Electronic Supplementary Materials

Heteroaryldisilenes: heteroaryl groups serve as electron acceptors for Si=Si double bonds in the intramolecular charge transfer transitions

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Contents

1. NMR Spectra

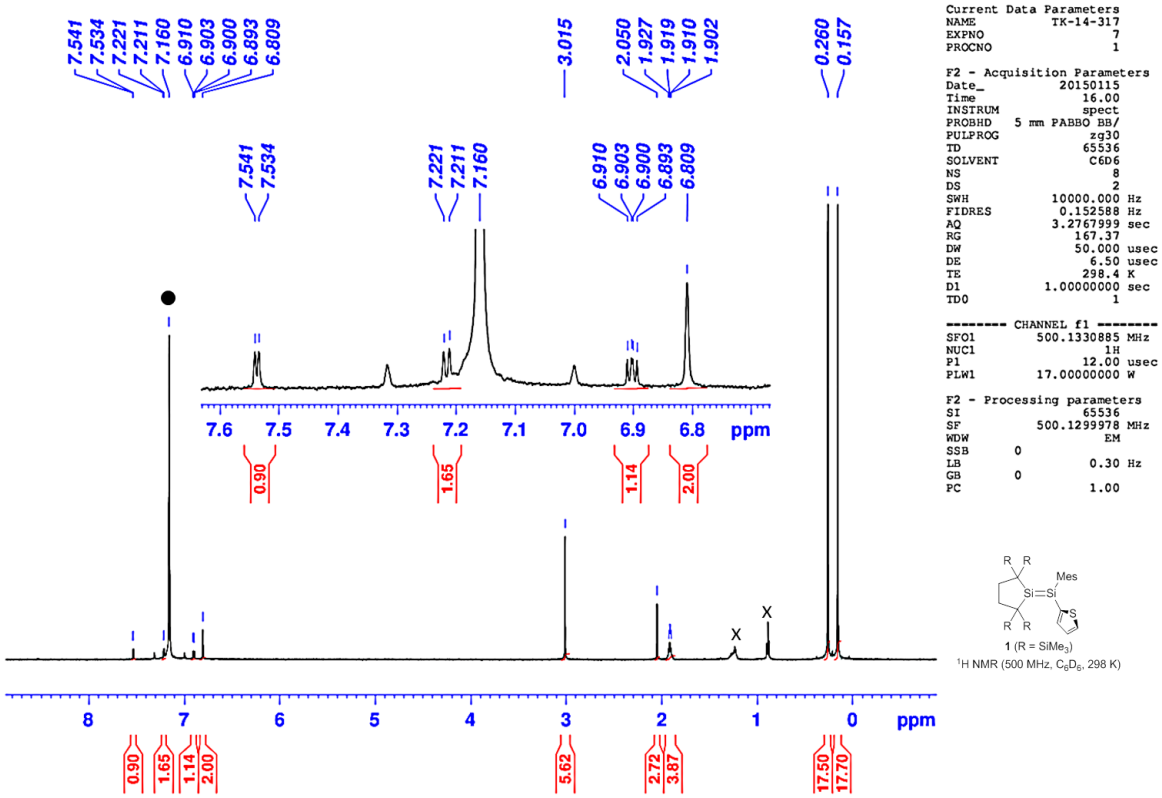


Figure S1. ^{1}H NMR spectrum of **1** in C_6D_6 at 298 K (● = C_6HD_5, x = hexane).

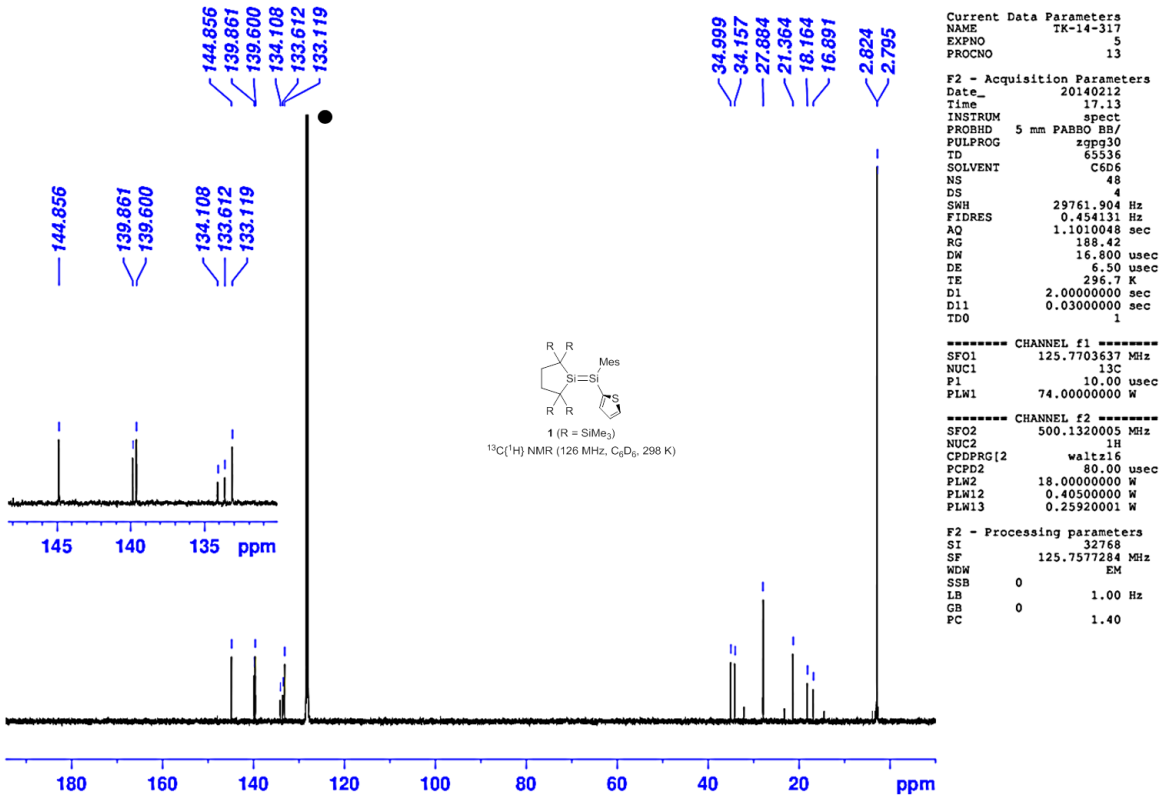


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6 at 298 (● = C_6D_6).

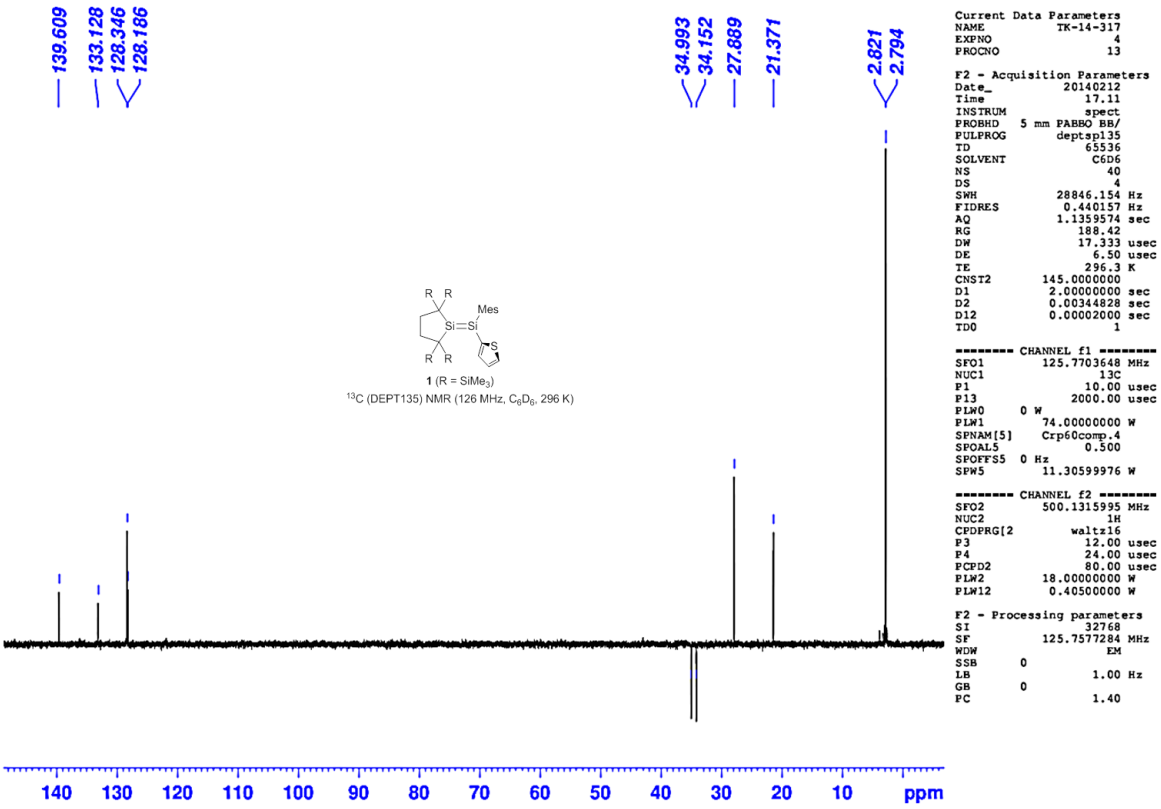


Figure S3. ^{13}C (DEPT135) NMR spectrum of **1** in C_6D_6 at 296 K.

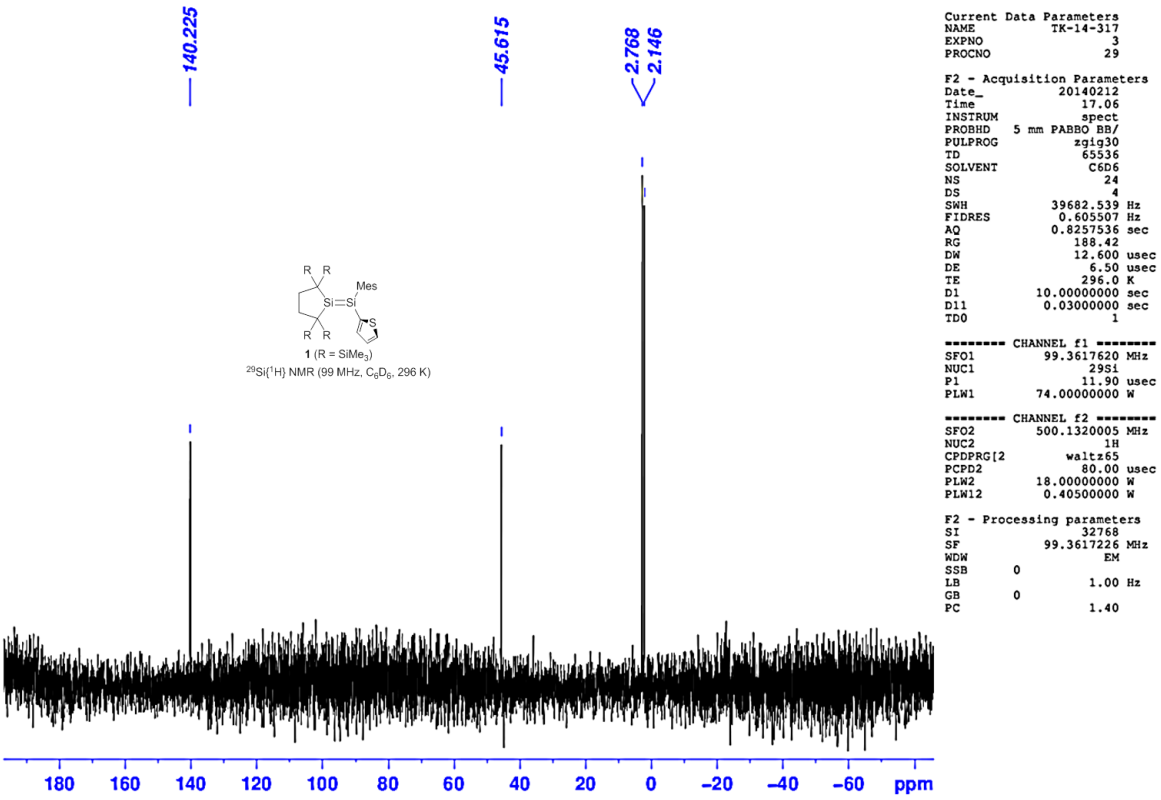


Figure S4. $^{29}Si\{^1H\}$ NMR spectrum of **1** in C_6D_6 at 296 K.

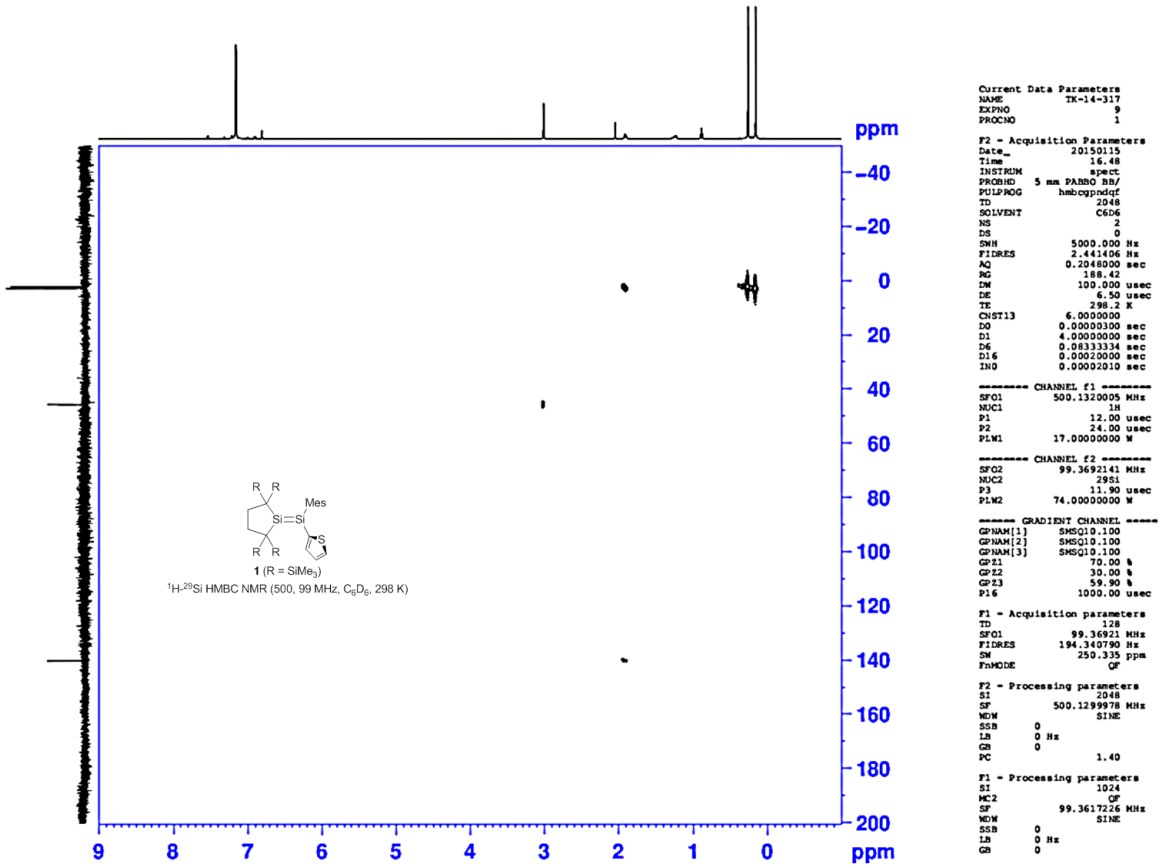


Figure S5. ^{1}H-^{29}Si HMBC NMR spectrum of **1** in C_6D_6 at 298 K.

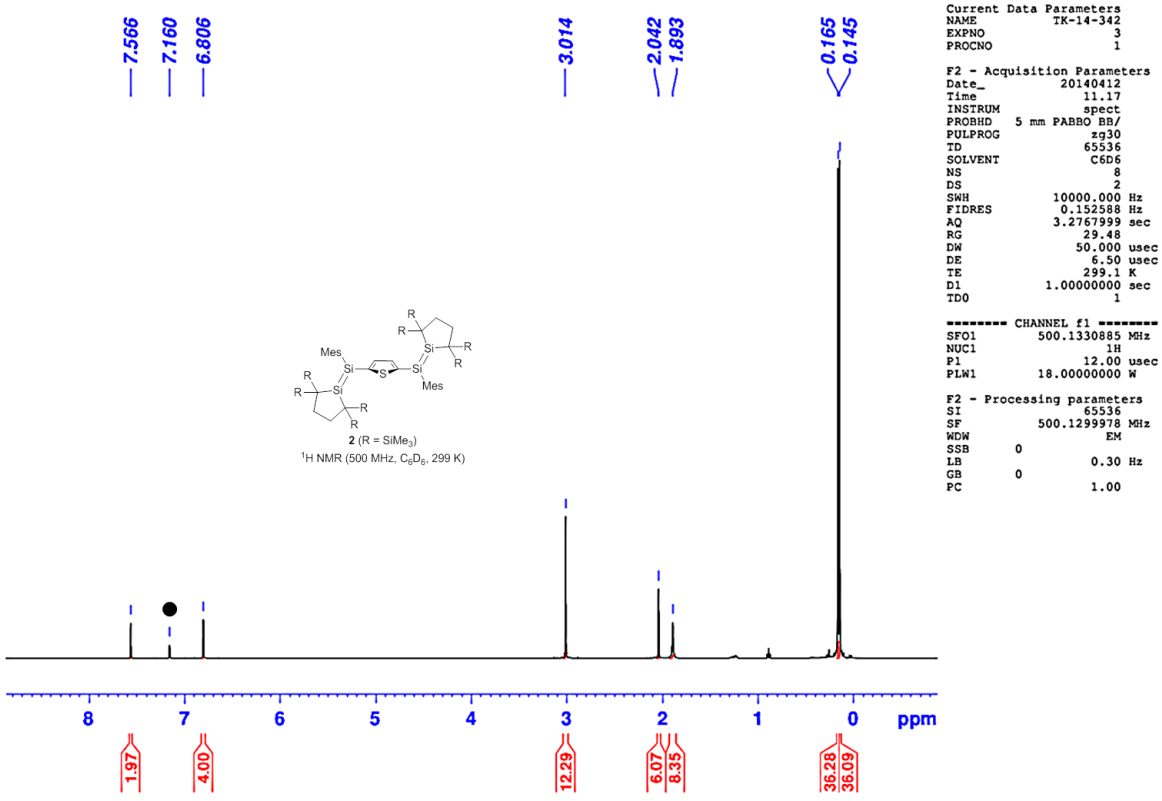


Figure S6. ^{1}H NMR spectrum of **2** in C_6D_6 at 299 K (● = C_6HD_5).

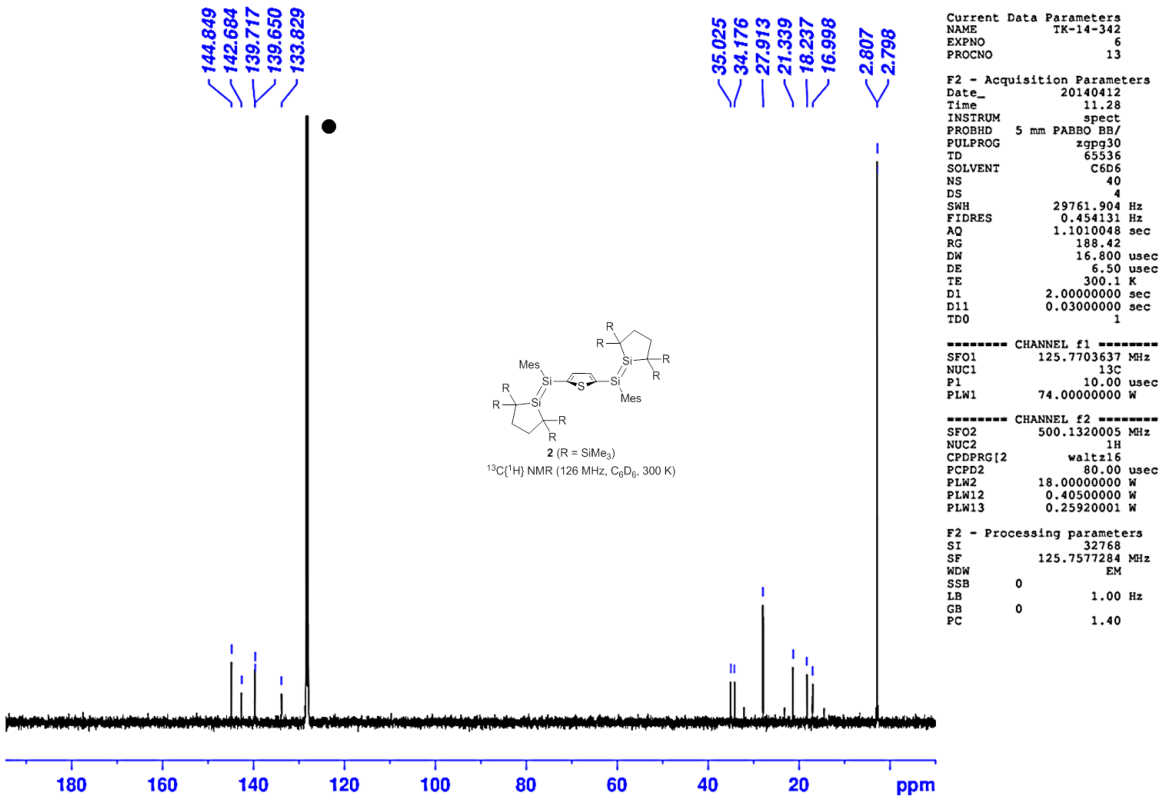


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 at 300 K (● = C_6D_6).

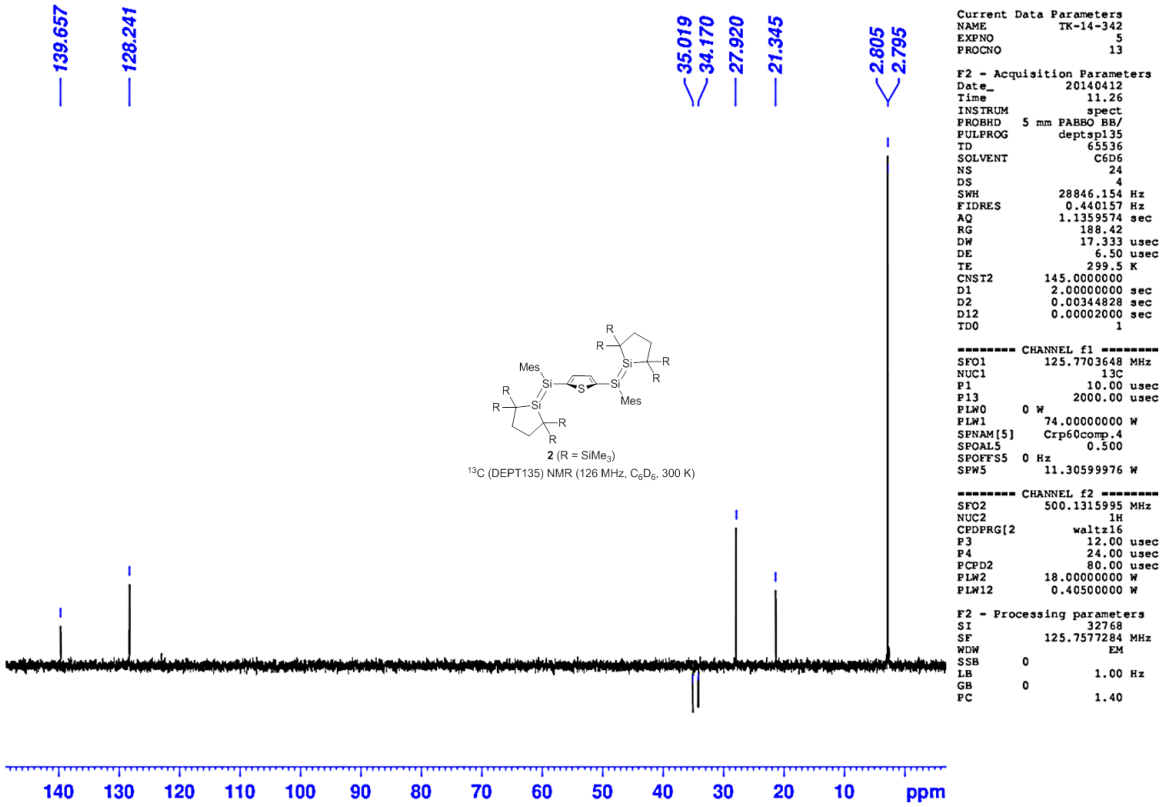


Figure S8. ^{13}C (DEPT135) NMR spectrum of **2** in C_6D_6 at 300 K.

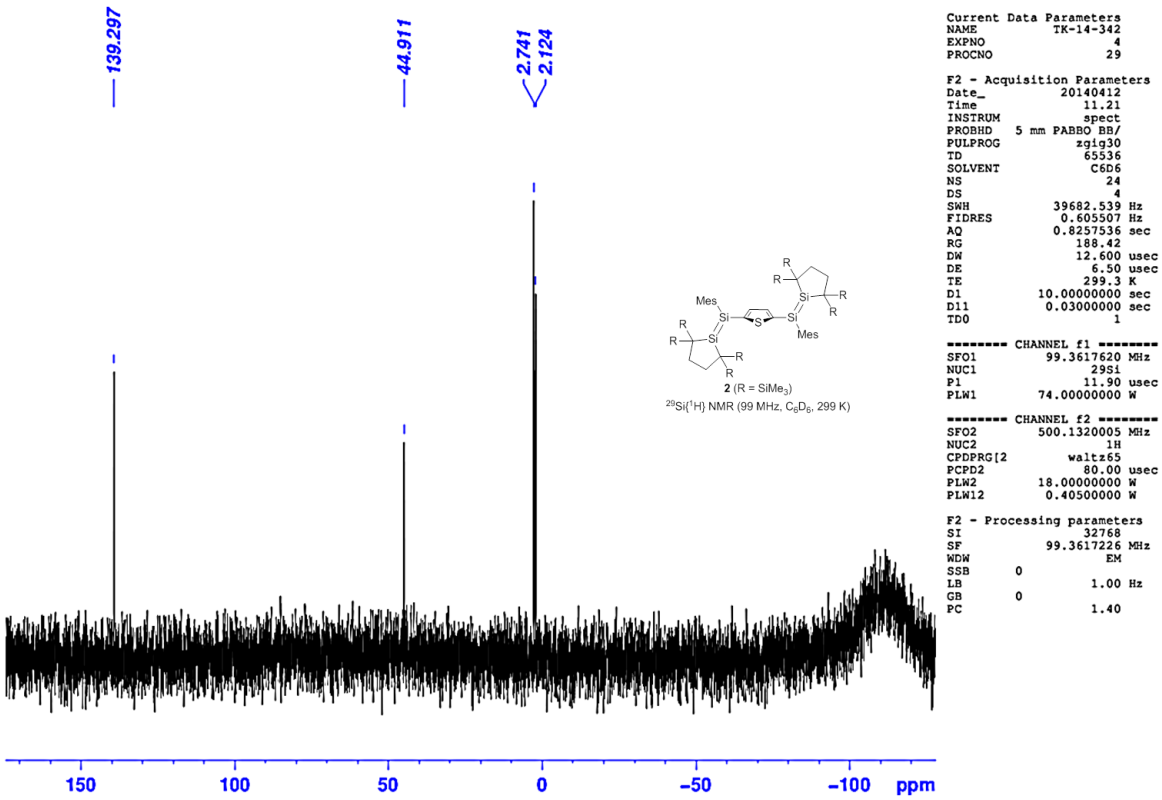


Figure S9. $^{29}Si\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 at 299 K.

