1655(1)	8029(1)	1937(1)	31(1)	
N(1)	2656(1)	10486(1)	1091(1)	30(1)	
H(1N)	1972(16)	10604(16)	874(11)	34(5)	
Si	2961(1)	10339(1)	2209(1)	30(1)	
Zn	2169(1)	8196(1)	668(1)	33(1)	

Table 3 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **2**.

	U11	U22	U33	U23	U13	U12
C(1)	38(1)	31(1)	45(1)	4(1)	14(1)	−2(1)
C(2)	63(1)	49(1)	42(1)	9(1)	20(1)	−3(1)
C(3)	73(1)	31(1)	77(1)	9(1)	33(1)	−1(1)
C(4)	38(1)	62(1)	62(1)	9(1)	17(1)	−9(1)
C(5)	59(1)	41(1)	47(1)	−16(1)	7(1)	3(1)
C(6)	32(1)	38(1)	43(1)	−2(1)	−1(1)	−3(1)
C(7)	33(1)	34(1)	38(1)	−1(1)	13(1)	2(1)
C(8)	32(1)	35(1)	31(1)	3(1)	4(1)	−4(1)
C(9)	46(1)	33(1)	43(1)	6(1)	8(1)	−3(1)
C(10)	55(1)	41(1)	52(1)	6(1)	9(1)	−18(1)
C(11)	43(1)	55(1)	49(1)	3(1)	2(1)	−22(1)
C(12)	28(1)	50(1)	46(1)	7(1)	7(1)	−7(1)
C(13)	42(1)	34(1)	43(1)	5(1)	17(1)	7(1)
C(14)	85(2)	54(1)	56(1)	−4(1)	26(1)	28(1)
C(15)	44(1)	37(1)	35(1)	−5(1)	−2(1)	4(1)
C(16)	48(1)	57(1)	36(1)	−11(1)	3(1)	−6(1)
N(2)	26(1)	32(1)	32(1)	1(1)	7(1)	−3(1)
N(1)	27(1)	27(1)	34(1)	0(1)	6(1)	−1(1)
Si	30(1)	27(1)	31(1)	−6(1)	5(1)	−1(1)
Zn	32(1)	32(1)	31(1)	−1(1)	4(1)	3(1)

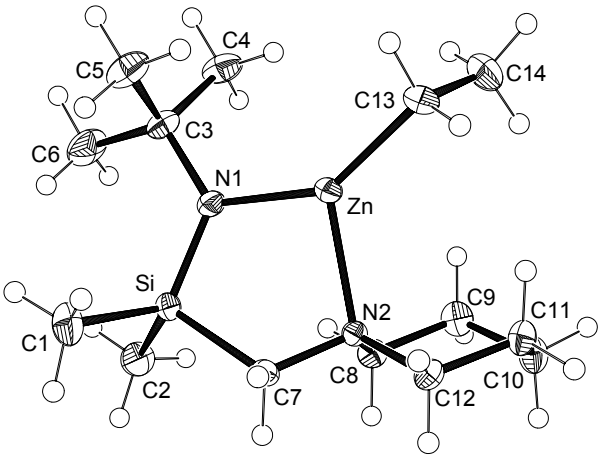

Fig. 3 ORTEP plot of **3** at 50 % probability level.

list of bond lengths [Å] and angles [°] for 3			
C(1)-Si	1.8780(15)	N(2)-C(7)-Si	113.86(8)
C(2)-Si	1.8798(15)	N(2)-C(8)-C(9)	111.78(10)
C(3)-N(1)	1.4771(16)	C(8)-C(9)-C(10)	110.80(11)
C(3)-C(4)	1.526(2)	C(11)-C(10)-C(9)	109.87(11)
C(3)-C(6)	1.535(2)	C(12)-C(11)-C(10)	110.96(11)
C(3)-C(5)	1.5372(19)	N(2)-C(12)-C(11)	112.01(10)
C(7)-N(2)	1.4903(15)	C(14)-C(13)-Zn	116.60(11)
C(7)-Si	1.9011(13)	C(3)-N(1)-Si	126.66(9)
C(8)-N(2)	1.4805(16)	C(3)-N(1)-Zn	118.36(8)
C(8)-C(9)	1.5200(18)	Si-N(1)-Zn	113.21(6)
C(9)-C(10)	1.5229(19)	C(8)-N(2)-C(12)	109.18(9)

C(10)-C(11)	1.5223(19)	C(8)-N(2)-C(7)	109.67(10)
C(11)-C(12)	1.5158(18)	C(12)-N(2)-C(7)	109.55(9)
C(12)-N(2)	1.4859(15)	C(8)-N(2)-Zn	109.48(7)
C(13)-C(14)	1.522(2)	C(12)-N(2)-Zn	117.41(8)
C(13)-Zn	1.9692(14)	C(7)-N(2)-Zn	101.18(7)
N(1)-Si	1.6958(11)	N(1)-Si-C(1)	117.28(7)
N(1)-Zn	1.9046(10)	N(1)-Si-C(2)	116.71(7)
N(2)-Zn	2.1672(10)	C(1)-Si-C(2)	106.23(7)
N(1)-C(3)-C(4)	109.65(11)	N(1)-Si-C(7)	102.36(5)
N(1)-C(3)-C(6)	111.92(11)	C(1)-Si-C(7)	103.66(7)
C(4)-C(3)-C(6)	107.99(12)	C(2)-Si-C(7)	109.60(6)
N(1)-C(3)-C(5)	110.00(11)	N(1)-Zn-C(13)	144.34(5)
C(4)-C(3)-C(5)	108.71(12)	N(1)-Zn-N(2)	93.27(4)
C(6)-C(3)-C(5)	108.50(12)	C(13)-Zn-N(2)	122.39(5)

Table 4 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for **3**.

