Supporting Information

for

Reduction of the dihalocyclopentasilanes. Quest for a homocyclic silylene

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Contents:

(1) Experimental details

Manipulation of air-sensitive compounds was performed under a controlled dry argon atmosphere using standard Schlenk techniques. Tetrahydrofuran (THF), hexane, and toluene were distilled from sodium–benzophenone. The starting material, 1,1,1,3,3,4,4,6,6,6-decamethyl-2,2,5,5-tetrakis(trimethylsilyl)hexa-silane **1**,[1] was prepared according to the literature procedures. All the other reagents were obtained from commercial suppliers and used without further purification. ^{1}H (400 MHz), ^{13}C (100.6 MHz) and ^{29}Si (79.5 MHz) NMR spectra were recorded on a Bruker AV-400 spectrometer at room temperature. Elemental analyses were carried out on an Elementar III Vario EI Analyzer. GC-MS spectrometry was performed with Agilent 7890a gas chromatography instrument coupled to an Agilent 5975c mass spectrometer and Agilent MSD ChemStation software.

Synthesis of 2a

Potassium tert-butoxide (7.39 g, 66 mmol) was added to a solution of **1** (18.33 g, 30 mmol) in 30 mL THF. The mixture was stirred at 60 ^{o}C overnight. After removing the solvent and adding 50 mL tolulene, $SiCl_4$ (3.8 mL, 33 mmol) in 50 mL toluene was introduced in 10 min at -50 ^{o}C. The mixture was slowly warmed to room temperature and stirred for 20 h. After aqueous workup and recrystallization from hexane, **2a** (10.32 g, 61%) was obtained as white crystals. ^{1}H NMR ($CDCl_3$, 400MHz): $\delta = 0.36$ (s, 12H, SiMe_2), 0.30 (s, 36H, SiMe_3). ^{13}C NMR ($CDCl_3$, 100.6 MHz): $\delta = 3.12$ (SiMe_3), -2.09 (SiMe_2). ^{29}Si NMR ($CDCl_{3,}$ 79.5 MHz): $\delta = 64.81$ (*Si*Cl_2), -5.77 (*Si*Me_3), -27.57 (*Si*Me_2), -113.26 (*Si*$(SiMe_3)_2$). GC-MS (m/z): 563.8 ([M^+]). Anal. Calcd for $C_{16}H_{48}Cl_2Si_9$ (564.23): C, 34.16; H, 8.61. Found: C, 34.24; H, 8.68%.

Synthesis of 2b

Potassium tert-butoxide (7.39 g, 66 mmol) was added to a solution of **1** (18.33 g, 30 mmol) in 30 mL THF. The mixture was stirred at 60 ^{o}C overnight. After removing the solvent and adding 50 mL tolulene, $SiBr_4$ (4.1 mL, 33 mmol) in 50 mL toluene was introduced in 10 min at -50 ^{o}C. The mixture was slowly warmed to room temperature and stirred for 20 h. After aqueous workup and recrystallization from hexane, **2b** (4.90 g, 25%) was obtained as white crystals. ^{1}H NMR ($CDCl_3$, 400MHz): δ = 0.37 (s, 12H, Si*Me*$_2$), 0.33 (s, 36H, Si*Me*$_3$). ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = 3.26 (Si*Me*$_3$), -2.01 (Si*Me*$_2$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ = 41.70 (*Si*Br$_2$), -4.72 (*Si*Me$_3$), -26.97 (*Si*Me$_2$), -109.04 (*Si*(SiMe$_3$)$_2$). GC-MS (m/z): 651.8 ([M$^+$]). Anal. Calcd for $C_{16}H_{48}Br_2Si_9$ (653.13): C, 29.42; H, 7.41. Found: C, 29.50; H, 7.49%.

Synthesis of 3

Freshly prepared KC_8 (324 mg, 2.4 mmol) and **2a** (564 mg, 1 mmol) was added 15 mL dry THF and stirred for 8h.The colour of the solution turned red slowly. The volatiles were removed by evaporation under reduced pressure at 0°C and the residue was dissolved in hexane. Filtration of the resulting salt gave a red solution, which was recrystallized under -20°C to give pure **3** (221 mg, 27%) as red crystals. Compound **3** is air and moisture sensitive. ^{1}H NMR (C_6D_6, 400MHz): δ = 0.34 (s, 18H, Si*Me*$_3$), 0.35 (s, 18H, Si*Me*$_3$), 0.39 (s, 9H, KSiSi*Me*$_3$), 0.40 (s, 6H, SiMe$_2$), 0.42 (s, 6H, SiMe$_2$), 1.42 (m, 6H, THF), 3.58 (m, 6H, THF). ^{13}C NMR (C_6D_6, 100.6 MHz): δ = -0.93 (Si*Me*$_2$), 4.23 (Si*Me*$_3$), 7.75 (Si*Me*$_3$), 25.64 (THF), 67.90 (THF). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ = -6.90 (*Si*Me$_3$), -9.94 (*Si*Me$_3$), -24.93 (*Si*Me$_2$), -120.99 (*Si*(SiMe$_3$)$_2$), -178.30 (*Si*K).

Synthesis of 4

Freshly prepared KC_8 (648 mg, 4.8 mmol) and **2b** (1.306 g, 2 mmol) was added 15 mL dry THF at -35 °C and stirred for 8h.The colour of the solution turned red slowly. The volatiles were removed by evaporation under the reduced pressure at -10 °C and the residue was dissolved in hexane. Filtration of the resulting salt gave a light yellow solution. After concentrated and stored in the refrigerator at -35°C for weeks, colourless crystals were obtained, which were identified as compound **4** (158 mg, 16%). ^{1}H NMR ($CDCl_3$, 400MHz): δ = 0.43 (s, 18H, Si*Me*$_3$), 0.46 (s, 18H, Si*Me*$_3$), 0.49 (s, 24H, Si*Me*$_3$ and Si*Me*$_2$, overlaped), 0.51 (s, 18H, Si*Me*$_3$), 0.58 (s, 6H, Si*Me*$_2$), 0.68 (s, 6H, Si*Me*$_2$), 0.80(s, 6H, Si*Me*$_2$). ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ = -2.15 (Si*Me*$_2$), -2.09 (Si*Me*$_2$), -1.90 (Si*Me*$_2$), 2.27 (Si*Me*$_3$), 2.70 (Si*Me*$_2$), 3.08 (Si*Me*$_3$), 3.24 (Si*Me*$_3$) 3.60 (Si*Me*$_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): -6.46 (*Si*Me$_3$), -7.15 (*Si*Me$_3$), -9.03 (*Si*Me$_3$), -9.85 (*Si*Me$_3$), -25.20 (*Si*Me$_2$), -27.60 (*Si*Me$_2$), -127.94 (*Si*(SiR)$_4$), -135.75 (*Si*(SiR)$_4$), -137.93 (*Si*(SiR)$_4$). Anal. Calcd for $C_{32}H_{96}Si_{18}$ (986.65): C, 38.96; H, 9.81. Found: C, 38.35; H, 9.72 %.

(2) ^{1}H, ^{13}C and ^{29}Si NMR Spectra of Compounds 2-4.

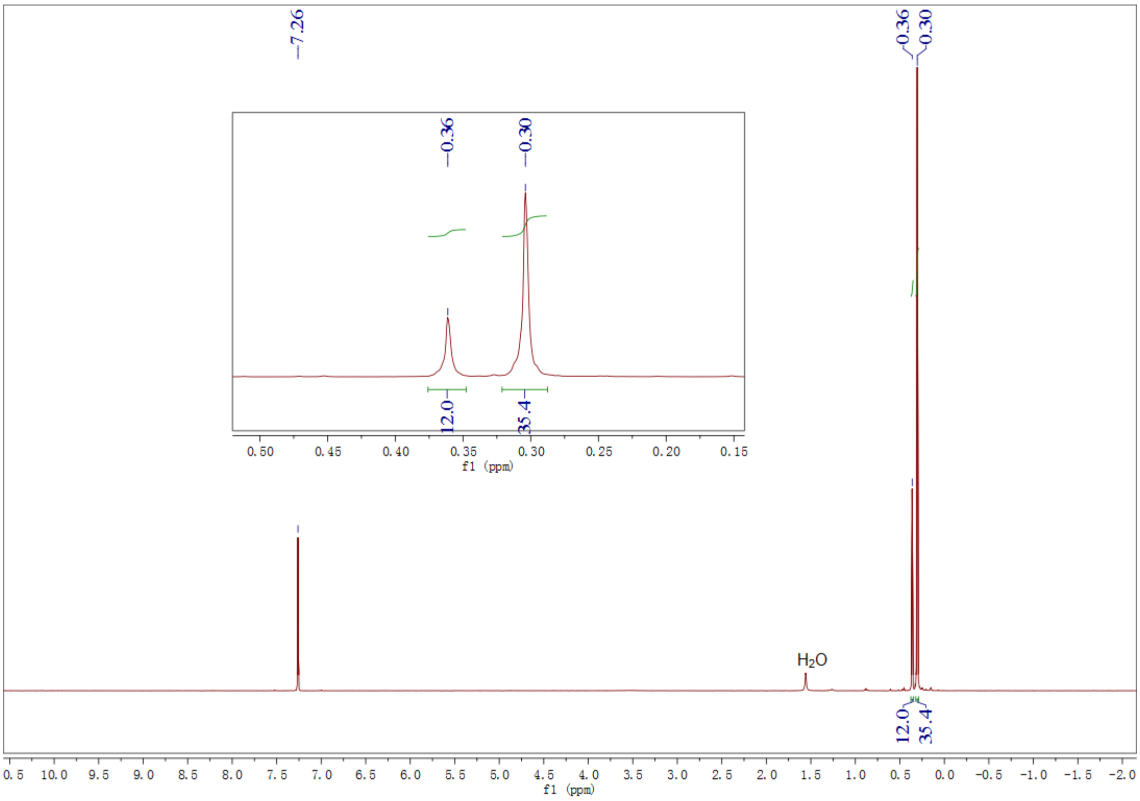


Figure S1. ^{1}H NMR spectrum of compound **2a** in $CDCl_3$.