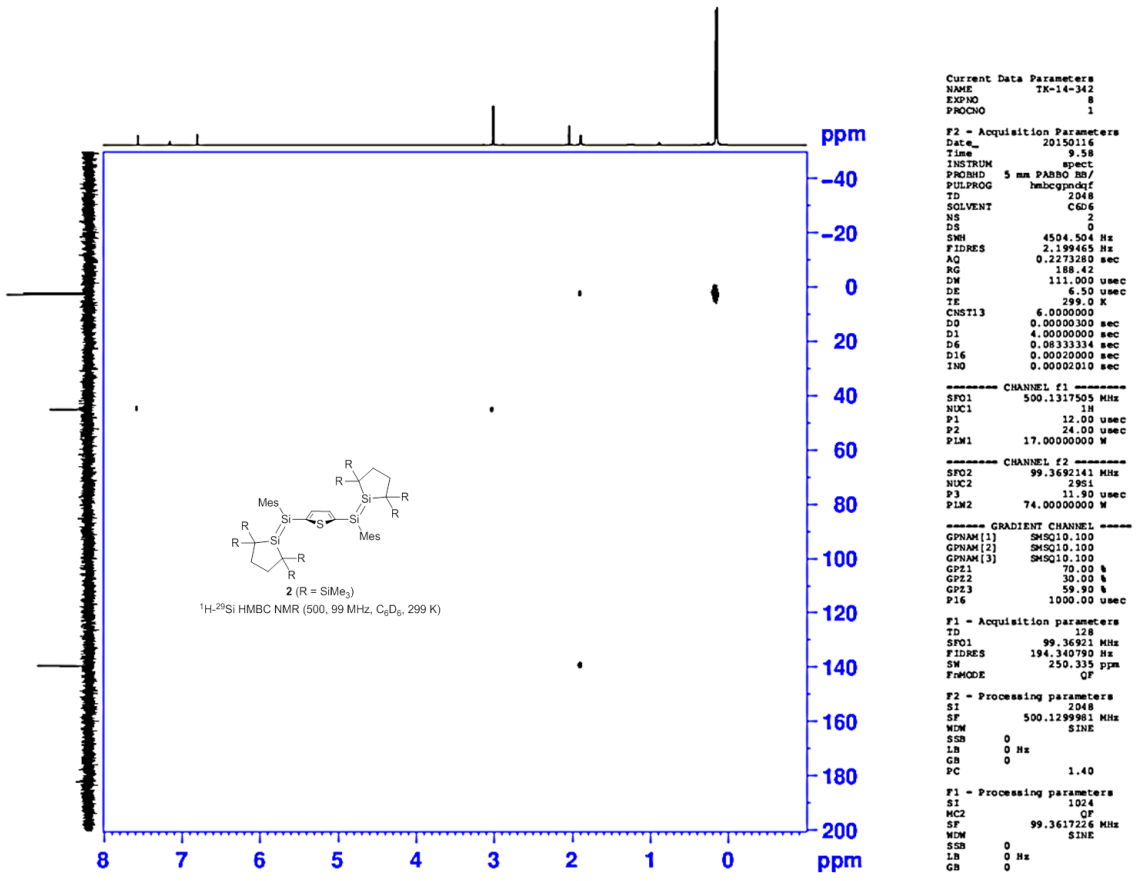


Figure S10. ^{1}H-^{29}Si HMBC NMR spectrum of **2** in C_6D_6 at 299 K.

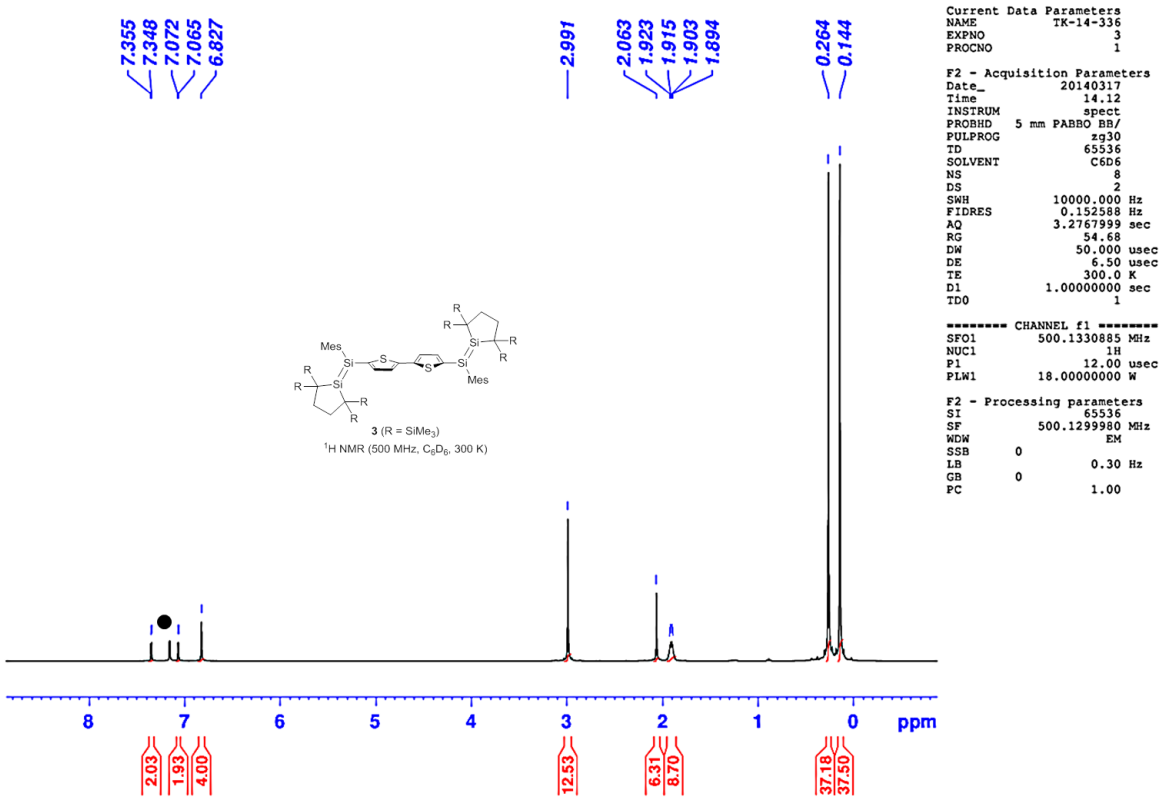


Figure S11. ^{1}H NMR spectrum of **3** in C_6D_6 at 300 (● = C_6HD_5).

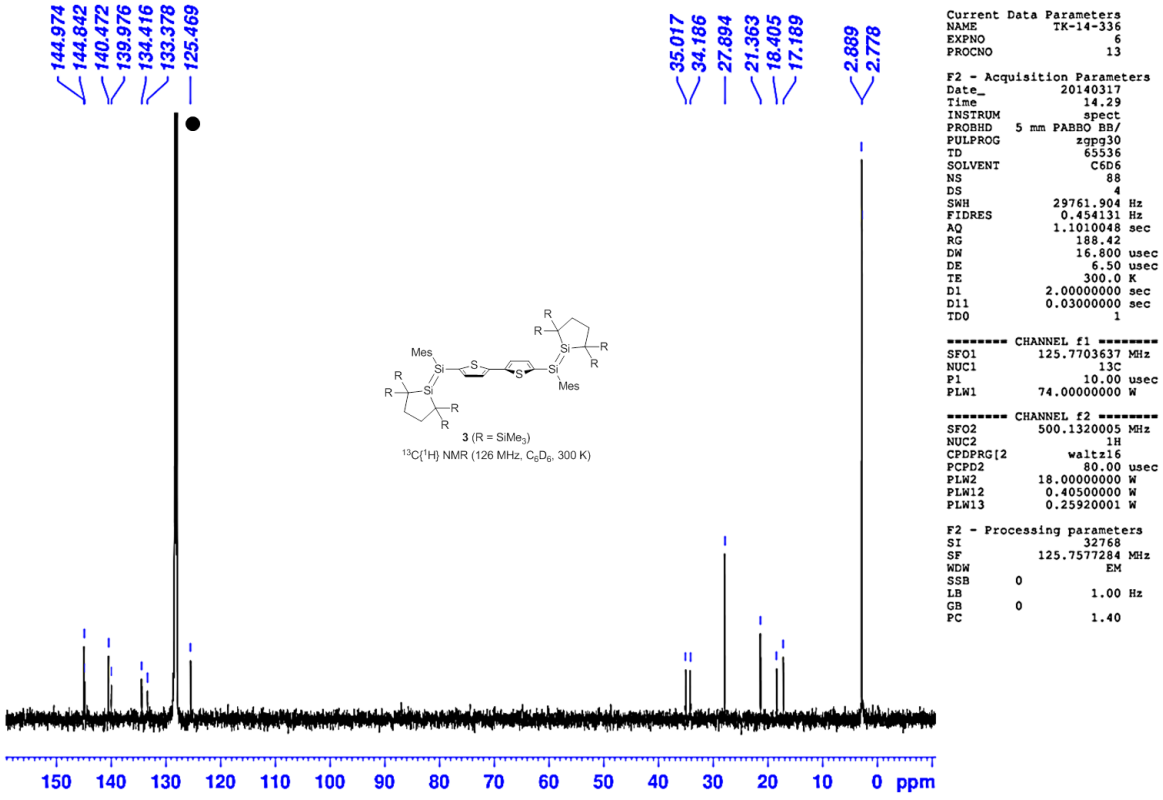


Figure S12. ^{13}C{^{1}H} NMR spectrum of **3** in C_6D_6 at 300 K (● = C_6D_6).

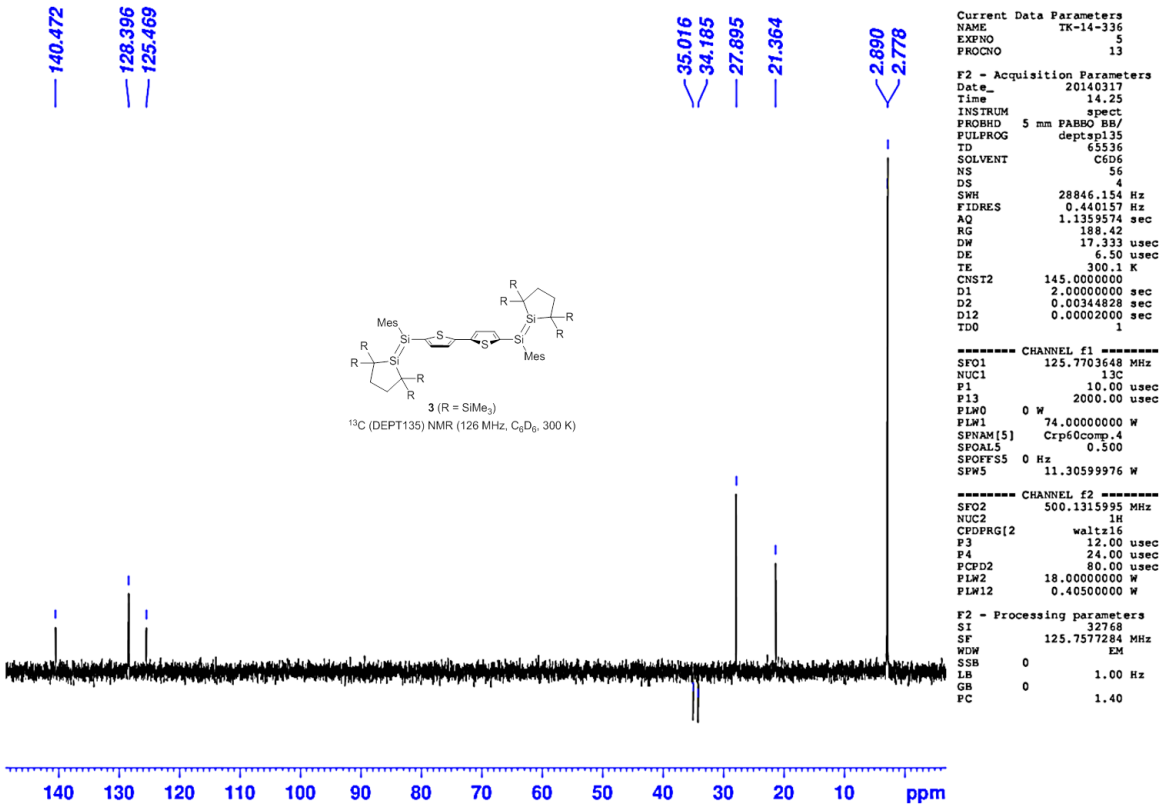


Figure S13. ^{13}C (DEPT135) NMR spectrum of **3** in C_6D_6 at 300 K.

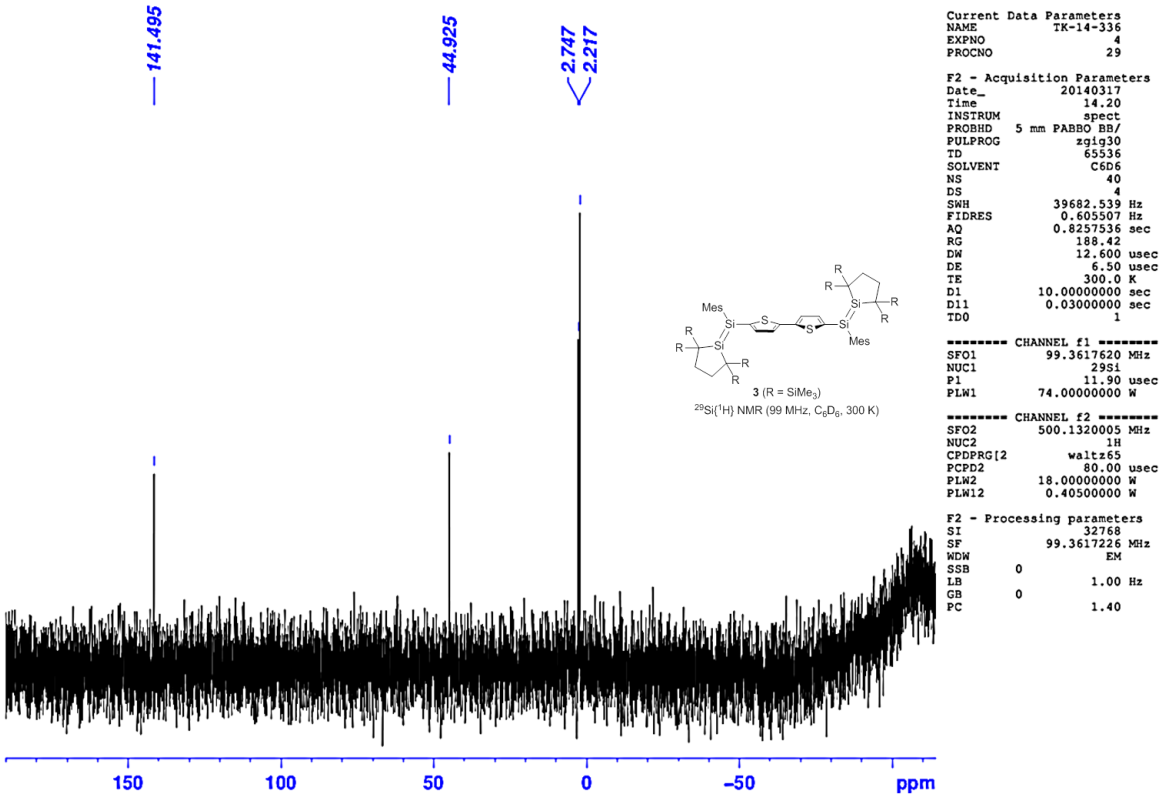


Figure S14. $^{29}Si\{^1H\}$ NMR spectrum of **3** in C_6D_6 at 300 K.

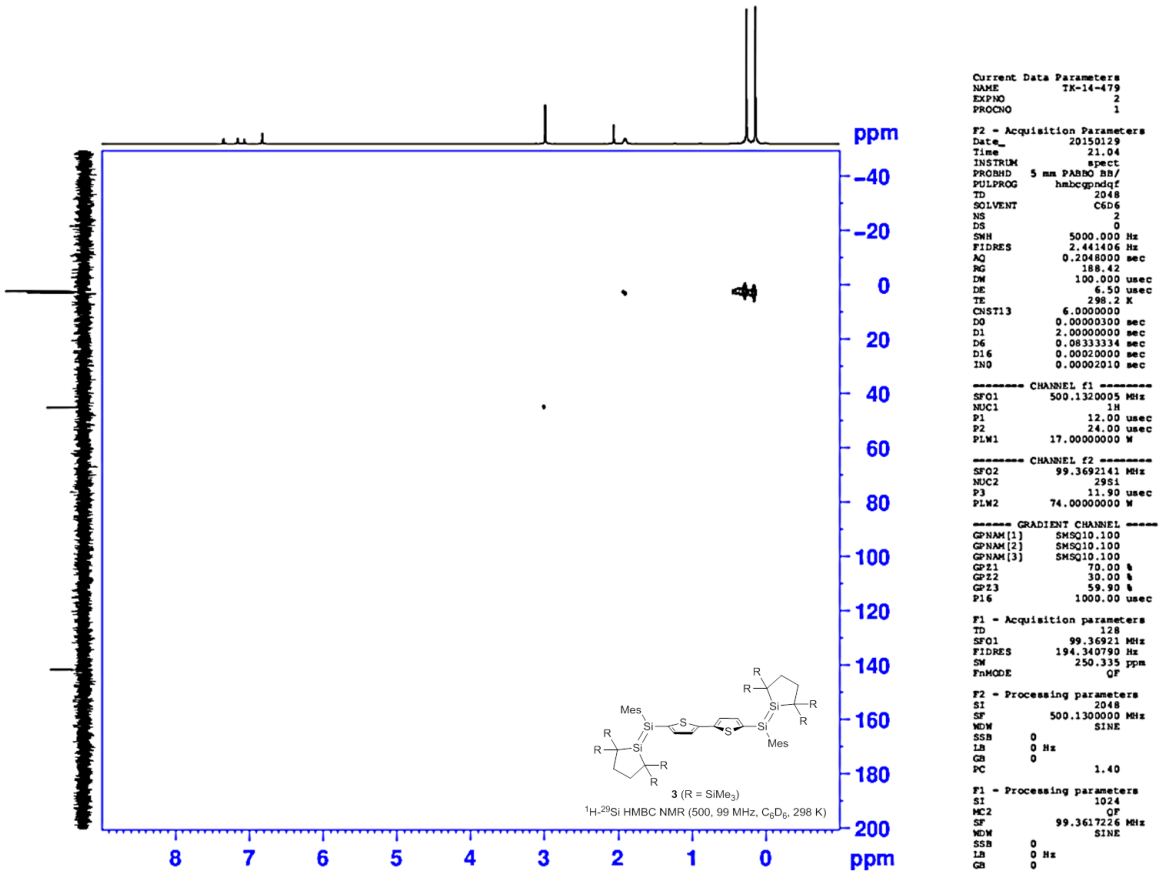


Figure S15. ^{1}H-^{29}Si HMBC NMR spectrum of **3** in C_6D_6 at 298 K.

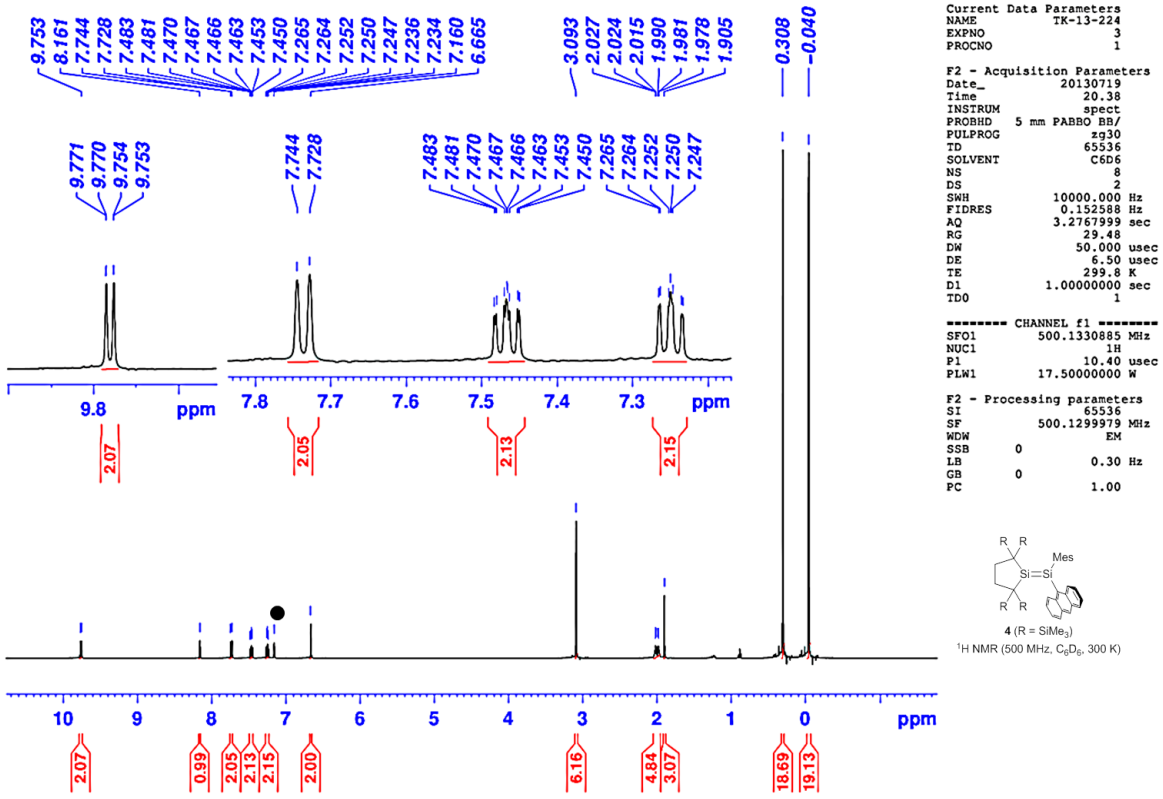


Figure S16. ^{1}H NMR spectrum of **4** in C_6D_6 at 300 K(● = C_6HD_5).

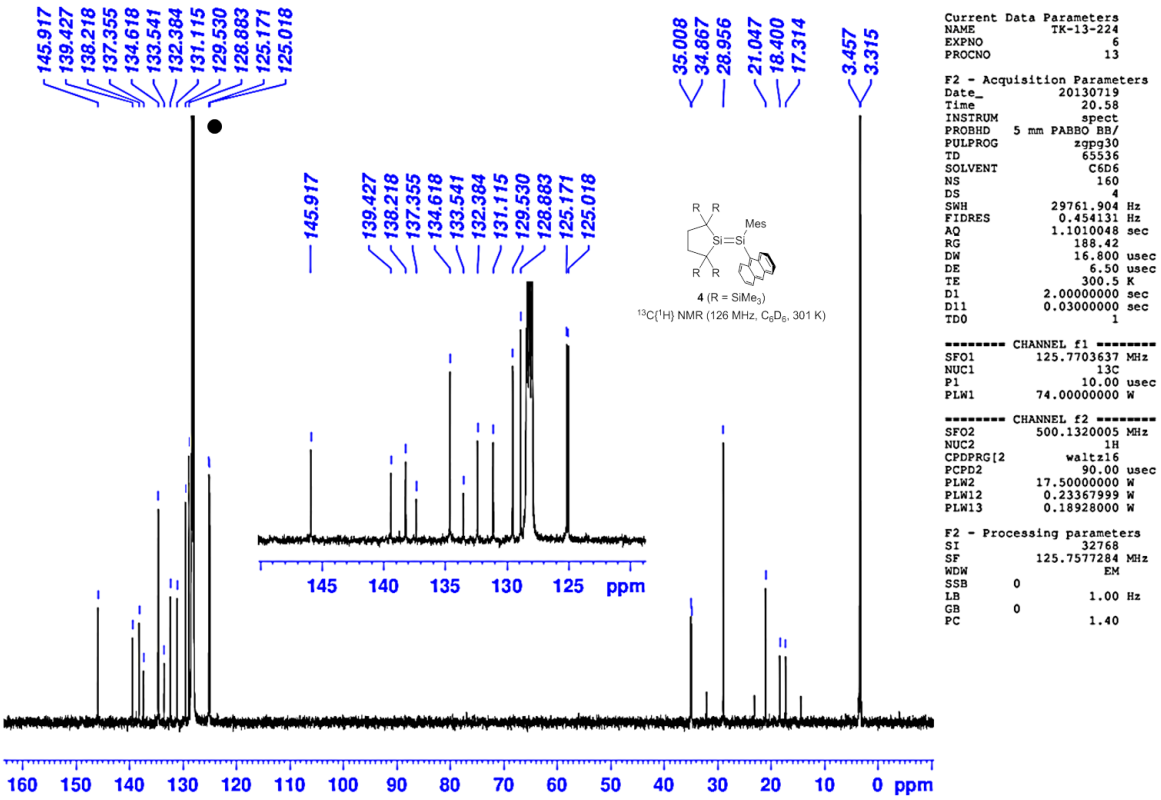


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at 301 K (● = C_6D_6).

