SUPPORTING INFORMATION of SYNTHESES, STRUCTURES, AND COMPUTATIONS

Facile Conversion of Bis-Silylene to Cyclic Silylene Isomers: Unexpected C–N and C–H Bond cleavage

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SUPPORTING INFORMATIONS of SYNTHESES

Materials and Methods

General.

The syntheses of air-sensitive compounds were performed under purified argon using Schlenk techniques and an inert atmosphere drybox (M-Braun LabMaster SP). Chemicals were purchased from Aldrich and Strem and used as received. The solvents were dried and distilled under argon from Na/benzophenone prior to use. ^{1}H NMR, ^{13}C{^{1}H} NMR, and ^{29}Si NMR spectra were recorded on a Bruker Avance III HD 400 MHz spectrometer and a Varian Unity Inova 500 MHz spectrometer. Infrared spectra were recorded using a Shimadzu IRPrestige-21 FTIR spectrophotometer. X-ray intensity data for **3·(toluene)$_{2.5}$** and **4·(toluene)$_2$** were collected at 100K on a Bruker D8 Quest PHOTON 100 CMOS X-ray diffractometer system with Incoatec Microfocus Source (IμS) monochromated Mo Kα radiation (λ = 0.71073 Å, sealed tube) using phi and omega-scan technique.

Synthesis of compound **3** in toluene: 6 mL of toluene was added to a Schlenk tube containing both **1** (0.316 g, 0.47 mmol) and **2** (0.252 g, 0.23 mmol) at room temperature. The resulting dark reddish brown solution was kept stationary in the Schlenk tube over three days, resulting in crystallization of **3·(toluene)$_{2.5}$.** X-ray quality yellow crystals of **3·(toluene)$_{2.5}$** (0.192 g, 52.5% yield) was isolated after solvent removal. Characterization of **3**: Mp: gradually decomposed (> 125°C). ^{1}H NMR (400.14 MHz, THF-d$_8$): δ 0.55 [d, 3H, CH(C*H*$_3$)$_2$], 0.87-1.32 [multiple d, 66H, CH(C*H*$_3$)$_2$], 1.47 [d, 3H, CH(C*H*$_3$)$_2$], 1.87 [m, 1H, C*H*(CH$_3$)$_2$], 2.16 [m, 1H, C*H*(CH$_3$)$_2$], 2.42 [m, 1H, C*H*(CH$_3$)$_2$], 2.55 [m, 1H, C*H*(CH$_3$)$_2$], 2.70 [m, 6H, C*H*(CH$_3$)$_2$], 2.78 [m, 1H, C*H*(CH$_3$)$_2$], 3.08 [m, 1H, C*H*(CH$_3$)$_2$], 4.61 (s, 1H, Si-*H*, $^{1}J_{\text{Si-H}}$ = 196 Hz and , $^{2}J_{\text{Si-H}}$ = 20 Hz based on ^{29}Si satellites), 6.30 (s, 1H, SC=C*H*), 6.97-7.55 (m, 18H, Ar-*H*), 8.02 (d, 2H, *H*C=C*H*). ^{13}C{^{1}H} NMR (100.63 MHz, THF-d$_8$): δ 22.0, 22.4, 23.29, 23.36, 23.40, 23.6, 24.0, 24.6, 24.8, 24.97, 26.08, 26.2, 26.9 [CH(*C*H$_3$)$_2$], 29.21, 29.50, 29.58, 29.68, 29.72, 29.83, 29.92, 29.95, 30.13, 30.71 [*C*H(CH$_3$)$_2$], 114.6, 123.90, 123.98, 124.09, 124.16, 124.60, 124.64, 124.8, 125.0, 125.1, 125.4, 126.2, 128.1, 129.1, 129.8, 129.9, 130.0, 130.1, 132.6, 132.8, 133.1, 135.0, 135.6, 136.0, 137.8, 138.2, 143.2, 146.9, 147.1, 147.6, 147.78, 147.83, 148.4, 149.0, 156.6, 167.6, 168.8 (imidazole-*C* and Ar-*C*). ^{29}Si NMR (THF-d$_8$, 99.3 MHz): δ -27.00 ($^{1}J_{\text{Si-H}}$ = 195 Hz), -72.98 ($^{2}J_{\text{Si-H}}$ = 20 Hz). IR (KBr): ν (Si-H, cm^{-1}): 2109(w). Crystal data for **3·(toluene)$_{2.5}$**: $C_{98.5}H_{126}N_6S_4Si_2$, fw = 1578.47, monoclinic, *C*2/c, *a* = 54.583(4) Å, *b* = 14.5630(12) Å, *c* = 25.285(2) Å, *V* = 18791(3) Å^3, *Z* = 4, R1 = 0.0997 for 10627 data ($I > 2\sigma(I)$), wR$_2$ = 0.2499 (all data).

Synthesis of compound **3** and **4** in THF: 4 mL of THF was added to a Schlenk tube containing both **1** (0.297 g, 0.44 mmol) and **2** (0.252 g, 0.22 mmol) at room temperature. The resulting dark reddish brown solution was then stirred at room temperature over one day. After THF removal, the residue was dissolved in 4 mL of toluene and kept at room temperature over two days. Yellow crystals of **3·(toluene)$_{2.5}$** (0.148 g, 42.7%) were isolated after toluene removal. Addition of hexane (1 mL) to the toluene filtrate induced

crystallization of **4·(toluene)$_2$** as colorless crystals (0.021 g, 6.2%, in terms of ^{1}H NMR data, which shows a 7:1 molar ratio of **3** to **4**). Characterization of **4**: ^{1}H NMR (400.14 MHz, THF-d$_8$): δ 0.62 [d, 3H, CH(C*H*$_3$)$_2$], 0.83 [d, 6H, CH(C*H*$_3$)$_2$], 0.90 [d, 3H, CH(C*H*$_3$)$_2$], 1.02-1.33 [multiple d, 60H, CH(C*H*$_3$)$_2$], 2.12 [m, 1H, C*H*(CH$_3$)$_2$], 2.45-2.86 [multiple m, 9H, C*H*(CH$_3$)$_2$], 3.28 [br, 2H, C*H*(CH$_3$)$_2$], 5.20 (s, 1H, SC=C*H*), 6.16 (s, 1H, SC=C*H*), 6.94-7.44 (m, 18H, Ar-*H*), 7.58 (d, 1H, HC=C*H*), 7.64 (d, 1H, *H*C=CH). ^{13}C{^{1}H} NMR (100.63 MHz, THF-d$_8$): δ 22.0, 24.05, 24.09, 24.15, 24.20, 24.27, 24.41, 24.45, 24.53, 24.54, 24.59, 24.92 [CH(*C*H$_3$)$_2$], 29.53, 29.55, 29.72, 29.75, 29.77, 29.83, 29.86, 29.90, 30.2, 30.3 [*C*H(CH$_3$)$_2$], 117.0, 121.2, 121.9, 124.0, 124.33, 124.39, 124.48, 124.52, 124.56, 124.74, 124.87, 124.93, 125.2, 125.3, 125.4, 130.1, 130.27, 130.33, 130.5, 130.7, 131.0, 131.3, 132.7, 133.1, 133.6, 134.4, 135.5, 135.6, 146.7, 147.41, 147.44, 147.48, 147.52, 148.08, 148.12, 148.2, 148.3, 148.5, 167.5, 168.2, 175.6 (imidazole-*C* and Ar-*C*). ^{29}Si NMR (THF-d$_8$, 99.3 MHz): δ 2.21, -56.73. Crystal data for **4·(toluene)$_2$**: $C_{95}H_{122}N_6S_4Si_2$, fw = 1532.40, monolinic, $P2_1/n$, a = 17.7211(15) Å, b = 27.855(2) Å, c = 18.2418(16) Å, β = 92.844(3)°, V = 8993.6(13) Å^3, Z = 4, R1 = = 0.0669 for 12920 data ($I > 2\sigma(I)$), wR_2 = 0.1883 (all data).