	x	**y**	**z**	**U(eq)**
C(1)	4435(2)	8943(2)	7783(2)	36(1)
C(2)	4682(2)	7338(2)	9726(1)	32(1)
C(3)	132(2)	6984(2)	8645(1)	23(1)
C(4)	−1436(2)	5783(2)	8910(1)	31(1)
C(5)	−455(2)	7776(2)	7779(2)	34(1)
C(6)	921(2)	8077(2)	9832(1)	40(1)
C(7)	4167(2)	5852(1)	7035(1)	18(1)
C(8)	3129(2)	3593(1)	7749(1)	20(1)
C(9)	1918(2)	2018(1)	7506(1)	25(1)
C(10)	2208(2)	1169(1)	6321(1)	27(1)
C(11)	2079(2)	1945(1)	5311(1)	24(1)
C(12)	3274(2)	3520(1)	5619(1)	19(1)
C(13)	−1526(2)	3415(2)	5699(1)	29(1)
C(14)	−2625(2)	2025(2)	6067(2)	41(1)
N(1)	1358(1)	6340(1)	8092(1)	20(1)
N(2)	2931(1)	4324(1)	6766(1)	15(1)
Si	3523(1)	7133(1)	8226(1)	19(1)
Zn	505(1)	4678(1)	6805(1)	18(1)

Table 5 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **3**.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	38(1)	20(1)	46(1)	5(1)	5(1)	5(1)
C(2)	31(1)	36(1)	24(1)	−7(1)	−7(1)	13(1)
C(3)	25(1)	28(1)	22(1)	5(1)	6(1)	16(1)
C(4)	28(1)	40(1)	36(1)	16(1)	14(1)	20(1)
C(5)	39(1)	39(1)	39(1)	18(1)	12(1)	26(1)
C(6)	44(1)	48(1)	31(1)	−6(1)	7(1)	27(1)
C(7)	15(1)	19(1)	20(1)	4(1)	2(1)	4(1)
C(8)	22(1)	24(1)	15(1)	5(1)	1(1)	10(1)
C(9)	31(1)	24(1)	22(1)	11(1)	4(1)	8(1)
C(10)	33(1)	18(1)	29(1)	5(1)	1(1)	7(1)
C(11)	29(1)	21(1)	20(1)	0(1)	2(1)	9(1)
C(12)	23(1)	21(1)	14(1)	4(1)	5(1)	10(1)
C(13)	19(1)	31(1)	34(1)	2(1)	−5(1)	9(1)
C(14)	24(1)	33(1)	52(1)	−2(1)	1(1)	0(1)
N(1)	18(1)	21(1)	20(1)	1(1)	2(1)	9(1)
N(2)	15(1)	16(1)	13(1)	3(1)	2(1)	5(1)
Si	18(1)	17(1)	19(1)	0(1)	−1(1)	6(1)
Zn	15(1)	20(1)	19(1)	2(1)	0(1)	5(1)

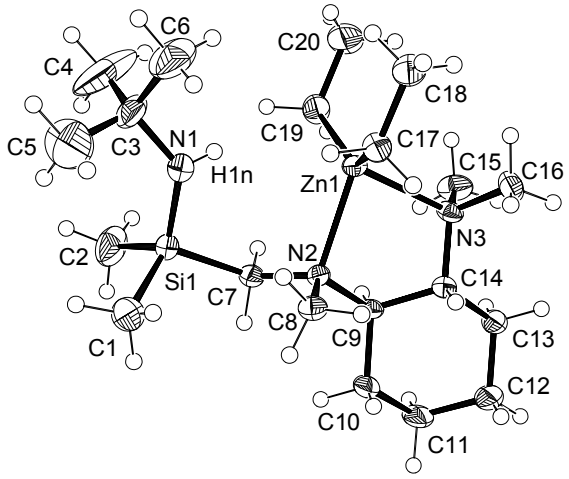

Fig. 4 ORTEP plot of (R_{C1},R_{C2},R_N)-**4** at 50 % probability level.

list of bond lengths [Å] and angles [°] for (R_{C1},R_{C2},R_N)-4			
C(1)-Si(1)	1.867(2)	C(11)-C(10)-C(9)	112.47(18)
C(2)-Si(1)	1.851(3)	C(10)-C(11)-C(12)	109.88(18)
C(3)-N(1)	1.468(3)	C(13)-C(12)-C(11)	109.17(19)
C(3)-C(5)	1.477(5)	C(12)-C(13)-C(14)	112.36(17)
C(3)-C(6)	1.500(4)	N(3)-C(14)-C(13)	112.69(16)
C(3)-C(4)	1.525(5)	N(3)-C(14)-C(9)	110.41(15)
C(7)-N(2)	1.478(2)	C(13)-C(14)-C(9)	112.16(15)
C(7)-Si(1)	1.893(2)	C(18)-C(17)-Zn(1)	113.77(15)
C(8)-N(2)	1.470(3)	C(20)-C(19)-Zn(1)	111.14(17)
C(9)-N(2)	1.497(2)	C(3)-N(1)-Si(1)	132.72(17)
C(9)-C(14)	1.525(3)	C(3)-N(1)-H(1N)	108.6(19)
C(9)-C(10)	1.536(3)	Si(1)-N(1)-H(1N)	113.4(19)
C(10)-C(11)	1.519(3)	C(8)-N(2)-C(7)	110.40(16)
C(11)-C(12)	1.519(3)	C(8)-N(2)-C(9)	112.69(15)
C(12)-C(13)	1.513(3)	C(7)-N(2)-C(9)	110.41(15)
C(13)-C(14)	1.520(3)	C(8)-N(2)-Zn(1)	106.28(12)
C(14)-N(3)	1.486(2)	C(7)-N(2)-Zn(1)	110.32(11)
C(15)-N(3)	1.470(3)	C(9)-N(2)-Zn(1)	106.58(10)
C(16)-N(3)	1.468(3)	C(16)-N(3)-C(15)	108.53(18)
C(17)-C(18)	1.530(3)	C(16)-N(3)-C(14)	110.55(16)
C(17)-Zn(1)	2.016(2)	C(15)-N(3)-C(14)	113.67(16)
C(19)-C(20)	1.520(3)	C(16)-N(3)-Zn(1)	107.19(12)
C(19)-Zn(1)	2.028(2)	C(15)-N(3)-Zn(1)	109.10(14)
N(1)-Si(1)	1.694(2)	C(14)-N(3)-Zn(1)	107.59(11)
N(1)-H(1N)	0.74(2)	N(1)-Si(1)-C(2)	116.05(11)
N(2)-Zn(1)	2.2377(15)	N(1)-Si(1)-C(1)	111.49(13)
N(3)-Zn(1)	2.2311(16)	C(2)-Si(1)-C(1)	106.52(15)
N(1)-C(3)-C(5)	109.4(2)	N(1)-Si(1)-C(7)	107.79(9)
N(1)-C(3)-C(6)	108.6(2)	C(2)-Si(1)-C(7)	102.51(11)
C(5)-C(3)-C(6)	109.6(3)	C(1)-Si(1)-C(7)	112.26(10)
N(1)-C(3)-C(4)	109.5(2)	C(17)-Zn(1)-C(19)	134.03(10)
C(5)-C(3)-C(4)	110.9(4)	C(17)-Zn(1)-N(3)	105.38(8)
C(6)-C(3)-C(4)	108.9(3)	C(19)-Zn(1)-N(3)	105.17(8)
N(2)-C(7)-Si(1)	122.44(13)	C(17)-Zn(1)-N(2)	107.57(7)
N(2)-C(9)-C(14)	112.10(15)	C(19)-Zn(1)-N(2)	110.44(8)