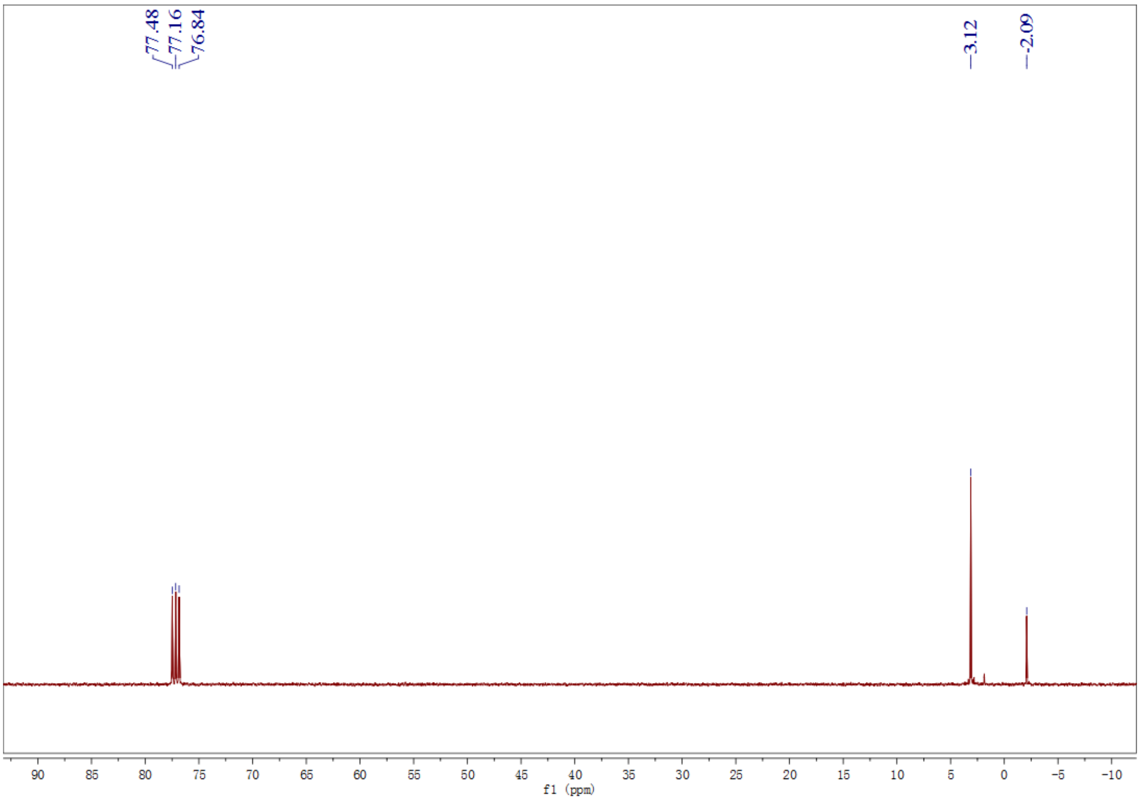


Figure S2. ^{13}C NMR spectrum of compound **2a** in $CDCl_3$.

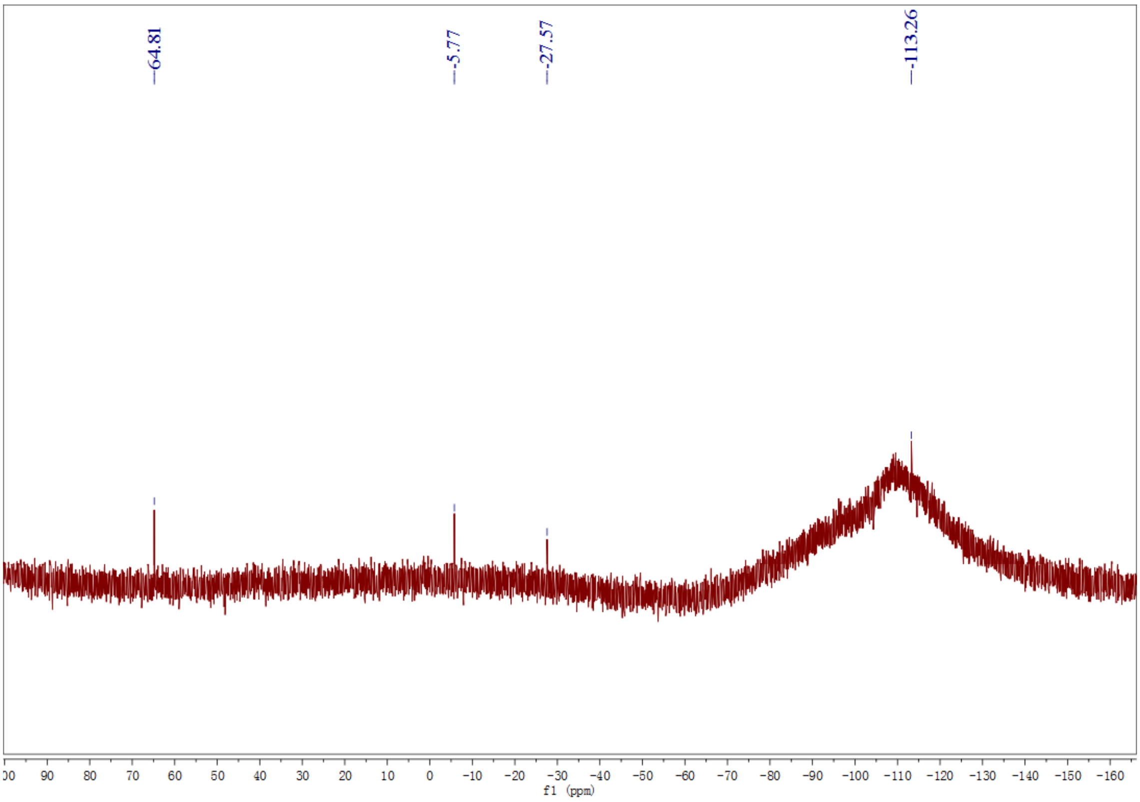


Figure S3. ^{29}Si NMR spectrum of compound **2a** in $CDCl_3$.

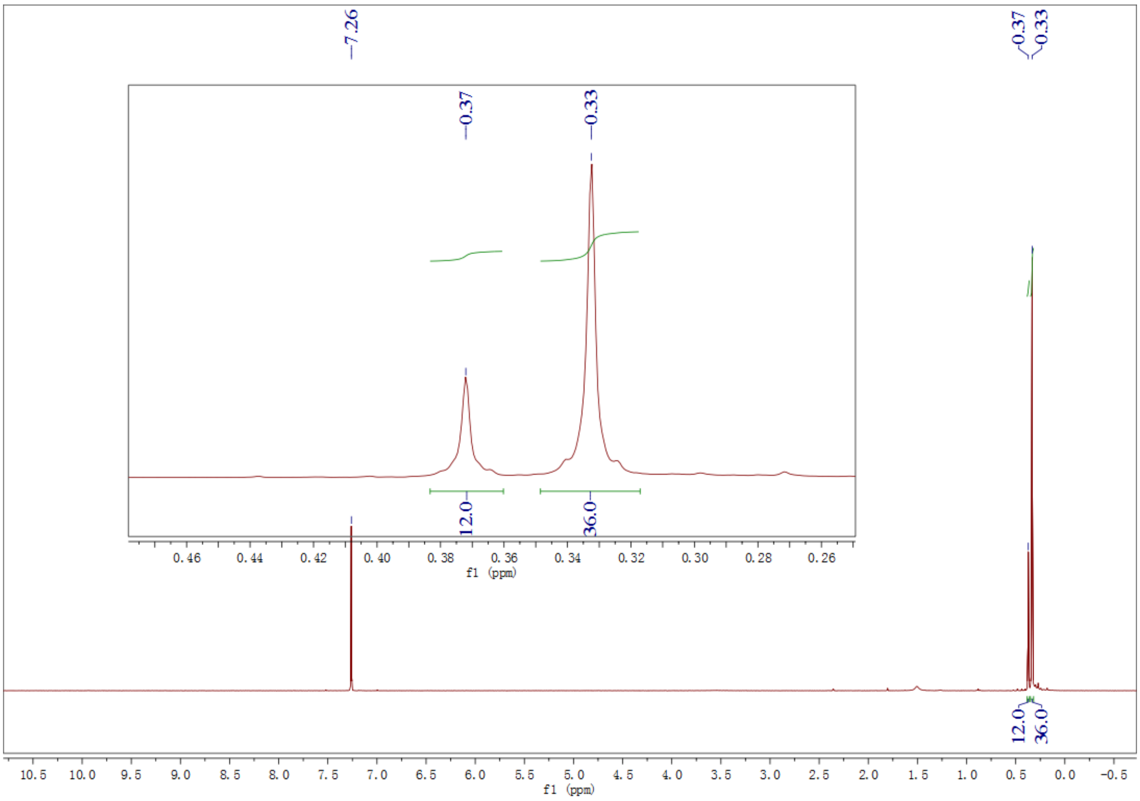


Figure S4. ^{1}H NMR spectrum of compound **2b** in $CDCl_3$.