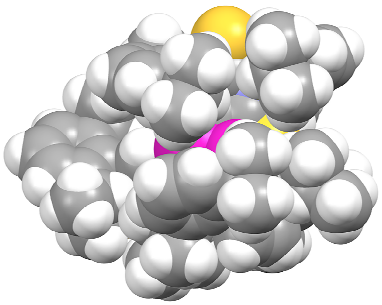
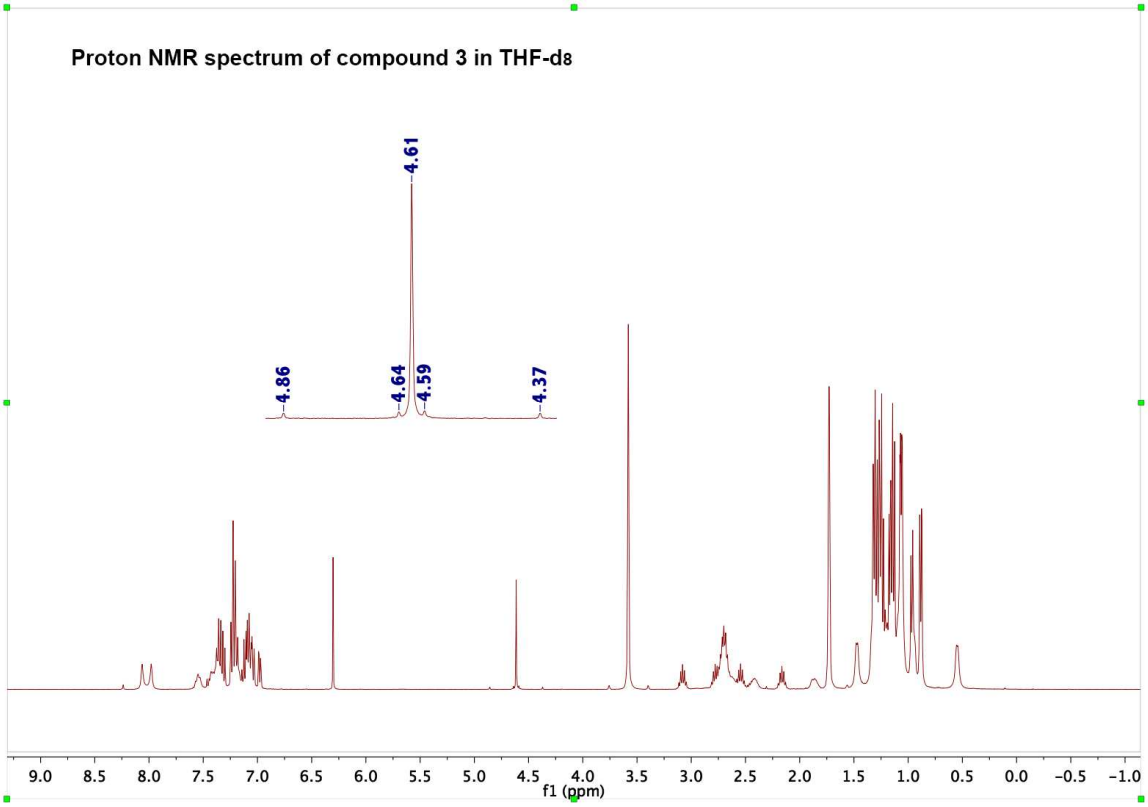
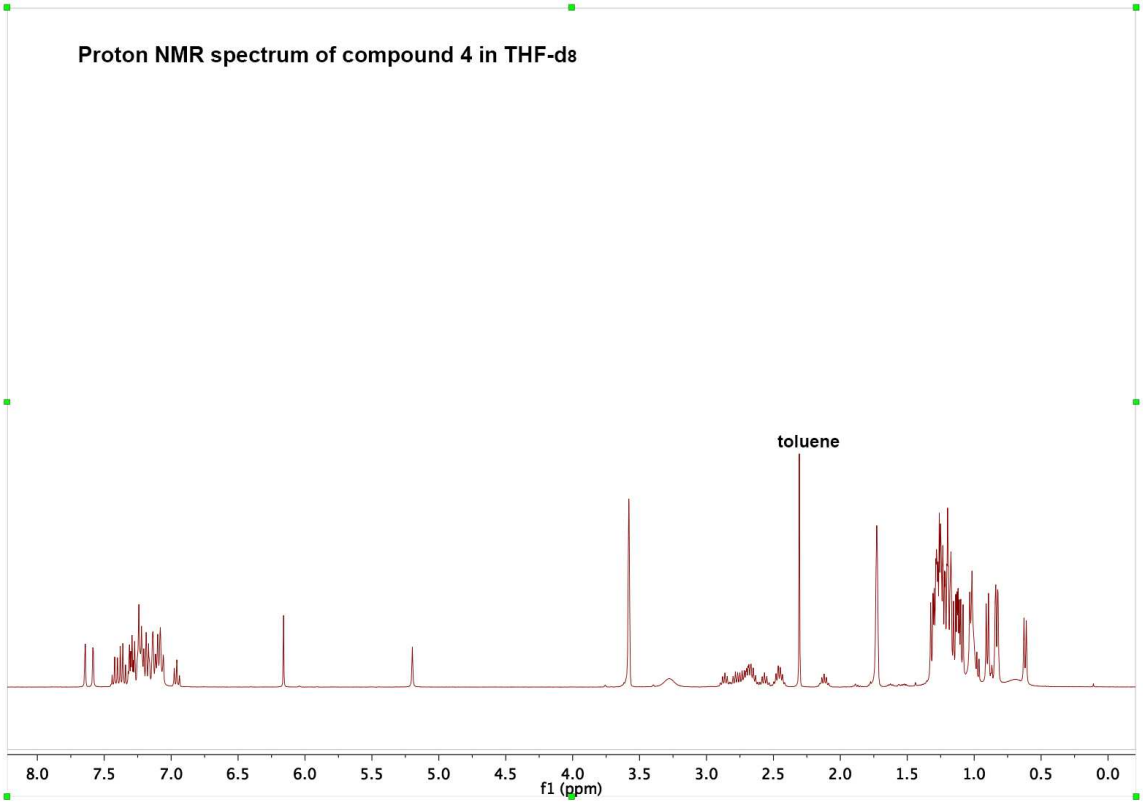


Figure S1. Space filling model of **3** (yellow, sulfur; purple, silicon; gray, carbon; white, hydrogen).


Proton NMR spectrum of compound 3 in THF-d8
4.61
4.86
4.64
4.59
4.37
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


Proton NMR spectrum of compound 4 in THF-d8
toluene
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

SUPPORTING INFORMATIONS of COMPUTATIONS

All computations employed the Gaussian09 programs:
For Gaussian 09: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, revision D.01; Gaussian, Inc., Wallingford CT, 2013.