N(2)-C(9)-C(10)	113.42(14)	N(3)-Zn(1)-N(2)	81.08(6)
C(14)-C(9)-C(10)	109.69(16)		

Table 6 Atomic coordinates (·104) and equivalent isotropic displacement parameters (Å2·103) for (R_{C1},R_{C2},R_N)-**4**.

	x	**y**	**z**	**U(eq)**
C(1)	2804(2)	4546(2)	8051(2)	61(1)
C(2)	3660(2)	2784(3)	9457(2)	59(1)
C(3)	995(2)	2894(3)	8870(2)	47(1)
C(4)	1286(3)	2250(6)	9701(2)	122(2)
C(5)	1050(3)	4350(4)	8938(4)	155(3)
C(6)	−8(2)	2489(4)	8422(2)	73(1)
C(7)	3196(1)	1546(2)	7870(1)	24(1)
C(8)	2225(2)	2234(2)	6541(1)	25(1)
C(9)	3203(1)	208(2)	6704(1)	22(1)
C(10)	3917(2)	957(2)	6382(1)	33(1)
C(11)	4503(2)	37(3)	6032(2)	43(1)
C(12)	3847(2)	−769(2)	5350(2)	42(1)
C(13)	3167(2)	−1557(2)	5669(1)	31(1)
C(14)	2579(1)	−681(2)	6045(1)	22(1)
C(15)	2332(2)	−2623(2)	6821(2)	39(1)
C(16)	1072(2)	−1862(2)	5688(2)	38(1)
C(17)	187(1)	742(2)	6399(1)	27(1)
C(18)	−728(1)	−20(3)	6344(1)	37(1)
C(19)	1689(2)	−1030(2)	8218(1)	36(1)
C(20)	892(2)	−1965(3)	8246(2)	60(1)
N(1)	1626(1)	2432(2)	8418(1)	33(1)
N(2)	2623(1)	1095(2)	7059(1)	20(1)
N(3)	1904(1)	−1446(2)	6354(1)	24(1)
Si(1)	2752(1)	2845(1)	8451(1)	29(1)
Zn(1)	1375(1)	−99(1)	7137(1)	22(1)

Table 7 Anisotropic Displacement parameters (Å2·103) for (R_{C1},R_{C2},R_N)-**4**.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	97(2)	30(2)	75(2)	−11(1)	56(2)	−13(1)
C(2)	41(2)	92(2)	40(2)	−25(2)	6(1)	−6(2)
C(3)	35(1)	68(2)	45(2)	−21(1)	22(1)	−1(1)
C(4)	67(2)	265(6)	48(2)	0(3)	37(2)	17(3)
C(5)	146(4)	88(3)	299(8)	−98(4)	169(5)	−31(3)
C(6)	41(2)	120(3)	64(2)	−15(2)	26(1)	5(2)
C(7)	20(1)	27(1)	26(1)	−1(1)	8(1)	−3(1)
C(8)	25(1)	23(1)	27(1)	6(1)	9(1)	3(1)
C(9)	20(1)	18(1)	30(1)	1(1)	13(1)	−1(1)
C(10)	31(1)	32(1)	43(1)	−10(1)	21(1)	−12(1)
C(11)	37(1)	43(1)	64(2)	−15(2)	36(1)	−15(1)
C(12)	49(2)	40(1)	53(2)	−15(1)	37(1)	−12(1)
C(13)	32(1)	27(1)	40(1)	−9(1)	21(1)	−5(1)
C(14)	23(1)	21(1)	23(1)	2(1)	8(1)	−1(1)
C(15)	47(2)	23(1)	59(2)	9(1)	32(1)	6(1)
C(16)	26(1)	39(1)	50(2)	−22(1)	14(1)	−8(1)
C(17)	21(1)	27(1)	33(1)	−2(1)	7(1)	5(1)
C(18)	22(1)	45(1)	44(1)	−6(2)	12(1)	5(1)
C(19)	52(2)	31(1)	26(1)	2(1)	12(1)	−8(1)
C(20)	85(2)	62(2)	41(2)	5(1)	30(2)	−31(2)
N(1)	35(1)	34(1)	34(1)	−8(1)	15(1)	−5(1)

N(2)	20(1)	20(1)	21(1)	1(1)	8(1)	0(1)
N(3)	18(1)	20(1)	35(1)	0(1)	11(1)	−1(1)
Si(1)	31(1)	29(1)	28(1)	−7(1)	13(1)	−5(1)
Zn(1)	20(1)	24(1)	22(1)	2(1)	8(1)	−1(1)

Computational Studies

All calculations were done without symmetry restrictions and modelled after the molecular structures in the crystal. Starting coordinates were obtained with Chem3DUltra 10.0, optimization was performed with Gaussian 03 Revision B.04 at the B3LYP/6-31+G(d) level.[5] Harmonic vibrational frequency analyses (to establish the nature of stationary points on the potential energy surface) were performed on the same level. Table 1 lists the total (SCF) and zero-point energies (ZPE) of all compounds. The vibrational frequency of all compounds analyses showed no imaginary frequencies for ground state structures and exactly one imaginary frequence for transition states.