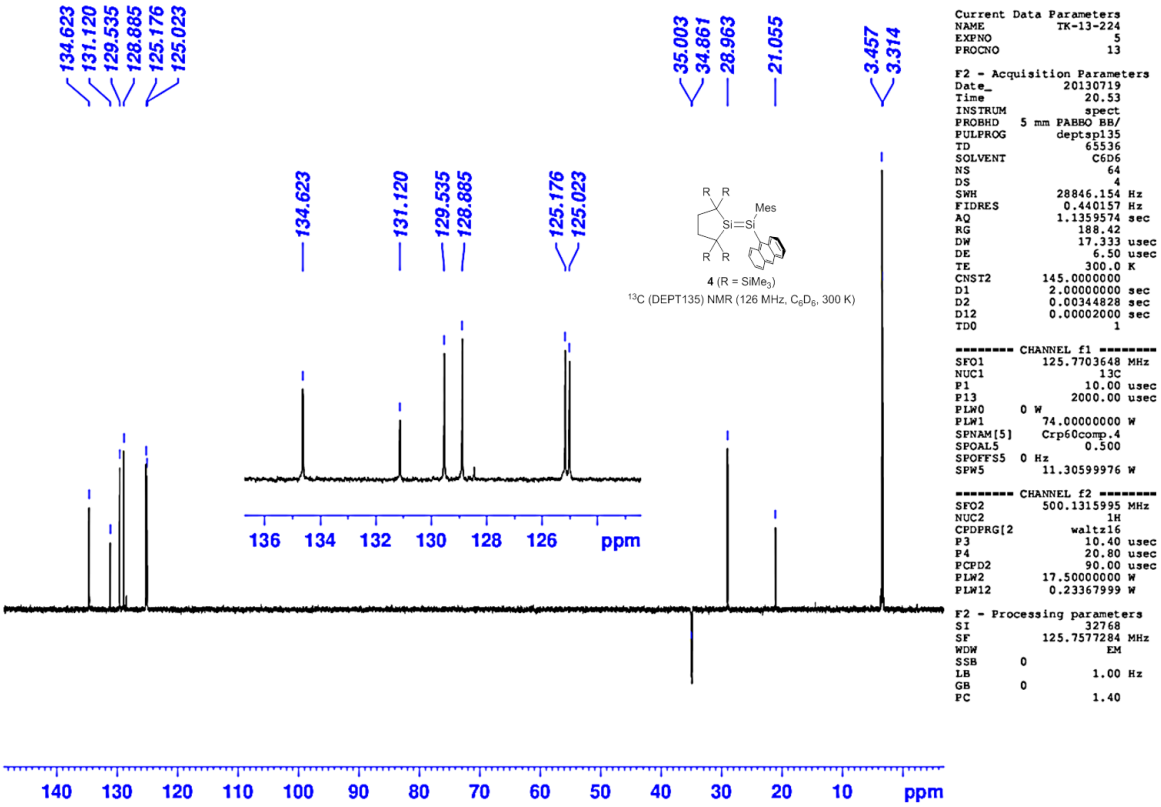
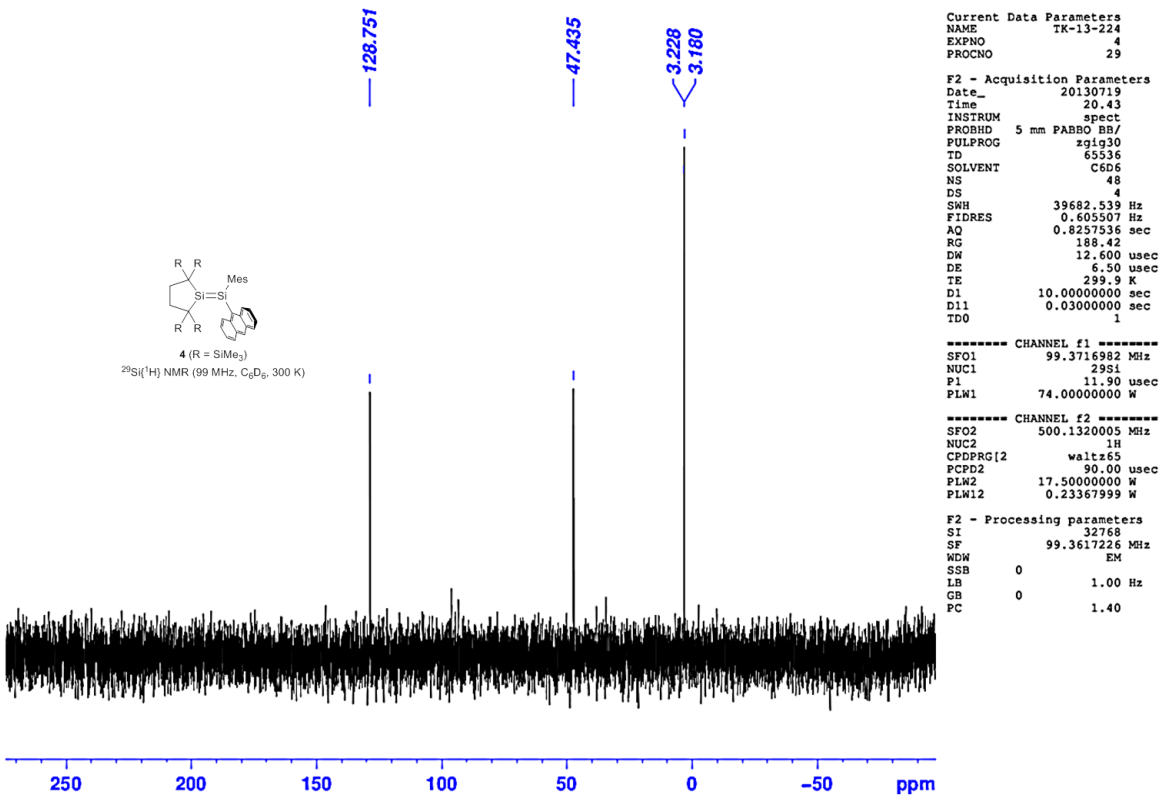


Figure S18. ^{13}C (DEPT135) NMR spectrum of **4** in C_6D_6 at 300 K.

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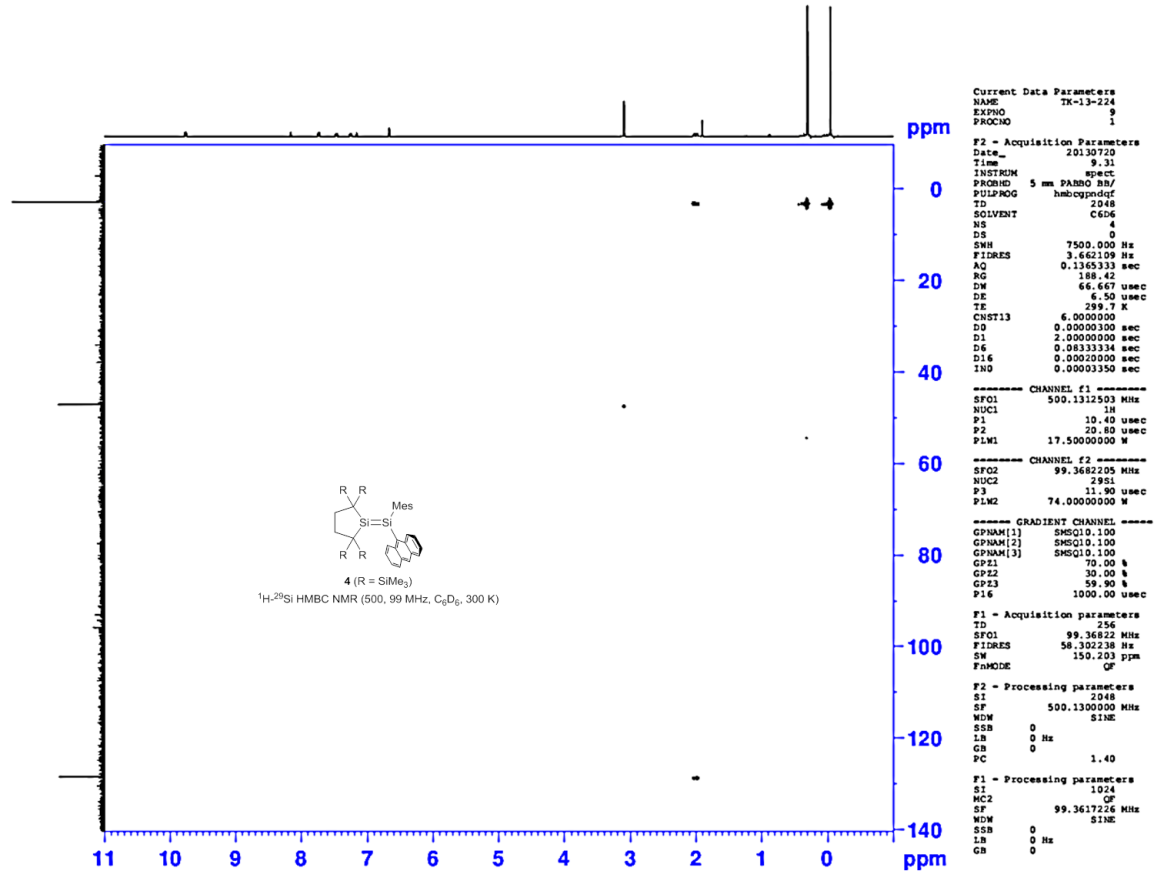


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F1 - Processing parameters
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Figure S20. ^{1}H-^{29}Si HMBC NMR spectrum of **4** in C_6D_6 at 300 K.

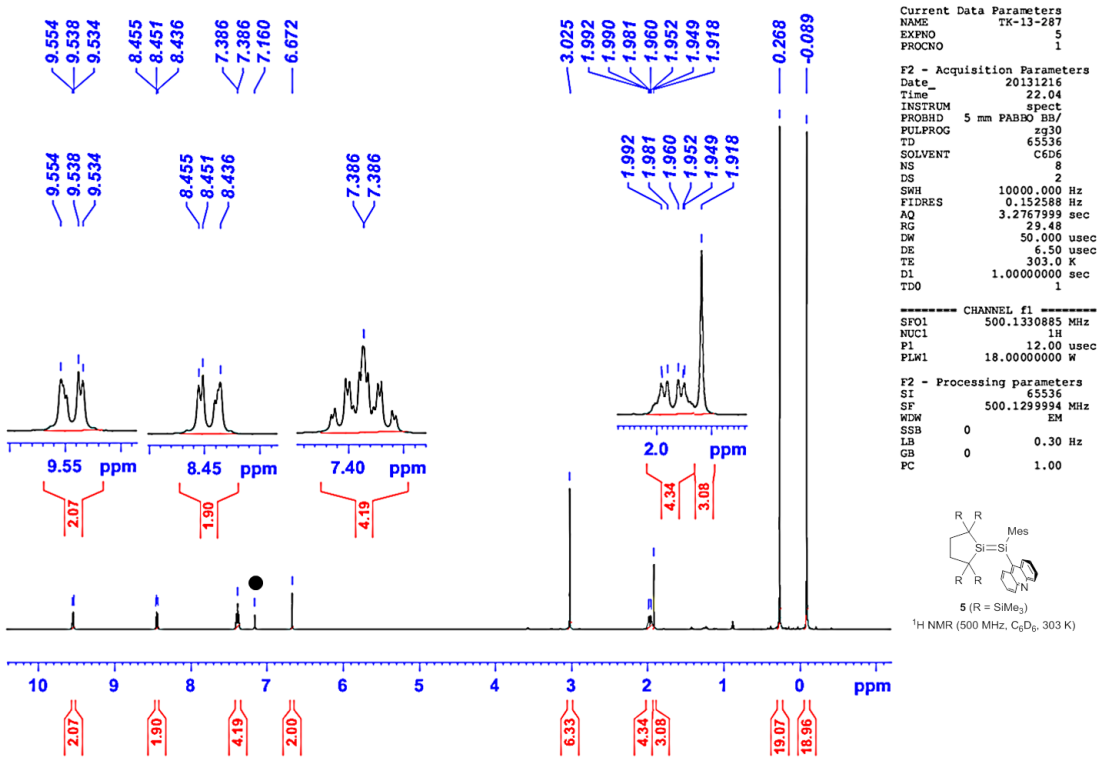


Figure S21. ^{1}H NMR spectrum of **5** in C_6D_6 at 303 (●= $C_6H\ D_5$).

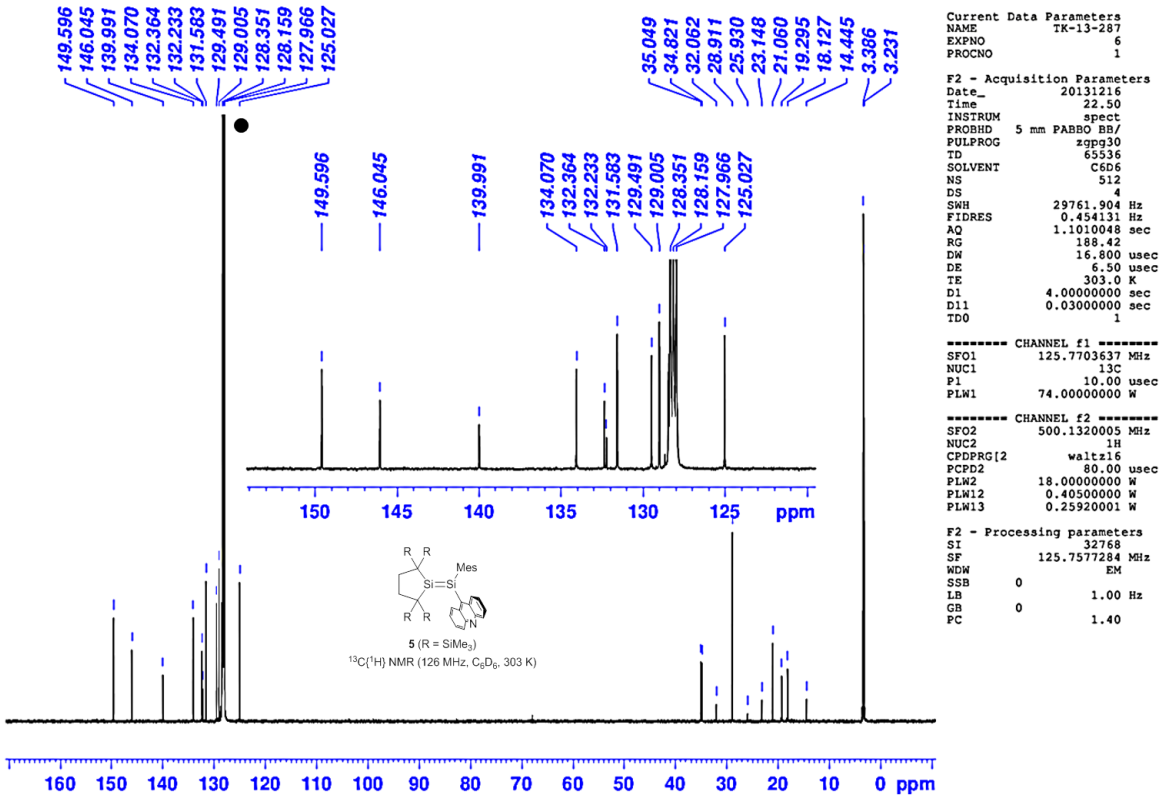


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 at 303 K (● = C_6D_6).

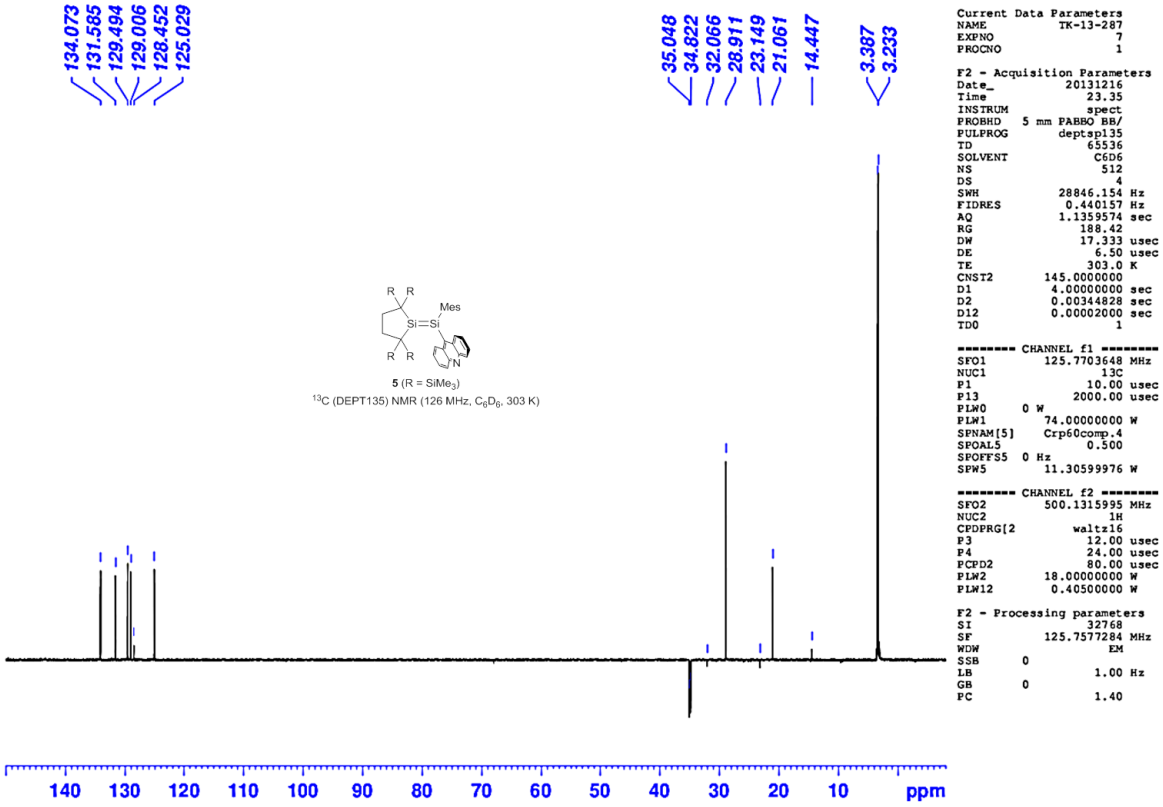


Figure S23. ^{13}C (DEPT135) NMR spectrum of **5** in C_6D_6 at 303 K.

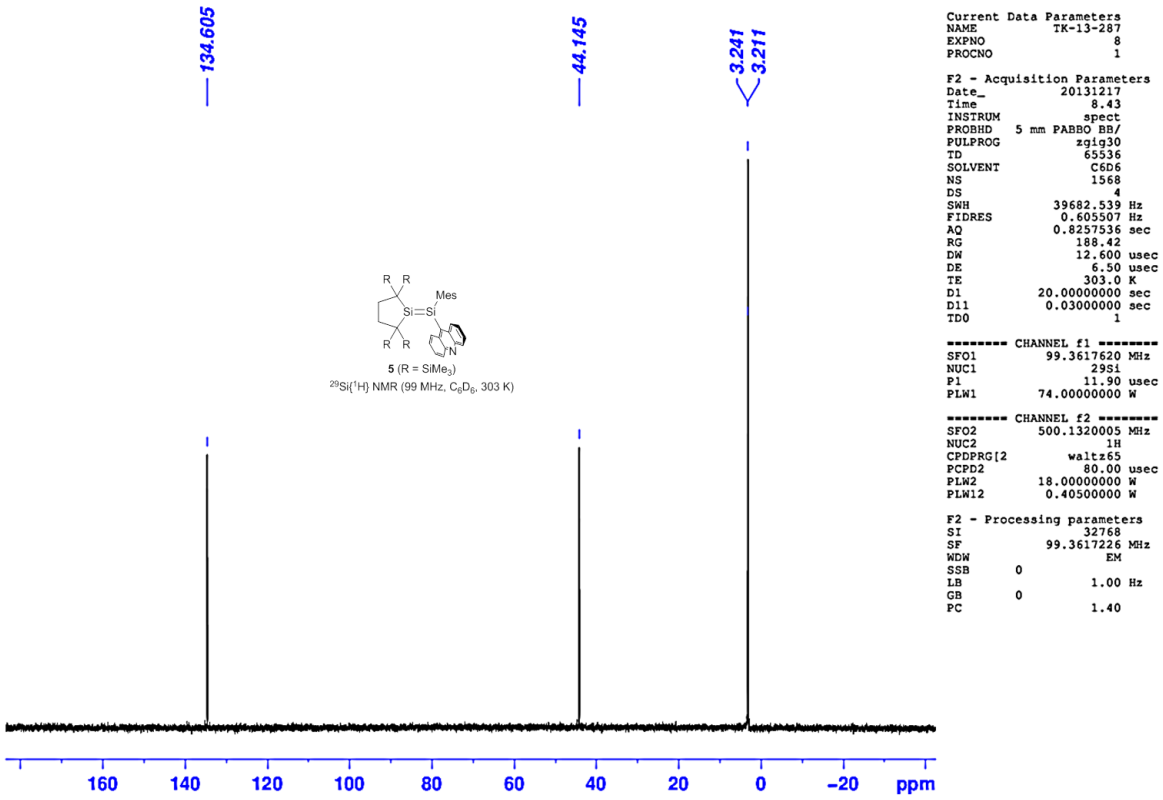


Figure S24. $^{29}Si\{^1H\}$ NMR spectrum of **5** in C_6D_6 at 303 K.

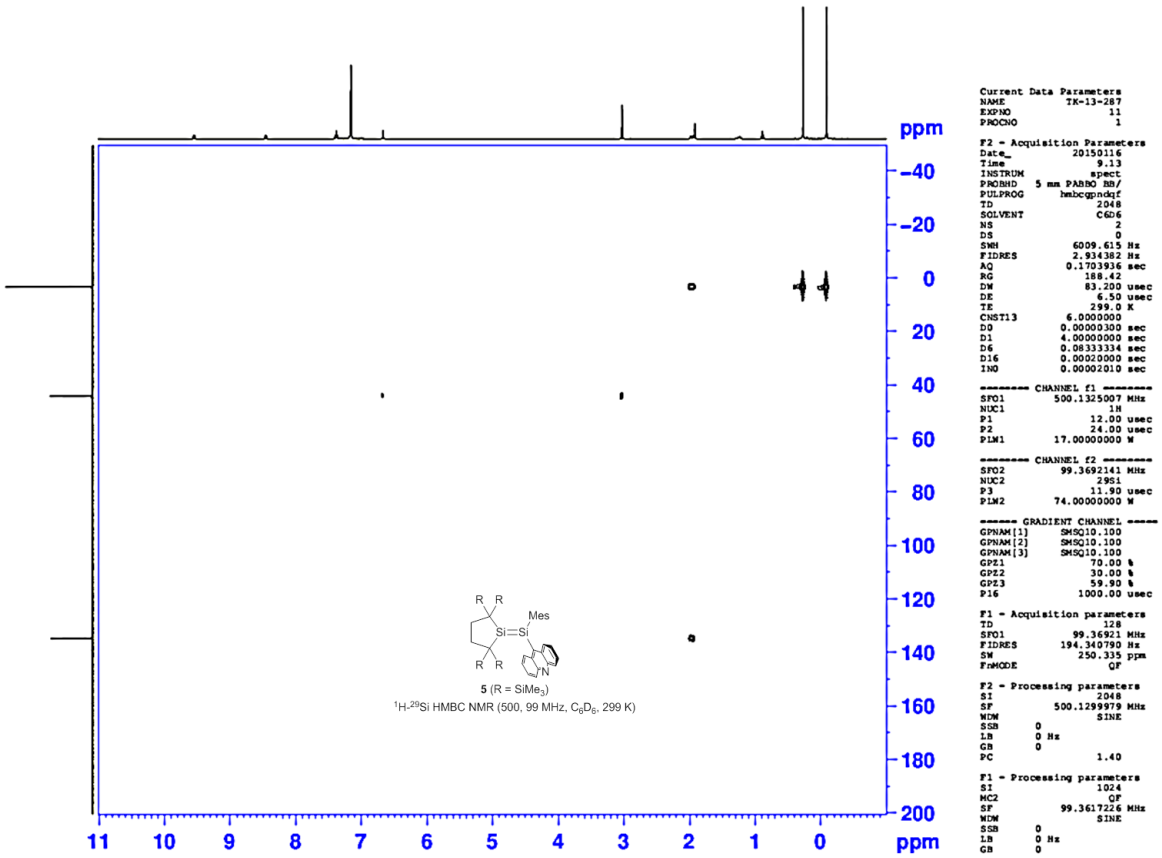


Figure S25. ^{1}H-^{29}Si HMBC NMR spectrum of **5** in C_6D_6 at 299 K.

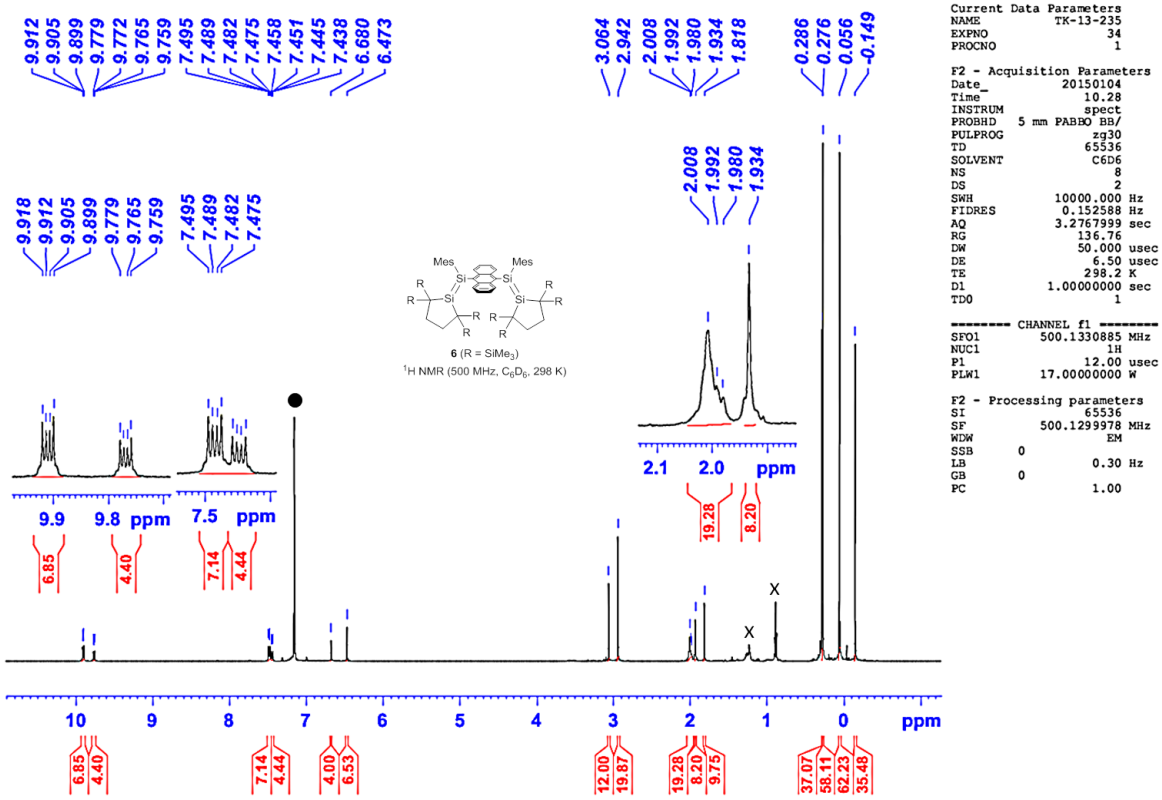


Figure S26. ^{1}H NMR spectrum of **6** in C_6D_6 at 298 (● = C_6HD_5, x = hexane).

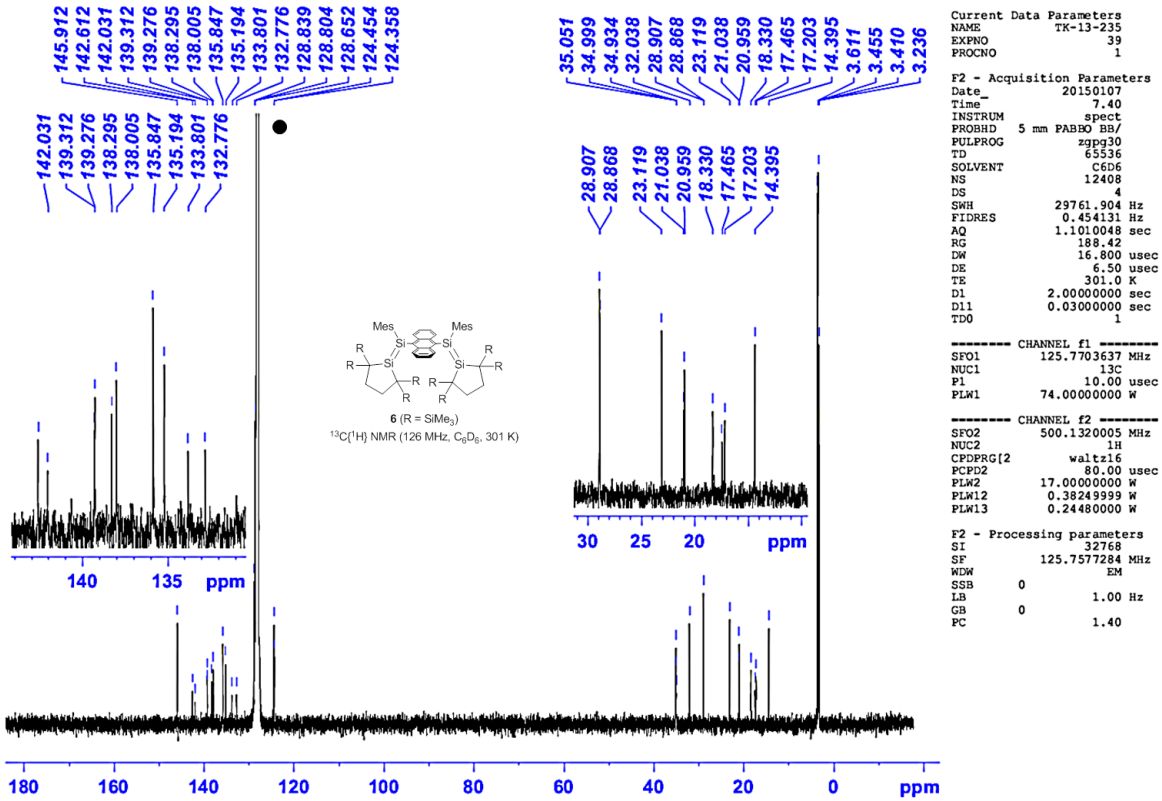


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in C_6D_6 at 301 K (● = C_6D_6).