Table S1. Coordinates of the B3LYP/6-311G** optimized geometry of **3-Ph**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.387431	-1.387577	1.784233
2	1	0	1.338119	-2.022833	3.126399
3	14	0	0.172392	0.659671	1.304897
4	16	0	4.254755	4.155696	-0.659143
5	16	0	3.488574	-0.884066	1.444070
6	16	0	-6.240078	-0.153653	-1.489716
7	16	0	-0.795919	-0.216765	-0.633805
8	7	0	-0.112476	-3.765584	1.029072
9	7	0	1.376961	-3.383528	-0.488284
10	7	0	4.069296	1.622252	0.389586
11	7	0	2.126312	2.575502	0.083784
12	7	0	-3.525045	-0.339167	-1.145576
13	7	0	-4.406176	1.341430	-0.058989
14	6	0	0.914992	-2.936859	0.706130
15	6	0	-0.288957	-4.723989	0.045940
16	1	0	-1.073828	-5.456792	0.103585
17	6	0	0.645477	-4.485372	-0.903041
18	1	0	0.848118	-4.973107	-1.839768
19	6	0	3.475905	2.795942	-0.061749
20	6	0	3.083309	0.717950	0.781526
21	6	0	1.851336	1.282484	0.596557
22	6	0	-4.737302	0.283502	-0.881461
23	6	0	-2.464646	0.342845	-0.515116
24	6	0	-3.021962	1.382400	0.147019
25	1	0	-2.564749	2.111720	0.789576
26	6	0	2.471200	-2.849031	-1.271602
27	6	0	3.684524	-3.531725	-1.275408
28	6	0	2.270669	-1.713585	-2.048327
29	6	0	4.726428	-3.053197	-2.062561
30	1	0	3.813667	-4.411025	-0.655587
31	6	0	3.324081	-1.241097	-2.827994
32	1	0	1.312405	-1.209121	-2.039981
33	6	0	4.547226	-1.906998	-2.835476
34	1	0	5.679317	-3.568507	-2.063433
35	1	0	3.183690	-0.350154	-3.427962
36	1	0	5.362883	-1.532706	-3.442635
37	6	0	-0.944589	-3.663644	2.205056
38	6	0	-0.818419	-4.621411	3.208606
39	6	0	-1.872196	-2.629826	2.297377
40	6	0	-1.636097	-4.534382	4.331433
41	1	0	-0.081468	-5.410281	3.115684
42	6	0	-2.678589	-2.549153	3.430777
43	1	0	-1.959404	-1.909577	1.493210
44	6	0	-2.562448	-3.498279	4.443565
45	1	0	-1.543049	-5.270446	5.120967
46	1	0	-3.397826	-1.743750	3.514688
47	1	0	-3.193418	-3.431120	5.321947
48	6	0	-3.382232	-1.480101	-1.997034
49	6	0	-2.739615	-1.349087	-3.225619
50	6	0	-3.886361	-2.714783	-1.592717

51	6	0	-2.588278	-2.463504	-4.047566
52	1	0	-2.370481	-0.378809	-3.533253
53	6	0	-3.740438	-3.822875	-2.421626
54	1	0	-4.406983	-2.792087	-0.647045
55	6	0	-3.088810	-3.700528	-3.648495
56	1	0	-2.092545	-2.359252	-5.005887
57	1	0	-4.150032	-4.779114	-2.115718
58	1	0	-2.984903	-4.563205	-4.297186
59	6	0	-5.290305	2.332901	0.462851
60	6	0	-4.919134	3.676508	0.380961
61	6	0	-6.486570	1.972272	1.084528
62	6	0	-5.742650	4.657173	0.927176
63	1	0	-3.996347	3.950333	-0.116018
64	6	0	-7.306445	2.961264	1.618422
65	1	0	-6.770577	0.931202	1.135096
66	6	0	-6.939555	4.303817	1.544637
67	1	0	-5.449357	5.698520	0.859806
68	1	0	-8.236970	2.677870	2.096902
69	1	0	-7.583270	5.068693	1.963594
70	6	0	1.120977	3.545071	-0.234422
71	6	0	0.243299	3.310637	-1.290041
72	6	0	1.022280	4.712874	0.521214
73	6	0	-0.743536	4.249115	-1.586949
74	1	0	0.332551	2.399952	-1.867594
75	6	0	0.038940	5.647684	0.216463
76	1	0	1.721566	4.884518	1.328947
77	6	0	-0.845349	5.418647	-0.837574
78	1	0	-1.424773	4.067103	-2.410105
79	1	0	-0.033893	6.558057	0.800240
80	1	0	-1.606122	6.153081	-1.077478
81	6	0	5.482909	1.406180	0.470989
82	6	0	6.093892	1.328065	1.720524
83	6	0	6.234851	1.273596	-0.694384
84	6	0	7.465158	1.098528	1.803095
85	1	0	5.497137	1.450942	2.615770
86	6	0	7.605499	1.053548	-0.604886
87	1	0	5.745020	1.362235	-1.654895
88	6	0	8.221999	0.961909	0.642205
89	1	0	7.940961	1.037451	2.775033
90	1	0	8.194098	0.960276	-1.510413
91	1	0	9.290714	0.791968	0.708048

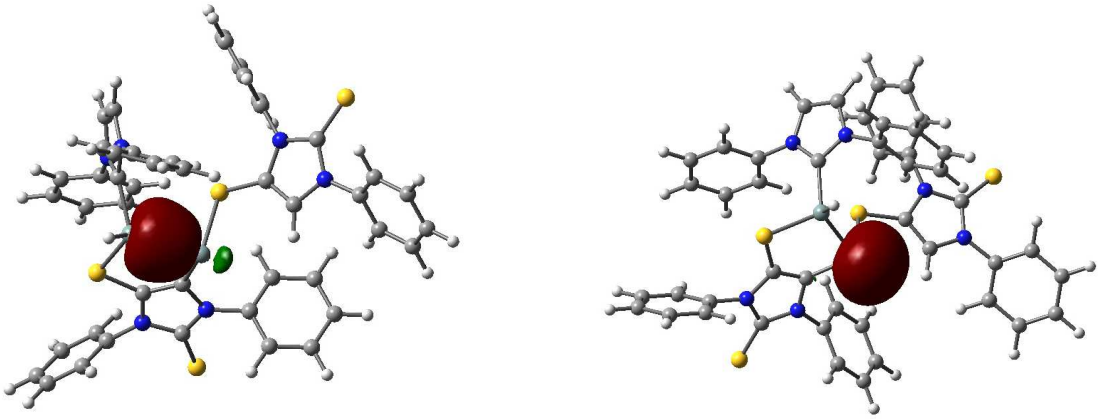

Figure S2. Selected natural bond orbitals (NBOs) of **3-Ph** model. (a) Si–Si σ bonding orbital; (b) silicon-based lone pair orbital.