Table 6 Results from Theoretical Studies.

Compound	**method/basis**	**Min./TS**	**SCF [Hartree]**	**ZPE [Hartree]**
66·EtLi	B3LYP/6-31+G(d)	Global Minimun	−959.960717852	−959.504387
66·EtLi (TS)	B3LYP/6-1+G(d)	Transition state (TS)	−959.951592925	−959.499021
66·Et_2Mg	B3LYP/6-31+G(d)	Global Minimun	−1231.75026078	−1231.228641
66·Et_2Mg (TS)	B3LYP/6-31+G(d)	Transition state (TS)	−1231.72521522	−1231.207591
66·Et_2Zn	B3LYP/6-31+G(d)	Global Minimum	−2810.82637397	−2810.303943
66·Et_2Zn (TS)	B3LYP/6-31+G(d)	Transition state (TS)	−2810.78027076	−2810.262282
(R_{C1},R_{C2},R_N)-4	B3LYP/6-31+G(d)	Global Minimum	−3023,41069825	−3022,756849
(R_{C1},R_{C2},R_N)-4 (TS)	B3LYP/6-31+G(d)	Transition state (TS)	−3023,35640282	−3022,707217

Table 7 Cartesian coordinates of **66·EtLi** and **66·EtLi (TS)** [B3LYP/6−31+G(d)].

66·EtLi				**TS**			
C	−1.75435500	3.61697800	1.10524100	**C**	0.32365300	3.54891100	−0.85744800
C	−0.56127300	3.10283500	0.26665200	**C**	−0.34906700	2.32979200	−1.53179800
C	−2.90444400	−0.15501500	0.87602800	**C**	2.99390300	−0.11623400	−1.05865100
C	−3.85786200	0.23509000	−0.25611300	**C**	3.95542700	0.69820900	−0.18783400
C	2.11159900	−0.64911400	2.73072400	**C**	−1.98560000	−1.65538000	−2.29066800
C	−0.65108400	−0.85467000	1.48363400	**C**	0.79841200	−1.17592900	−1.23445600
C	3.97018700	0.36968200	−0.47246000	**C**	−3.87216100	0.22629300	0.25772700
N	1.48493700	0.37829800	−0.08142200	**N**	−1.36925200	0.23541000	0.07238800
N	−1.56760400	−0.53990500	0.36055300	**N**	1.73216800	−0.42613200	−0.34659300
C	2.44963900	1.94357000	−1.70133200	**C**	−2.50688300	2.11617700	1.17233100
Si	1.22780600	−0.93923900	1.08223800	**Si**	−1.05084000	−1.30842500	−0.67269600
Li	−0.54919500	1.13579400	−0.32161200	**Li**	0.44436000	1.10861800	−0.00668300
C	2.56991100	0.52938000	−1.10187700	**C**	−2.52703300	0.59175800	0.92658300
C	−3.99085300	−0.89388600	−1.28610700	**C**	4.25653400	−0.02453900	1.13195200

C	−1.68812300	−1.67229500	−0.57962100	**C**	2.02063700	−1.18793900	0.88812000
C	−2.60186900	−1.33634100	−1.76332600	**C**	2.94769100	−0.41432100	1.83161100
C	1.73706400	−2.64704600	0.44874500	**C**	−1.29669400	−2.84772200	0.41753100
H	−1.74293300	4.70126500	1.33112200	**H**	0.55950900	4.38454600	−1.53883300
H	−1.81480500	3.10794000	2.08192000	**H**	1.29089800	3.29609700	−0.37741500
H	−2.71667000	3.42463100	0.60291400	**H**	−0.31083800	3.96859000	−0.06269500
H	0.36797400	3.39864600	0.79984400	**H**	0.28247700	1.99212100	−2.37607900
H	−0.51765300	3.70773700	−0.66303000	**H**	−1.28433600	2.66943400	−2.00341800
H	1.38460600	1.27834900	0.40590300	**H**	−1.08035100	1.14231000	−0.70316100
H	−2.76784400	0.68986800	1.55766600	**H**	2.73787000	0.43934000	−1.96722300
H	−3.33241400	−0.99372300	1.45895500	**H**	3.48111900	−1.05789300	−1.37601900
H	−4.83493600	0.48833000	0.17404400	**H**	4.87873900	0.88370400	−0.75103300
H	−3.47966300	1.14571600	−0.74076500	**H**	3.51059200	1.68223500	0.02033100
H	1.89787100	0.35118500	3.12796800	**H**	−1.92960600	−0.79305400	−2.96653800
H	1.79543700	−1.37938600	3.48802900	**H**	−1.56940200	−2.52471100	−2.81921300
H	3.19958800	−0.73726600	2.62228600	**H**	−3.04718500	−1.86273300	−2.10741300
H	−0.76441700	−0.04975100	2.22282500	**H**	0.78396100	−0.64774700	−2.19647500
H	−0.96985700	−1.78144600	2.00138000	**H**	1.20599100	−2.18323500	−1.44673200
H	4.11510500	1.09393400	0.33790700	**H**	−3.95395200	0.70142900	−0.72665000
H	4.11379600	−0.63604800	−0.05975400	**H**	−3.96574900	−0.85807200	0.11890600
H	4.75743300	0.53571800	−1.21844700	**H**	−4.72352200	0.55341500	0.86916100
H	2.56951700	2.71553000	−0.93223500	**H**	−2.59094100	2.67364900	0.23421600
H	3.22226300	2.10019400	−2.46306000	**H**	−3.33816800	2.41105300	1.82411400
H	1.46973000	2.09630300	−2.16658800	**H**	−1.57359500	2.42107600	1.66385600
H	−4.50711300	−1.75070600	−0.82765900	**H**	4.84138400	−0.93297900	0.92484400
H	−4.60544900	−0.57256000	−2.13621700	**H**	4.87232600	0.60482300	1.78647800
H	−2.07972100	−2.56172500	−0.04745600	**H**	2.48240200	−2.15925300	0.62512500
H	−0.68869600	−1.92909500	−0.94259300	**H**	1.07145700	−1.40569800	1.38554200
H	−2.14200800	−0.53356900	−2.35799300	**H**	2.43261700	0.49171800	2.18520300
H	−2.67307200	−2.21426400	−2.41825000	**H**	3.14660600	−1.02755400	2.71967000
H	2.82344300	−2.72910400	0.32564900	**H**	−2.36174800	−3.04502200	0.59331400
H	1.44313700	−3.38896100	1.20371100	**H**	−0.89054100	−3.72732400	−0.10140800
H	1.26869900	−2.93957400	−0.49593800	**H**	−0.80794000	−2.78314600	1.39591800
C	2.37871400	−0.50332400	−2.22606000	**C**	−2.43717300	−0.11019700	2.29861700
H	2.49783500	−1.52982700	−1.86754000	**H**	−2.49506300	−1.19851300	2.20062900
H	1.38251200	−0.40738100	−2.67357100	**H**	−1.48924600	0.13656500	2.79273700
H	3.12177800	−0.34281000	−3.01620500	**H**	−3.25737000	0.20871100	2.95578000