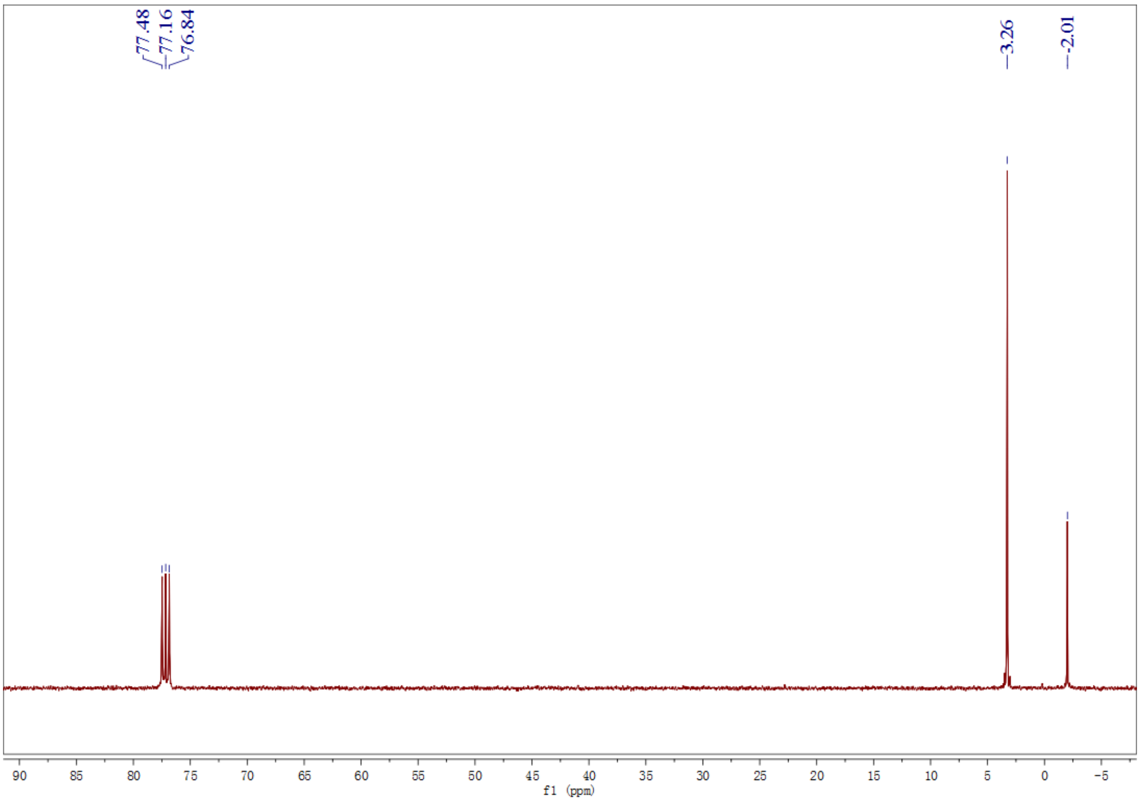


Figure S5. ^{13}C NMR spectrum of compound **2b** in CDCl$_3$.

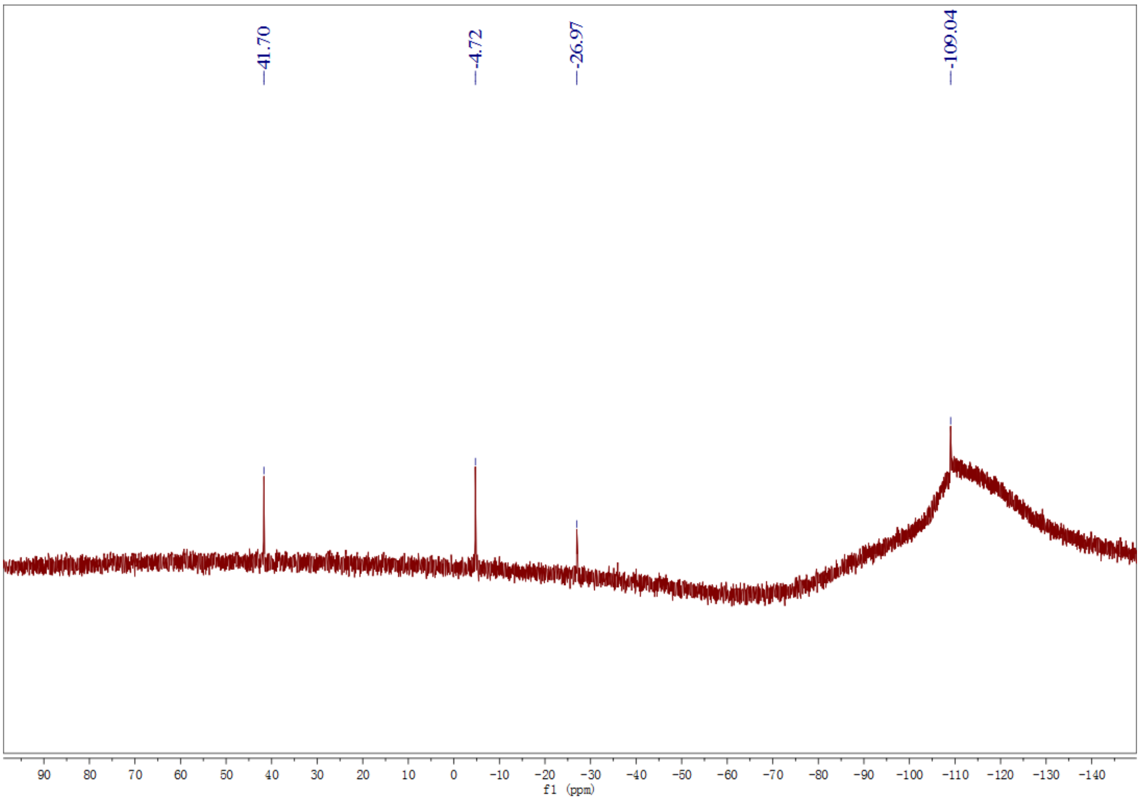


Figure S6. ^{29}Si NMR spectrum of compound **2b** in CDCl$_3$.

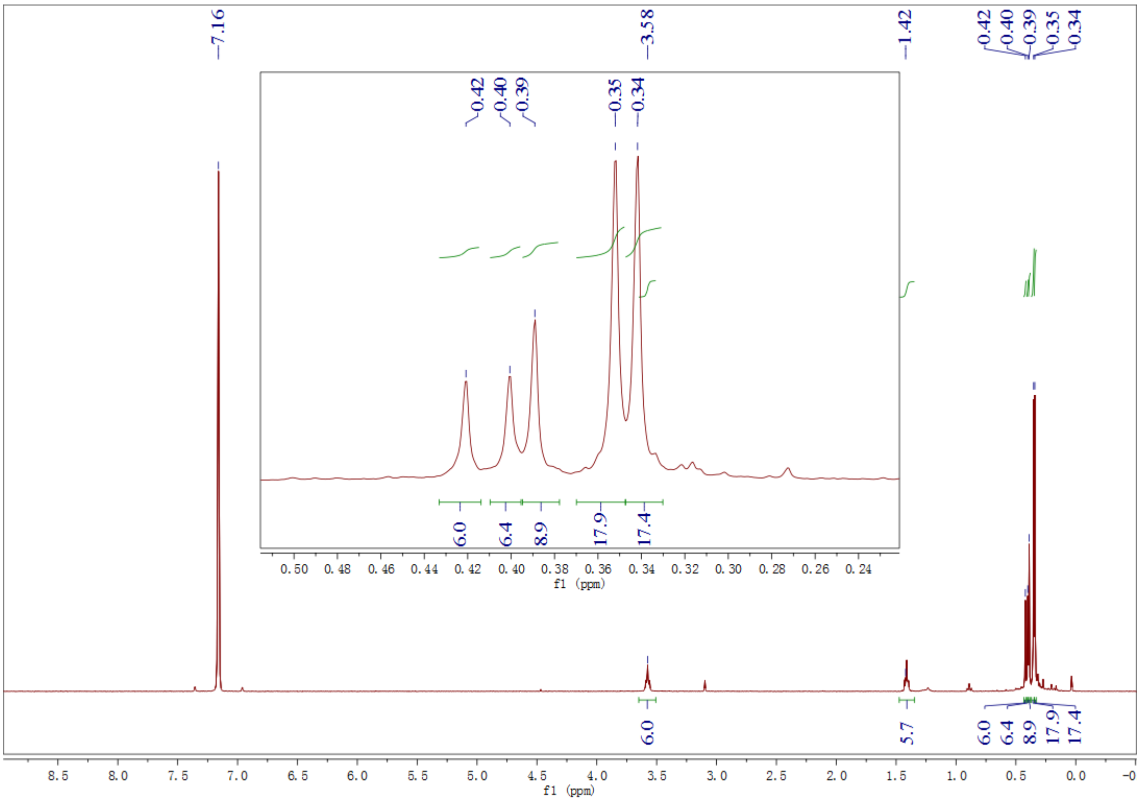


Figure S7. ^{1}H NMR spectrum of compound **3** in C_6D_6.