Table S2. Coordinates of the B3LYP/6-311G** optimized geometry of **4-Ph**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.045221	-0.052694	0.817932
2	14	0	-1.144493	2.142873	1.010551
3	16	0	5.842521	-0.421259	-1.948281
4	16	0	1.931852	0.332962	1.882100
5	16	0	-3.293949	-1.391307	-3.995108
6	16	0	-2.710367	2.774088	-0.387234
7	7	0	-1.967816	1.165090	2.372985
8	7	0	-1.756044	-0.746683	3.397636
9	7	0	3.918692	0.152022	-0.083753
10	7	0	4.287912	-1.993502	-0.291492
11	7	0	-2.802691	0.734496	-2.327577
12	7	0	-4.320431	-0.642823	-1.552623
13	6	0	-1.220267	0.035979	2.420516
14	6	0	-2.987919	1.095817	3.301832
15	1	0	-3.699294	1.890020	3.450278
16	6	0	-2.856408	-0.090636	3.950462
17	1	0	-3.409675	-0.510535	4.772552
18	6	0	-1.305133	-2.050273	3.780910
19	6	0	0.059475	-2.302278	3.911719
20	6	0	0.482172	-3.575279	4.285862
21	1	0	1.542697	-3.772247	4.389762
22	6	0	-0.445218	-4.583220	4.539819
23	1	0	-0.109082	-5.569940	4.835463
24	6	0	-1.807093	-4.319194	4.410528
25	1	0	-2.534216	-5.100581	4.597311
26	6	0	-2.242463	-3.054838	4.025187
27	6	0	-0.573765	3.773519	1.752432
28	6	0	-1.484746	4.732532	2.230633
29	6	0	-1.038040	5.932897	2.774802
30	1	0	-1.754416	6.660877	3.139332
31	6	0	0.328713	6.200210	2.845424
32	1	0	0.676674	7.136519	3.267608
33	6	0	1.244298	5.265193	2.370697
34	1	0	2.307927	5.468298	2.419445
35	6	0	0.798537	4.060739	1.828749
36	6	0	4.696636	-0.759934	-0.773519
37	6	0	3.041760	-0.505726	0.800945
38	6	0	3.284684	-1.828989	0.661269
39	1	0	2.846620	-2.667830	1.170858
40	6	0	4.743410	-3.273722	-0.731783
41	6	0	6.103869	-3.580738	-0.739165
42	6	0	6.515628	-4.848668	-1.136717
43	1	0	7.573285	-5.085602	-1.146527
44	6	0	5.580651	-5.809569	-1.518845
45	1	0	5.909113	-6.795099	-1.828396
46	6	0	4.223878	-5.496650	-1.508279
47	1	0	3.490429	-6.233580	-1.814601
48	6	0	3.802043	-4.227188	-1.120987
49	6	0	4.010521	1.571554	-0.265313
50	6	0	4.940315	2.300181	0.470647

51	6	0	5.025267	3.678752	0.296049
52	1	0	5.753832	4.247832	0.862075
53	6	0	4.183615	4.322460	-0.609741
54	1	0	4.254146	5.395483	-0.747544
55	6	0	3.255208	3.585932	-1.343062
56	1	0	2.600472	4.080800	-2.050730
57	6	0	3.168606	2.206560	-1.173937
58	6	0	-3.473472	-0.438888	-2.633760
59	6	0	-3.232402	1.237170	-1.085255
60	6	0	-4.169129	0.377584	-0.621866
61	1	0	-4.766721	0.424309	0.270663
62	6	0	-5.207444	-1.748509	-1.369796
63	6	0	-6.195589	-2.025901	-2.313395
64	6	0	-7.071534	-3.083976	-2.093729
65	1	0	-7.837567	-3.302677	-2.828516
66	6	0	-6.968872	-3.858880	-0.939290
67	1	0	-7.654306	-4.682346	-0.775129
68	6	0	-5.978836	-3.576849	-0.001781
69	1	0	-5.885316	-4.183570	0.891654
70	6	0	-5.091669	-2.524930	-0.217504
71	6	0	-1.804697	1.325761	-3.172271
72	6	0	-2.098378	2.493427	-3.870598
73	6	0	-1.126086	3.068250	-4.685231
74	1	0	-1.351358	3.978008	-5.229485
75	6	0	0.125573	2.469345	-4.808060
76	1	0	0.878299	2.911673	-5.450621
77	6	0	0.408169	1.294273	-4.112299
78	1	0	1.376729	0.819187	-4.217203
79	6	0	-0.555995	0.719869	-3.288593
80	1	0	6.823311	-2.829102	-0.446504
81	1	0	2.750116	-3.967570	-1.137633
82	1	0	2.460140	1.621831	-1.747227
83	1	0	5.594501	1.784431	1.162504
84	1	0	0.777475	-1.512716	3.727638
85	1	0	-3.299500	-2.855890	3.895120
86	1	0	1.526663	3.342864	1.469405
87	1	0	-2.552887	4.548158	2.173592
88	1	0	-4.297689	-2.316114	0.489786
89	1	0	-6.264559	-1.422970	-3.208142
90	1	0	-0.354900	-0.196192	-2.748371
91	1	0	-3.080447	2.940835	-3.779255

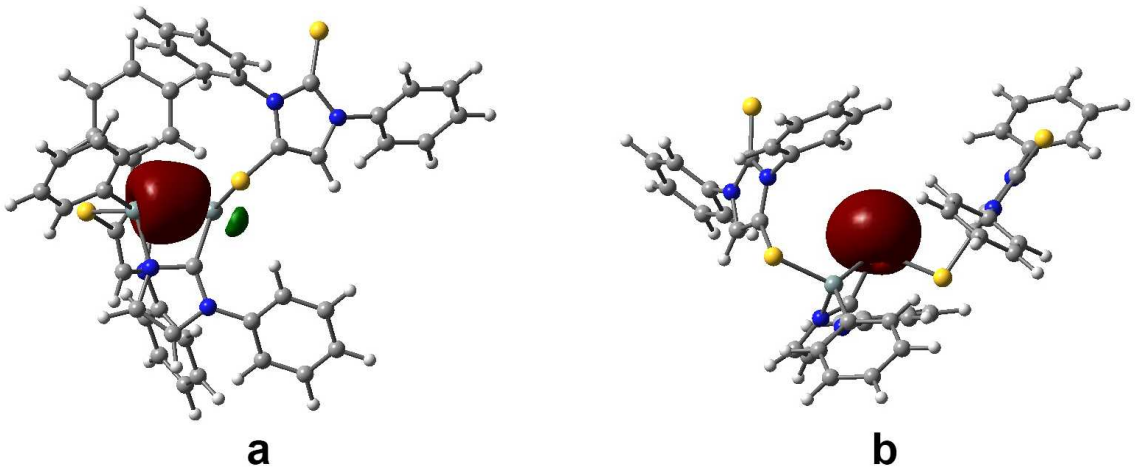

Figure S3. Selected natural bond orbitals (NBOs) of **4-Ph** model. (a) Si–Si σ bonding orbital; (b) silicon-based lone pair orbital.

Table S3. Coordinates of the B3LYP/6-311G** optimized geometry of **6a-Me**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.861435	0.778311	0.323968
2	14	0	1.404025	1.163877	0.548358
3	16	0	-6.439893	-2.260126	0.650029
4	16	0	-1.700070	-0.273744	-1.453475
5	16	0	7.668400	-0.596674	-0.613908
6	16	0	2.135120	-0.633474	-0.492772
7	7	0	-1.838135	3.338312	1.334822
8	7	0	-1.872520	3.369103	-0.828879
9	7	0	-4.195392	-1.043023	-0.401159
10	7	0	-3.916321	-3.150535	0.085346
11	7	0	4.910743	-0.543636	-0.769651
12	7	0	5.681337	-0.994477	1.220317
13	6	0	-1.540323	2.584053	0.236221
14	6	0	-2.338883	4.569076	0.957332
15	1	0	-2.626106	5.317298	1.675299
16	6	0	-2.370671	4.584036	-0.396770
17	1	0	-2.699131	5.345528	-1.082469
18	6	0	-4.847742	-2.143259	0.108381
19	6	0	-2.872042	-1.371335	-0.722455
20	6	0	-2.714789	-2.684453	-0.418770
21	6	0	6.080507	-0.710709	-0.061468
22	6	0	3.808464	-0.721562	0.071051
23	6	0	4.299492	-1.007843	1.304088
24	1	0	3.778424	-1.221220	2.220422
25	6	0	6.605436	-1.245251	2.313637
26	1	0	7.243868	-2.098172	2.077959
27	1	0	7.243582	-0.374699	2.474141
28	1	0	6.027066	-1.451996	3.213681
29	6	0	4.855263	-0.230080	-2.188220
30	1	0	4.293500	-0.996412	-2.724734
31	1	0	4.379569	0.739673	-2.346481
32	1	0	5.881454	-0.199794	-2.549912
33	6	0	-1.645272	2.923753	2.723298
34	1	0	-1.736055	1.837645	2.775787
35	1	0	-0.655132	3.212978	3.078163
36	1	0	-2.410754	3.393306	3.341087
37	6	0	-1.649544	3.033930	-2.233543
38	1	0	-0.684415	2.535743	-2.330052
39	1	0	-2.426481	2.368281	-2.606700
40	1	0	-1.639961	3.958201	-2.809865
41	6	0	-4.819868	0.254073	-0.580753
42	1	0	-4.395811	0.987177	0.109838
43	1	0	-4.678127	0.598173	-1.606396
44	1	0	-5.881283	0.132762	-0.370407
45	6	0	-4.185225	-4.506159	0.536555
46	1	0	-4.996653	-4.943016	-0.047652
47	1	0	-3.278438	-5.097107	0.411907
48	1	0	-4.483725	-4.500378	1.586057
49	1	0	-1.845370	-3.310143	-0.517285