Table 8 Cartesian coordinates of **66·Et_2Mg** and **66·Et_2Mg (TS)** [B3LYP/6−31+G(d)].

66·Et_2Mg				**TS**			
C	−1.73405000	2.33268300	2.89035400	**C**	0.92586100	2.86515400	2.32736100
C	−0.48472200	1.63342700	2.30752500	**C**	0.38200300	1.44887500	2.06136800
C	−2.48963500	−1.22527100	1.13753800	**C**	−2.55916900	−0.91310200	1.44593700
C	−3.72010400	−0.57700800	0.50059400	**C**	−3.79425300	−0.18134000	0.91686100
C	2.73725900	−2.31643800	1.61475600	**C**	2.59012900	−2.47612300	1.36606200
C	−0.15727400	−1.84176700	0.93924900	**C**	−0.32766700	−1.77862000	1.02938900
C	4.21986000	0.52864800	−0.10008800	**C**	3.88061300	0.80406600	0.34826600
N	1.73632500	0.24509600	0.23385500	**N**	1.53902800	0.06103200	−0.10051900
N	−1.28212000	−1.13916600	0.26740400	**N**	−1.45721900	−0.99370200	0.44282900
C	2.67938300	2.50387600	−0.00625400	**C**	2.36188600	2.16411600	−1.11453100
Si	1.62008400	−1.54281900	0.29602700	**Si**	1.37884900	−1.66639900	0.14841100
Mg	−0.52456300	1.07089700	0.20152900	**Mg**	−0.45651100	0.97896600	−0.08328600
C	2.81234200	1.04052500	−0.46713800	**C**	2.73962200	0.73004600	−0.69182700
C	−4.02897800	−1.20307200	−0.86492000	**C**	−4.31567500	−0.83564300	−0.36903700
C	−1.56568500	−1.76253400	−1.05153500	**C**	−1.96182800	−1.66560600	−0.78835100
C	−2.78003000	−1.14751400	−1.75231300	**C**	−3.17860600	−0.95794700	−1.39104300