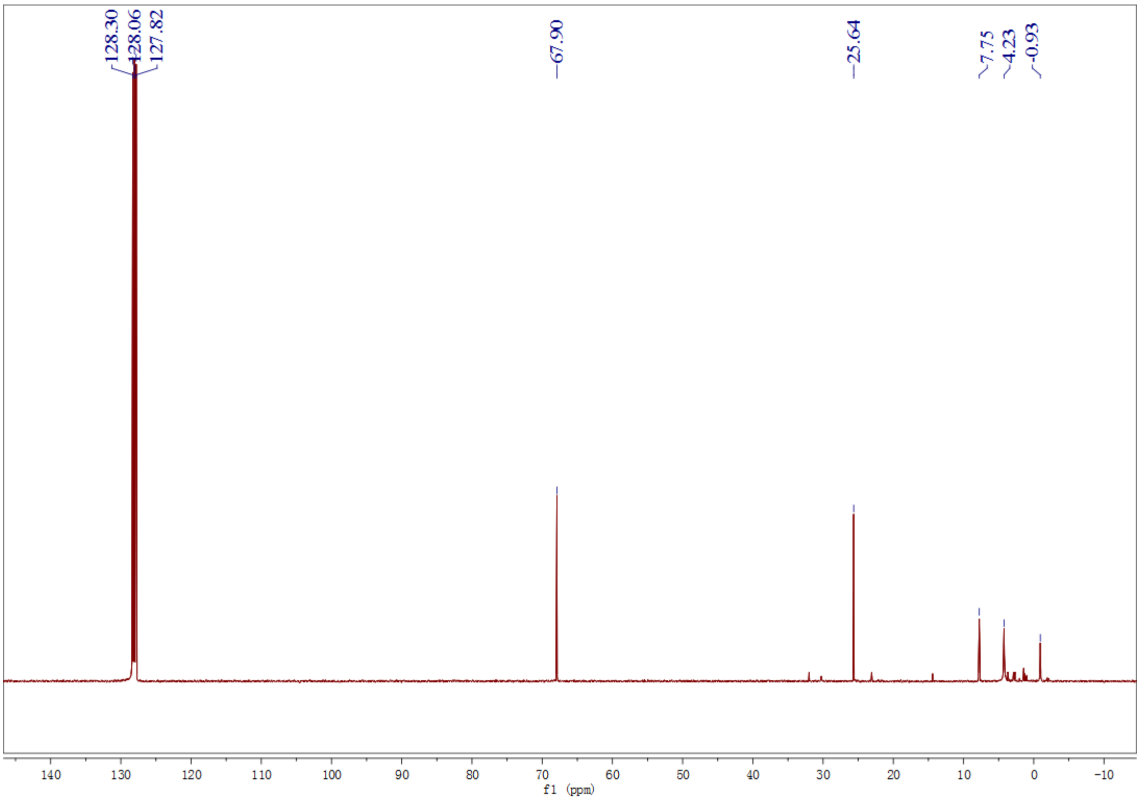


Figure S8. ^{13}C NMR spectrum of compound **3** in C_6D_6.

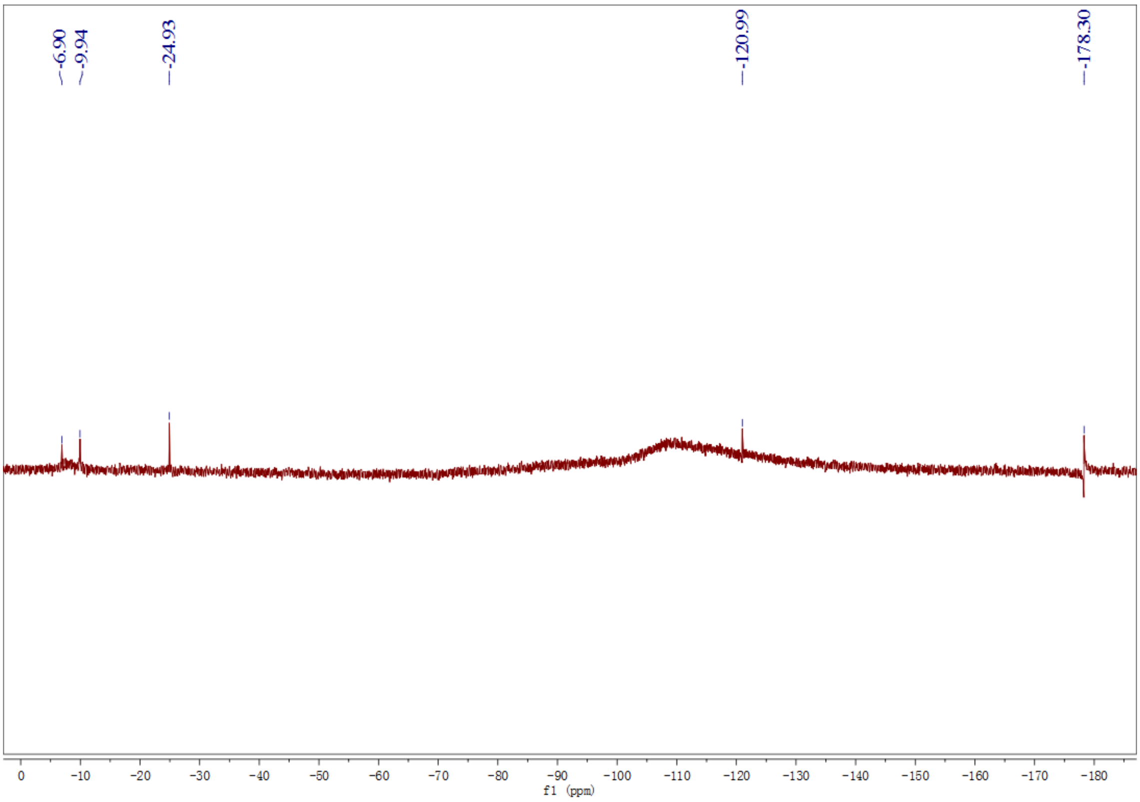


Figure S9. ^{29}Si NMR spectrum of compound **3** in C_6D_6.