Table S4. Coordinates of the B3LYP/6-311G** optimized geometry of **6b-Me**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.789509	0.051029	-0.267888
2	14	0	1.240906	-0.605695	-1.163549
3	16	0	-6.918749	-0.956565	1.224945
4	16	0	-2.357878	-0.130770	-1.832857
5	16	0	7.045167	-2.221312	0.988714
6	16	0	2.496178	0.803021	0.025327
7	7	0	-0.560637	2.321335	1.545514
8	7	0	-1.026878	3.043660	-0.440583
9	7	0	-4.666264	-0.302337	-0.232245
10	7	0	-5.102101	-2.438562	-0.183315
11	7	0	4.662012	-0.862483	0.674030
12	7	0	6.217506	-0.269351	-0.736144
13	6	0	-0.799089	1.902449	0.269746
14	6	0	-0.634275	3.697067	1.624958
15	1	0	-0.465550	4.229381	2.544692
16	6	0	-0.936426	4.148895	0.383428
17	1	0	-1.090077	5.149752	0.019294
18	6	0	-5.557687	-1.225609	0.267372
19	6	0	-3.667152	-0.946354	-0.973338
20	6	0	-3.954381	-2.271718	-0.938679
21	6	0	5.966269	-1.118561	0.312598
22	6	0	4.119162	0.128419	-0.150686
23	6	0	5.096465	0.491449	-1.019632
24	1	0	5.079857	1.225790	-1.805324
25	6	0	7.491262	-0.207961	-1.433452
26	1	0	8.288251	0.061678	-0.738601
27	1	0	7.729708	-1.180939	-1.866024
28	1	0	7.417402	0.540417	-2.222049
29	6	0	3.966333	-1.555794	1.744735
30	1	0	3.498965	-0.832644	2.414300
31	1	0	3.200166	-2.221452	1.340657
32	1	0	4.707453	-2.142988	2.283987
33	6	0	-0.224360	1.450398	2.670760
34	1	0	-0.686980	0.476205	2.506659
35	1	0	0.857041	1.325111	2.739306
36	1	0	-0.609475	1.893693	3.588645
37	6	0	-1.255727	3.115875	-1.881876
38	1	0	-0.583757	2.418334	-2.382395
39	1	0	-2.283190	2.851747	-2.128385
40	1	0	-1.039544	4.130496	-2.213508
41	6	0	-4.784832	1.128309	-0.021399
42	1	0	-3.977042	1.495375	0.616462
43	1	0	-4.756743	1.651120	-0.978660
44	1	0	-5.739895	1.303006	0.471515
45	6	0	-5.755442	-3.703727	0.110496
46	1	0	-6.778488	-3.695528	-0.268755
47	1	0	-5.189242	-4.503040	-0.366510
48	1	0	-5.791384	-3.866539	1.188828
49	1	0	-3.428717	-3.098275	-1.383085

SUPPORTING INFORMATIONS of X-RAY

Compound 3·(toluene)$_{2.5}$

Table S5. Sample and crystal data for **3·(toluene)$_{2.5}$**

Identification code	**3·(toluene)$_{2.5}$**
Chemical formula	$C_{197}H_{252}N_{12}S_8Si_4$
Formula weight	3156.94 g/mol
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal size	0.180 x 0.350 x 0.400 mm
Crystal system	monoclinic
Space group	C2/c (No. 15)
Unit cell dimensions	a = 54.583(4) Å α = 90°
	b = 14.5630(12) Å β = 110.778(2)°
	c = 25.285(2) Å γ = 90°
Volume	18791(3) Å^3
Z	4
Density (calculated)	1.116 g/cm^3
Absorption coefficient	0.174 mm^{-1}
F(000)	6808

Table S6. Data collection and structure refinement for **3·(toluene)$_{2.5}$**

Theta range for data collection	2.14 to 25.25°	
Index ranges	-65<=h<=65, -17<=k<=16, -30<=l<=29	
Reflections collected	119971	
Independent reflections	16953 [R(int) = 0.1164]	
Coverage of independent reflections	99.7%	
Max. and min. transmission	0.7454 and 0.6277	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	16953 / 274 / 1065	
Goodness-of-fit on F^2	1.094	
Δ/σ_{max}	0.001	
Final R indices	10627 data; I>2σ(I)	R1 = 0.0997, wR2 = 0.2247
	all data	R1 = 0.1544, wR2 = 0.2499
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0507P)^2+195.1683P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.538 and -0.389 eÅ^{-3}	
R.M.S. deviation from mean	0.082 eÅ^{-3}	

Table S7. Bond lengths (Å) for **3·(toluene)$_{2.5}$**

Si1-H1	1.441(19)	Si1-C1	1.909(6)
Si1-S2	2.183(2)	Si1-Si2	2.349(2)
Si2-C30	1.941(6)	Si2-S4	2.263(2)
S1-C28	1.669(6)	S2-C29	1.768(6)
S3-C55	1.675(6)	S4-C56	1.752(6)
N1-C1	1.345(7)	N1-C2	1.374(7)
N1-C16	1.454(7)	N2-C1	1.340(7)
N2-C3	1.381(7)	N2-C4	1.462(7)
N3-C28	1.375(7)	N3-C29	1.388(7)
N3-C43	1.444(7)	N4-C28	1.368(7)
N4-C30	1.386(7)	N4-C31	1.443(7)
N5-C55	1.362(7)	N5-C56	1.407(7)
N5-C70	1.440(7)	N6-C55	1.367(7)
N6-C57	1.381(7)	N6-C58	1.447(7)
C2-C3	1.330(8)	C4-C9	1.398(9)
C4-C5	1.403(9)	C5-C6	1.382(9)
C5-C13	1.496(9)	C6-C7	1.402(10)
C7-C8	1.358(10)	C8-C9	1.409(8)
C9-C10	1.505(9)	C10-C11	1.509(9)
C10-C12	1.515(10)	C13-C15	1.521(9)
C13-C14	1.522(9)	C16-C17	1.384(8)
C16-C21	1.409(8)	C17-C18	1.393(8)
C17-C25	1.532(8)	C18-C19	1.365(9)
C19-C20	1.380(9)	C20-C21	1.381(8)
C21-C22	1.514(8)	C22-C23	1.512(9)
C22-C24	1.518(9)	C25-C27	1.508(8)
C25-C26	1.522(8)	C29-C30	1.364(7)
C31-C36	1.398(8)	C31-C32	1.404(9)
C32-C33	1.419(8)	C32-C40	1.490(9)
C33-C34	1.357(10)	C34-C35	1.369(9)
C35-C36	1.400(8)	C36-C37	1.528(9)
C37-C39	1.520(9)	C37-C38	1.539(9)
C40-C41	1.511(9)	C40-C42	1.532(9)
C43-C48	1.377(8)	C43-C44	1.395(9)
C44-C45	1.387(8)	C44-C52	1.501(9)