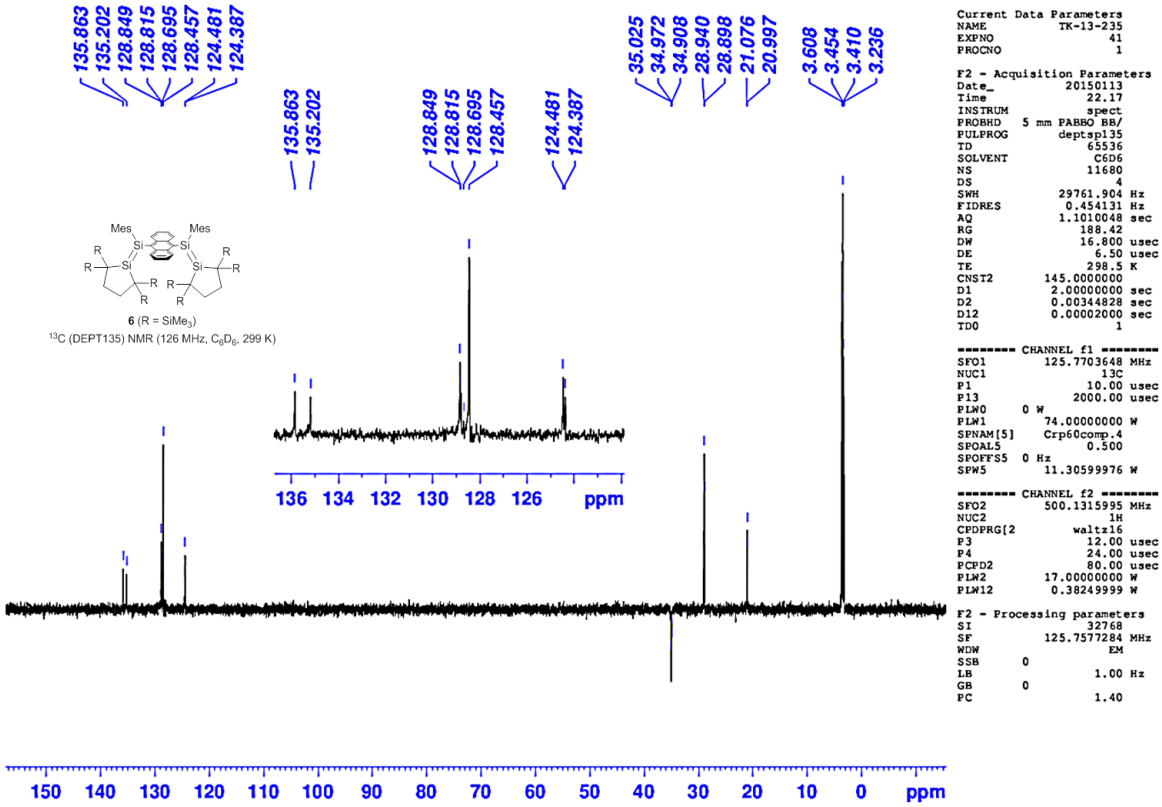
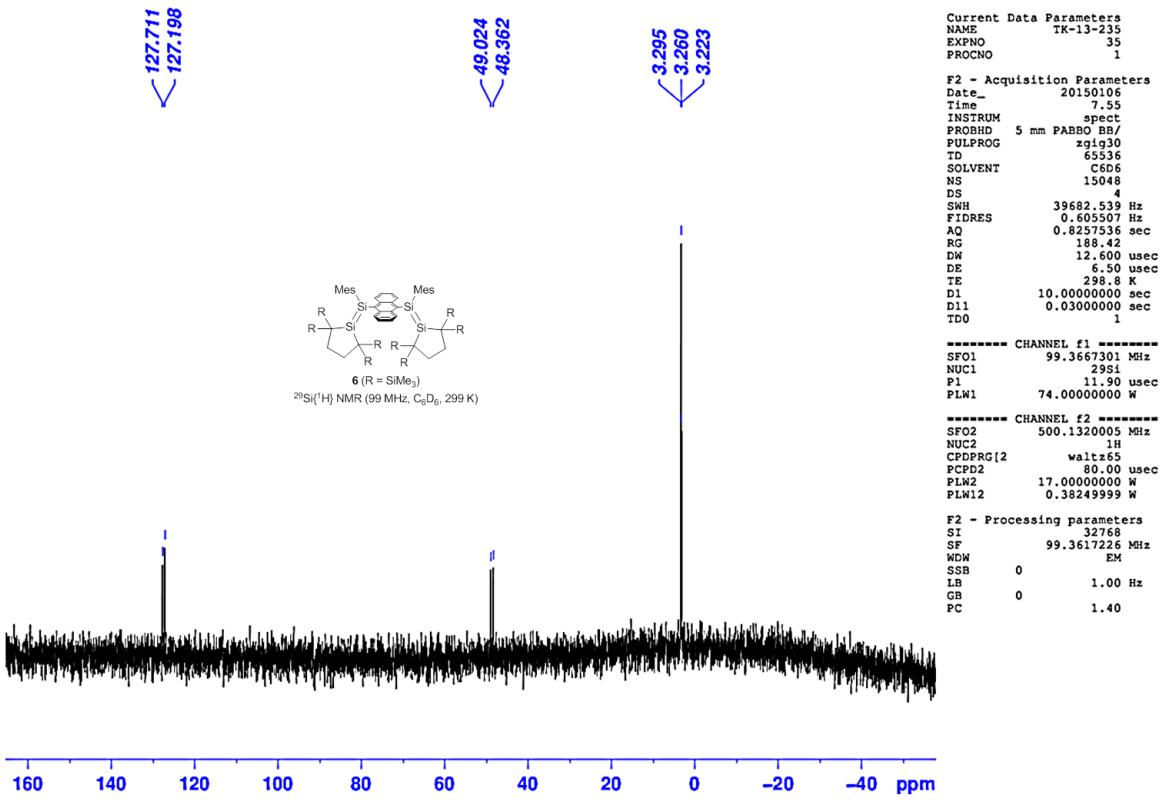


Figure S28. ^{13}C (DEPT135) NMR spectrum of **6** in C_6D_6 at 299 K.

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F2 - Processing parameters
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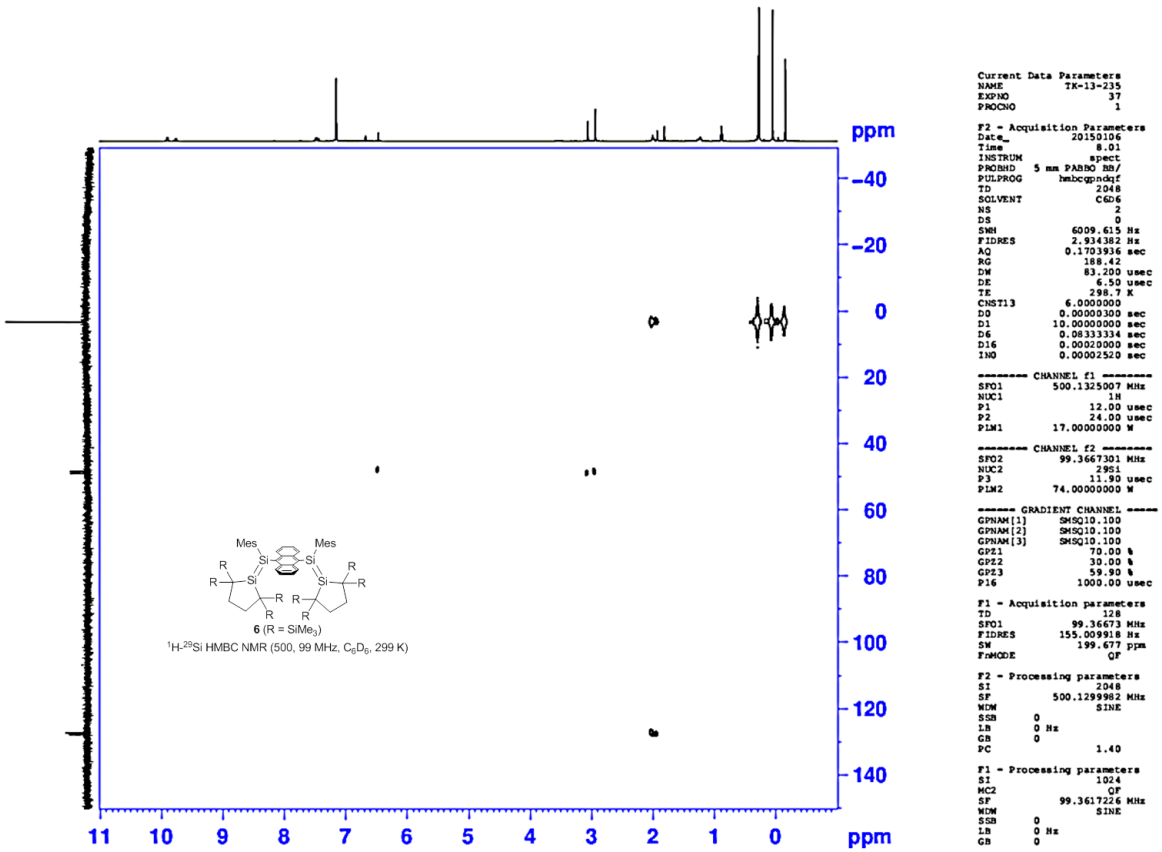
Figure S29. $^{29}Si\{^{1}H\}$ NMR spectrum of **6** in C_6D_6 at 299 K.

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D1                10.00000000 sec
D6                 0.08333334 sec
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NUC1                       1H
P1                       12.00 usec
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PLW1              17.00000000 W

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NUC2                      29Si
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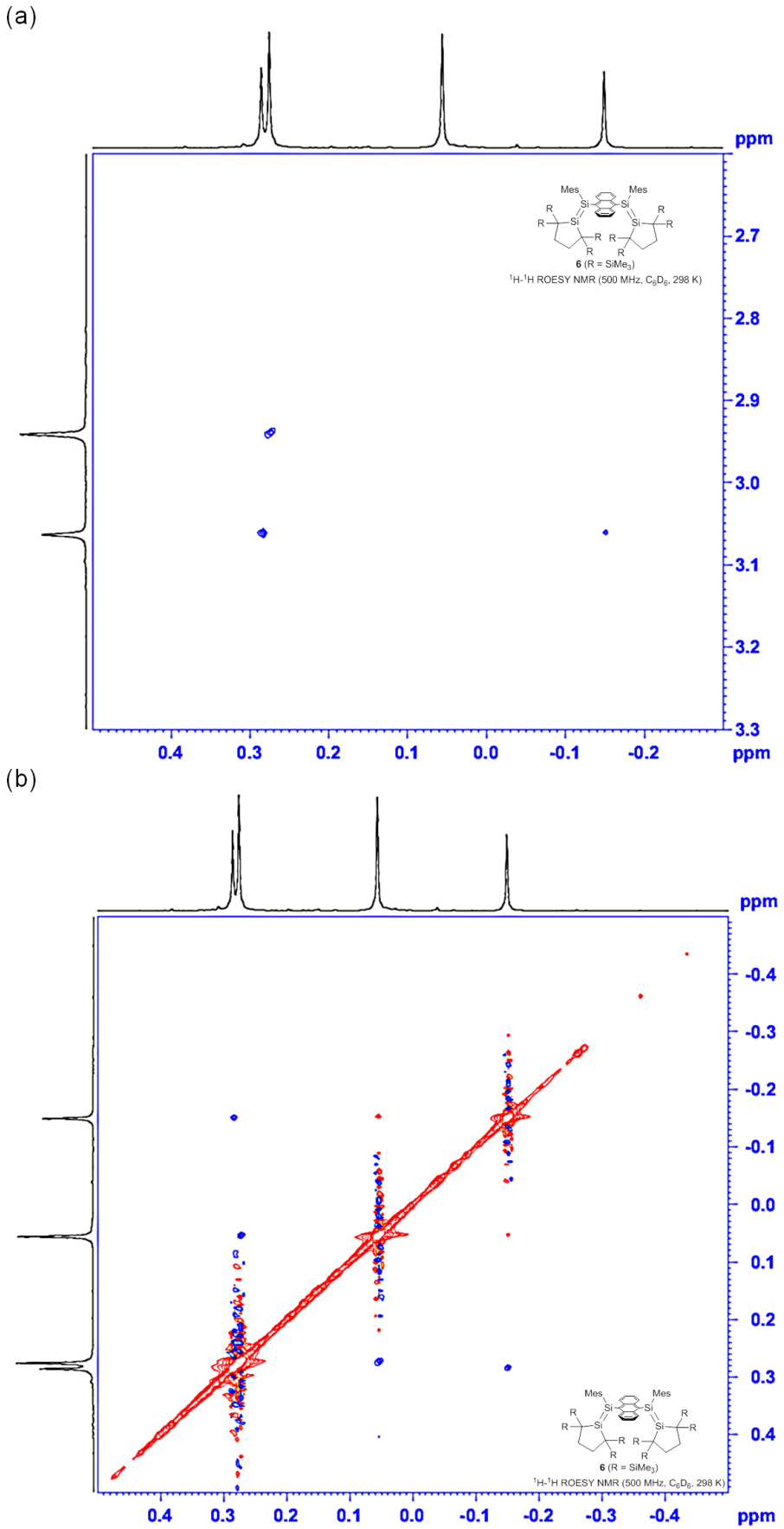
Figure S30. ^{1}H-^{29}Si HMBC NMR spectrum of **6** in C_6D_6 at 299 K.

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RG                       188.42
DW                      200.000 usec
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TE                      298.3 K
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GB                0
PC                        1.00