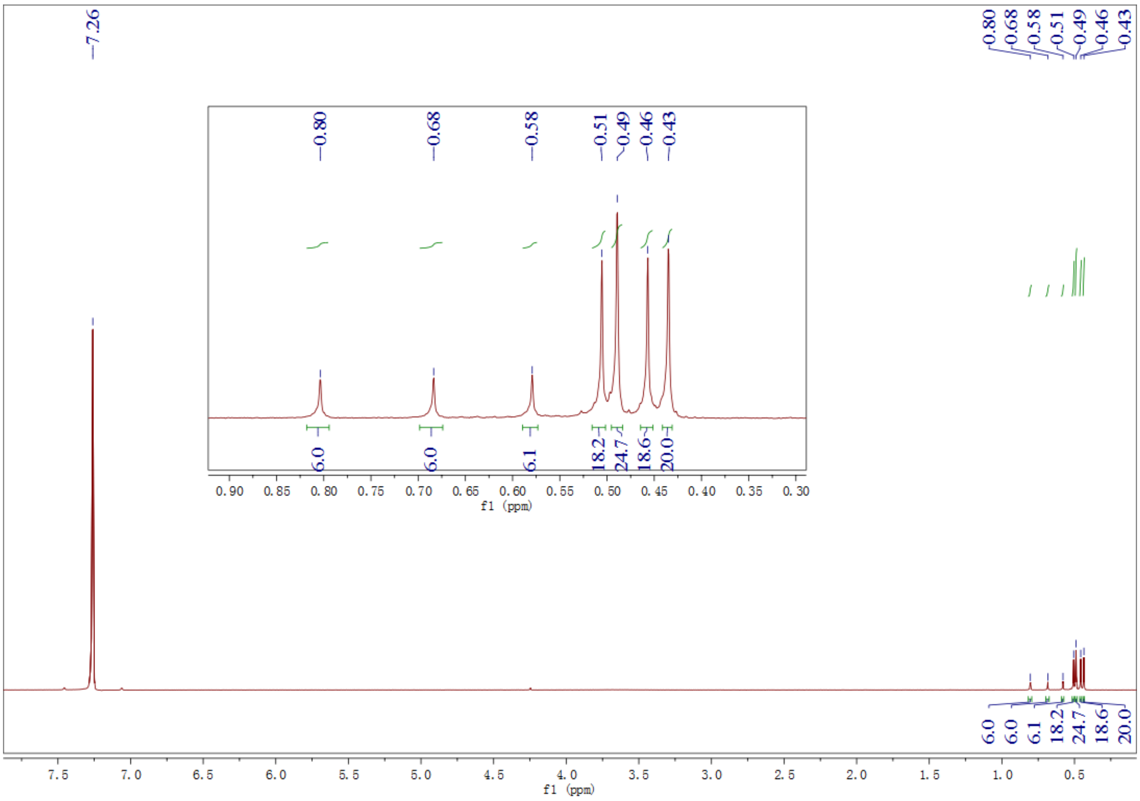


Figure S10. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

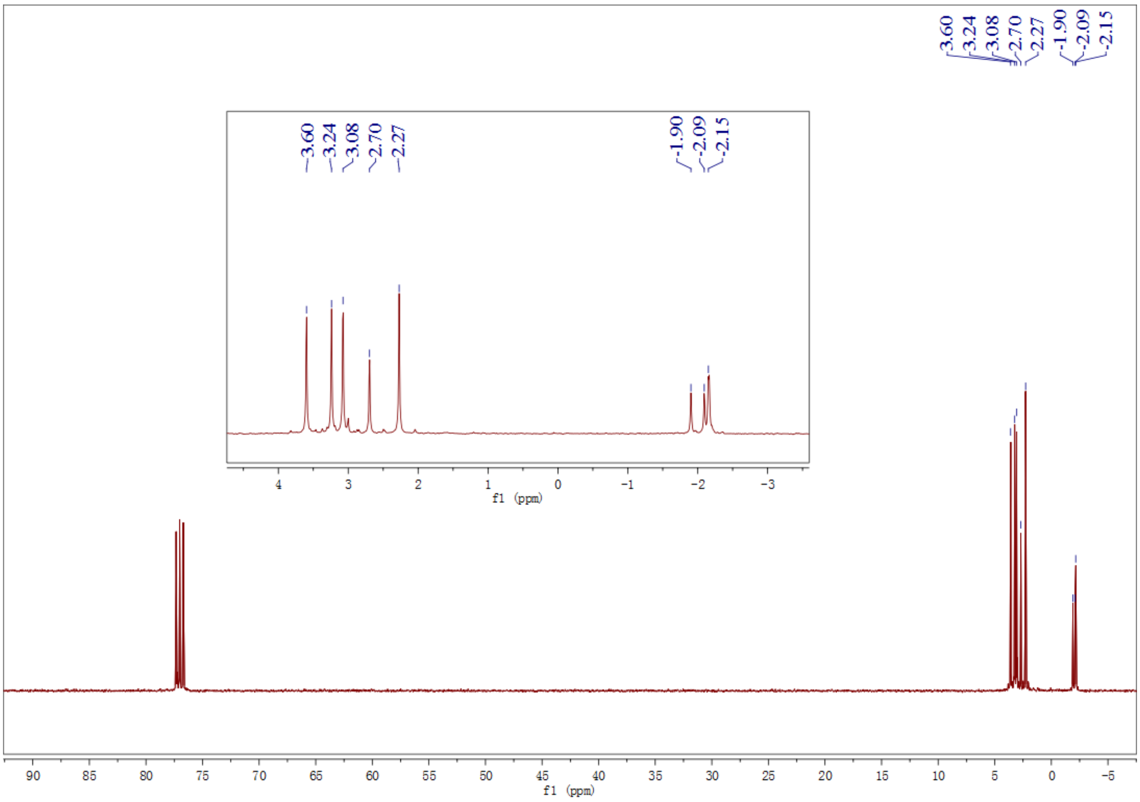


Figure S11. ^{13}C NMR spectrum of compound **4** in CDCl$_3$.

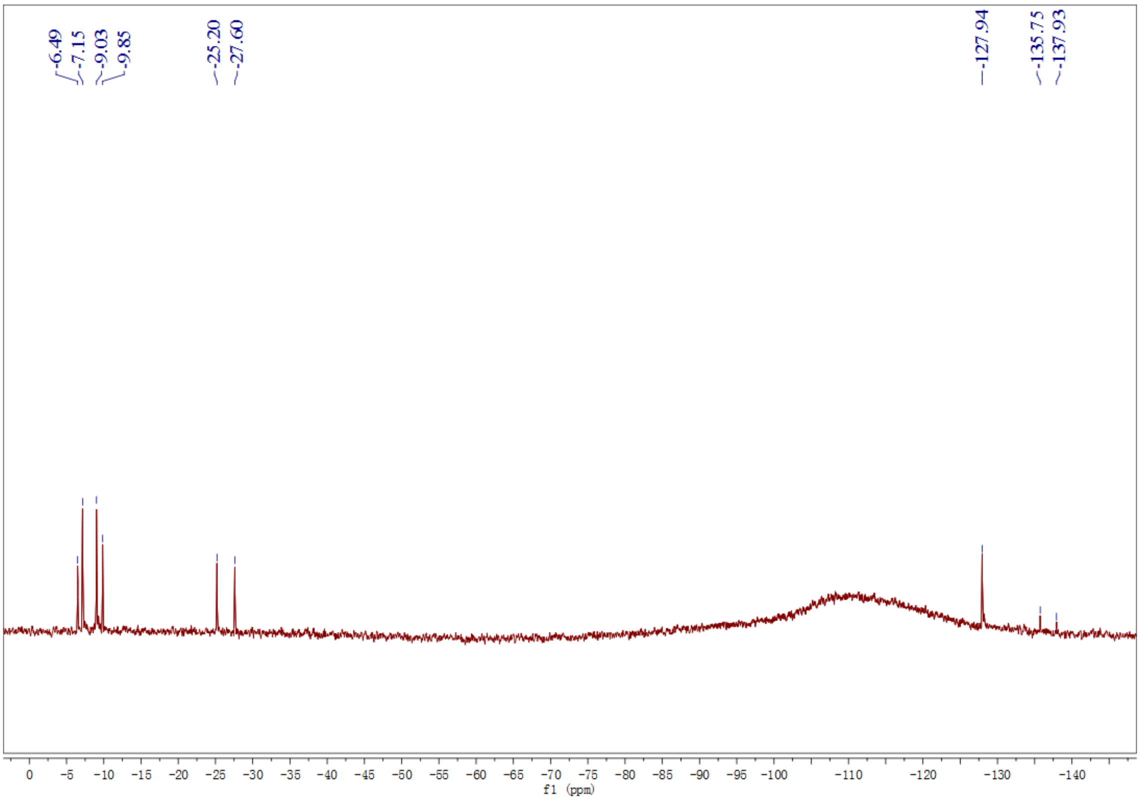


Figure S12. ^{29}Si NMR spectrum of compound **4** in CDCl$_3$.

(3) X-ray crystallography

Diffraction data of **2a**, **2b**, **3** and **4** were collected on a Bruker Smart Apex II CCD diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct method and subsequently refined on F^2 by using full-matrix least-squares techniques (SHELXTL).[2] Absorption corrections were applied empirically using the SADABS program.[3] The non-hydrogen atoms were refined anisotropically, and hydrogen atoms were located at calculated positions. A summary of the crystallographic data and selected experimental information are given in Table S1. The perspective drawing of **2a**, **2b**, **3** and **4** is shown in figure S1-S4.

Table S1. Summary of Crystallographic Data for **2a**, **2b**, **3** and **4**.

	2a	**2b**	**3**	**4**
Empirical formula	$C_{16}H_{48}Cl_2Si_9$	$C_{16}H_{48}Br_2Si_9$	$C_{31}H_{81}O_3Si_{10}K$	$C_{32}H_{96}Si_{18}$
Formula weight	564.25	653.17	821.96	986.71
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	*C2/c*	*C2/c*	P2(1)/c	*C2/c*
a (Å)	16.581(4)	16.3991(19)	10.925(3)	27.289(2)
b (Å)	9.272(2)	9.4161(11)	25.574(7)	12.4843(10)
c (Å)	22.553(5)	22.631(3)	18.928(5)	20.2377(16)
α (deg)	90	90	90	90
β (deg)	95.961(4)	95.312(3)	96.712(5)	113.0010(10)
γ (deg)	90	90	90	90
V (Å^3)	3448.6(14)	3479.6(7)	5252 (2)	6346.6(9)
Z	4	4	4	2
D_c (g/cm^{-3})	1.087	1.247	1.040	1.033
μ (mm^{-1})	0.506	2.644	0.354	0.379
F(000)	1216	1360	1800	2160
θ range (^{o})	2.52 ~ 25.50	1.81 ~ 26.00	1.88 ~ 27.55	2.28 ~ 27.49
Ref. collected	13337	25067	34999	14986

completeness to θ (°)	99.5%	99.9%	99.5%	99.6%
Max./min. trans.	0.9418/ 0.9056	0.9418/ 0.9056	0.745 / 0.377	0.7456 / 0.6532
Data / restraints / parameters	3210 / 0 / 131	3423 / 0 / 131	12071 / 0 / 455	5038 / 0 / 207
Goodness of fit on F^2	1.043	1.016	1.017	0.996
Final R indices [$I > 2\sigma(I)$][a]	$R_1 = 0.0344$ $wR_2 = 0.1178$	$R_1 = 0.0380$ $wR_2 = 0.0925$	$R_1 = 0.0625$ $wR_2 = 0.1574$	$R_1 = 0.0532$ $wR_2 = 0.1216$
R indices (all data)	$R_1 = 0.0439$ $wR_2 = 0.1332$	$R_1 = 0.0502$ $wR_2 = 0.1024$	$R_1 = 0.1210$ $wR_2 = 0.1892$	$R_1 = 0.1076$ $wR_2 = 0.1480$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e/Å^3)	0.360 and 0.251	1.022 and -0.674	0.546 and -0.357	0.690 and -0.206

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$; $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma wF_o^2]^{1/2}$.