C45-C46	1.368(9)	C46-C47	1.366(10)
C47-C48	1.413(8)	C48-C49	1.513(9)
C49-C51	1.503(10)	C49-C50	1.532(9)
C52-C54	1.479(12)	C52-C53	1.531(10)
C56-C57	1.345(8)	C58-C63	1.390(8)
C58-C59	1.407(8)	C59-C60	1.401(8)
C59-C67	1.514(9)	C60-C61	1.367(9)
C61-C62	1.394(9)	C62-C63	1.401(8)
C63-C64	1.517(8)	C64-C65	1.515(9)
C64-C66	1.512(9)	C67-C68	1.525(9)
C67-C69	1.538(9)	C70-C71	1.364(8)
C70-C75	1.421(8)	C71-C72	1.406(8)
C71-C79	1.530(9)	C72-C73	1.385(9)
C73-C74	1.367(9)	C74-C75	1.392(8)
C75-C76	1.511(9)	C76-C77	1.511(10)
C76-C78	1.533(9)	C79-C80	1.533(10)
C79-C81	1.546(10)	C82-C83	1.368(9)
C82-C87	1.408(9)	C82-C88	1.481(10)
C83-C84	1.374(10)	C84-C85	1.360(11)
C85-C86	1.390(10)	C86-C87	1.356(10)
C89-C94	1.418(14)	C89-C90	1.410(16)
C89-C95	1.533(16)	C90-C91	1.433(16)
C91-C92	1.412(15)	C92-C93	1.383(15)
C93-C94	1.401(15)	C89'-C90'	1.41(2)
C89'-C94'	1.446(16)	C89'-C95'	1.51(2)
C90'-C91'	1.43(2)	C91'-C92'	1.41(2)
C92'-C93'	1.38(2)	C93'-C94'	1.42(2)
C96-C97	1.369(11)	C96-C97	1.369(11)
C96-C100	1.473(14)	C97-C98	1.405(14)
C98-C99	1.478(16)	C99-C98	1.478(16)

Table S8. Bond angles (°) for **3·(toluene)$_{2.5}$**

H1-Si1-C1	97(2)	H1-Si1-S2	108(2)
C1-Si1-S2	108.65(18)	H1-Si1-Si2	112(2)
C1-Si1-Si2	123.89(18)	S2-Si1-Si2	106.57(9)
C30-Si2-S4	98.50(18)	C30-Si2-Si1	77.33(17)
S4-Si2-Si1	93.40(8)	C29-S2-Si1	83.0(2)
C56-S4-Si2	102.0(2)	C1-N1-C2	109.9(5)
C1-N1-C16	124.7(4)	C2-N1-C16	124.8(5)
C1-N2-C3	109.3(5)	C1-N2-C4	125.7(5)
C3-N2-C4	124.2(5)	C28-N3-C29	109.3(4)
C28-N3-C43	124.3(4)	C29-N3-C43	126.4(5)
C28-N4-C30	112.7(4)	C28-N4-C31	124.4(4)
C30-N4-C31	122.5(4)	C55-N5-C56	110.3(5)
C55-N5-C70	123.1(5)	C56-N5-C70	126.2(5)
C55-N6-C57	109.8(5)	C55-N6-C58	123.2(5)
C57-N6-C58	127.0(5)	N2-C1-N1	106.2(5)
N2-C1-Si1	133.1(4)	N1-C1-Si1	120.6(4)
C3-C2-N1	106.9(5)	C2-C3-N2	107.6(5)
C9-C4-C5	124.6(6)	C9-C4-N2	118.0(5)
C5-C4-N2	117.3(5)	C6-C5-C4	116.2(6)
C6-C5-C13	120.5(6)	C4-C5-C13	123.4(5)
C5-C6-C7	121.1(6)	C8-C7-C6	121.0(6)
C7-C8-C9	121.1(6)	C4-C9-C8	116.0(6)
C4-C9-C10	122.8(5)	C8-C9-C10	121.2(6)
C9-C10-C11	112.9(6)	C9-C10-C12	109.3(5)
C11-C10-C12	112.6(6)	C5-C13-C15	110.7(6)
C5-C13-C14	112.3(5)	C15-C13-C14	110.4(6)
C17-C16-C21	123.6(5)	C17-C16-N1	119.3(5)
C21-C16-N1	117.1(5)	C18-C17-C16	117.0(5)
C18-C17-C25	120.8(5)	C16-C17-C25	122.1(5)
C19-C18-C17	121.0(6)	C18-C19-C20	120.5(6)
C19-C20-C21	121.7(6)	C20-C21-C16	116.1(6)
C20-C21-C22	120.8(5)	C16-C21-C22	123.0(5)
C23-C22-C21	109.6(5)	C23-C22-C24	110.2(6)
C21-C22-C24	114.0(5)	C27-C25-C26	110.3(5)
C27-C25-C17	110.2(5)	C26-C25-C17	113.1(5)

N4-C28-N3	104.3(5)	N4-C28-S1	129.2(4)
N3-C28-S1	126.5(4)	C30-C29-N3	109.3(5)
C30-C29-S2	127.9(5)	N3-C29-S2	122.7(4)
C29-C30-N4	104.4(5)	C29-C30-Si2	127.4(4)
N4-C30-Si2	127.4(4)	C36-C31-C32	124.4(5)
C36-C31-N4	118.3(5)	C32-C31-N4	117.1(5)
C31-C32-C33	115.3(6)	C31-C32-C40	122.5(5)
C33-C32-C40	122.1(6)	C34-C33-C32	121.2(6)
C33-C34-C35	121.7(6)	C34-C35-C36	121.0(6)
C31-C36-C35	116.3(6)	C31-C36-C37	121.7(5)
C35-C36-C37	122.0(6)	C39-C37-C36	113.0(5)
C39-C37-C38	111.1(6)	C36-C37-C38	110.8(5)
C32-C40-C41	111.2(5)	C32-C40-C42	113.8(5)
C41-C40-C42	110.2(6)	C48-C43-C44	124.2(5)
C48-C43-N3	117.8(6)	C44-C43-N3	117.9(5)
C43-C44-C45	116.7(6)	C43-C44-C52	122.6(6)
C45-C44-C52	120.7(6)	C46-C45-C44	121.1(6)
C47-C46-C45	121.0(6)	C46-C47-C48	120.8(6)
C43-C48-C47	116.2(6)	C43-C48-C49	122.6(5)
C47-C48-C49	121.3(6)	C51-C49-C48	111.9(6)
C51-C49-C50	110.2(7)	C48-C49-C50	112.5(6)
C54-C52-C44	111.2(7)	C54-C52-C53	110.6(7)
C44-C52-C53	113.4(6)	N5-C55-N6	105.4(5)
N5-C55-S3	127.4(4)	N6-C55-S3	127.1(4)
C57-C56-N5	105.9(5)	C57-C56-S4	135.0(5)
N5-C56-S4	119.0(4)	C56-C57-N6	108.5(5)
C63-C58-C59	123.4(5)	C63-C58-N6	118.5(5)
C59-C58-N6	118.1(5)	C60-C59-C58	116.5(6)
C60-C59-C67	120.0(6)	C58-C59-C67	123.6(5)
C61-C60-C59	122.2(6)	C60-C61-C62	119.6(6)
C63-C62-C61	121.3(6)	C58-C63-C62	117.1(6)
C58-C63-C64	122.1(5)	C62-C63-C64	120.7(5)
C65-C64-C63	110.8(5)	C65-C64-C66	109.6(6)
C63-C64-C66	114.4(5)	C59-C67-C68	111.6(5)
C59-C67-C69	110.0(5)	C68-C67-C69	111.2(6)
C71-C70-C75	122.7(5)	C71-C70-N5	119.9(5)
C75-C70-N5	117.4(5)	C70-C71-C72	118.6(6)