F1 - Processing parameters
SI                         1024
MC2                States-TPPI
SF                  500.1299974 MHz
WDW                       QSINE
SSB                           2
LB                0 Hz
GB                0
```

Figure S31. ^{1}H-^{1}H ROESY NMR spectrum of **6** in C_6D_6 at 298 K.

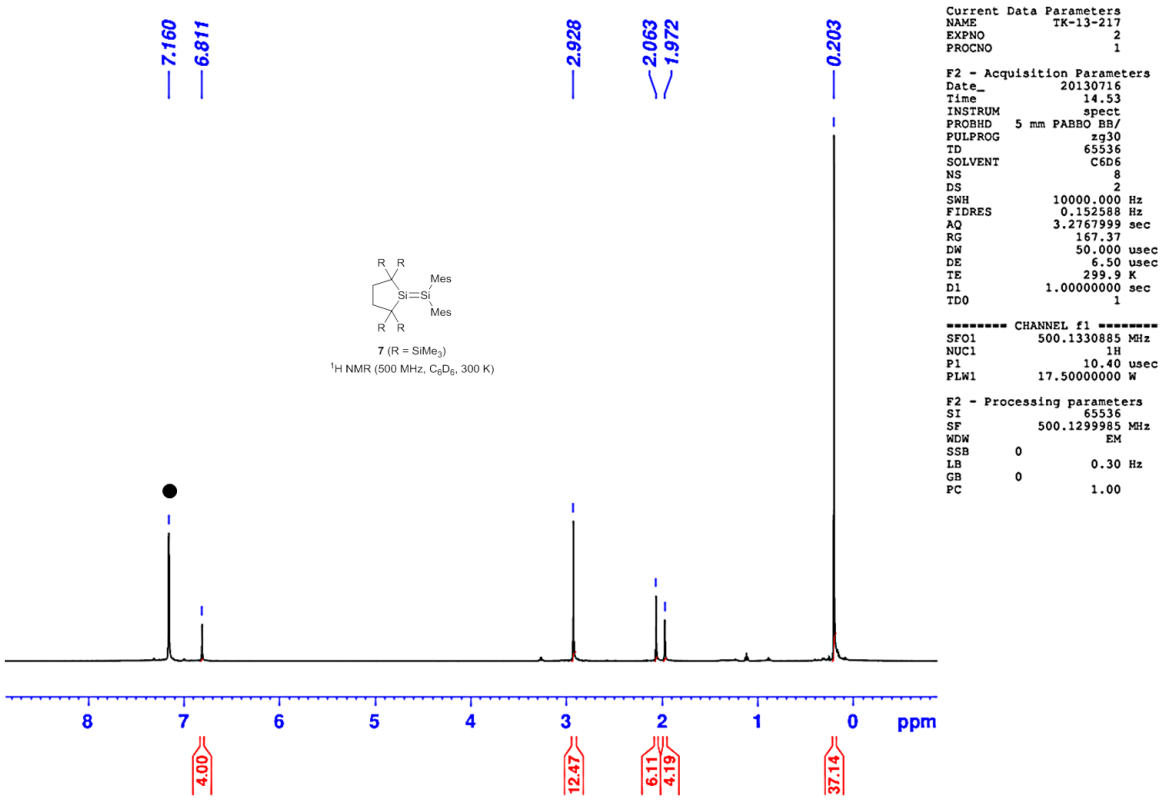


Figure S32. ^{1}H NMR spectrum of **7** in C_6D_6 at 300 (● = C_6HD_5).

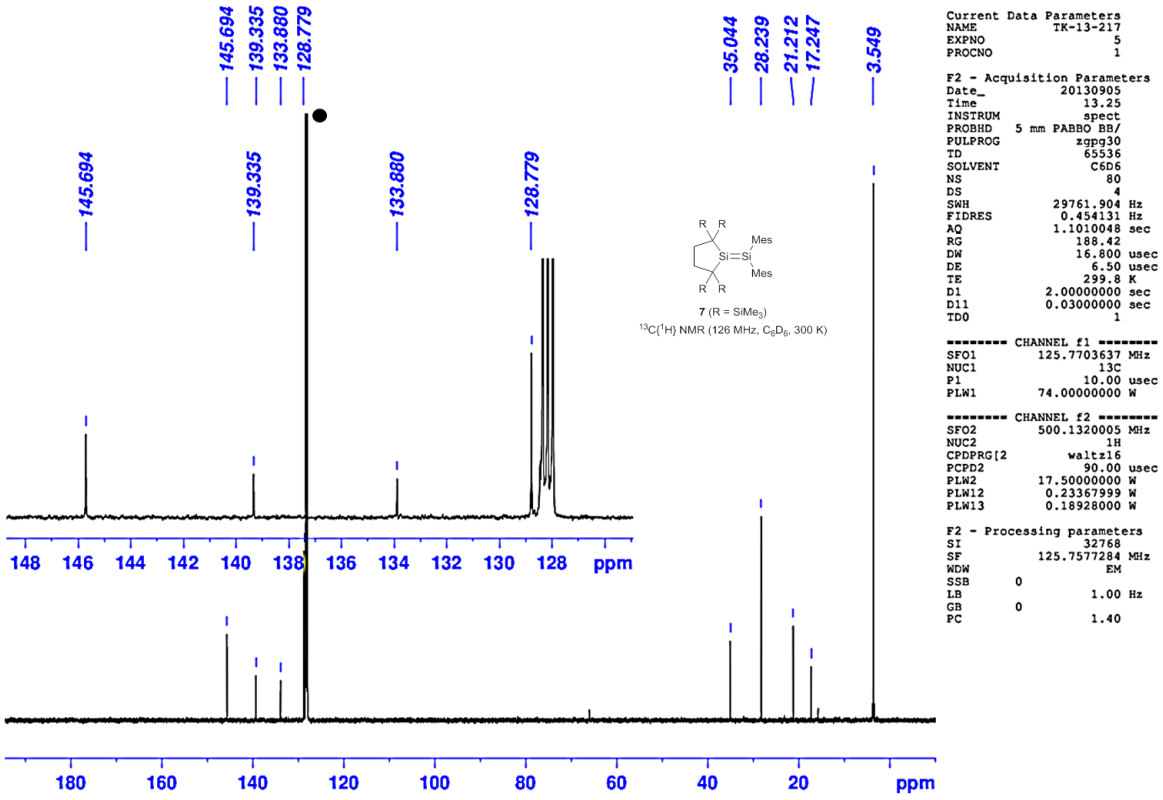


Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of **7** in C_6D_6 at 300 K (● = C_6D_6).

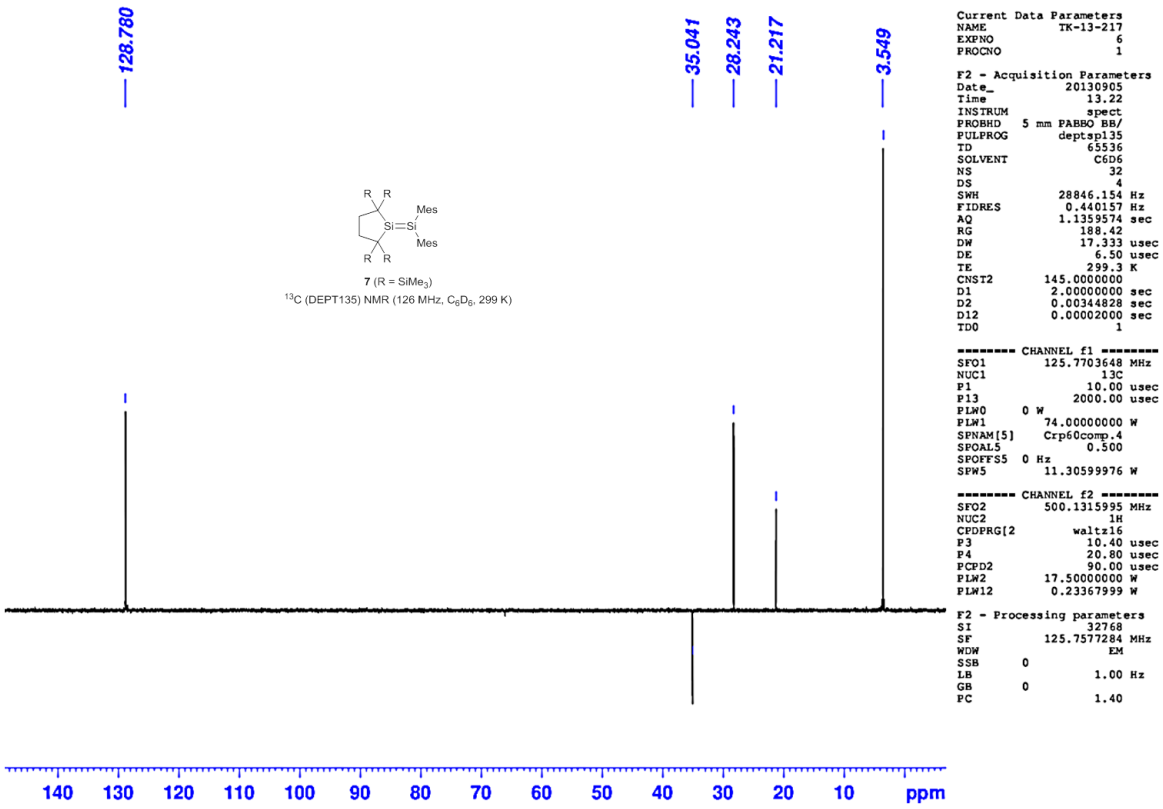


Figure S34. ^{13}C (DEPT135) NMR spectrum of **7** in C_6D_6 at 299 K.

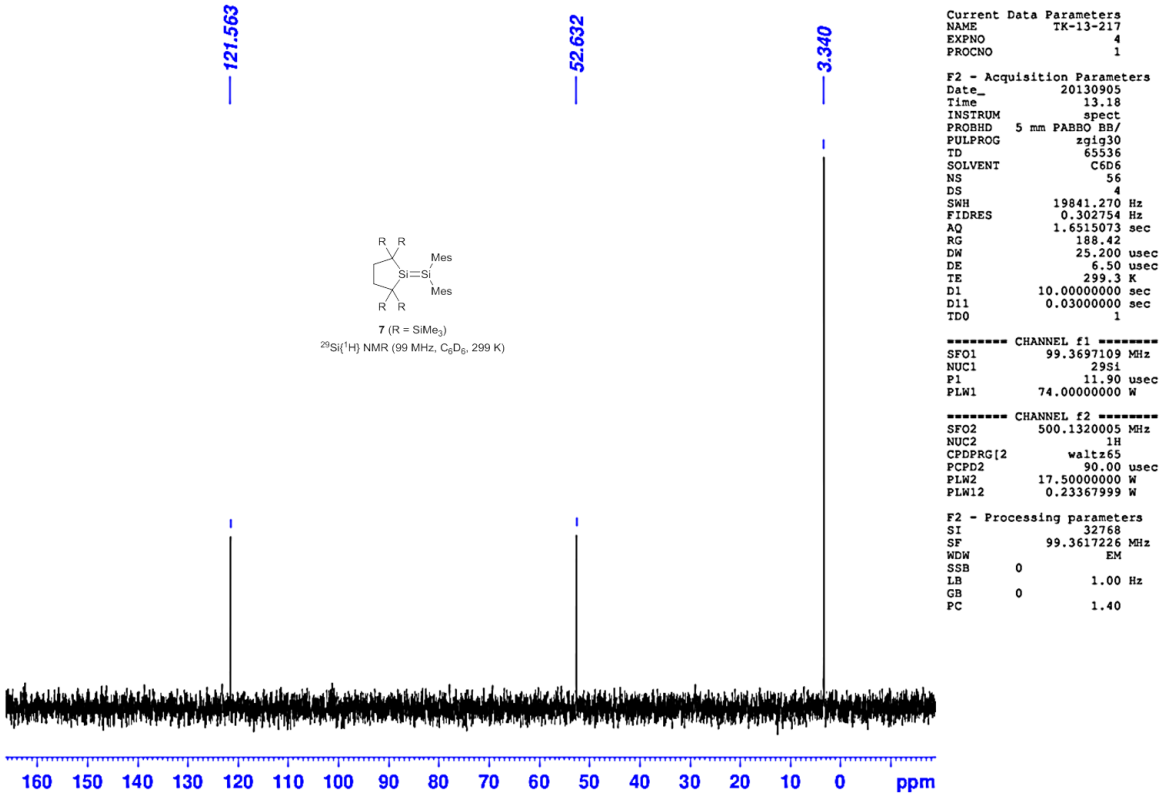


Figure S35. $^{29}Si\{^1H\}$ NMR spectrum of **7** in C_6D_6 at 299 K.

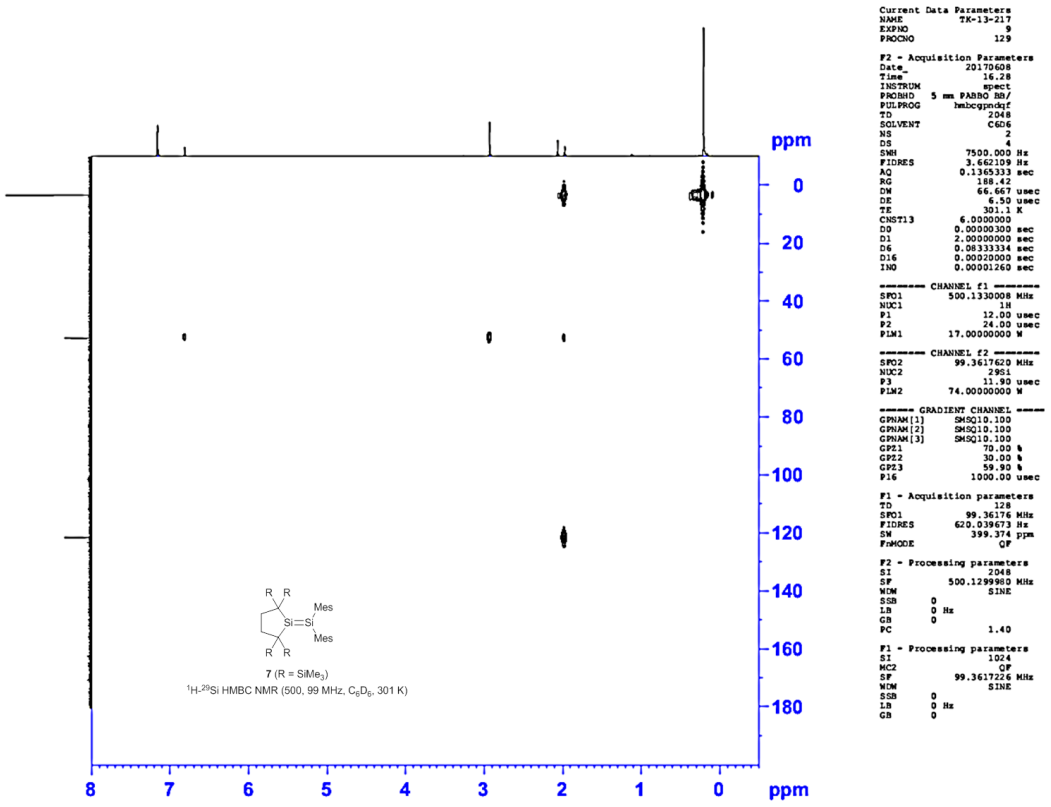


Figure S36. ^{1}H-^{29}Si HMBC NMR spectrum of **7** in C_6D_6 at 301 K.

2. Equilibrium between *anti*-6 and *syn*-6

Figures S37-S46 show ^{1}H NMR spectra of **6** measured at 50 °C to –40 °C in toluene-d_8. The equilibrium constants (K_{eq}) between ***anti*-6** and ***syn*-6** at various temperatures were determined by using the integral ratio of *o*-Me signals. The K_{eq} values at various temperatures were summarized in Table S1. A plot of ln(K_{eq}) at various temperatures was shown in Figure S47.

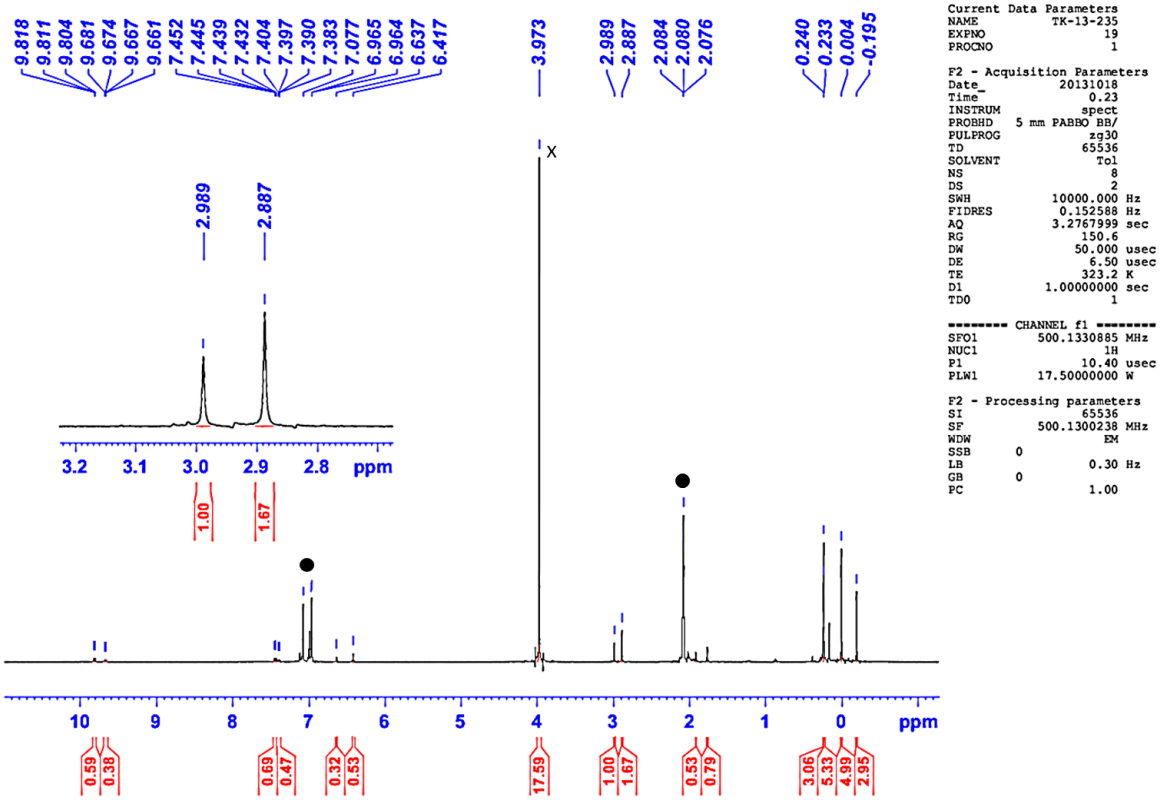


Figure S37. ^{1}H NMR spectrum of **6** in C_7D_8 at 323 K (● = C_7HD_7, x = ferrocene).

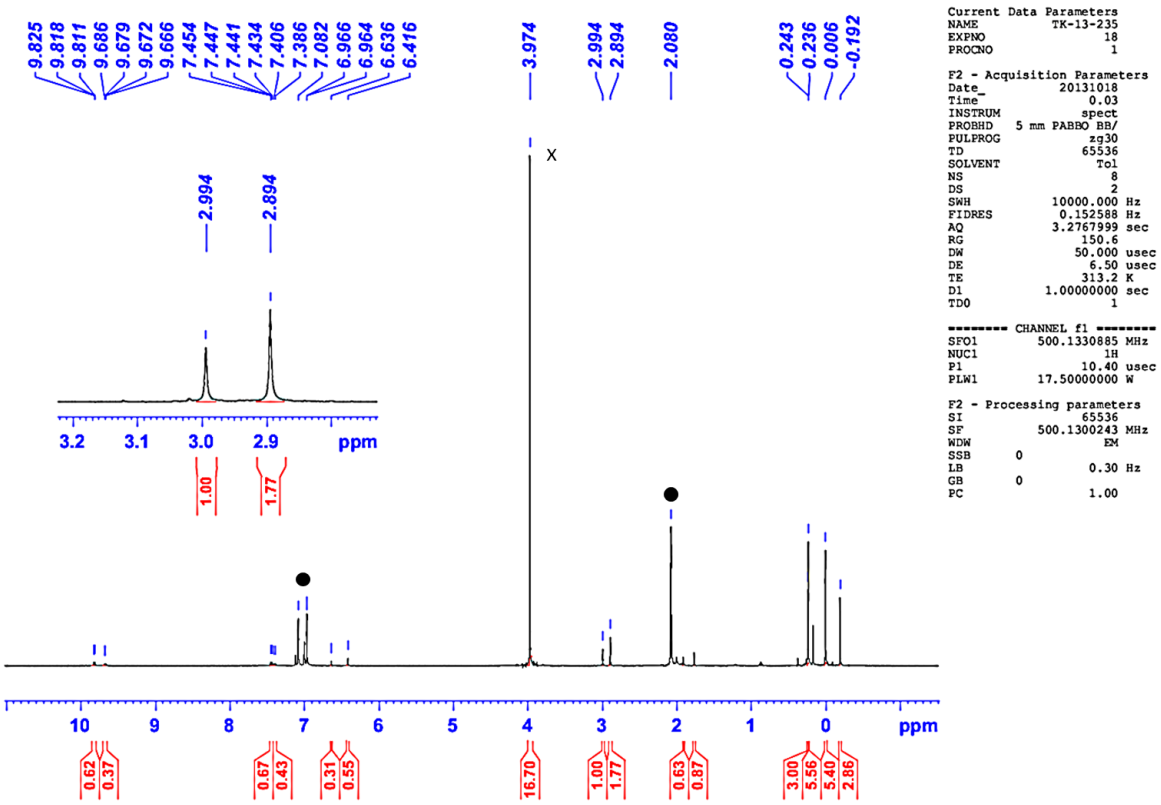


Figure S38. ^{1}H NMR spectrum of **6** in C_7D_8 at 313 K (● = C_7HD_7, x = ferrocene).

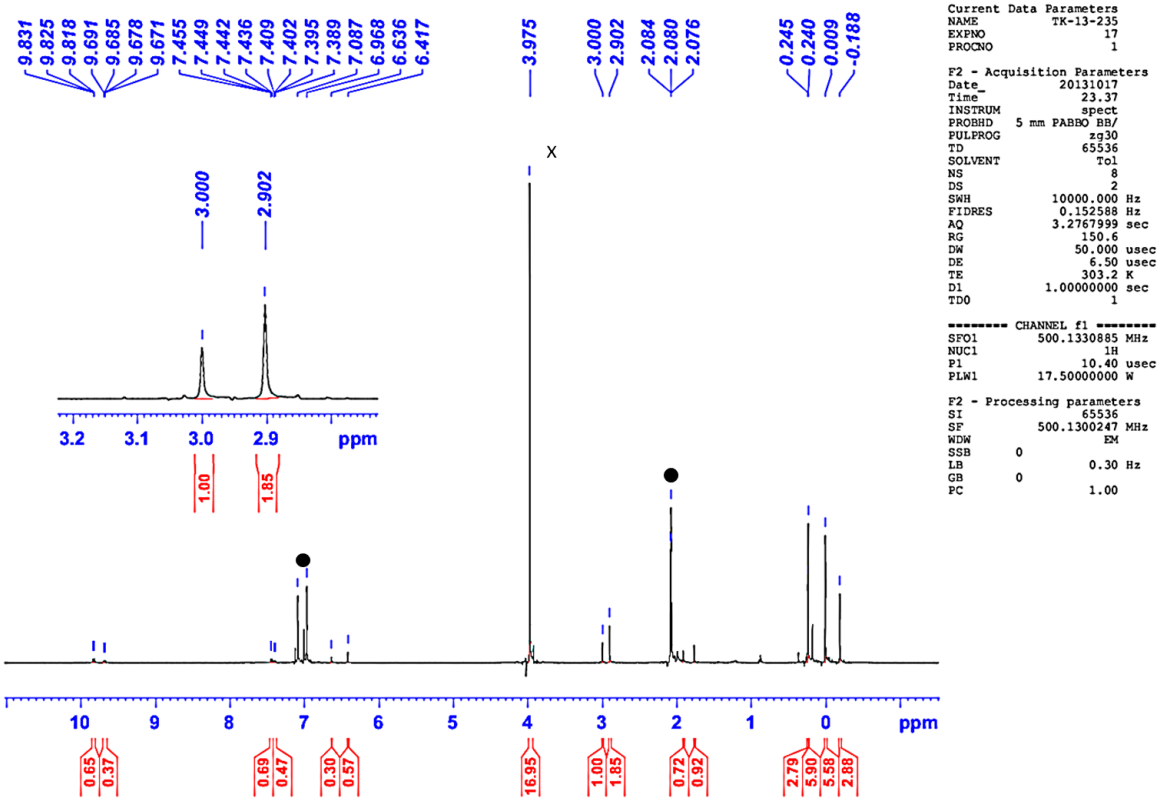


Figure S39. ^{1}H NMR spectrum of **6** in C_7D_8 at 303 K (● = C_7HD_7, x = ferrocene).

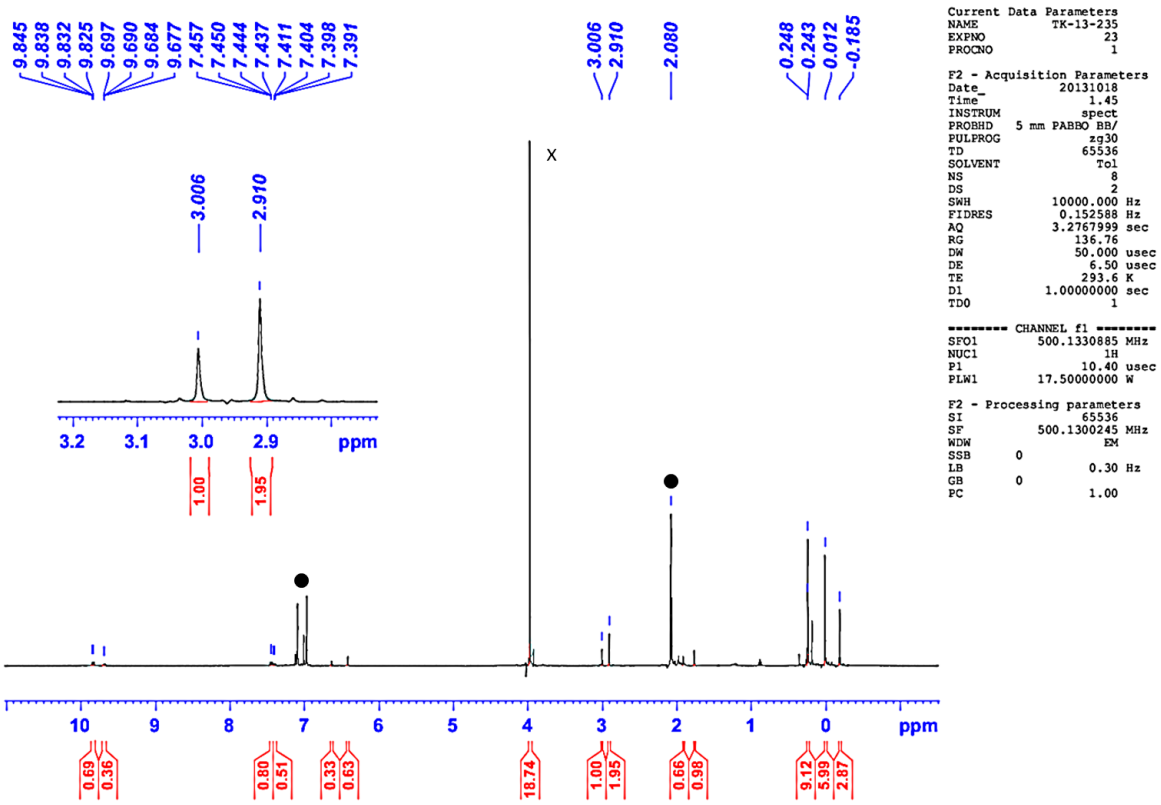


Figure S40. ^{1}H NMR spectrum of **6** in C_7D_8 at 293 K (● = C_7HD_7, x = ferrocene).

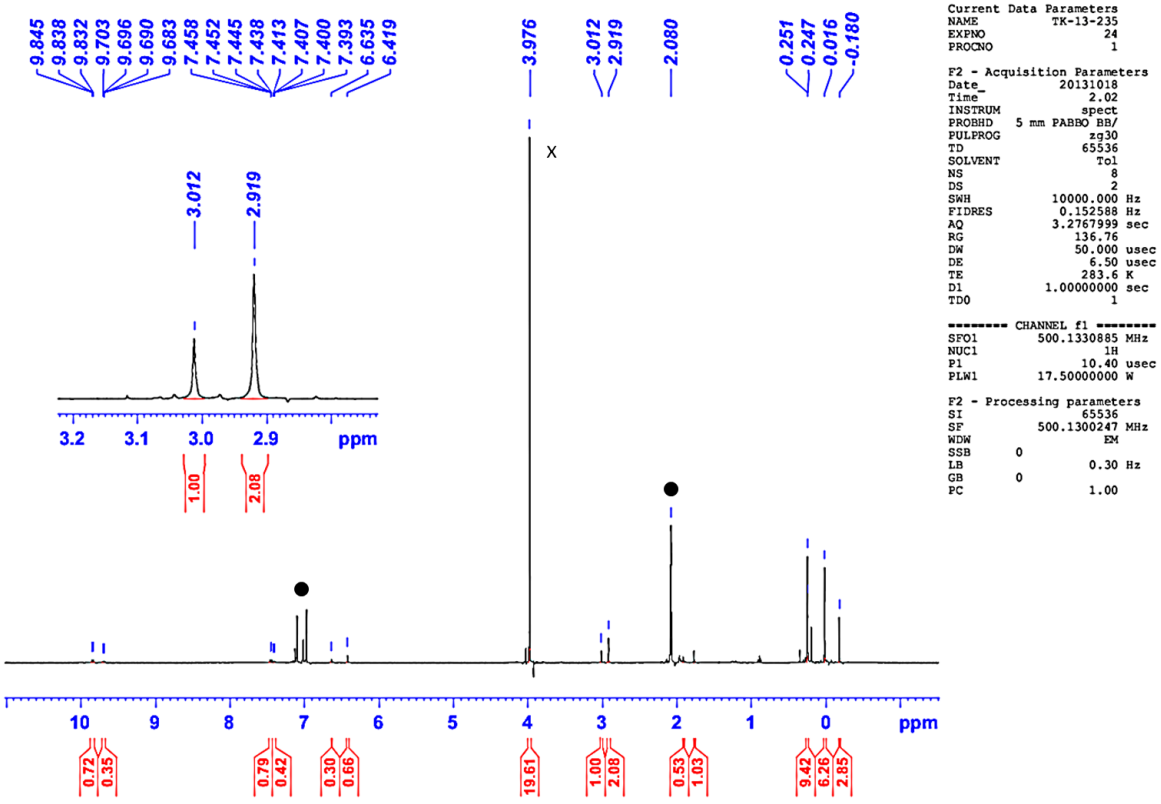
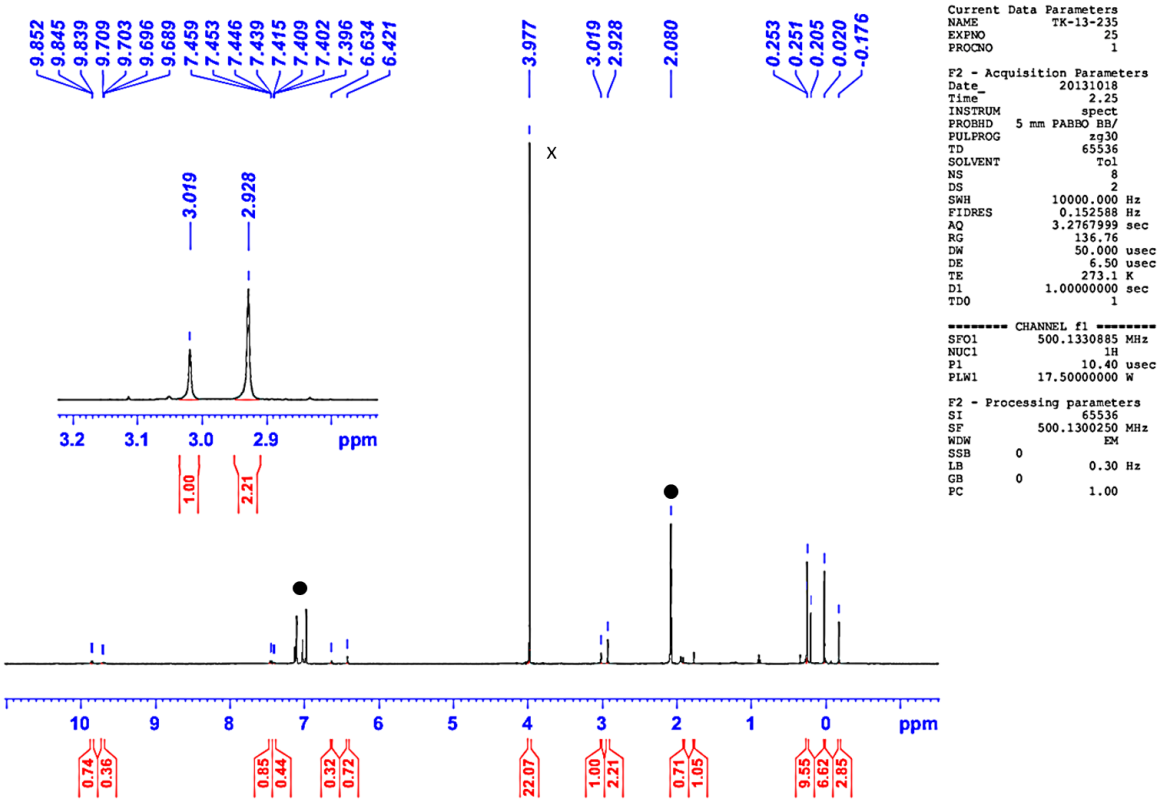


Figure S41. ^{1}H NMR spectrum of **6** in C_7D_8 at 283 K (● = C_7HD_7, x = ferrocene).




```
Current Data Parameters
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EXPNO                        25
PROCNO                        1

F2 - Acquisition Parameters
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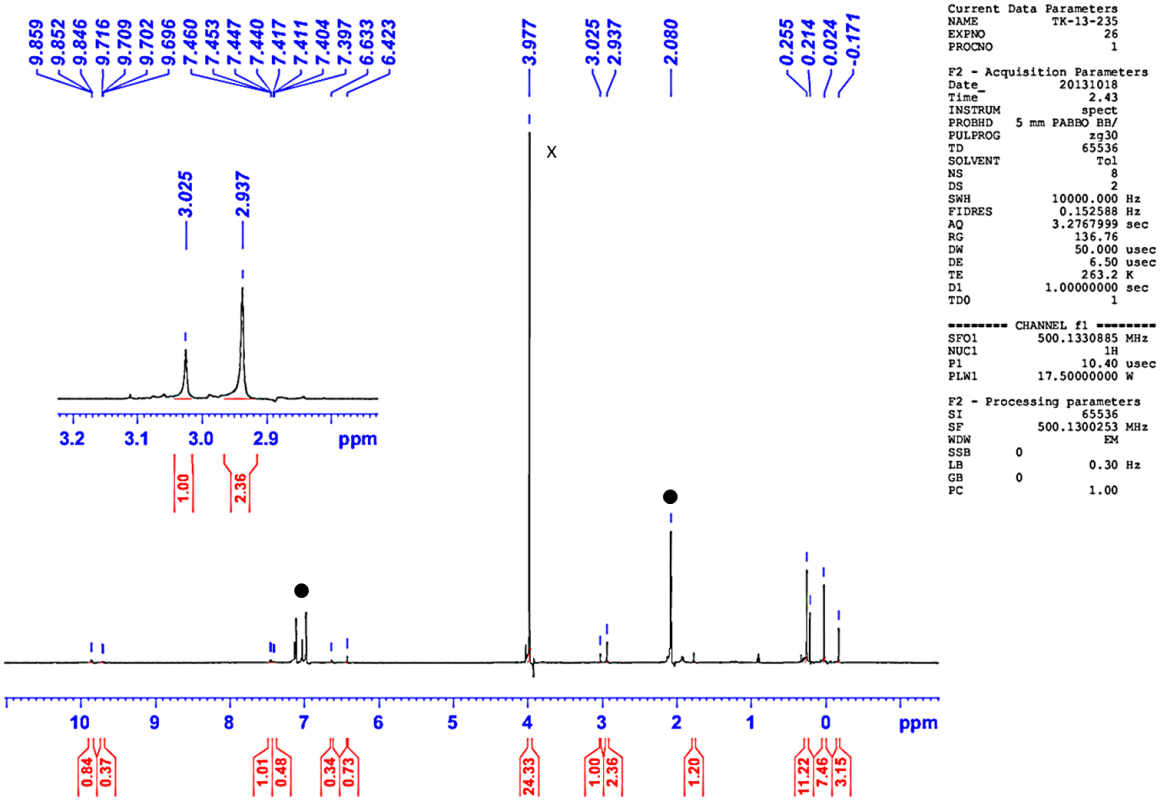
Time                     2.25
INSTRUM                 spect
PROBHD     5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                  Tol
NS                         8
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                    136.76
DW                    50.000 usec
DE                     6.50 usec
TE                    273.1 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1              500.1330885 MHz
NUC1                      1H
P1                     10.40 usec
PLW1              17.50000000 W

F2 - Processing parameters
SI                     65536
SF                500.1300250 MHz
WDW                       EM
SSB                0
LB                     0.30 Hz
GB                 0
PC                     1.00
```

Figure S42. ^{1}H NMR spectrum of **6** in C_7D_8 at 273 K (● = C_7HD_7, x = ferrocene).