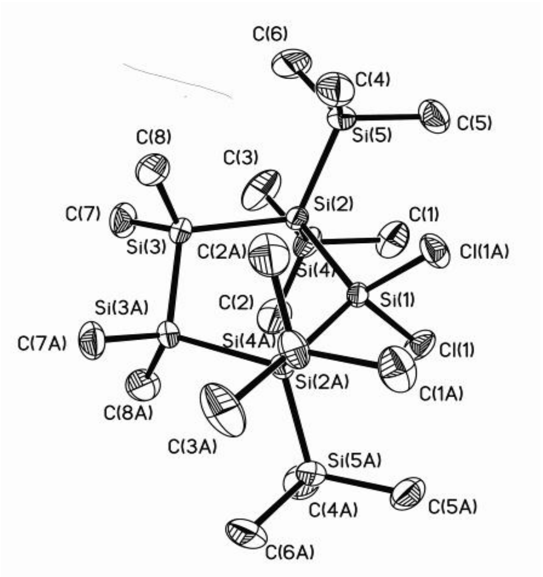


Figure S13. Molecular structure of compound **2a** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level). Selected bond lengths (Å) and angles (°): Si(1)- Cl(1) 2.0896(8), Si(1)-Cl(1A) 2.0896(8), Si(1)-Si(2A) 2.3474(7), Si(1)-Si(2) 2.3474(7), Si(2)-Si(5) 2.3527(10), Si(2)-Si(4) 2.3578(9), Si(2)-Si(3) 2.3651(9), Si(3)-Si(3A) 2.3519(13); Cl(1)-Si(1)-Cl(1A) 102.26(6), Cl(1)-Si(1)-Si(2A) 109.29(2), Cl(1A)-Si(1)-Si(2A) 111.12(2), Cl(1)-Si(1)-Si(2) 111.12(2), Cl(1A)-Si(1)-Si(2) 109.29(2), Si(2A)-Si(1)-Si(2) 113.22(4), Si(1)-Si(2)-Si(5) 107.94(3), Si(1)-Si(2)-Si(4) 110.40(3), Si(5)-Si(2)-Si(4) 111.31(4), Si(1)-Si(2)-Si(3) 102.54(3), Si(5)-Si(2)-Si(3) 111.13(3), Si(4)-Si(2)-Si(3) 113.07(3), Si(3A)-Si(3)-Si(2) 107.43(2).

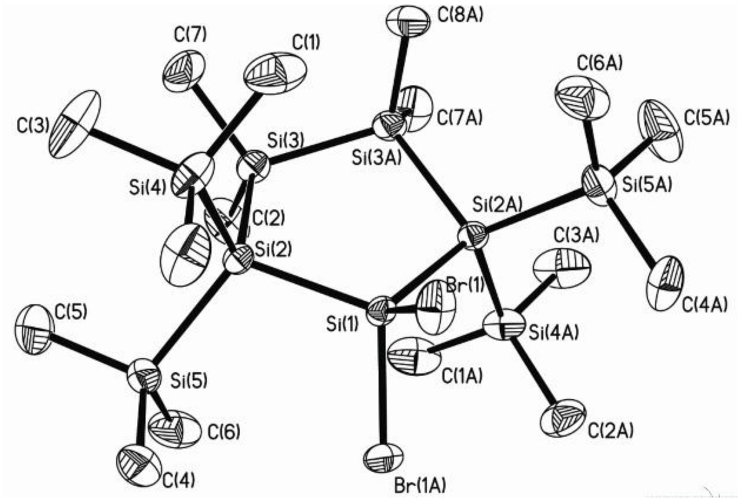


Figure S14. Molecular structure of compound **2b** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level). Selected bond lengths (Å) and angles (°): Br(1)-Si(1) 2.2604(7), Si(1)-Br(1A) 2.2604(7), Si(1)-Si(2) 2.3526(9), Si(1)-Si(2A) 2.3526(9), Si(2)-Si(5) 2.3560(12), Si(2)-Si(4) 2.3581(12), Si(2)-Si(3) 2.3628(11), Si(3)-Si(3A) 2.3541(18); Br(1A)-Si(1)-Br(1) 102.06(5), Br(1A)-Si(1)-Si(2) 109.25(2), Br(1)-Si(1)-Si(2) 111.03(2), Br(1A)-Si(1)-Si(2A) 111.03(2), Br(1)-Si(1)-Si(2A) 109.25(2), Si(2)-Si(1)-Si(2A) 113.62(5), Si(1)-Si(2)-Si(5) 111.11(4), Si(1)-Si(2)-Si(4) 108.83(4), Si(5)-Si(2)-Si(4) 110.76(5), Si(1)-Si(2)-Si(3) 101.88(4), Si(5)-Si(2)-Si(3) 112.80(5), Si(4)-Si(2)-Si(3) 111.09(5), Si(3A)-Si(3)-Si(2) 107.33(3).

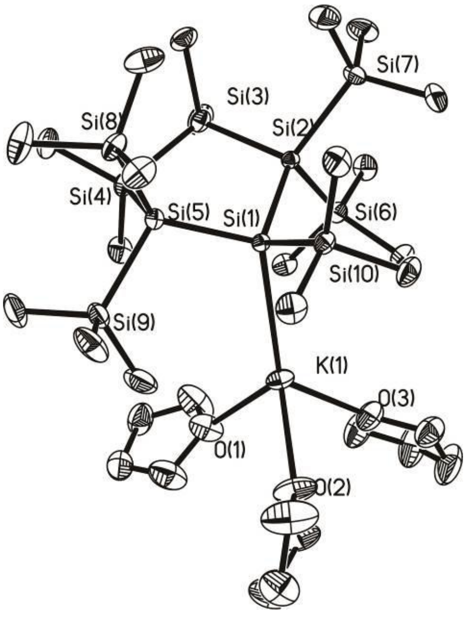


Figure S15. Molecular structure of compound **3** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level). Selected bond lengths (Å) and angles (°): Si(1)-K(1) 3.4220(15), Si(1)-Si(10) 2.3356(14), Si(1)-Si(5) 2.3661(13), Si(1)-Si(2) 2.3818(14), Si(2)-Si(7) 2.3495(14), Si(2)-Si(6) 2.3512(14), Si(2)-Si(3) 2.3591(14), Si(3)-Si(4) 2.3460(15), Si(4)-Si(5) 2.3549(14), Si(5)-Si(8) 2.3502(15), Si(5)-Si(9) 2.3528(15), K(1)-O(2) 2.629(4), K(1)-O(3) 2.659(3), K(1)-O(1) 2.713(4); Si(10)-Si(1)-Si(5) 108.43(5), Si(10)-Si(1)-Si(2) 109.93(5), Si(5)-Si(1)-Si(2) 104.10(5), Si(10)-Si(1)-K(1) 108.05(4), Si(5)-Si(1)-K(1)114.45(4), Si(2)-Si(1)-K(1)111.78(4), Si(7)-Si(2)-Si(6) 105.82(5), Si(7)-Si(2)-Si(3) 107.13(6), Si(6)-Si(2)-Si(3) 107.99(5), Si(7)-Si(2)-Si(1) 127.18(5), Si(6)-Si(2)-Si(1) 101.49(5), Si(3)-Si(2)-Si(1) 106.03(5), Si(4)-Si(3)-Si(2) 104.55(5), Si(3)-Si(4)-Si(5) 104.69(5), Si(8)-Si(5)-Si(9) 103.72(6), Si(8)-Si(5)-Si(4) 109.94(5), Si(9)-Si(5)-Si(4) 106.08(6), Si(8)-Si(5)-Si(1) 126.73(6), Si(9)-Si(5)-Si(1) 109.16(6), Si(4)-Si(5)-Si(1)99.81(5), O(2)-K(1)-O(3) 81.37(12), O(2)-K(1)-O(1) 88.83(13), O(3)-K(1)-O(1) 89.19(12), O(2)-K(1)-Si(1) 124.84(9), O(3)-K(1)-Si(1) 130.00(9), O(1)-K(1)-Si(1) 127.92(9).