C70-C71-C79	122.4(5)	C72-C71-C79	119.0(6)
C73-C72-C71	119.9(6)	C74-C73-C72	120.5(6)
C73-C74-C75	121.8(6)	C74-C75-C70	116.5(6)
C74-C75-C76	120.5(6)	C70-C75-C76	123.0(5)
C75-C76-C77	111.3(5)	C75-C76-C78	111.8(6)
C77-C76-C78	111.8(6)	C80-C79-C71	111.1(6)
C80-C79-C81	111.2(6)	C71-C79-C81	111.8(6)
C83-C82-C87	118.3(7)	C83-C82-C88	121.6(7)
C87-C82-C88	120.1(7)	C82-C83-C84	120.6(7)
C85-C84-C83	121.5(7)	C84-C85-C86	118.3(7)
C87-C86-C85	121.0(7)	C86-C87-C82	120.2(7)
C94-C89-C90	125.1(18)	C94-C89-C95	111.8(18)
C90-C89-C95	123.0(18)	C89-C90-C91	112.9(17)
C92-C91-C90	126.(2)	C91-C92-C93	114.0(19)
C92-C93-C94	125.7(18)	C89-C94-C93	113.7(18)
C90'-C89'-C94'	120(3)	C90'-C89'-C95'	120(3)
C94'-C89'-C95'	117(3)	C91'-C90'-C89'	106(2)
C90'-C91'-C92'	124(3)	C93'-C92'-C91'	114(3)
C94'-C93'-C92'	125(3)	C93'-C94'-C89'	109(3)
C97-C96-C97	119.5(15)	C97-C96-C100	120.3(7)
C97-C96-C100	120.3(7)	C98-C97-C96	121.0(13)
C97-C98-C99	118(2)	C98-C99-C98	115(2)

Compound 4·(toluene)$_2$

Table S9. Sample and crystal data for **4·(toluene)$_2$**.

Identification code	**4·(toluene)$_2$**
Chemical formula	$C_{95}H_{122}N_6S_4Si_2$
Formula weight	1532.40 g/mol
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal size	0.120 x 0.220 x 0.340 mm
Crystal system	monoclinic
Space group	$P2_1/n$ (No. 14)
Unit cell dimensions	a = 17.7211(15) Å
	b = 27.855(2) Å
	c = 18.2418(16) Å
Volume	8993.6(13) Å^3
Z	4
Density (calculated)	1.132 g/cm^3
Absorption coefficient	0.179 mm^{-1}
F(000)	3304

Table S10. Data collection and structure refinement for **4·(toluene)$_2$**.

Theta range for data collection	2.14 to 25.25°	
Index ranges	-21<=h<=21, -33<=k<=33, -21<=l<=21	
Reflections collected	253811	
Independent reflections	16265 [R(int) = 0.0871]	
Max. and min. transmission	0.7456 and 0.6302	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	16265 / 205 / 998	
Goodness-of-fit on F^2	1.068	
Δ/σ_{max}	0.001	
Final R indices	12920 data; I>2σ(I)	R1 = 0.0669, wR2 = 0.1760
	all data	R1 = 0.0859, wR2 = 0.1883
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0857P)^2+13.8780P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.834 and -0.637 eÅ^{-3}	
R.M.S. deviation from mean	0.066 eÅ^{-3}	

Table S11. Bond lengths (Å) for **4·(toluene)$_2$**.

Si1-C1	1.952(3)	Si1-S2	2.2181(11)
Si1-Si2	2.4164(11)	Si2-N1	1.838(3)
Si2-C16	1.889(3)	Si2-S4	2.1502(11)
S1-C28	1.677(3)	S2-C29	1.743(3)
S3-C55	1.664(3)	S4-C56	1.747(3)
N1-C1	1.355(4)	N1-C2	1.389(4)
N2-C1	1.346(4)	N2-C3	1.384(4)
N2-C4	1.440(4)	N3-C28	1.364(4)
N3-C29	1.413(4)	N3-C43	1.437(4)
N4-C28	1.361(4)	N4-C30	1.383(4)
N4-C31	1.441(4)	N5-C55	1.368(4)
N5-C56	1.395(4)	N5-C70	1.442(4)
N6-C55	1.356(4)	N6-C57	1.392(4)
N6-C58	1.439(4)	C2-C3	1.348(5)
C4-C9	1.392(5)	C4-C5	1.399(5)
C5-C6	1.391(5)	C5-C13	1.518(5)
C6-C7	1.378(5)	C7-C8	1.374(5)
C8-C9	1.393(5)	C9-C10	1.515(5)
C10-C11	1.504(7)	C10-C12	1.520(6)
C13-C14	1.514(5)	C13-C15	1.521(6)
C16-C21	1.407(5)	C16-C17	1.409(5)
C17-C18	1.402(5)	C17-C25	1.514(5)
C18-C19	1.369(6)	C19-C20	1.371(6)
C20-C21	1.395(5)	C21-C22	1.519(5)
C22-C23	1.516(6)	C22-C24	1.526(5)
C25-C27	1.525(5)	C25-C26	1.529(5)
C29-C30	1.344(4)	C31-C32	1.399(5)
C31-C36	1.397(5)	C32-C33	1.389(5)
C32-C40	1.513(6)	C33-C34	1.365(6)
C34-C35	1.373(6)	C35-C36	1.396(5)
C36-C37	1.516(5)	C37-C38	1.515(6)
C37-C39	1.533(6)	C40-C41	1.523(6)
C40-C42	1.532(6)	C43-C48	1.391(4)
C43-C44	1.399(4)	C44-C45	1.396(5)
C44-C52	1.525(5)	C45-C46	1.377(5)
C46-C47	1.379(5)	C47-C48	1.397(4)

C48-C49	1.515(5)	C49-C50	1.528(5)
C49-C51	1.532(5)	C52-C53	1.520(5)
C52-C54	1.525(6)	C56-C57	1.348(4)
C58-C63	1.388(5)	C58-C59	1.387(4)
C59-C60	1.392(5)	C59-C67	1.502(14)
C59-C67'	1.536(12)	C60-C61	1.384(5)
C61-C62	1.361(5)	C62-C63	1.395(5)
C63-C64	1.517(5)	C64-C65	1.540(6)
C64-C66	1.529(7)	C67-C69	1.528(14)
C67-C68	1.535(12)	C67'-C69'	1.522(11)
C67'-C68'	1.535(13)	C70-C75	1.398(5)
C70-C71	1.387(5)	C71-C72	1.390(5)
C71-C79	1.520(5)	C72-C73	1.386(6)
C73-C74	1.368(6)	C74-C75	1.389(5)
C75-C76	1.516(14)	C75-C76'	1.537(15)
C76-C78	1.507(12)	C76-C77	1.521(15)
C76'-C78'	1.527(12)	C76'-C77'	1.535(13)
C79-C81	1.524(5)	C79-C80	1.516(6)
C82-C83	1.39	C82-C87	1.39
C82-C88	1.426(8)	C83-C84	1.39
C84-C85	1.39	C85-C86	1.39
C86-C87	1.39	C89-C90	1.39
C89-C94	1.39	C89-C95	1.436(10)
C90-C91	1.39	C91-C92	1.39
C92-C93	1.39	C93-C94	1.39

Table S12. Bond angles (°) for **4·(toluene)$_2$**.