```
Current Data Parameters
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EXPNO                        26
PROCNO                        1

F2 - Acquisition Parameters
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Time                     2.43
INSTRUM                 spect
PROBHD     5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                  Tol
NS                         8
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                    136.76
DW                    50.000 usec
DE                     6.50 usec
TE                    263.2 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1              500.1330885 MHz
NUC1                      1H
P1                     10.40 usec
PLW1              17.50000000 W

F2 - Processing parameters
SI                     65536
SF                500.1300253 MHz
WDW                       EM
SSB                0
LB                     0.30 Hz
GB                 0
PC                     1.00
```

Figure S43. ^{1}H NMR spectrum of **6** in C_7D_8 at 263 K (● = C_7HD_7, x = ferrocene).

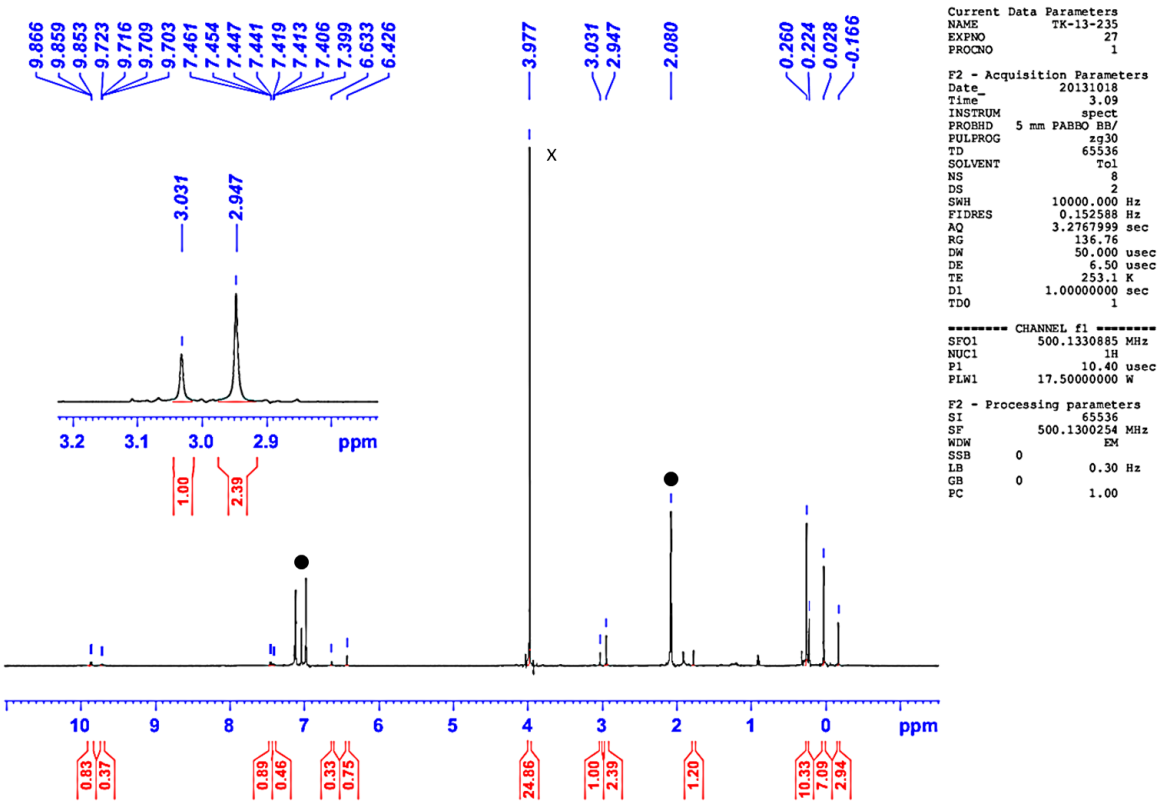


Figure S44. ^{1}H NMR spectrum of **6** in C_7D_8 at 253 K (● = C_7HD_7, x = ferrocene).

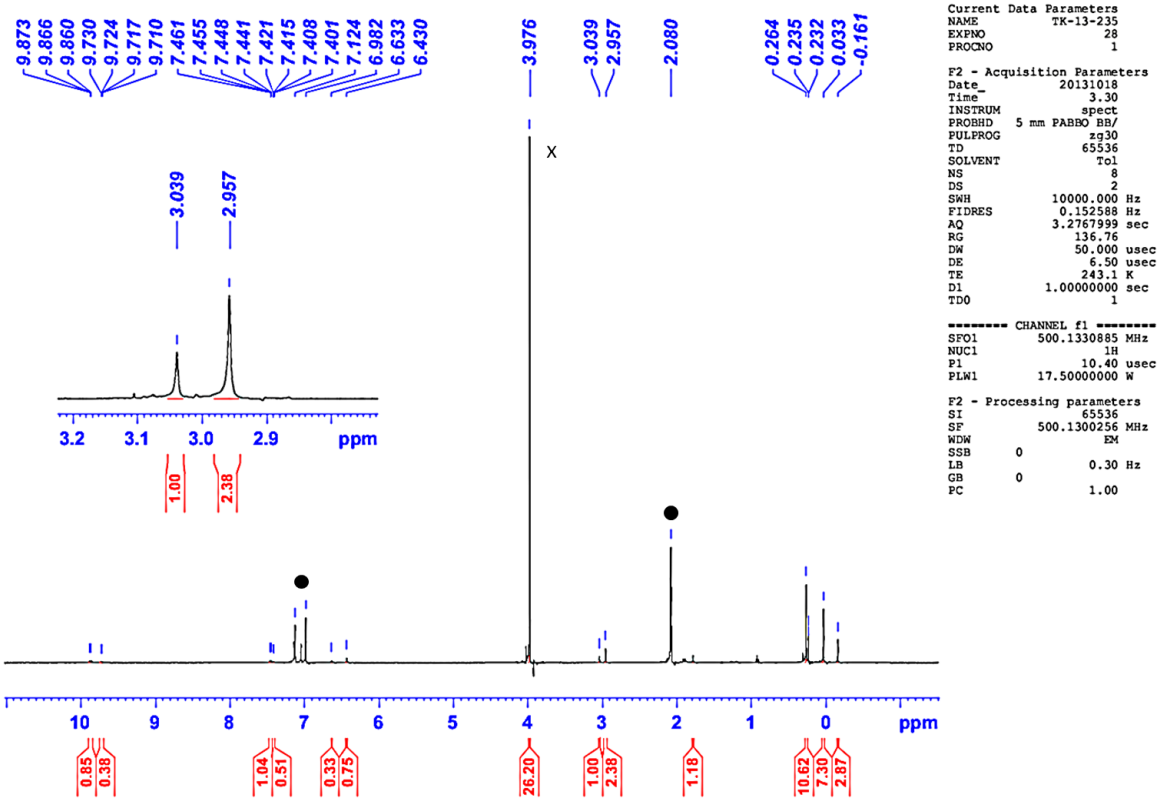


Figure S45. ^{1}H NMR spectrum of **6** in C_7D_8 at 243 K (● = C_7HD_7, x = ferrocene).

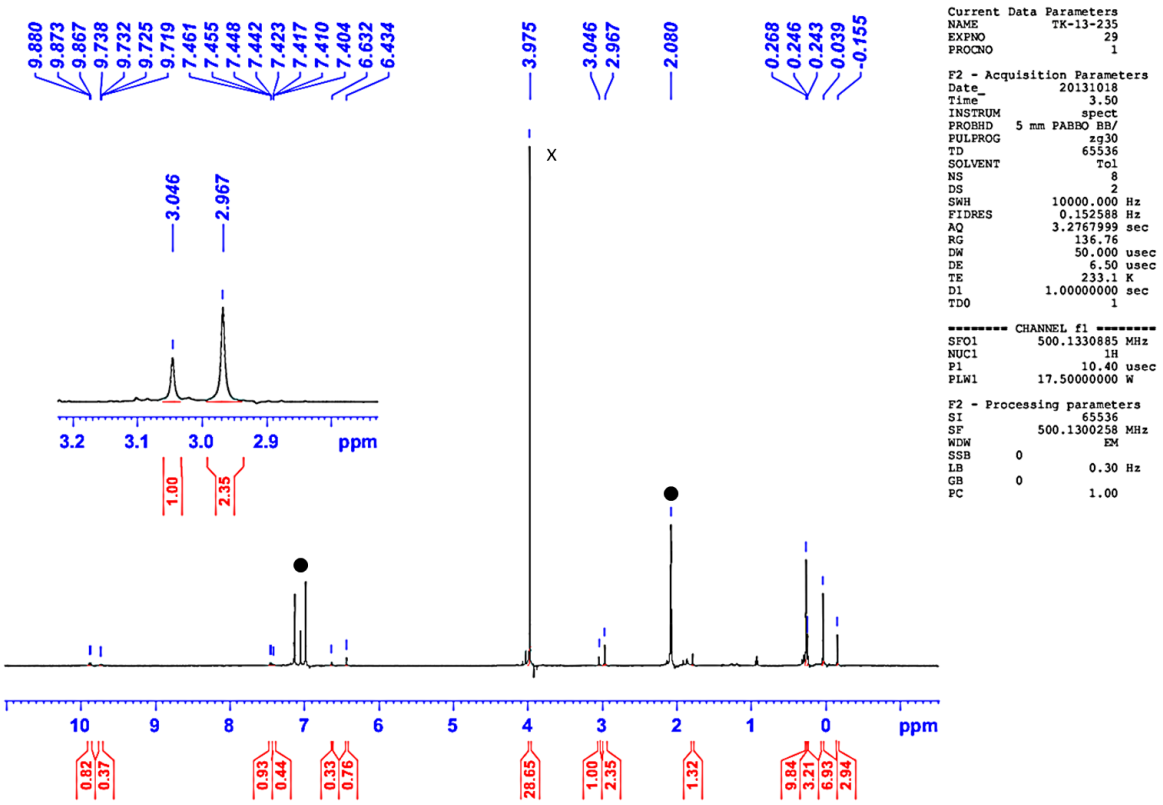


Figure S46. ^{1}H NMR spectrum of **6** in C_7D_8 at 233 K (● = C_7HD_7, x = ferrocene).

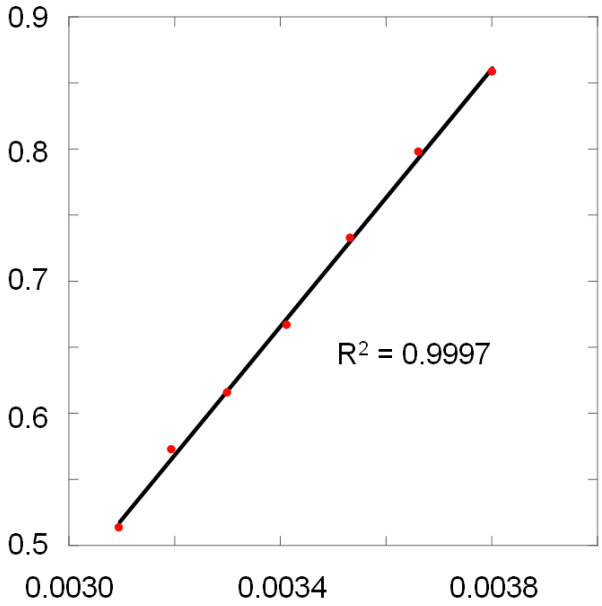


Figure S47. A plot of ln(K_{eq}) vs 1/T.

Table S1. Equilibrium Constant K_{eq} in Toluene-d_8 at Various Temperatures

T / K	K_{eq}	ln(K_{eq})
323	1.67	0.513
313	1.77	0.573
303	1.85	0.616
293	1.95	0.667
283	2.08	0.733
273	2.21	0.798
263	2.36	0.858
253	2.39	0.869
243	2.38	0.869
233	2.35	0.855

3. X-ray Analysis

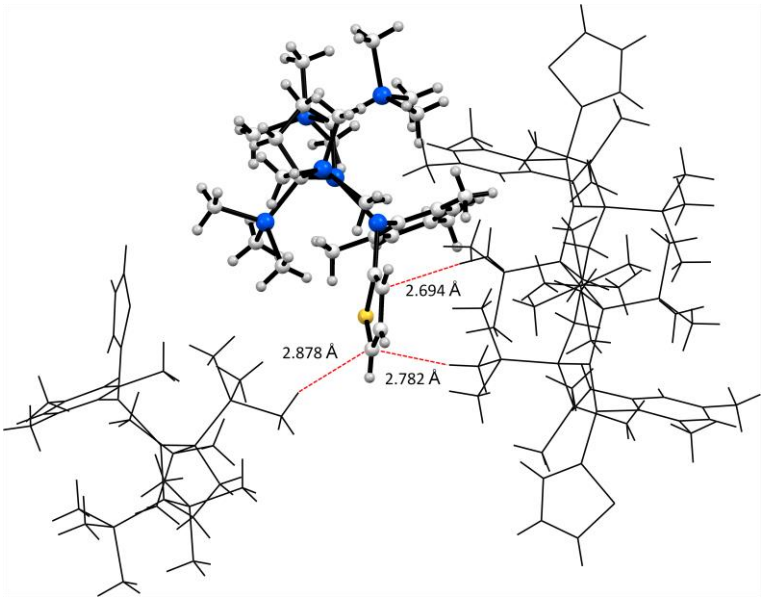


Figure S48. Packing diagram of **1**.

Table S2. Crystal data of **1-5** and **7**.

	1	**2**	**3**·4($C_5H_{10}O$)	**4**·($C_4H_{10}O_2$)	**5**	7
empirical formula	$C_{29}H_{54}SSi_6$	$C_{54}H_{104}SSi_{12}$	$C_{78}H_{146}O_4S_2Si_{12}$	$C_{43}H_{70}O_2Si_6$	$C_{38}H_{59}NSi_6$	$C_{34}H_{62}Si_6$
formula weight	603.32	1122.51	1549.14	787.53	698.4	639.37
Temperature (K)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
crystal system	monoclinic	triclinic	monoclinic	triclinic	monoclinic	monoclinic
space group	$P2_1/n$	P-1	$P2_1/c$	P-1	$P2_1/c$	$P2_1/c$
a (Å)	13.9334(13)	11.8362(12)	16.030(3)	11.4296(11)	12.2262(11)	11.3903(3)
b (Å)	16.8620(16)	17.6788(17)	30.312(6)	13.7384(13)	16.6001(16)	17.1318(4)
c (Å)	14.7774(14)	18.7605(18)	9.521(2)	15.2495(15)	20.3560(19)	19.8809(5)
α (deg.)	90	84.1110(10)	90	77.0900(10)	90	90
β (deg.)	90.0935(10)	81.8700(10)	93.418(3)	82.3360(10)	103.6680(10)	90.9660(10)
γ (deg.)	90	89.7240(10)	90	79.2250(10)	90	90
V (Å^3)	3471.9(6)	3865.5(7)	4617.9(17)	2282.4(4)	4014.4(6)	3878.93(17)
Z	4	2	2	2	4	4
density (Mg/m^3)	1.154	0.964	1.114	1.146	1.156	1.095
absorption coefficient (mm^{-1})	0.318	0.255	0.256	0.216	0.234	0.236
F(000)	1312	1224	1692	856	1512	1400
Theta range for data collection(deg.)	1.832 to 25.999	1.514 to 26.500	1.273 to 25.000	1.376 to 25.499	1.601 to 26.495	1.569 to 27.494
Index ranges	-17<=h<=16, -17<=k<=20, -18<=l<=15	-14<=h<=14, -22<=k<=22, -23<=l<=23	-19<=h<=19, -36<=k<=36, -11<=l<=11	-13<=h<=13, -16<=k<=16, -18<=l<=18	-12<=h<=15, -19<=k<=20, -25<=l<=23	-10<=h<=14 -22<=k<=22 -25<=l<=25
Refrections collected	17762	41666	40728	22849	21223	28627
Independent reflections	6781	15902	8100	8479	8265	8901
[R(int)]	[0.0222]	[0.0177]	[0.0975]	[0.0137]	[0.0120]	[0.0462]
Goodness-of-fit on F^2	1.018	1.044	1.079	1.023	1.032	1.010
Final R indices [I>2σ(I)]	0.0304	0.0296	0.0728	0.0316	0.0285	0.0386
R indices (all data)	0.0839	0.0844	0.1991	0.0843	0.0806	0.1006

4. UV-vis Absorption Spectra

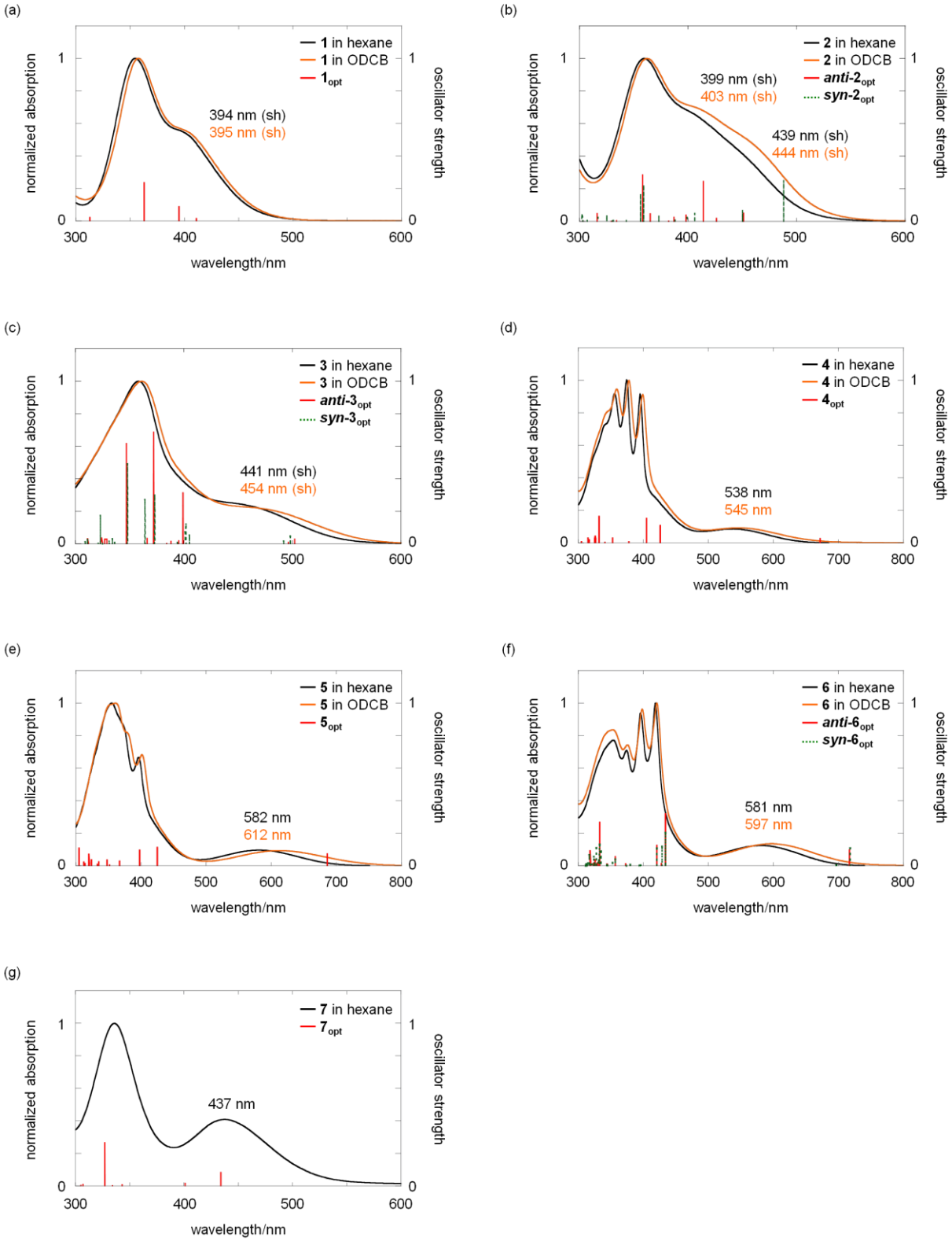
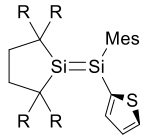


Figure S49. UV-vis absorption spectra of (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5**, (f) **6** and (g) **7** in hexane (black) and o-dichlorobenzene (orange) with oscillator strength (red and green) calculated at B3LYP/6-31+G(d)//B3PW91-D3/&-31G(d) level of theory.

4. Theoretical Calculations

Table S3. Atomic Coordinate of $\mathbf{1}_{opt}$ Calculated at the B3PW91-D3/6-31G(d) Level.



1 (R = $SiMe_3$)

Atom	x	y	z
Si	-0.70628800	1.27156300	0.56795400
Si	0.53101800	-0.43274000	-0.02741800
C	0.04560700	2.98201900	0.37861500
C	0.59838300	3.74041500	1.39293500
H	0.66711000	3.37959400	2.41307500
C	1.07215900	5.01737900	0.98470500
H	1.53936100	5.73435200	1.65161000
C	0.86976400	5.24452300	-0.35030300
H	1.12761800	6.12690000	-0.92324000
S	0.09871500	3.90497500	-1.10417500
C	-2.58350200	1.27121700	0.29997800
C	-3.43205500	1.08817800	1.42178100
C	-4.81472000	1.03991300	1.24771300
H	-5.45251000	0.89102800	2.11770100
C	-5.40329700	1.16750000	-0.01195900
C	-4.56707800	1.38635600	-1.10297100
H	-5.00644900	1.51485100	-2.09123700
C	-3.17591900	1.45665200	-0.97013500
C	-2.88066100	0.91433100	2.81507400
H	-3.67242600	1.00965300	3.56598300
H	-2.10649300	1.65609900	3.04418300
H	-2.42248500	-0.07283400	2.93877800
C	-6.89499400	1.05513700	-0.17920400
H	-7.20897600	0.00301900	-0.18304700
H	-7.23111400	1.50197300	-1.12052600
H	-7.42838500	1.54848000	0.64111200
C	-2.37797100	1.78963600	-2.20247000
H	-2.81360400	1.32980400	-3.09550000
H	-1.33996100	1.45246400	-2.12033400
H	-2.36248000	2.87470200	-2.36214300
C	2.43019100	-0.52524100	-0.03195200
C	2.63784000	-2.02790600	-0.43316800
H	2.64004600	-2.13429800	-1.52331400
H	3.61964300	-2.39526400	-0.10246000
C	1.52229600	-2.92317900	0.13808300
H	1.69566900	-3.06186900	1.21184500
H	1.58805800	-3.92605900	-0.30756000
C	0.11199200	-2.28927700	-0.09600700
Si	3.10484000	0.62705600	-1.41571200
C	3.51805100	2.36574000	-0.80950800
H	3.74181100	2.99304900	-1.68112300
H	4.38460000	2.40119900	-0.14222900

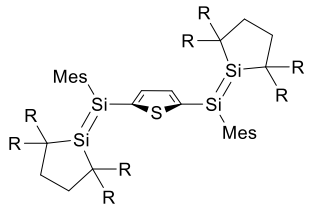
H	2.67041700	2.82161500	-0.29006600
C	1.86600800	0.84906500	-2.83076100
H	1.08549700	1.56585400	-2.55944400
H	1.37297200	-0.08038100	-3.13175600
H	2.39427900	1.24433700	-3.70837600
C	4.65363200	-0.14779700	-2.18253600
H	4.41881300	-1.08289100	-2.70386000
H	5.43429600	-0.36056500	-1.44667000
H	5.07148400	0.54440800	-2.92415600
Si	3.33965600	-0.20582100	1.62296100
C	2.77792900	1.34693100	2.52207000
H	1.71680900	1.26221600	2.78186800
H	2.90942600	2.25907100	1.93580400
H	3.34965300	1.44951400	3.45281700
C	3.13887000	-1.62727100	2.85363200
H	3.74608800	-1.39382900	3.73762700
H	3.49451300	-2.58519800	2.45852600
H	2.10622800	-1.74834600	3.18765300
C	5.21298500	-0.12932500	1.33531400
H	5.53851900	0.71601000	0.72269600
H	5.57828100	-1.04899500	0.86294200
H	5.71075700	-0.04441900	2.30944200
Si	-1.07506700	-2.85263000	1.29875400
C	-0.57864600	-2.13251400	2.97820100
H	-0.29958200	-1.07455800	2.93774900
H	0.25862400	-2.69736700	3.40242300
H	-1.42007700	-2.23721100	3.67493600
C	-2.86522200	-2.38942400	0.93160100
H	-3.49201800	-2.63818200	1.79674700
H	-3.26589400	-2.92899100	0.06723900
H	-2.98433800	-1.32002300	0.73583100
C	-0.94931900	-4.72478000	1.56747800
H	-1.39111000	-4.96590100	2.54262800
H	0.09679000	-5.05203100	1.59527600
H	-1.46924000	-5.31784500	0.81174800
Si	-0.58148400	-2.79379800	-1.81422400
C	-1.83387200	-1.54967400	-2.46657500
H	-1.31617200	-0.69604600	-2.91440400
H	-2.49832100	-1.16097700	-1.68881800
H	-2.45321400	-2.01214100	-3.24495000
C	-1.37905600	-4.51303400	-1.79052900
H	-2.30219900	-4.56680900	-1.20628700
H	-0.68893500	-5.27413100	-1.40957300
H	-1.62712600	-4.78254900	-2.82505800
C	0.78025700	-2.99132500	-3.11791800
H	0.30473900	-3.32000400	-4.05093700
H	1.50542700	-3.76304900	-2.83455100
H	1.33081000	-2.07331400	-3.33932300

E(RB3LYP) = -3272.28946234 A.U.

Zero-point correction= 0.760777 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -3271.609432

Table S4. Atomic Coordinate of ***anti*-2$_{opt}$** Calculated at the B3PW91-D3/6-31G(d) Level.



2 (R = $SiMe_3$)

Atom	x	y	z
S	-0.00981500	0.13567900	0.02153200
C	1.21728200	-0.23540700	1.18646700
C	0.71235800	-0.00739900	2.45427300
H	1.28980600	-0.18480600	3.35476000
C	-0.62405700	0.46856900	2.46566500
H	-1.17188800	0.69041300	3.37560800
C	-1.18514900	0.59935900	1.20828300
Si	2.86404000	-0.99778300	0.71890300
Si	4.39435800	0.40660300	0.02243200
Si	-2.91964100	1.17270300	0.78577600
Si	-4.22259500	-0.43522900	0.06787400
C	2.49560800	-2.67937600	-0.08713700
C	1.89969600	-2.81738100	-1.36114200
C	1.48878400	-4.08452000	-1.79662700
H	1.03583300	-4.17548800	-2.78324300
C	1.63136500	-5.22239400	-1.00901100
C	2.23449300	-5.07916000	0.24329800
H	2.36345400	-5.95839200	0.87250600
C	2.66424200	-3.83959200	0.71300900
C	1.63789600	-1.66280500	-2.29147500
H	1.95624200	-1.90689500	-3.31062900
H	2.16575500	-0.75907000	-1.97798400
H	0.56854400	-1.43064200	-2.32983600
C	1.12693000	-6.56323700	-1.47051800
H	0.94863200	-6.57829200	-2.55056400
H	0.17913000	-6.81240700	-0.97560100
H	1.83628900	-7.36357800	-1.23114600
C	3.28504700	-3.76185300	2.08674400
H	2.68529700	-3.13713100	2.76117700
H	4.28915400	-3.32414000	2.05395700
H	3.36568400	-4.75583300	2.53980400
C	4.55910400	2.23717500	0.49975600
C	5.94157000	2.56949600	-0.16700800
H	5.80005400	2.85408300	-1.21527900
H	6.41369300	3.43990000	0.31006900
C	6.89697500	1.36044800	-0.11746400
H	7.27903100	1.25206400	0.90429200
H	7.77679600	1.55879100	-0.74632000
C	6.16808500	0.04808800	-0.55488000
Si	4.66532100	2.68813900	2.35803800
C	6.32292900	2.20585200	3.13034300
H	6.32097000	2.55324300	4.17148700
H	7.17854300	2.67508300	2.63250800

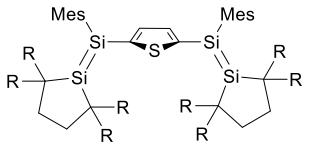
H	6.47667600	1.12447900	3.14586300
C	4.59787000	4.57104600	2.57398800
H	3.64318500	5.01890100	2.28380700
H	5.39131100	5.06544100	2.00101500
H	4.76610800	4.80572900	3.63253900
C	3.34300200	1.88861100	3.42679400
H	3.48150400	2.20956100	4.46676000
H	3.44461700	0.79826000	3.39201800
H	2.32571500	2.14247200	3.12134200
Si	3.13573300	3.21413000	-0.35849200
C	3.77144800	4.92215100	-0.87329500
H	4.55681800	4.84727200	-1.63422100
H	4.17006100	5.49980700	-0.03447000
H	2.94359100	5.49406700	-1.31073200
C	1.59610700	3.42158800	0.71302000
H	0.78514200	3.82243000	0.09159600
H	1.73925900	4.10759100	1.55363200
H	1.24907800	2.46470500	1.11256100
C	2.54239300	2.37024400	-1.94820600
H	1.87026900	1.53810100	-1.71833100
H	3.35003800	1.98151800	-2.57679500
H	1.97939300	3.10034100	-2.54479700
Si	6.26665300	-0.17861300	-2.45709900
C	6.21102500	1.47468400	-3.38157800
H	6.30254600	1.26319700	-4.45470000
H	7.04803000	2.12673700	-3.10637100
H	5.28271200	2.03467100	-3.23796300
C	4.87125600	-1.25452000	-3.12474000
H	4.53493700	-2.01859100	-2.41733700
H	5.19062200	-1.75919900	-4.04474200
H	4.00710900	-0.63027400	-3.37059200
C	7.92109700	-0.92275900	-3.00307500
H	8.04244100	-1.97190900	-2.71683500
H	8.77399600	-0.35993900	-2.60789800
H	7.97033200	-0.87184200	-4.09822500
Si	6.92346100	-1.46866100	0.34313800
C	6.61202800	-1.44641000	2.21050400
H	5.58429800	-1.18716500	2.48319900
H	7.29493500	-0.75118000	2.71081200
H	6.82544200	-2.44703800	2.60832900
C	6.24394600	-3.08619800	-0.35154400
H	6.52201400	-3.24470800	-1.39882400
H	5.15132600	-3.13263000	-0.29067200
H	6.64317900	-3.92737900	0.22832500
C	8.81411000	-1.44845000	0.21112600
H	9.22578700	-2.11203700	0.98185000
H	9.20973100	-0.44365500	0.40219300
H	9.19678400	-1.78330500	-0.75555100
C	-2.90953000	2.93606200	0.08058200
C	-3.45948700	3.98215300	0.86628400
C	-3.43038000	5.29472500	0.39730200
H	-3.85960700	6.08521800	1.01104400
C	-2.86646500	5.62423400	-0.83685800
C	-2.30866500	4.59746000	-1.59227200
H	-1.85147300	4.83287900	-2.55252400
C	-2.31126300	3.26686100	-1.15734500
C	-4.09768600	3.71737500	2.20752400
H	-4.30704200	4.65398700	2.73534400

H	-3.45667200	3.10331600	2.85138600
H	-5.04486300	3.17908700	2.09704000
C	-2.88312100	7.04417700	-1.33606300
H	-3.86765300	7.30238700	-1.74776000
H	-2.14365500	7.20280400	-2.12776800
H	-2.67434200	7.75482000	-0.52839500
C	-1.62152200	2.25770700	-2.03532400
H	-1.79975200	2.46970300	-3.09488400
H	-1.96485900	1.23912600	-1.83251300
H	-0.53835500	2.28116600	-1.86854800
C	-5.99054100	-0.32871200	-0.62018300
C	-6.56044200	-1.72902900	-0.21872400
H	-7.03937000	-1.66697100	0.76559400
H	-7.34730600	-2.05523400	-0.91390300
C	-5.44764800	-2.79527500	-0.16106800
H	-5.19059400	-3.08042800	-1.18795400
H	-5.83279300	-3.71053200	0.31033800
C	-4.17247900	-2.26802100	0.58681200
Si	-7.04439600	1.05736600	0.18099200
C	-6.86615000	1.10940200	2.06511500
H	-5.83683100	0.97709600	2.41399700
H	-7.49523200	0.34413100	2.53206500
H	-7.22576700	2.08122000	2.42674500
C	-6.61351200	2.76166200	-0.50417200
H	-6.84777900	2.85927900	-1.56922200
H	-5.55418000	3.00471300	-0.37621200
H	-7.19359700	3.52207400	0.03323400
C	-8.89121400	0.72023900	-0.08008200
H	-9.46131600	1.34076200	0.62283900
H	-9.13624200	-0.32613200	0.13754600
H	-9.24633300	0.94763600	-1.08774100
Si	-5.96079700	-0.10910400	-2.52661600
C	-4.69651900	1.17735400	-3.07511000
H	-4.98569200	1.60029800	-4.04510900
H	-3.71628700	0.70588600	-3.19596100
H	-4.57864900	2.00273300	-2.36675400
C	-7.66000200	0.35988800	-3.22222500
H	-7.98314800	1.37013900	-2.95420800
H	-8.43719900	-0.34328900	-2.90254100
H	-7.60168200	0.31132300	-4.31705100
C	-5.55190300	-1.72573000	-3.41972600
H	-5.58487000	-1.53960300	-4.50072700
H	-6.27755500	-2.51733400	-3.20123200
H	-4.55271200	-2.09792800	-3.18125400
Si	-2.60159200	-3.14890500	-0.10343000
C	-2.05515800	-2.43951200	-1.76884500
H	-1.89089100	-1.35798200	-1.75014100
H	-2.76943300	-2.66761100	-2.56618300
H	-1.10651900	-2.92385400	-2.02952900
C	-2.98783300	-4.96524500	-0.48310100
H	-2.09497200	-5.41018900	-0.94119900
H	-3.81048600	-5.06851800	-1.19981000
H	-3.23575300	-5.55347300	0.40432200
C	-1.12203000	-3.10305300	1.06210600
H	-0.23478800	-3.43339900	0.50959000
H	-1.24434600	-3.76860500	1.92244500
H	-0.91318200	-2.10047300	1.44081600
Si	-4.34156000	-2.63083900	2.46376400

C	-3.19116500	-1.61038600	3.54778600
H	-3.40539200	-0.54190700	3.43384400
H	-2.13535200	-1.76678200	3.31496700
H	-3.35629700	-1.88212100	4.59791900
C	-6.09558800	-2.34870000	3.11082700
H	-6.11417000	-2.64408700	4.16773000
H	-6.83842600	-2.96214900	2.58881000
H	-6.40449100	-1.30384200	3.05645100
C	-4.05572600	-4.47299600	2.81738500
H	-3.03025900	-4.81108900	2.64643300
H	-4.72524300	-5.10119500	2.21809200
H	-4.29382700	-4.65751500	3.87257800

E(RB3LYP) = -5991.69289379 A.U.
Zero-point correction= 1.454358 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -5990.370879

Table S5. Atomic Coordinate of ***syn*-2$_{opt}$** Calculated at the B3PW91-D3/6-31G(d) Level.



2 (R = $SiMe_3$)

Atom	x	y	z
S	0.08720400	0.77381400	-0.04113800
C	1.32414800	0.31826900	-1.17828700
C	0.71496000	-0.17174100	-2.32111200
H	1.27874400	-0.50257600	-3.18640400
C	-0.70172900	-0.15905800	-2.27594900
H	-1.33054600	-0.47808100	-3.10156300
C	-1.22467900	0.33474800	-1.09273300
Si	3.13907200	0.75611400	-0.96763100
Si	4.47110100	-0.61228700	0.09087800
Si	-2.99668300	0.83458800	-0.76418100
Si	-4.48353800	-0.59803100	-0.03788900
C	3.35781200	2.63751200	-0.85426800
C	3.00783900	3.39135700	0.28918800
C	3.24499500	4.77078100	0.30783200
H	2.98267400	5.33444500	1.20214300
C	3.79173800	5.44264700	-0.78098100
C	4.08508700	4.70026500	-1.92680200
H	4.49190900	5.21011700	-2.79881900
C	3.87834100	3.32290100	-1.98249000
C	2.32582700	2.79745600	1.49338500
H	2.70548600	3.23856400	2.42084200
H	2.46466100	1.71356700	1.55193200
H	1.24767200	2.99395900	1.44952100
C	4.07402700	6.92024300	-0.72849900
H	3.50518300	7.41230900	0.06711900
H	3.82497700	7.40936800	-1.67700200
H	5.13885000	7.10790800	-0.53740800
C	4.24281400	2.59556500	-3.25291800
H	3.45093200	1.90666500	-3.57055800

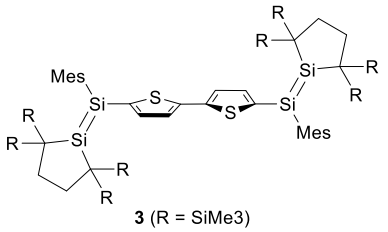
H	5.15185000	1.99875400	-3.12132200
H	4.42356800	3.30069100	-4.07148900
C	4.27356900	-2.49143700	0.26380500
C	5.61565400	-2.85798000	0.98798900
H	5.49771400	-2.77626400	2.07329200
H	5.89307100	-3.90541100	0.80345700
C	6.76389200	-1.92801500	0.55282100
H	7.09555300	-2.22301700	-0.45010300
H	7.63106700	-2.07848000	1.21185700
C	6.31181000	-0.43073100	0.54402100
Si	4.14931000	-3.51350600	-1.34920300
C	5.79881600	-3.61995600	-2.26702900
H	5.65898300	-4.27020600	-3.14008600
H	6.59649900	-4.05944400	-1.65809600
H	6.13391700	-2.64678500	-2.63241400
C	3.74462600	-5.32207900	-0.94193600
H	2.76318900	-5.47247200	-0.48341900
H	4.49853800	-5.74974400	-0.26997900
H	3.77028200	-5.90470500	-1.87131500
C	2.90737100	-2.84174200	-2.59276000
H	2.87130000	-3.51060700	-3.46177300
H	3.23364400	-1.85427800	-2.93854300
H	1.89507700	-2.74035000	-2.19544700