C	1.98474800	−2.38327200	−1.35524600	**C**	1.39077000	−2.74913600	−1.41740800
C	−0.99820800	2.14951200	−1.61887600	**C**	−1.34858300	2.45541300	−1.35240400
C	−2.36125400	2.87661800	−1.66769000	**C**	−2.73688000	3.05868100	−1.05352900
H	−1.62315800	2.65465800	3.94042400	**C**	3.25173400	−0.01018300	−1.94246400
H	−2.62095200	1.68093700	2.86011300	**H**	0.69167500	3.24058100	3.33539100
H	−1.99497200	3.23178600	2.31376700	**H**	0.52141900	3.59772600	1.61520900
H	−0.23239500	0.77867300	2.96785400	**H**	2.01931300	2.89857700	2.22637900
H	0.37029100	2.32657000	2.43359900	**H**	−0.71355700	1.46660900	2.24742100
H	1.71554700	0.56909200	1.20686700	**H**	1.14556300	0.68932700	0.94980000
H	−2.24476000	−0.73524700	2.08441100	**H**	0.75287100	0.76649100	2.84434500
H	−2.69950500	−2.28959600	1.35273500	**H**	−2.16270700	−0.41037100	2.33384100
H	−4.56810600	−0.69089700	1.18770800	**H**	−2.83389500	−1.94041600	1.74571500
H	−3.55089400	0.50209200	0.38596200	**H**	−4.56370700	−0.18806100	1.69930400
H	2.60741400	−1.83207100	2.59081100	**H**	−3.54763700	0.87035100	0.72401600
H	2.50382500	−3.38190600	1.74424400	**H**	2.67939800	−1.90041000	2.29520000
H	3.79745200	−2.24374300	1.34654600	**H**	2.25629800	−3.48972900	1.62869800
H	−0.14446700	−1.50041500	1.98278500	**H**	3.59505300	−2.57125400	0.93638300
H	−0.36050000	−2.92914800	0.98245300	**H**	−0.16527200	−1.39322400	2.04339300
H	4.37950300	0.55503400	0.98479500	**H**	−0.63559800	−2.83302100	1.14950700
H	4.37968300	−0.49967900	−0.44485300	**H**	3.55517600	1.34325200	1.24480600
H	4.99030400	1.15326100	−0.56819900	**H**	4.20398200	−0.19626500	0.65612300
H	2.79880900	2.59320900	1.08096800	**H**	4.75316600	1.32738900	−0.06365800
H	3.45325500	3.11947600	−0.47868800	**H**	1.98041800	2.74552000	−0.26879300
H	1.70426900	2.91929500	−0.27901100	**H**	3.23890800	2.69254100	−1.50810800
H	−4.34152900	−2.24939900	−0.72636500	**H**	1.59640900	2.15412600	−1.89893700
H	−4.86508000	−0.68302300	−1.34799400	**H**	−4.71237000	−1.83554300	−0.13680800
H	−1.72844600	−2.84758400	−0.90638900	**H**	−5.14591900	−0.25379100	−0.78697900
H	−0.67835100	−1.64770600	−1.67933000	**H**	−2.22235100	−2.71003300	−0.53792200
H	−2.55451500	−0.10771700	−2.01270300	**H**	−1.14566800	−1.70449700	−1.51513900
H	−2.94535900	−1.68763000	−2.69358800	**H**	−2.88508400	0.03923500	−1.74101500
H	3.05813000	−2.37328400	−1.57925600	**H**	−3.50542300	−1.52375200	−2.27281700
H	1.68024500	−3.43605800	−1.28402300	**H**	2.41203100	−3.03223600	−1.69846600
H	1.46111500	−1.94412400	−2.20925300	**H**	0.83872700	−3.68058300	−1.23074200
H	−0.21121400	2.91497500	−1.75101100	**H**	0.93798100	−2.25942600	−2.28656100
H	−0.90521400	1.51421400	−2.51945100	**H**	−0.61526600	3.28073900	−1.35823300
H	−2.47393300	3.57724900	−0.82777900	**H**	−1.34321500	2.08597400	−2.39414400
H	−3.20795900	2.17622000	−1.59850200	**H**	−2.79169600	3.47563300	−0.03731700
H	−2.52247600	3.46285700	−2.58892900	**H**	−3.53948600	2.31040900	−1.12860500
C	2.60608000	0.97030100	−1.98861000	**H**	−3.01478700	3.87463000	−1.74132800
H	2.77609300	−0.03816200	−2.37660900	**H**	3.63670100	−1.00691000	−1.69836500
H	1.59476000	1.28621500	−2.26112600	**H**	2.45684100	−0.12148500	−2.68863500
H	3.31884500	1.63648800	−2.48862200	**H**	4.07354200	0.55067500	−2.40536100

Table 9 Cartesian coordinates of **66·Et_2Zn** and **66·Et_2Zn (TS)** [B3LYP/6−31+G(d)].

66·Et_2Zn				**TS**			
C	1.81756600	−2.38279500	2.64901800	**C**	0.86732800	2.76689200	2.30259900
C	0.56931300	−1.67961900	2.07689900	**C**	0.30357700	1.36092100	2.03752100
C	2.44404500	1.31313000	1.23503100	**C**	−2.50116800	−1.00795700	1.44443200
C	3.71887200	0.71612800	0.63622700	**C**	−3.74182200	−0.28701900	0.91610700
C	−2.71704900	2.66064700	1.44178600	**C**	2.64350100	−2.56402500	1.36444100
C	0.11275100	1.86186100	0.95682700	**C**	−0.27474700	−1.87629100	1.03119700
C	−4.45707800	−0.34544700	0.21257700	**C**	3.90761900	0.74754500	0.42731400
N	−1.95626600	−0.09311300	0.28171300	**N**	1.58397600	−0.00779300	−0.05634100
N	1.28405000	1.22396200	0.31501700	**N**	−1.40152400	−1.09479400	0.44133000
C	−2.92798500	−2.33439400	0.14549700	**C**	2.42050100	2.10192800	−1.06847700
Si	−1.64979800	1.64620100	0.24036600	**Si**	1.42974700	−1.73493600	0.15935700