C1-Si1-S2	100.20(9)	C1-Si1-Si2	67.84(9)
S2-Si1-Si2	99.66(4)	N1-Si2-C16	114.67(14)
N1-Si2-S4	108.31(9)	C16-Si2-S4	100.11(10)
N1-Si2-Si1	78.78(9)	C16-Si2-Si1	126.58(10)
S4-Si2-Si1	125.49(5)	C29-S2-Si1	98.24(11)
C56-S4-Si2	104.53(11)	C1-N1-C2	108.7(3)
C1-N1-Si2	100.11(19)	C2-N1-Si2	151.2(2)
C1-N2-C3	109.0(3)	C1-N2-C4	124.1(3)
C3-N2-C4	126.9(3)	C28-N3-C29	109.9(2)
C28-N3-C43	123.1(2)	C29-N3-C43	127.0(2)
C28-N4-C30	110.1(2)	C28-N4-C31	125.6(3)
C30-N4-C31	124.1(3)	C55-N5-C56	110.5(2)
C55-N5-C70	123.4(2)	C56-N5-C70	126.0(2)
C55-N6-C57	110.6(2)	C55-N6-C58	123.9(2)
C57-N6-C58	125.2(2)	N2-C1-N1	107.4(3)
N2-C1-Si1	139.9(2)	N1-C1-Si1	110.4(2)
C3-C2-N1	107.2(3)	C2-C3-N2	107.6(3)
C9-C4-C5	123.4(3)	C9-C4-N2	118.4(3)
C5-C4-N2	118.2(3)	C4-C5-C6	116.7(3)
C4-C5-C13	122.3(3)	C6-C5-C13	120.9(3)
C7-C6-C5	121.3(3)	C8-C7-C6	120.4(3)
C7-C8-C9	121.2(3)	C4-C9-C8	116.9(3)
C4-C9-C10	123.2(3)	C8-C9-C10	119.9(3)
C9-C10-C11	112.4(4)	C9-C10-C12	110.7(4)
C11-C10-C12	111.0(4)	C5-C13-C14	113.1(3)
C5-C13-C15	110.1(3)	C14-C13-C15	109.7(3)
C21-C16-C17	119.9(3)	C21-C16-Si2	118.3(2)
C17-C16-Si2	121.8(2)	C16-C17-C18	118.8(3)
C16-C17-C25	123.2(3)	C18-C17-C25	118.1(3)
C19-C18-C17	120.8(4)	C18-C19-C20	120.4(4)
C19-C20-C21	121.2(4)	C16-C21-C20	118.7(3)
C16-C21-C22	122.2(3)	C20-C21-C22	118.8(3)
C21-C22-C23	110.1(3)	C21-C22-C24	114.4(3)
C23-C22-C24	110.9(3)	C17-C25-C27	112.4(3)
C17-C25-C26	111.7(3)	C27-C25-C26	111.0(3)
N3-C28-N4	105.6(2)	N3-C28-S1	128.3(2)

N4-C28-S1	126.1(2)	C30-C29-N3	106.1(3)
C30-C29-S2	129.7(2)	N3-C29-S2	124.2(2)
C29-C30-N4	108.3(3)	C32-C31-C36	123.1(3)
C32-C31-N4	118.2(3)	C36-C31-N4	118.6(3)
C33-C32-C31	116.8(4)	C33-C32-C40	121.0(3)
C31-C32-C40	122.1(3)	C32-C33-C34	121.6(4)
C35-C34-C33	120.4(3)	C34-C35-C36	121.3(4)
C35-C36-C31	116.7(4)	C35-C36-C37	121.0(4)
C31-C36-C37	122.4(3)	C36-C37-C38	111.5(4)
C36-C37-C39	113.6(3)	C38-C37-C39	109.1(4)
C32-C40-C41	112.2(3)	C32-C40-C42	110.8(3)
C41-C40-C42	110.4(3)	C48-C43-C44	122.5(3)
C48-C43-N3	118.4(3)	C44-C43-N3	119.0(3)
C45-C44-C43	117.1(3)	C45-C44-C52	120.9(3)
C43-C44-C52	122.0(3)	C44-C45-C46	121.3(3)
C45-C46-C47	120.4(3)	C46-C47-C48	120.5(3)
C43-C48-C47	118.0(3)	C43-C48-C49	122.8(3)
C47-C48-C49	119.1(3)	C48-C49-C50	110.2(3)
C48-C49-C51	111.2(3)	C50-C49-C51	111.5(3)
C44-C52-C53	112.2(3)	C44-C52-C54	112.4(3)
C53-C52-C54	110.1(4)	N6-C55-N5	105.0(2)
N6-C55-S3	127.4(2)	N5-C55-S3	127.7(2)
C57-C56-N5	106.6(3)	C57-C56-S4	134.5(2)
N5-C56-S4	118.9(2)	C56-C57-N6	107.3(3)
C63-C58-C59	123.7(3)	C63-C58-N6	117.9(3)
C59-C58-N6	118.4(3)	C60-C59-C58	116.5(3)
C60-C59-C67	120.2(8)	C58-C59-C67	123.3(8)
C60-C59-C67'	123.9(8)	C58-C59-C67'	119.6(8)
C59-C60-C61	121.3(3)	C62-C61-C60	120.3(3)
C61-C62-C63	121.0(3)	C58-C63-C62	117.1(3)
C58-C63-C64	122.5(3)	C62-C63-C64	120.3(3)
C65-C64-C63	111.1(4)	C65-C64-C66	112.1(3)
C63-C64-C66	111.6(4)	C59-C67-C69	114.5(13)
C59-C67-C68	111.9(11)	C69-C67-C68	109.7(11)
C69'-C67'-C59	109.5(10)	C69'-C67'-C68'	110.1(10)
C59-C67'-C68'	110.9(13)	C75-C70-C71	124.6(3)
C75-C70-N5	116.9(3)	C71-C70-N5	118.5(3)

C70-C71-C72	116.5(3)	C70-C71-C79	121.8(3)
C72-C71-C79	121.7(3)	C73-C72-C71	120.6(4)
C74-C73-C72	121.0(3)	C73-C74-C75	121.2(4)
C70-C75-C74	116.1(3)	C70-C75-C76	120.3(9)
C74-C75-C76	123.4(9)	C70-C75-C76'	123.8(9)
C74-C75-C76'	120.0(9)	C78-C76-C75	109.4(13)
C78-C76-C77	111.2(13)	C75-C76-C77	106.4(14)
C78'-C76'-C75	118.0(18)	C78'-C76'-C77'	108.6(12)
C75-C76'-C77'	113.4(12)	C71-C79-C81	111.7(3)
C71-C79-C80	111.5(3)	C81-C79-C80	111.7(3)
C83-C82-C87	120.0	C83-C82-C88	115.8(7)
C87-C82-C88	124.2(7)	C84-C83-C82	120.0
C83-C84-C85	120.0	C86-C85-C84	120.0
C85-C86-C87	120.0	C86-C87-C82	120.0
C90-C89-C94	120.0	C90-C89-C95	105.1(9)
C94-C89-C95	134.9(9)	C89-C90-C91	120.0
C92-C91-C90	120.0	C91-C92-C93	120.0
C94-C93-C92	120.0	C93-C94-C89	120.0