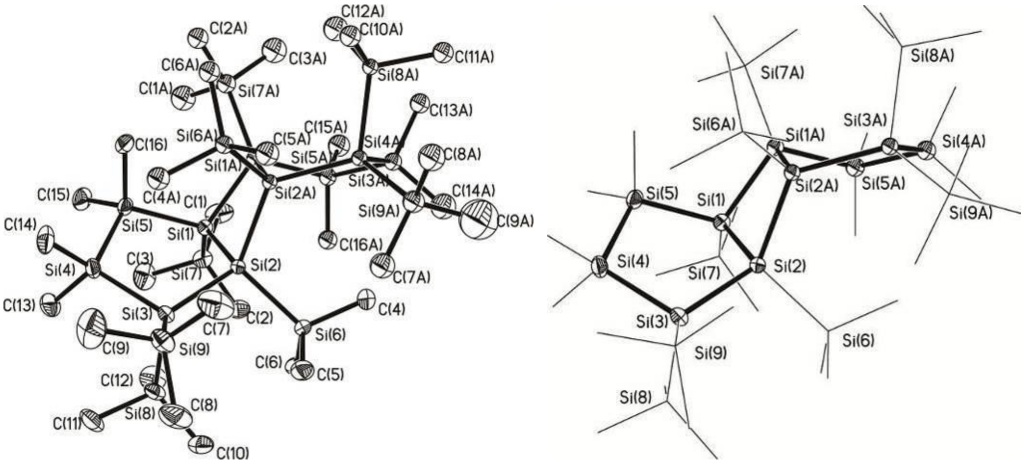
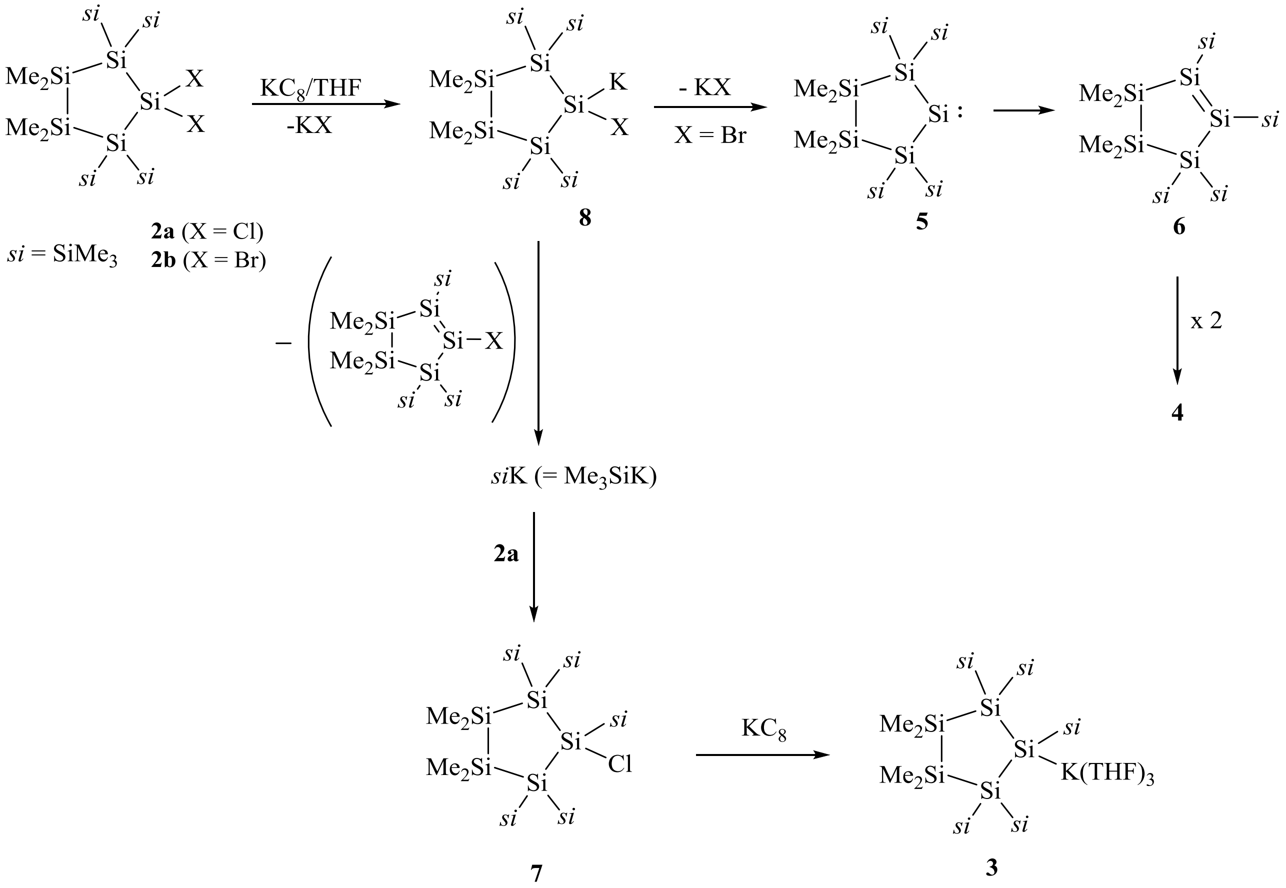


Figure S16. Molecular structure of compound **4** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level). Selected bond lengths (Å) and angles (°): Si(1)-Si(5) 2.3755(7), Si(1)-Si(1A) 2.3865(9), Si(1)-Si(7) 2.3949(7), Si(1)-Si(2) 2.4063(6), Si(2)-Si(6) 2.3803(7), Si(2)-Si(3) 2.4370(6), Si(2)-Si(2A) 2.4902(8), Si(3)-Si(9) 2.3850(8), Si(3)-Si(8) 2.3925(7), Si(3)-Si(4) 2.3928(7), Si(4)-Si(5) 2.3526(8); Si(5)-Si(1)-Si(1A) 106.54(3), Si(5)-Si(1)-Si(7) 109.87(3), Si(1A)-Si(1)-Si(7) 118.83(2), Si(5)-Si(1)-Si(2) 101.58(2), Si(1A)-Si(1)-Si(2) 90.001(15), Si(7)-Si(1)-Si(2) 126.92(3), Si(6)-Si(2)-Si(1) 123.73(3), Si(6)-Si(2)-Si(3) 103.52(2), Si(1)-Si(2)-Si(3) 104.40(2), Si(6)-Si(2)-Si(2A) 112.43(3), Si(1)-Si(2)-Si(2A) 87.583(15), Si(3)-Si(2)-Si(2A) 126.34(3), Si(9)-Si(3)-Si(8) 103.28(3), Si(9)-Si(3)-Si(4) 113.50(3), Si(8)-Si(3)-Si(4) 101.02(3), Si(9)-Si(3)-Si(2) 119.53(3), Si(8)-Si(3)-Si(2) 112.31(3), Si(4)-Si(3)-Si(2) 105.78(2), Si(5)-Si(4)-Si(3) 105.82(3), Si(4)-Si(5)-Si(1) 108.53(3).

(4) Possible mechanism for the formation of compounds 3 and 4.

The reduction of **2** to **8** will be took place quickly. When X = Br, the elimination of KBr from **8** afford compound **5**, which isomerized to **6** and then dimerized to **4**. When X = Cl, the elimination of KCl from **8** to **5** may be slow because Cl is not a good leaving group for the α-elimination.[4] Then, trimethylsilyl potassium may be eliminated. Once Me_3SiK is formed, it may react with the starting materials **2a** to give **7**, which will be reduced by C_8K to afford **3**. This mechanism was strengthened by the observation of **7** in the experiments.

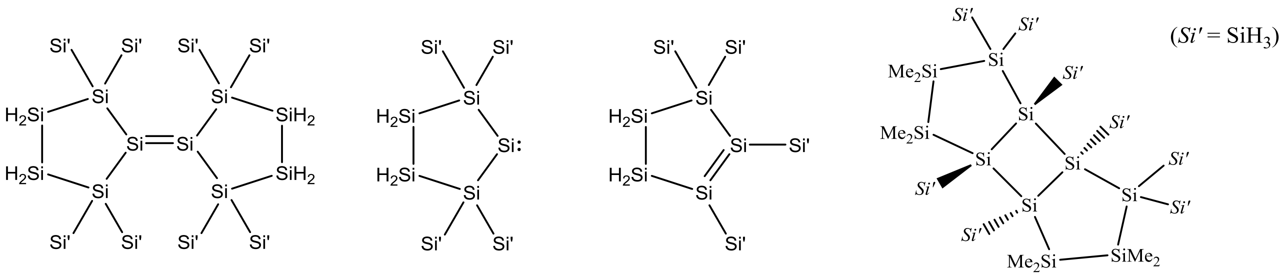


Scheme S1. Possible mechanism for the formation of compounds **3** and **4**.

(5) Theoretical study of model compounds

All DFT calculations were carried out using a Gaussian 03 program.[4] Geometry optimization was carried out at the B3LYP/6-31G(d, p) level. Model compounds ($SiMe_3$ and $SiMe_2$ was changed to SiH_3 and SiH_2 respectively) and relative energy are shown in Scheme S2. Atomic coordinates of optimized structures of **4’-7’** are shown in Table S2-S5.