Zn	0.64900100	−1.21391600	0.11713300	**C**	2.78449500	0.66874800	−0.63307700
C	−3.09575000	−0.86827900	−0.29553400	**C**	−4.26219300	−0.94852700	−0.36655400
C	4.07212700	1.39886300	−0.69055100	**C**	−1.90480200	−1.76970500	−0.78697200
C	1.60011700	1.89297900	−0.96615900	**C**	−3.12632000	−1.07172100	−1.38988700
C	2.86476600	1.34448200	−1.63388300	**C**	1.45084200	−2.80076200	−1.42044200
C	−1.88690200	2.38658300	−1.48263100	**C**	3.32604500	−0.07022000	−1.87398300
C	0.81702300	−1.77334000	−1.80344800	**H**	0.62236000	3.14578100	3.30650700
C	2.08685400	−2.57555400	−2.15409400	**H**	0.48071600	3.49973600	1.58188400
H	1.70373600	−2.65898200	3.70949400	**H**	1.96203900	2.78523700	2.21773100
H	2.71318100	−1.74955500	2.58177100	**H**	−0.79017400	1.39318800	2.20133400
H	2.04498700	−3.30771100	2.10215800	**H**	0.65794600	0.66613200	2.81743700
H	0.34973300	−0.78834200	2.68774900	**H**	1.08525300	0.63824600	0.98171600
H	−0.29723100	−2.34673400	2.21412300	**H**	−2.10415200	−0.49720500	2.32670000
H	−1.75750100	−0.45415500	1.21534600	**H**	−2.77067000	−2.03452300	1.75204500
H	2.17534800	0.79107900	2.15848400	**H**	−4.50966400	−0.29684700	1.70022800
H	2.62313800	2.37503000	1.49594100	**H**	−3.49964500	0.76480600	0.72191700
H	4.53371500	0.82404400	1.36372700	**H**	2.72889100	−2.00683900	2.30528300
H	3.57799900	−0.36164100	0.47563900	**H**	2.31311600	−3.58410800	1.60620300
H	−2.64197300	2.28251500	2.46954800	**H**	3.64991600	−2.64718100	0.93559000
H	−2.40389300	3.71357600	1.45469700	**H**	−0.12271000	−1.49657400	2.04859800
H	−3.77659500	2.63822800	1.16091300	**H**	−0.57833900	−2.93312300	1.14192500
H	0.04946800	1.46636300	1.97996500	**H**	3.56619000	1.29349200	1.31378500
H	0.29748400	2.94907100	1.07859800	**H**	4.22248800	−0.25110300	0.74865000
H	−4.50150400	−0.36927500	1.30827100	**H**	4.78919300	1.26597800	0.02796500
H	−4.63322200	0.68683100	−0.11186300	**H**	2.00471200	2.68192700	−0.23893300
H	−5.28129400	−0.95831900	−0.17400100	**H**	3.31315600	2.62857700	−1.42849400
H	−2.94650300	−2.42372400	1.23964300	**H**	1.68607900	2.08852200	−1.88076700
H	−3.74275700	−2.95034900	−0.25208800	**H**	−4.65398800	−1.94912300	−0.12925200
H	−1.97917900	−2.74581800	−0.21404200	**H**	−5.09654500	−0.37308300	−0.78584600
H	4.34804700	2.44710700	−0.49946600	**H**	−2.16172100	−2.81436100	−0.53279800
H	4.94432600	0.92084700	−1.15374300	**H**	−1.08907500	−1.80544700	−1.51307100
H	1.72124500	2.98068200	−0.78809900	**H**	−2.83691700	−0.07647800	−1.74674900
H	0.74593500	1.76770000	−1.63536900	**H**	−3.45287800	−1.64438200	−2.26738800
H	2.68598400	0.30963600	−1.94469600	**H**	2.47384700	−3.07721600	−1.70209400
H	3.05548100	1.92522100	−2.54583900	**H**	0.90061200	−3.73595000	−1.24697300
H	−2.95204900	2.50645300	−1.71538500	**H**	0.99936600	−2.30104700	−2.28472700
H	−1.43863900	3.38855800	−1.50906500	**H**	3.71316900	−1.06409000	−1.62142300
H	−1.43361400	1.79343500	−2.28256800	**H**	2.54497200	−0.18830300	−2.63362300
H	−0.06048200	−2.40043200	−2.02559300	**H**	4.15246000	0.49499500	−2.32363900
H	0.72903600	−0.90527100	−2.47430500	**Zn**	−0.45110400	0.88715300	−0.11859300
H	2.16730800	−3.48679500	−1.54627300	**C**	−1.22752200	2.26274400	−1.35701300
H	3.00541500	−1.99871000	−1.97602200	**C**	−2.56983500	2.92612700	−1.00229200
H	2.11241100	−2.89196400	−3.20913100	**H**	−0.45734800	3.04361300	−1.42295000
C	−3.05822700	−0.80386600	−1.83225600	**H**	−1.28685700	1.82908300	−2.36716100
H	−3.26888200	0.20328700	−2.20384900	**H**	−2.55225300	3.37516600	−0.00028100
H	−2.07931300	−1.11330700	−2.21040700	**H**	−3.40458400	2.21322000	−1.01929500
H	−3.81936600	−1.47211100	−2.25233500	**H**	−2.83244500	3.72982600	−1.70764700

Table 10 Cartesian coordinates of **(R_{C1},R_{C2},R_N)-4** and **(R_{C1},R_{C2},R_N)-4 (TS)** [B3LYP/6−31+G(d)].

(R_{C1},R_{C2},R_N)-4				**TS**			
C	−3.05850700	1.37434000	1.64040000	**C**	−2.55780500	1.38746800	2.05197200
C	0.35799100	3.15619800	2.40499000	**C**	2.02928000	1.43674200	3.01374500
C	0.29662300	1.68758200	1.93551100	**C**	0.87753200	1.18759800	2.01638400
C	−4.53368500	−0.60519700	0.05580900	**C**	−4.53647100	0.15601300	0.21948900
C	−3.95345800	−3.04598800	0.02877700	**C**	−4.52551300	−2.32376600	−0.14006800
C	2.84468100	−2.44948800	2.03666200	**C**	2.50329500	−2.70367600	1.90552400