Si	2.76851100	-2.84149600	1.40470700
C	3.13151100	-4.36626700	2.46744900
H	3.93756800	-4.17499500	3.18511100
H	3.41396300	-5.23857800	1.87050800
H	2.23523300	-4.62854200	3.04320100
C	1.16877800	-3.10731400	0.44939200
H	0.36915700	-3.30169000	1.17165900
H	1.18716500	-3.94241900	-0.25522200
H	0.89462000	-2.20235400	-0.10294400
C	2.37768800	-1.41676800	2.59160200
H	1.82557000	-0.62824100	2.06952000
H	3.25681000	-0.95711300	3.05381600
H	1.73528500	-1.79511400	3.39785500
Si	6.52673800	0.35629200	2.28085300
C	6.19747800	-0.87799900	3.68094400
H	6.36191300	-0.35777800	4.63332100
H	6.89292600	-1.72479200	3.64938900
H	5.17879600	-1.27481200	3.69769300
C	5.38647400	1.83136800	2.53636200
H	5.28075200	2.45441100	1.64308000
H	5.76351400	2.46234700	3.35067700
H	4.38691700	1.48572200	2.81632600
C	8.31321000	0.89899500	2.60551200
H	8.63183800	1.75037500	1.99666200
H	9.02286300	0.07977700	2.44482100
H	8.38948600	1.19926600	3.65832700
Si	7.33010200	0.52696100	-0.76575100
C	6.92607700	-0.04684800	-2.52429300
H	5.85469300	-0.18242700	-2.70451300
H	7.43813900	-0.98967400	-2.74590000
H	7.30116200	0.69701600	-3.23868000
C	7.06493900	2.38922700	-0.64339200
H	7.44804100	2.80154700	0.29594700
H	6.00853700	2.66304300	-0.71724200
H	7.59372100	2.88863700	-1.46449100

C	9.17747200	0.14111400	-0.58784700
H	9.68665300	0.44712600	-1.51052800
H	9.34777800	-0.93499200	-0.46462200
H	9.66051500	0.65759000	0.24474500
C	-3.08668800	2.60392300	-0.08923000
C	-2.86770100	2.91129500	1.27723500
C	-3.13128100	4.20062300	1.74538300
H	-2.97904400	4.41672400	2.80214200
C	-3.58090800	5.21698600	0.90275000
C	-3.70135600	4.93135500	-0.45619200
H	-3.99788800	5.72325800	-1.14274800
C	-3.44305300	3.65656100	-0.96633700
C	-2.27285700	1.92902400	2.25271200
H	-2.73712200	2.00721300	3.24102300
H	-1.20073000	2.12924200	2.37525400
H	-2.37252800	0.89668100	1.90758000
C	-3.93351600	6.57525900	1.44640000
H	-4.98695100	6.60679800	1.75472300
H	-3.78934500	7.36032900	0.69648600
H	-3.32934300	6.82751500	2.32457300
C	-3.47672500	3.48373700	-2.46437900
H	-4.36381800	3.94622800	-2.90983500
H	-3.46513500	2.42742800	-2.75583200
H	-2.59229500	3.95573800	-2.91091200
C	-4.47751700	-2.49320300	-0.10391100
C	-6.00897400	-2.80447400	-0.15621300
H	-6.34064200	-2.85854600	-1.19946500
H	-6.23146300	-3.78920900	0.27899600
C	-6.83623900	-1.72115500	0.56723800
H	-6.76233300	-1.89206800	1.64740300
H	-7.90074900	-1.84508200	0.32223300
C	-6.34142500	-0.27534800	0.21525200
Si	-3.59956500	-3.26688800	-1.62441500
C	-3.91259600	-2.31117300	-3.22850800
H	-3.83999900	-1.22543500	-3.10039900
H	-4.89630700	-2.54334000	-3.65011300
H	-3.16295700	-2.61636400	-3.96975400
C	-1.73078500	-3.38683600	-1.41537600
H	-1.41798600	-4.00251300	-0.56903400
H	-1.27737200	-2.40053900	-1.29113700
H	-1.30243100	-3.82989800	-2.32337900
C	-4.30251600	-4.99836700	-1.93011400
H	-3.86572300	-5.40212500	-2.85214000
H	-5.38939600	-4.96861300	-2.06863900
H	-4.08432900	-5.70165200	-1.12205600
Si	-3.67746000	-3.15051400	1.51655200
C	-2.11944300	-2.18048500	1.95956600
H	-1.46615000	-2.78412200	2.60154900
H	-2.38340200	-1.27586100	2.51794200
H	-1.54313400	-1.86649800	1.08433500
C	-3.29508800	-5.00675400	1.43502700
H	-2.54999700	-5.29533400	0.68944800
H	-4.20895100	-5.58064800	1.24093700
H	-2.91956700	-5.31780000	2.41829100
C	-4.85440000	-3.04871800	2.99442900
H	-4.33976700	-3.47073600	3.86723500
H	-5.76365100	-3.63974100	2.83508700
H	-5.14475800	-2.02734600	3.24718300

Si	-6.66192100	0.90420900	1.69636900
C	-5.43457500	0.62340200	3.11700500
H	-4.46106300	0.25382800	2.78125500
H	-5.83479300	-0.08100800	3.85440100
H	-5.26137200	1.57601700	3.63204500
C	-8.36289500	0.55758500	2.45568000
H	-8.44385500	1.11422400	3.39811700
H	-8.48630200	-0.50536500	2.69379900
H	-9.19775200	0.85950500	1.81836400
C	-6.57087600	2.72944300	1.22871900
H	-6.73546300	3.32539300	2.13523300
H	-7.32931100	3.02429400	0.49677200
H	-5.58827900	3.00328400	0.83354000
Si	-7.25334200	0.35858800	-1.34589700
C	-6.40518900	1.82326100	-2.16929900
H	-5.58735100	1.46943900	-2.80380700
H	-5.98531900	2.53864000	-1.45773600
H	-7.12334800	2.35535100	-2.80577500
C	-7.43022200	-0.97982100	-2.66783000
H	-7.95633200	-0.54540000	-3.52744900
H	-8.01717700	-1.83878700	-2.32408300
H	-6.46034500	-1.33715300	-3.02131400
C	-9.03961600	0.83891900	-0.92819900
H	-9.11690500	1.74648400	-0.32168000
H	-9.56439400	0.03321000	-0.40212500
H	-9.57619900	1.02233400	-1.86763400

E(RB3LYP) = -5991.68224830 A.U.
Zero-point correction= 1.453842 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -5990.362545

Table S6. Atomic Coordinate of ***anti*-3$_{opt}$** Calculated at the B3PW91-D3/6-31G(d) Level.



3 (R = SiMe3)

Atom	x	y	z
Si	4.98197100	1.10416900	0.56039700
Si	6.14937600	-0.70157800	0.13520200
C	3.11636000	0.89230900	0.58137300
C	2.32678600	0.77256900	1.71060500
H	2.74170200	0.79918800	2.71186300
C	0.94517200	0.60865300	1.45122100
H	0.18731100	0.51102000	2.22187700
C	0.64505800	0.60995700	0.10425300
C	5.51687100	2.80471100	-0.08722300
C	6.06229400	3.73981300	0.82929300
C	6.50182000	4.98315500	0.37582200
H	6.92495000	5.68737600	1.09052500

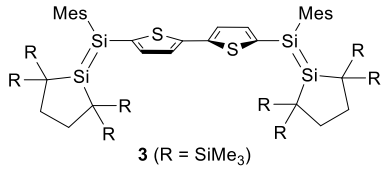
C	6.42261700	5.34646900	-0.96984000
C	5.85114000	4.43901600	-1.85742900
H	5.75597900	4.71182500	-2.90754100
C	5.38454100	3.18719300	-1.44190500
C	6.20975400	3.42177900	2.29658600
H	7.01950300	2.70407300	2.46679000
H	5.29774900	2.97779500	2.71271500
H	6.43927900	4.32435400	2.87319400
C	6.95576300	6.67243800	-1.44232400
H	6.75707100	7.46682900	-0.71426500
H	6.51232800	6.96880000	-2.39854000
H	8.04367300	6.62724200	-1.58386400
C	4.70327100	2.32476500	-2.47052300
H	3.64922400	2.61214100	-2.56852900
H	4.73351900	1.26501800	-2.19888900
H	5.16932900	2.43523300	-3.45504300
C	5.65689700	-2.50145200	0.50041800
C	6.97703300	-3.24225900	0.08665500
H	7.05805400	-4.21780700	0.58651200
H	6.96815100	-3.46506600	-0.98580000
C	8.22226200	-2.38965300	0.39334800
H	9.10779800	-2.84778600	-0.06990500
H	8.40675500	-2.40952700	1.47392900
C	8.02878300	-0.91388500	-0.08615900
C	4.25442100	-2.03683600	-2.30003000
H	3.61996700	-2.54993300	-3.03457000
H	5.25504000	-1.94473400	-2.73356700
H	3.85642200	-1.02740000	-2.16402800
C	2.50830900	-2.74393700	0.06900100
H	2.39285800	-1.73168500	0.46511700
H	2.27027900	-3.44985100	0.87064900
H	1.75780500	-2.87019100	-0.72075700
C	4.41196200	-4.83347300	-1.15172100
H	4.44541500	-5.50041600	-0.28561100
H	5.31923100	-5.00288500	-1.74284400
H	3.55693300	-5.13155600	-1.77126300
C	4.03043600	-1.80147100	3.15272100
H	3.06238700	-1.74940900	2.64963900
H	4.44854600	-0.78944000	3.19040900
H	3.86537200	-2.14027000	4.18309100
C	4.58236900	-4.73934700	2.40094900
H	4.45413200	-5.00920100	3.45673300
H	5.29524500	-5.45109600	1.96797100
H	3.61896200	-4.88250500	1.90376300
C	6.77699900	-3.00921200	3.42226800
H	7.23673500	-2.02569600	3.54052800
H	7.53876200	-3.71260300	3.06855200
H	6.45963500	-3.34628000	4.41743500
C	8.19866500	-2.28105800	-2.94554500
H	7.13964700	-2.53977300	-3.02548300
H	8.73338000	-3.15386300	-2.55312900
H	8.56923600	-2.10439100	-3.96345900
C	10.42519100	-0.52066800	-2.12207600
H	10.65503900	-0.55160700	-3.19475300
H	10.97260800	-1.34149900	-1.64542300
H	10.81526900	0.42266300	-1.72920600
C	7.68866000	0.72659100	-2.75919600
H	7.59609500	1.60272600	-2.11014700

H	6.67959000	0.43617400	-3.06693900
H	8.24033000	1.02532700	-3.65903700
C	10.82159300	-0.41324800	1.24527300
H	11.46825100	-0.25490600	0.37928900
H	10.81206400	-1.48630700	1.47027900
H	11.28185800	0.09429100	2.10246600
C	9.13580800	2.00691900	0.33047700
H	9.65057100	2.66215300	1.04387400
H	8.14053500	2.42632400	0.15774800
H	9.68205300	2.05616200	-0.61706900
C	8.39230700	0.32251700	2.79630400
H	8.70918100	-0.56275000	3.35830000
H	7.30137600	0.39745600	2.85086000
H	8.82018400	1.19473700	3.30679400
Si	4.22113200	-3.01025200	-0.67635000
Si	5.24574100	-2.96464200	2.31343100
Si	8.55105400	-0.72342700	-1.92488100
Si	9.06185200	0.25608500	1.02649900
S	2.09335100	0.82001900	-0.83131000
Si	-4.86830500	-0.63928700	-1.02166900
Si	-6.25011600	0.62356000	0.11898100
C	-3.06923600	-0.10008700	-1.01765200
C	-2.41329400	0.55544600	-2.04388100
H	-2.91032400	0.82476900	-2.96913300
C	-1.05966800	0.87104300	-1.77453100
H	-0.41352800	1.41403300	-2.45673000
C	-0.64629100	0.45089700	-0.52708900
C	-5.06405900	-2.52557500	-1.07236100
C	-5.55359500	-3.12639800	-2.26037700
C	-5.74616300	-4.50645600	-2.31390300
H	-6.12930000	-4.95183800	-3.23075500
C	-5.47025700	-5.33151900	-1.22199300
C	-4.95498500	-4.74011700	-0.07204400
H	-4.70864400	-5.36808100	0.78304700
C	-4.73246300	-3.36172300	0.01852100
C	-5.90421500	-2.30879600	-3.47865600
H	-6.82554300	-1.73808700	-3.32020400
H	-5.11905400	-1.58447400	-3.72549000
H	-6.05745300	-2.95128100	-4.35245600
C	-5.73978400	-6.81098700	-1.28719700
H	-5.49297000	-7.22024300	-2.27322600
H	-5.16223200	-7.36051600	-0.53670200
H	-6.80176700	-7.02241200	-1.10523700
C	-4.08636200	-2.84558400	1.27628600
H	-2.99651400	-2.95314500	1.21447900
H	-4.30577100	-1.78638400	1.44245800
H	-4.42502700	-3.40276200	2.15582400
C	-6.08192700	2.48715900	0.45714000
C	-7.45199000	2.77037800	1.16827200
H	-7.73508500	3.82857900	1.07800100
H	-7.36784900	2.58319500	2.24415400
C	-8.57460100	1.87695600	0.60852500
H	-9.46683700	1.96155600	1.24528800
H	-8.87291500	2.25833700	-0.37528300
C	-8.10472400	0.39090000	0.48287600
C	-4.34728600	1.27680000	2.81526400
H	-3.72580300	1.58651100	3.66583200
H	-5.27179200	0.85269900	3.21883400

H	-3.81800300	0.47822600	2.28805900
C	-2.98279300	3.11853200	0.83794700
H	-2.75718200	2.37093800	0.07315100
H	-2.93838700	4.10580100	0.36791300
H	-2.18165700	3.06891200	1.58546900
C	-5.05179000	4.22006400	2.83428900
H	-5.28416700	5.14084100	2.29182900
H	-5.90430700	3.98651600	3.48232300
H	-4.19175900	4.42252100	3.48480400
C	-4.63896800	3.12982700	-2.31521100
H	-3.62832400	3.07354700	-1.90501700
H	-4.89478400	2.14577900	-2.72335500
H	-4.63505300	3.85082100	-3.14220200
C	-5.56405400	5.42473400	-0.47736800
H	-5.58672900	6.08581100	-1.35281200
H	-6.33122300	5.78234200	0.21961700
H	-4.58917200	5.54643200	0.00304800
C	-7.55414700	3.82411500	-2.00806800
H	-7.86186700	2.88716600	-2.47734500
H	-8.37749300	4.19209400	-1.38612800
H	-7.39776800	4.55813700	-2.80894100
C	-8.18274300	0.56030700	3.65148900
H	-7.17831300	0.97111900	3.78156500
H	-8.89276500	1.39546500	3.63977600
H	-8.40655900	-0.04319300	4.54050100
C	-10.16819500	-1.17123200	2.31503500
H	-10.27806600	-1.58169100	3.32691100
H	-10.89141200	-0.35459400	2.21184500
H	-10.44147600	-1.96019500	1.60860700
C	-7.21348500	-2.01509400	2.31697700
H	-7.06100600	-2.56305500	1.38193100
H	-6.23322800	-1.67078500	2.66055200
H	-7.60298900	-2.71724900	3.06436300
C	-10.91643300	-0.10100900	-0.81278000
H	-11.42845300	-0.69188400	-0.05004000
H	-11.10252600	0.95898200	-0.60295600
H	-11.38367200	-0.32757200	-1.77951600
C	-8.77377000	-2.32002700	-0.97652500
H	-9.24969600	-2.74917000	-1.86677500
H	-7.71083600	-2.57456600	-1.01720400
H	-9.19882200	-2.82097800	-0.10065700
C	-8.59309100	0.27106900	-2.63109200
H	-9.10350100	1.22762500	-2.78778600
H	-7.51701200	0.42585300	-2.76041700
H	-8.93764700	-0.40820200	-3.42120700
Si	-4.63112300	2.77209000	1.68832900
Si	-5.93032100	3.65543100	-1.05391700
Si	-8.38567900	-0.55394900	2.13153500
Si	-9.05944400	-0.45661300	-0.94665000
S	-1.94283000	-0.36869600	0.28797000

E(RB3LYP) = -6543.40148423 A.U.
Zero-point correction= 1.501047 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -6542.042851

Table S7. Atomic Coordinate of ***syn*-3$_{opt}$** Calculated at the B3PW91-D3/6-31G(d) Level.



3 (R = $SiMe_3$)

Atom	x	y	z
Si	5.08345900	1.55386000	0.50730300
Si	5.31067700	-0.62019200	0.32680200
C	3.28753900	2.10216400	0.54781000
C	2.59757500	2.57673200	1.64927600
H	3.08129700	2.74647500	2.60566300
C	1.21276200	2.78000600	1.43278600
H	0.52067200	3.12930600	2.19225700
C	0.81551500	2.45911900	0.15050600
C	6.24476200	2.76279600	-0.37815600
C	7.24740500	3.42734300	0.37157300
C	8.13579100	4.29235900	-0.26911200
H	8.90527000	4.78978300	0.31925900
C	8.06996700	4.53227200	-1.64187700
C	7.05769600	3.90622500	-2.36573800
H	6.97293200	4.09853700	-3.43429900
C	6.14021400	3.04187500	-1.76152700
C	7.41076900	3.21372700	1.85583500
H	7.88596000	2.24984500	2.06580400
H	6.44769400	3.21300200	2.37918700
H	8.03738200	3.99539000	2.29861000
C	9.07455000	5.42519700	-2.31939800
H	9.38855800	6.24571400	-1.66499200
H	8.67224200	5.85936900	-3.24068400
H	9.97711900	4.86114800	-2.58956300
C	5.03782900	2.48010300	-2.61758200
H	4.16317200	3.14149700	-2.59718000
H	4.71112000	1.49697100	-2.26331300
H	5.35485200	2.37838600	-3.66052300
C	4.14503000	-1.96303000	1.01283000
C	4.95095600	-3.24980100	0.61856300
H	4.67353200	-4.10160100	1.25563900
H	4.69640900	-3.55287100	-0.40394500
C	6.47302100	-3.01816700	0.69170200
H	6.99689100	-3.85757100	0.21229000
H	6.78022600	-3.03803400	1.74370000
C	6.88032100	-1.65216100	0.04572600
C	2.61048700	-1.47979100	-1.72545300
H	1.63589800	-1.12089100	-2.07713300
H	2.88017400	-2.34965600	-2.33479100
H	3.34050500	-0.68572700	-1.91267200
C	1.18174700	-0.84310800	0.93531100
H	1.62934700	0.07162700	1.32747600
H	0.66867900	-1.34592000	1.76048100
H	0.42158500	-0.54241300	0.20828800
C	1.73201000	-3.71916900	0.04746700
H	1.34536000	-4.05942300	1.01169500
H	2.46408600	-4.45429300	-0.30551400

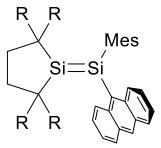
H	0.89814100	-3.72571800	-0.66556300
C	3.46113900	-0.24637400	3.62499100
H	2.50928000	0.15500000	3.26883900
H	4.24639400	0.47488700	3.37258800
H	3.40913900	-0.32630200	4.71811300
C	2.48603200	-3.15790700	3.39827300
H	2.46451600	-3.22890100	4.49303400
H	2.68796200	-4.16279500	3.00954400
H	1.48785500	-2.85965700	3.06737400
C	5.35224200	-2.59576900	3.87732300
H	6.23156200	-1.95711900	3.78181500
H	5.62610600	-3.61603900	3.58652100
H	5.07785500	-2.62257300	4.93963800
C	5.97259700	-3.03229200	-2.64346400
H	4.94581500	-2.66592500	-2.56765500
H	6.01372900	-4.04376200	-2.22391800
H	6.21778500	-3.10927700	-3.71044500
C	8.89465900	-2.68352600	-2.15065600
H	8.94774300	-2.94968100	-3.21397300
H	9.01373600	-3.60732000	-1.57335600
H	9.74658800	-2.03267300	-1.93121200
C	7.14445000	-0.23087400	-2.77521400
H	7.42003500	0.63936500	-2.17390900
H	6.13043400	-0.06292200	-3.15084200
H	7.81671200	-0.26980200	-3.64117000
C	9.72547500	-2.35185100	1.14343000
H	10.24651300	-2.62394900	0.22261700
H	9.26758500	-3.25923300	1.55434300
H	10.47902700	-2.01205200	1.86525500
C	9.23940600	0.45250100	-0.02439400
H	10.08858900	0.83503300	0.55550600
H	8.54912800	1.28569200	-0.18616400
H	9.62059300	0.14403000	-1.00342400
C	8.09092800	-0.39892200	2.69063700
H	8.08633900	-1.25252700	3.37665000
H	7.14430500	0.14061900	2.79966100
H	8.90077200	0.26574400	3.01723200
Si	2.44709900	-1.96463400	0.10085700
Si	3.86106600	-1.94408900	2.91406600
Si	7.21666000	-1.86253800	-1.83228400
Si	8.44441400	-0.97314000	0.92091100
S	2.17900500	1.93417700	-0.78495100
Si	-4.81714600	1.51468500	-0.54998700
Si	-5.36291200	-0.60830400	-0.37668800
C	-2.99020400	1.89891400	-0.68723500
C	-2.31564600	2.15975800	-1.86696500
H	-2.81355400	2.15115100	-2.83124900
C	-0.93297300	2.41940700	-1.70736400
H	-0.25405300	2.63892500	-2.52507100
C	-0.52330000	2.36741000	-0.39092800
C	-5.79403500	2.73347000	0.52730600
C	-5.78011600	2.67869700	1.94494900
C	-6.68762500	3.44891900	2.67456000
H	-6.68191600	3.37926200	3.76147400
C	-7.59778100	4.30637200	2.05467300
C	-7.53525000	4.43057600	0.66851900
H	-8.19767400	5.13418900	0.16610200
C	-6.64108800	3.67840300	-0.09920600

C	-4.75492100	1.88965000	2.71587100
H	-5.14636700	1.54248800	3.67715800
H	-4.40222900	1.02054900	2.15466500
H	-3.87959000	2.51939900	2.92112600
C	-8.61953000	5.06276100	2.85983100
H	-8.23526200	5.33013500	3.85019500
H	-8.93128600	5.98323900	2.35509600
H	-9.51920400	4.45210700	3.01297700
C	-6.56907100	3.97703600	-1.57602900
H	-6.06077200	4.93666700	-1.73525100
H	-6.00402200	3.21212500	-2.12070100
H	-7.56380600	4.04737900	-2.02842300
C	-7.13270400	-1.30048900	-0.39150100
C	-6.84911000	-2.83889400	-0.49706500
H	-7.69188200	-3.36642400	-0.96611200
H	-6.75329600	-3.27446400	0.50312100
C	-5.55465800	-3.12884000	-1.28428000
H	-5.27015200	-4.18248000	-1.15036200
H	-5.76074400	-3.01050200	-2.35409700
C	-4.39421800	-2.16880700	-0.85916500
C	-6.89548900	-0.88164600	2.75088600
H	-7.19125300	-0.06391500	3.41868800
H	-6.96117700	-1.81582800	3.31961700
H	-5.84616200	-0.71508700	2.48842700
C	-8.93227000	0.76986800	1.22407200
H	-8.22766500	1.59588700	1.08733000
H	-9.70790600	0.84845500	0.45620100
H	-9.41478900	0.91247500	2.19935200
C	-9.33244900	-2.25077900	1.61380600
H	-10.15066200	-2.28379200	0.88991000
H	-8.86886800	-3.24358800	1.64502400
H	-9.76801800	-2.06248700	2.60336800