Scheme S2 Relative energy of model compound **4’-7’**.



7' (-57.4 kcal/mol)　**5'** (0 kcal/mol)　**6'** (-11.4 kcal/mol)　**4'** (-84.7 kcal/mol)

Talbe S2 Atomic Coordinates of **5’**.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	14	0	2.504132	-2.205971	-0.294562
2	1	0	3.044148	-2.512297	-1.646004
3	1	0	3.572793	-2.443355	0.712647
4	1	0	1.385881	-3.148722	-0.016507
5	14	0	3.610164	1.378041	-0.848401
6	1	0	4.775856	1.181347	0.056361
7	1	0	4.019902	1.018750	-2.233028
8	1	0	3.243345	2.820150	-0.825190
9	14	0	-3.613165	-1.373967	-0.850766
10	1	0	-4.023873	-1.009895	-2.233865
11	1	0	-3.248562	-2.816704	-0.832298
12	1	0	-4.777546	-1.178153	0.055864
13	14	0	-0.000003	-0.000271	-1.762618
14	14	0	-2.500090	2.206943	-0.290678
15	1	0	-3.032659	2.519350	-1.643697
16	1	0	-3.573646	2.442236	0.711816
17	1	0	-1.381747	3.146757	-0.003277

18	14	0	1.777221	0.056761	-0.161124
19	14	0	1.096783	0.426068	2.078268
20	1	0	1.081146	1.886287	2.379137
21	1	0	1.991842	-0.235850	3.069392
22	14	0	-1.097657	-0.430670	2.077385
23	1	0	-1.082025	-1.891428	2.375696
24	1	0	-1.992955	0.229462	3.069487
25	14	0	-1.777521	-0.057500	-0.161543

(energy with zero point energy: -2615.067138 hartree)

Talbe S3 Atomic Coordinates of **6’**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	4.318352	0.281968	0.007930
2	1	0	4.402684	1.765493	0.014886
3	1	0	5.007736	-0.248682	1.214853
4	1	0	5.026764	-0.238053	-1.192456
5	14	0	-3.129577	0.660843	-1.668916
6	1	0	-3.483771	2.083458	-1.408716
7	1	0	-2.488003	0.571036	-3.007600
8	1	0	-4.387371	-0.135242	-1.689556
9	14	0	-2.680340	0.007260	2.123726
10	1	0	-2.891995	1.431386	2.500870
11	1	0	-4.002861	-0.677334	2.125885
12	1	0	-1.815729	-0.630495	3.152473
13	14	0	2.070384	-0.369713	-0.011620
14	14	0	1.309733	-2.584302	-0.012511
15	1	0	1.552122	-3.244048	1.302212
16	1	0	1.992703	-3.409642	-1.049174
17	14	0	-1.006828	-2.384531	-0.455608
18	1	0	-1.257143	-2.685228	-1.893802
19	1	0	-1.803635	-3.352955	0.350887
20	14	0	-1.665671	-0.148704	-0.003075
21	14	0	0.381883	1.002104	-0.028951
22	14	0	0.567898	3.336555	0.014165
23	1	0	2.003370	3.720748	0.016304
24	1	0	-0.091080	3.934915	-1.177941
25	1	0	-0.085480	3.893929	1.228935

(energy with zero point energy: -2615.085294 hartree)

Talbe S4 Atomic Coordinates of **7’**.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	14	0	-2.523476	2.724458	2.333976
2	1	0	-1.164746	3.016778	2.857648
3	1	0	-3.343141	3.965113	2.420398
4	1	0	-3.149163	1.688792	3.200306
5	14	0	-1.944915	3.657198	-1.431638
6	1	0	-3.018061	4.686845	-1.356341
7	1	0	-0.646911	4.317650	-1.140606
8	1	0	-1.908379	3.109874	-2.813070
9	14	0	-1.942815	-3.656100	1.433151
10	1	0	-0.644005	-4.315308	1.142880
11	1	0	-1.907055	-3.107408	2.814060
12	1	0	-3.014750	-4.687067	1.358722
13	14	0	-1.094631	-0.000107	-0.000965
14	14	0	-2.523345	-2.726936	-2.333358
15	1	0	-1.164676	-3.018303	-2.857715
16	1	0	-3.341861	-3.968442	-2.418368
17	1	0	-3.150601	-1.692476	-3.199995
18	14	0	-2.449218	1.939199	0.105620
19	14	0	-4.614076	1.109705	-0.391605
20	1	0	-4.839289	1.122225	-1.865075
21	1	0	-5.672681	1.947315	0.240537
22	14	0	-4.613764	-1.110985	0.391501
23	1	0	-4.839054	-1.123561	1.864957
24	1	0	-5.672107	-1.948897	-0.240684
25	14	0	-2.448645	-1.939944	-0.105635
26	1	0	3.017373	-4.686072	-1.357881
27	14	0	1.944043	-3.656539	-1.432113
28	1	0	0.646289	-4.317304	-1.140656
29	1	0	1.906674	-3.108580	-2.813268
30	14	0	2.449085	-1.939157	0.105577
31	14	0	2.525536	-2.725220	2.333590
32	14	0	4.613707	-1.109594	-0.392685
33	14	0	1.094403	0.000187	0.000902
34	1	0	1.167396	-3.017021	2.859085
35	1	0	3.344705	-3.966302	2.418516
36	1	0	3.152938	-1.690129	3.199373
37	14	0	4.613770	1.110917	0.390894
38	1	0	4.838146	-1.121751	-1.866275
39	1	0	5.672597	-1.947430	0.238682
40	14	0	2.448521	1.939845	-0.105619
41	1	0	4.839306	1.123211	1.864314
42	1	0	5.671934	1.949027	-0.241319

43	14	0	2.521957	2.725718	-2.333789
44	14	0	1.943713	3.657336	1.432048
45	1	0	1.162967	3.017314	-2.857188
46	1	0	3.340800	3.966936	-2.419954
47	1	0	3.148195	1.690718	-3.200512
48	1	0	3.016300	4.687567	1.356799
49	1	0	0.645325	4.317169	1.141303
50	1	0	1.907639	3.109757	2.813392

(energy with zero point energy: -5230.225798 hartree)

Talbe S5 Atomic Coordinates of **4’**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-1.015058	1.897663	-0.627796
2	14	0	-0.978529	-0.504347	-0.703366
3	14	0	-3.026961	-1.220599	0.287469
4	14	0	-3.578440	0.524172	1.791411
5	14	0	-2.915091	2.492425	0.664616
6	14	0	-0.753168	-1.453667	-2.853305
7	14	0	-0.989281	3.077963	-2.668930
8	14	0	-4.704679	-1.256798	-1.380242
9	14	0	-2.963869	-3.357924	1.285701
10	14	0	1.015058	1.897663	0.627796
11	14	0	0.978529	-0.504347	0.703366
12	14	0	3.026961	-1.220599	-0.287469
13	14	0	3.578440	0.524172	-1.791411
14	14	0	2.915091	2.492426	-0.664616
15	14	0	0.753168	-1.453667	2.853305
16	14	0	0.989281	3.077963	2.668930
17	14	0	4.704679	-1.256798	1.380242
18	14	0	2.963869	-3.357924	-1.285701
19	1	0	-0.849596	4.538920	-2.420956
20	1	0	0.144906	2.636383	-3.524777
21	1	0	-2.257114	2.846502	-3.412876
22	1	0	2.631215	3.619531	-1.597136
23	1	0	0.849596	4.538920	2.420956
24	1	0	4.011864	2.929685	0.246753
25	1	0	2.257114	2.846502	3.412876
26	1	0	5.029880	0.527693	-2.130109
27	1	0	2.811313	0.381639	-3.060604
28	1	0	6.034513	-1.496060	0.755583
29	1	0	4.759233	0.037936	2.111675

30	1	0	4.450212	-2.341211	2.366604
31	1	0	2.551751	-4.383011	-0.288476
32	1	0	4.315076	-3.718400	-1.795575
33	1	0	2.006999	-3.396117	-2.421409
34	1	0	0.775117	-2.939474	2.789778
35	1	0	-0.511507	-1.023903	3.505539
36	1	0	1.890277	-1.004552	3.702134
37	1	0	-2.006998	-3.396117	2.421409
38	1	0	-4.315076	-3.718400	1.795575
39	1	0	-2.551752	-4.383011	0.288476
40	1	0	-6.034513	-1.496060	-0.755583
41	1	0	-4.450212	-2.341211	-2.366604
42	1	0	-4.759233	0.037937	-2.111675
43	1	0	-5.029880	0.527693	2.130109
44	1	0	-2.811313	0.381639	3.060604
45	1	0	-4.011864	2.929685	-0.246753
46	1	0	-2.631215	3.619531	1.597136
47	1	0	-0.144906	2.636383	3.524777
48	1	0	-1.890277	-1.004552	-3.702134
49	1	0	-0.775117	-2.939474	-2.789778
50	1	0	0.511507	-1.023902	-3.505539

(energy with zero point energy: -5230.269180 hartree)

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