C	−4.92987400	−1.98410100	−0.48503500	**C**	−5.24025400	−1.01282100	−0.47786000
C	−2.07352100	−1.28862800	0.14524300	**C**	−2.29461200	−1.06395600	0.08340200
C	0.28203300	−1.64913200	0.71724900	**C**	−0.04213200	−1.97226900	0.49125400
C	4.75105000	0.75849500	0.97899000	**C**	4.73882300	−0.37831000	0.21753900
C	−3.08318200	−0.19530400	−0.29949100	**C**	−3.03079400	0.28274000	−0.13007600
C	−2.52122500	−2.67711400	−0.37539700	**C**	−3.05700500	−2.23977800	−0.57266700
C	−3.31112800	2.23515000	−0.58843600	**C**	−2.72797500	2.70718100	0.06736900
C	4.17171600	0.20953500	−0.34487000	**C**	3.52549400	0.26808700	−0.49132900
C	4.13315700	1.34181400	−1.39019300	**C**	3.61405300	1.79316100	−0.27492500
C	−0.33243500	−1.23870000	−1.62885900	**C**	−0.64501800	−1.27885700	−1.77058000
C	0.04151500	3.64302400	−1.99804400	**C**	0.36341500	3.73102000	−1.59904300
C	2.48783900	−3.19541900	−0.89266700	**C**	2.37211800	−3.14805300	−1.08298800
C	−0.07523000	2.11161800	−1.85866000	**C**	0.13188300	2.22382500	−1.81505100
C	5.07088900	−0.92312500	−0.86533000	**C**	3.63551500	0.00353100	−2.01061300
H	0.72878900	3.26533300	3.43752700	**H**	1.66200700	1.69001300	4.01914400
H	−2.68460900	0.55262600	2.25446400	**H**	−2.33116300	0.40769800	2.47919800
H	−4.14206600	1.48027800	1.80572500	**H**	−3.58367500	1.66834200	2.34473900
H	−2.56877800	2.28953600	1.98163400	**H**	−1.87130200	2.10829500	2.50343100
H	−0.32673300	1.11184400	2.63879700	**H**	0.32785000	2.13773200	1.91550200
H	−4.64554600	−0.62763200	1.14779000	**H**	−4.64222700	0.01140400	1.30288500
H	−0.62811300	3.64250700	2.37404800	**H**	2.66871100	2.26669700	2.69042200
H	−4.03178200	−3.11908300	1.12400600	**H**	−4.59521200	−2.51397300	0.94155800
H	2.67832800	−1.72129200	2.83998200	**H**	2.27939900	−2.06949600	2.77249400
H	1.30400200	1.25418100	2.03789100	**H**	0.17272200	0.47598200	2.47052900
H	−2.08799200	−1.32410700	1.24213700	**H**	−2.27584500	−1.25346200	1.16226900
H	−5.95867700	−2.21839700	−0.18244800	**H**	−6.29278400	−1.04947200	−0.16822900
H	1.01767800	3.75691200	1.76430500	**H**	2.67497200	0.55418300	3.11569200
H	0.18038200	−1.16086700	1.69465200	**H**	−0.24869200	−1.74454900	1.54401700
H	2.36802600	−3.39399600	2.33361600	**H**	2.03901800	−3.68503400	2.08000700
H	−5.22806500	0.15925900	−0.31341600	**H**	−5.04073000	1.10028600	−0.01827000
H	4.11695200	1.56167300	1.37326300	**H**	4.68296600	−0.21885400	1.30052300
H	−4.20742400	−4.03614400	−0.37122300	**H**	−5.00761600	−3.17375100	−0.63991300
H	3.92420300	−2.63869000	1.98020000	**H**	3.58906000	−2.85861500	1.88371600
H	4.80714300	−0.02928800	1.73884700	**H**	4.78536700	−1.45883100	0.03403900
H	−4.41156500	2.25896600	−0.52667400	**H**	−3.78230200	2.96908000	0.26631600
H	−0.03098600	−2.69932600	0.87180800	**H**	−0.39560600	−3.00528900	0.32394300
H	−1.81968300	−3.44238400	−0.02263400	**H**	−2.53905200	−3.17945700	−0.34549600
H	−2.93233600	3.19800800	−0.23244500	**H**	−2.10143600	3.47122600	0.53724500
H	5.76023400	1.16574200	0.83311000	**H**	5.68183300	0.05389800	−0.14268500
H	−4.91957400	−1.97721300	−1.58539400	**H**	−5.23860100	−0.86367400	−1.56814300
H	2.17557900	0.49864200	0.08830600	**H**	1.65805400	0.48311200	1.00848600
H	−3.01579000	−0.10796900	−1.39162500	**H**	−2.95105400	0.54178300	−1.19483300
H	−2.46863700	−2.68848800	−1.47180600	**H**	−3.04049200	−2.12791100	−1.66396600
H	−3.01187700	2.12025600	−1.63260500	**H**	−2.55268500	2.74165800	−1.00999000
H	3.47832400	2.15690000	−1.05833000	**H**	3.60915400	2.04612700	0.78929000
H	−0.87406000	4.15816600	−1.67337400	**H**	−0.38289100	4.17308500	−0.92693700
H	0.85797200	4.04270300	−1.38102100	**H**	1.34486900	3.93376500	−1.15187600
H	5.16196300	−1.73878000	−0.13757200	**H**	3.63452400	−1.06759500	−2.23495900
H	1.88166700	−4.08014900	−0.65543400	**H**	1.95678300	−4.13799500	−0.84668300
H	5.13399000	1.76069700	−1.55349000	**H**	4.54289500	2.18438600	−0.70828700
H	−0.29131600	−2.31305200	−1.86089000	**H**	−0.82232400	−2.33150200	−2.03149800
H	3.53689400	−3.51323700	−0.88120000	**H**	3.46099400	−3.26683000	−1.14349800
H	6.08111100	−0.54149500	−1.05276300	**H**	4.56494100	0.42663300	−2.41522700
H	−1.07352600	−0.76763700	−2.27933800	**H**	−1.31134900	−0.64563900	−2.36225000
H	0.63698000	−0.79454900	−1.86133000	**H**	0.38269500	−1.02746900	−2.03973800
H	−0.86917800	1.74876500	−2.53236800	**H**	−0.83895200	2.07690800	−2.31432700
H	3.74857100	0.97094400	−2.34654400	**H**	2.77760800	2.30927200	−0.75517400

H	0.85016800	1.65458700	−2.24205400	**H**	0.87829700	1.85177300	−2.53243300
H	2.24645500	−2.88601000	−1.91553800	**H**	2.01535800	−2.86728600	−2.08012800
H	0.23570700	3.96973600	−3.03315200	**H**	0.32071900	4.30098100	−2.54089200
H	4.68348200	−1.33608700	−1.80309100	**H**	2.79489600	0.46466600	−2.54050500
N	−2.72077200	1.15739700	0.22278600	**N**	−2.35656000	1.39073800	0.59724000
N	−0.65210400	−0.96274300	−0.21568800	**N**	−0.84102800	−1.01318700	−0.32583600
N	2.78825300	−0.27900000	−0.14851200	**N**	2.23661700	−0.24242400	0.04692600
Si	2.16768900	−1.82128400	0.37612000	**Si**	1.87354600	−1.92104600	0.28697900
Zn	−0.36710300	1.42908900	0.02866600	**Zn**	0.23448300	0.99037300	−0.21881300

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