C	-8.22005800	1.10685800	-2.17492400
H	-8.22030200	1.68713200	-1.24945300
H	-7.34430200	1.41039300	-2.75569000
H	-9.11680000	1.37599900	-2.74716600
C	-9.96588500	-1.38058300	-1.71582900
H	-10.48962500	-1.21403100	-2.66559500
H	-10.00151900	-2.45577600	-1.50599300
H	-10.53044500	-0.86400600	-0.93332300
C	-7.57387300	-1.52220100	-3.51213000
H	-6.54515000	-1.23002000	-3.73798200
H	-7.63754100	-2.61588700	-3.51471100
H	-8.20896000	-1.15415700	-4.32805600
C	-4.64744600	-3.71300000	1.90827300
H	-5.40404600	-3.04325700	2.32152800
H	-5.15321000	-4.57918600	1.46658300
H	-4.04178300	-4.08234200	2.74591300
C	-2.30257400	-4.28707400	0.20557200
H	-1.89422500	-4.71295300	1.13076700
H	-2.83789100	-5.08951900	-0.31517500
H	-1.45610700	-3.98457500	-0.41505300
C	-2.52001500	-1.55998900	1.62580900
H	-1.89056000	-0.93965900	0.98478800
H	-3.19856200	-0.89142000	2.16623300
H	-1.87039800	-2.04442100	2.36551800
C	-2.89854800	-3.62892900	-3.16612800
H	-2.39070300	-4.36501700	-2.53775100

H	-3.85054200	-4.06241700	-3.49323600
H	-2.28476100	-3.47457600	-4.06257300
C	-1.47373600	-1.29816300	-1.77344800
H	-0.84990000	-1.17009900	-2.66669700
H	-1.55240300	-0.32096800	-1.29038100
H	-0.94557500	-1.97527800	-1.09668100
C	-3.80575600	-0.81647800	-3.67735100
H	-4.52212300	-1.33789400	-4.32145900
H	-4.28534000	0.08916100	-3.29170900
H	-2.96224400	-0.51115800	-4.30930700
Si	-8.05620400	-0.90111300	1.24550300
Si	-8.18485200	-0.75462100	-1.89702200
Si	-3.47623100	-2.87661600	0.67910700
Si	-3.15723600	-1.95725200	-2.31381500
S	-1.87002200	1.98915000	0.64322600

E(RB3LYP) = -6543.40538519 A.U.
Zero-point correction= 1.501597 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -6542.043832

Table S8. Atomic Coordinate of $\mathbf{4}_{opt}$ Calculated at the B3PW91-D3/6-31G(d) Level.



4 (R = $SiMe_3$)

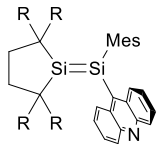
Atom	x	y	z
Si	-0.99466400	-0.63951300	0.04841800
Si	0.53020700	0.88947600	-0.09714800
C	-0.80465800	-2.51343600	0.37350000
C	-2.25639400	-3.00031800	0.04296300
H	-2.33838600	-3.22331500	-1.02857500
H	-2.48684000	-3.94054300	0.56264100
C	-3.31771400	-1.94063700	0.39639500
H	-3.46146500	-1.94722500	1.48410500
H	-4.28618000	-2.23150900	-0.03434600
C	-2.89676100	-0.50873300	-0.07703100
Si	0.38525500	-3.41112900	-0.83220200
Si	-0.32293300	-2.87006000	2.20273500
Si	-3.45696300	-0.15361600	-1.87724300
Si	-3.67005900	0.75964900	1.12609400
C	0.05166300	-2.88479100	-2.62167200
H	-0.19563100	-1.82432400	-2.72526000
H	-0.77163400	-3.47409000	-3.04060600
H	0.94275900	-3.08087800	-3.22782900
C	0.01781900	-5.27173300	-0.86802500
H	0.53118600	-5.70427400	-1.73665800
H	-1.05351400	-5.46693800	-0.99468800
H	0.35996400	-5.80947300	0.01910200
C	2.20862700	-3.17379400	-0.38979600
H	2.81331300	-3.09639000	-1.30015600
H	2.58286200	-4.02362500	0.19098800
H	2.38989500	-2.26568400	0.18967700
C	0.91205200	-1.62343500	2.88938500

H	0.45069700	-0.64321500	3.04500500
H	1.77079300	-1.47137500	2.22886200
H	1.29204400	-1.97796000	3.85566300
C	0.42103300	-4.59678500	2.44780300
H	1.36615500	-4.75499300	1.92127600
H	-0.27757400	-5.38619800	2.14978100
H	0.61705400	-4.72107400	3.52053300
C	-1.82990300	-2.90256700	3.34759100
H	-1.49451400	-3.23781900	4.33724600
H	-2.59169200	-3.61237500	3.00501400
H	-2.30039700	-1.92651700	3.47453900
C	-3.42743500	-1.70439900	-2.95810700
H	-3.84896200	-1.44698800	-3.93810200
H	-4.04583700	-2.50640800	-2.53850900
H	-2.42275900	-2.09560800	-3.12443100
C	-2.38652900	1.16191000	-2.70364200
H	-1.45493100	0.71117600	-3.06113700
H	-2.11794000	1.98211400	-2.02978500
H	-2.91146600	1.58761200	-3.56767300
C	-5.26948100	0.39573300	-1.98260200
H	-5.46958300	1.37508400	-1.53862800
H	-5.93919900	-0.33450600	-1.51462000
H	-5.53924000	0.45450700	-3.04478900
C	-3.47542600	2.53158900	0.51217000
H	-3.80703900	3.23194700	1.28849500
H	-4.07964600	2.72037100	-0.38114700
H	-2.43910200	2.77648800	0.26538900
C	-5.51442800	0.40813000	1.39240600
H	-5.84170100	0.94500600	2.29205900
H	-5.69485100	-0.65899100	1.56823000
H	-6.15241800	0.72774300	0.56547700
C	-2.94409300	0.58692700	2.86937400
H	-1.88335100	0.31969900	2.88113000
H	-3.49493900	-0.17697300	3.42915000
H	-3.05908800	1.53098600	3.41464100
C	0.24972300	2.76608800	-0.17929100
C	-0.16871400	3.52928500	0.93529200
C	-0.30542400	4.91837200	0.82011700
H	-0.63603000	5.48258800	1.69124800
C	-0.03909500	5.59288500	-0.36464100
C	0.39461600	4.83836300	-1.45765200
H	0.62115900	5.34591700	-2.39405900
C	0.54859300	3.45607800	-1.38666700
C	1.05719100	2.73375500	-2.60526500
H	1.15666000	3.41449600	-3.45685100
H	0.38129700	1.92556500	-2.90192600
H	2.03987400	2.28513100	-2.42187300
C	-0.48907700	2.93869700	2.28374400
H	0.24530800	3.26053700	3.03309700
H	-0.50085900	1.84709800	2.25757700
H	-1.47368700	3.27049100	2.62980300
C	-0.22145600	7.08199200	-0.48345400
H	-0.36806900	7.55077600	0.49484600
H	-1.09631400	7.32168500	-1.10157800
H	0.64704900	7.55291600	-0.95857000
C	2.38006700	0.44402500	-0.13477200
C	3.18557200	0.71813900	1.00172100
C	2.65136900	1.28083900	2.19862600

H	1.58691400	1.48044900	2.23548800
C	3.43296400	1.54741600	3.28904400
H	2.98555400	1.97328300	4.18341200
C	4.82456800	1.26048300	3.26653500
H	5.43500700	1.47492000	4.13977500
C	5.38504600	0.70715000	2.14888200
H	6.44728600	0.47415700	2.11861200
C	4.59699700	0.42009000	0.99352600
C	5.16555100	-0.15467700	-0.14279300
H	6.22787900	-0.39342600	-0.14326300
C	4.40534000	-0.43119900	-1.27854200
C	5.00058500	-1.02912600	-2.43003900
H	6.06150100	-1.26741800	-2.39556000
C	4.26251800	-1.29691000	-3.54966900
H	4.72759300	-1.75158800	-4.42042300
C	2.87999200	-0.97124400	-3.57408200
H	2.29335900	-1.17695500	-4.46549100
C	2.27750500	-0.40794100	-2.48221500
H	1.21712700	-0.17986600	-2.50014400
C	2.99598900	-0.11647000	-1.28501200

E(RB3LYP) = -3258.72457584 A.U.
Zero-point correction= 0.888674 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -3257.923624

Table S9. Atomic Coordinate of $\mathbf{5}_{\mathbf{opt}}$ Calculated at the B3PW91-D3/6-31G(d) Level.



5 (R = $SiMe_3$)

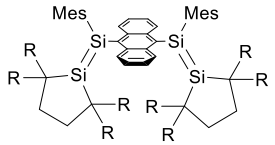
Atom	x	y	z
Si	-0.68488700	-0.86646600	0.03085100
Si	0.26295000	1.08901900	0.09358700
C	0.05836300	-2.53644200	0.59528200
C	-1.27355600	-3.25183200	1.02417200
H	-1.15503800	-4.34115900	1.05220000
H	-1.55138700	-2.95070800	2.04324900
C	-2.42185300	-2.86162700	0.07991500
H	-3.36104800	-3.32383900	0.40637900
H	-2.20843600	-3.27985600	-0.91431700
C	-2.54554200	-1.29837100	-0.00064300
C	2.12937500	1.20653700	-0.22985300
C	2.78742300	0.56814600	-1.31081100
C	2.11120900	-0.08148000	-2.38678500
H	1.02645100	-0.07986300	-2.37807800
C	2.79432300	-0.69157700	-3.40431100
H	2.24555200	-1.17119000	-4.21005600
C	4.21486200	-0.71246200	-3.40942100
H	4.74307200	-1.21696000	-4.21434800
C	4.91150400	-0.08829700	-2.41197600
H	5.99699300	-0.06952600	-2.39005500
C	4.23321100	0.59081200	-1.35365100
C	2.93888000	1.91403400	0.69186700

C	2.40812400	2.62904100	1.80557400
H	1.33125200	2.65233000	1.94431300
C	3.22139800	3.28567500	2.68919800
H	2.78722900	3.82560100	3.52652000
C	4.63326500	3.26210300	2.52359000
H	5.26586900	3.78532300	3.23598000
C	5.19046300	2.57832300	1.47855300
H	6.26457500	2.53264200	1.32549300
C	4.37167700	1.88637800	0.53534100
C	-0.66979800	2.70962900	-0.18247500
C	-0.70102800	3.31163700	-1.46977600
C	-1.40956500	4.49304200	-1.66420900
H	-1.43272900	4.93802400	-2.65773800
C	-2.10746700	5.11643200	-0.62448500
C	-2.05798100	4.53229300	0.63553000
H	-2.58182600	5.00700700	1.46405800
C	-1.34688300	3.35003500	0.87926100
C	-0.02087800	2.66973900	-2.64905000
H	-0.12567000	3.28172700	-3.55052600
H	-0.45844100	1.68554800	-2.85923400
H	1.04867800	2.51590800	-2.47027700
C	-2.88696700	6.37833900	-0.87877400
H	-3.31357900	6.78393800	0.04391700
H	-3.71273300	6.19527100	-1.57773800
H	-2.25229400	7.15239000	-1.32676200
C	-1.33257600	2.84598100	2.30099400
H	-0.89354500	3.59577700	2.97113200
H	-0.75687500	1.92084200	2.40009600
H	-2.34667200	2.64094600	2.66154700
Si	0.94561300	-3.55786200	-0.78717500
C	0.61716600	-5.40598400	-0.51762900
H	-0.42975800	-5.65995100	-0.72179200
H	0.86260200	-5.76000700	0.48745700
H	1.23180300	-5.97115200	-1.22963000
C	2.81694700	-3.30615600	-0.85375700
H	3.19980000	-3.95305500	-1.65356600
H	3.34158800	-3.57312000	0.06767900
H	3.08700700	-2.28055600	-1.11781900
C	0.33551600	-3.23677500	-2.54385900
H	1.01635700	-3.74355300	-3.23940100
H	0.32589700	-2.17743100	-2.80573400
H	-0.66704800	-3.63965900	-2.71011500
Si	1.24594500	-2.42939200	2.10605900
C	2.76824700	-1.33819900	1.86894100
H	2.55904900	-0.32790900	2.23416100
H	3.12676500	-1.24812100	0.84317000
H	3.58895100	-1.74328700	2.47418700
C	1.79078200	-4.18277300	2.58787400
H	2.34572600	-4.12692100	3.53279400
H	2.43952300	-4.66940300	1.85357000
H	0.92361700	-4.83257400	2.75619600
C	0.43153200	-1.76153800	3.67232000
H	1.19778700	-1.78338600	4.45830700
H	-0.41578800	-2.35572500	4.02722400
H	0.10901600	-0.72397400	3.55693500
Si	-3.38721800	-0.77264900	-1.64748700
C	-2.57220000	-1.53926800	-3.16858900
H	-3.15396300	-1.21820700	-4.04229300

H	-2.56538000	-2.63285000	-3.16632900
H	-1.54575100	-1.18849400	-3.30934700
C	-3.38806100	1.09209000	-1.96088800
H	-2.63933400	1.62543000	-1.37177600
H	-4.35956700	1.54528200	-1.74186500
H	-3.16498100	1.28002000	-3.01776100
C	-5.17589600	-1.39862400	-1.68267800
H	-5.82259000	-0.88424200	-0.96451700
H	-5.23258200	-2.47468700	-1.48028000
H	-5.59306300	-1.22806000	-2.68299800
Si	-3.60036500	-0.63650600	1.46946600
C	-2.68441900	-0.46739300	3.10740900
H	-3.33878300	0.04821400	3.82186000
H	-1.76520100	0.11311800	3.01439200
H	-2.42773100	-1.43870400	3.53860100
C	-5.01163900	-1.84649300	1.84072300
H	-4.63281800	-2.76221100	2.30990100
H	-5.59581300	-2.13333200	0.96205700
H	-5.69506000	-1.37484900	2.55811400
C	-4.35516800	1.06184600	1.12361500
H	-5.16002300	1.02629700	0.38309800
H	-3.61812000	1.79466100	0.78196900
H	-4.78838500	1.43381100	2.06073200
N	4.99022600	1.21878200	-0.44662300

E(RB3LYP) = -3274.75598268 A.U.
Zero-point correction= 0.876653 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -3273.967491

Table S10. Atomic Coordinate of ***syn*-6$_{opt}$** Calculated at the B3PW91-D3/6-31G(d) Level.



***syn*-6** (R = $SiMe_3$)

Atom	x	y	z
Si	-4.56729000	-0.64852200	-0.31120800
Si	-3.34435200	1.04733800	0.25201500
C	-4.03477100	-2.44074100	-0.70973800
C	-5.38768600	-3.01252700	-1.25355900
H	-5.46965600	-2.81008600	-2.32926500
H	-5.42716700	-4.10523200	-1.15082600
C	-6.60596800	-2.38363500	-0.55199000
H	-6.70319400	-2.84187900	0.44031100
H	-7.52285600	-2.65113400	-1.09584500
C	-6.46658600	-0.83041000	-0.41062000
Si	-2.75451600	-2.59453900	-2.12650100
Si	-3.42474300	-3.35796000	0.87355100
Si	-7.15993300	0.10184000	-1.93646200
Si	-7.39654100	-0.31028300	1.17582600
C	-3.95849200	2.72263900	0.89982600
C	-4.46153700	2.89377300	2.21045500
C	-4.84621700	4.16623900	2.65074200
H	-5.23710900	4.27109300	3.66202300

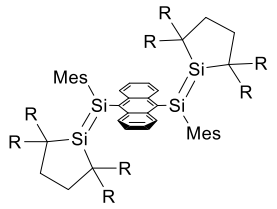
C	-4.74899900	5.29039000	1.84023000
C	-4.23182400	5.12073900	0.55347600
H	-4.13498500	5.98924600	-0.09619100
C	-3.83351700	3.87466200	0.07552000
C	-3.25433300	3.79618600	-1.31152700
H	-3.30974600	4.76437300	-1.81941700
H	-3.78920400	3.06614300	-1.92718200
H	-2.20161500	3.49310800	-1.28843900
C	-4.61580300	1.76962900	3.20194600
H	-3.90496700	1.88266800	4.03042700
H	-4.45364500	0.79357100	2.73956500
H	-5.62199400	1.76713200	3.63422800
C	-5.19687800	6.64637200	2.31519000
H	-5.37097600	6.65912000	3.39588000
H	-6.13250700	6.94412000	1.82434300
H	-4.45200700	7.41616900	2.08225200
C	-1.44729900	1.01291000	0.08318000
C	-0.79502700	1.05046600	-1.17356600
C	-1.52513200	1.10663400	-2.39851700
H	-2.60762500	1.14181500	-2.33135000
C	-0.91027000	1.09458700	-3.61966600
H	-1.50597200	1.13789800	-4.52737300
C	0.50207200	0.99995000	-3.69780900
H	0.99480900	0.95616200	-4.66562100
C	1.24160500	0.95912700	-2.54898400
H	2.32008600	0.86342300	-2.60377800
C	0.64773000	1.01227600	-1.25274000
C	1.44730200	1.01286800	-0.08321100
C	0.79503600	1.05045700	1.17353300
C	1.52514300	1.10663600	2.39848700
H	2.60763900	1.14175600	2.33132000
C	0.91028100	1.09469500	3.61963500
H	1.50598600	1.13800800	4.52734000
C	-0.50206800	1.00015600	3.69778100
H	-0.99480900	0.95645000	4.66559600
C	-1.24160200	0.95930800	2.54895900
H	-2.32008600	0.86367000	2.60375300
C	-0.64772500	1.01233500	1.25270700
Si	3.34434800	1.04730900	-0.25208300
Si	4.56731000	-0.64848000	0.31129400
C	3.95843000	2.72266000	-0.89984000
C	4.03477300	-2.44071300	0.70974500
C	6.46661000	-0.83039700	0.41064600
C	4.46137900	2.89382400	-2.21049100
C	3.83354200	3.87467100	-0.07549000
C	5.38769500	-3.01251700	1.25355300
Si	2.75453400	-2.59454700	2.12653700
Si	3.42476200	-3.35792600	-0.87357600
C	6.60598500	-2.38362400	0.55199800
Si	7.15997800	0.10184700	1.93647500
Si	7.39655500	-0.31024800	-1.17580100
C	4.84604700	4.16629400	-2.65078800
C	4.61556700	1.76968800	-3.20200200
C	4.23183400	5.12074800	-0.55345000
C	3.25449000	3.79619200	1.31161100
H	5.46967800	-2.81008900	2.32926000
H	5.42716100	-4.10522100	1.15081100
H	6.70322900	-2.84184500	-0.44031000

H	7.52286700	-2.65113200	1.09586000
H	5.23687300	4.27115900	-3.66209300
C	4.74889600	5.29042600	-1.84025000
H	3.90465900	1.88272200	-4.03042300
H	4.45345500	0.79362500	-2.73962000
H	5.62172500	1.76720600	-3.63436700
H	4.13507200	5.98924000	0.09624900
H	3.31001900	4.76436400	1.81951900
H	3.78937200	3.06609800	1.92719200
H	2.20174900	3.49319400	1.28861800
C	5.19660500	6.64645500	-2.31523400
H	5.37221900	6.65879500	-3.39568200
H	6.13132100	6.94506500	-1.82318200
H	4.45089100	7.41588000	-2.08374000
C	-6.87915700	-0.85195100	-3.54389600
H	-5.82436100	-0.94831400	-3.80565000
H	-7.31899500	-1.85537700	-3.50652800
H	-7.37468800	-0.30872800	-4.35852100
C	-6.38693500	1.81300500	-2.12443500
H	-6.23182500	2.32239200	-1.16765900
H	-5.41068900	1.72639300	-2.61266700
H	-7.02442500	2.44930900	-2.75057300
C	-9.04562500	0.29656400	-1.87860100
H	-9.40297000	0.96620200	-1.09096300
H	-9.36862400	0.71677300	-2.83962300
H	-9.54753100	-0.67009500	-1.75831700
C	-2.77179000	-4.35109000	-2.84051100
H	-2.21164900	-4.34311700	-3.78459800
H	-2.30851100	-5.09549000	-2.18870900
H	-3.79095700	-4.68286700	-3.07053300
C	-3.24839800	-1.52517300	-3.60981200
H	-2.36559200	-1.36227500	-4.23826400
H	-4.00033200	-2.03786200	-4.21982200
H	-3.64081600	-0.54369500	-3.32869400
C	-0.99356600	-2.18528800	-1.58147700
H	-0.50136900	-1.55722100	-2.33043600
H	-0.96105300	-1.64167300	-0.63444400
H	-0.39375800	-3.09380900	-1.46591400
C	-2.54236700	-2.21562500	2.08427700
H	-3.23566500	-1.55303400	2.61080800
H	-2.00900900	-2.81615000	2.83146500
H	-1.80500800	-1.58108300	1.58521000
C	-4.84486000	-4.21521300	1.78617000
H	-5.42332900	-4.87462800	1.12906500
H	-4.41076000	-4.84117300	2.57602000
H	-5.53342700	-3.51598100	2.26429200
C	-2.22329900	-4.78172400	0.51430100
H	-1.31165600	-4.47785600	-0.00715200
H	-1.92215000	-5.20342700	1.48200300
H	-2.69709700	-5.58619400	-0.05813500
C	-9.13570000	-1.06496100	1.21991300
H	-9.51295200	-1.00194900	2.24874900
H	-9.85585100	-0.56072400	0.57169800
H	-9.11681800	-2.12644600	0.94609100
C	-7.55482400	1.56195400	1.33192000
H	-7.97413200	1.81830300	2.31256700
H	-6.59482600	2.07580500	1.23682700
H	-8.22490100	1.97377700	0.57001300

C	-6.57048700	-1.04003300	2.71875400
H	-6.96340500	-2.04409200	2.91364800
H	-5.48210700	-1.11119400	2.64088700
H	-6.80549000	-0.42589800	3.59571400
C	2.54230300	-2.21562300	-2.08427200
H	1.80495800	-1.58106100	-1.58519900
H	3.23558700	-1.55304300	-2.61082900
H	2.00892100	-2.81615100	-2.83143800
C	2.22341800	-4.78177600	-0.51436600
H	1.92230300	-5.20348800	-1.48207400
H	2.69726600	-5.58621800	0.05806400
H	1.31175000	-4.47797300	0.00707800
C	4.84491500	-4.21505600	-1.78625500
H	5.42347700	-4.87443800	-1.12920400
H	4.41083500	-4.84103600	-2.57610300
H	5.53338300	-3.51574600	-2.26439800
C	0.99355800	-2.18540300	1.58152500
H	0.50131100	-1.55738200	2.33048200
H	0.96099800	-1.64179900	0.63448300
H	0.39381700	-3.09397400	1.46598700
C	3.24837600	-1.52511000	3.60981100
H	2.36555400	-1.36214400	4.23822500
H	4.00027000	-2.03779100	4.21987700
H	3.64084000	-0.54366400	3.32864900
C	2.77190600	-4.35107600	2.84059900
H	2.21174700	-4.34310300	3.78467600
H	2.30868700	-5.09553400	2.18882000
H	3.79108800	-4.68278200	3.07065700
C	6.57045600	-1.03988400	-2.71875800
H	6.96333600	-2.04394600	-2.91371200
H	5.48207400	-1.11100100	-2.64087600
H	6.80546800	-0.42570800	-3.59568700
C	7.55490200	1.56199100	-1.33180300
H	7.97429600	1.81836200	-2.31240800
H	6.59490300	2.07585200	-1.23678100
H	8.22491600	1.97378500	-0.56982600
C	9.13568200	-1.06499400	-1.21995800
H	9.51292800	-1.00190400	-2.24879100
H	9.85585400	-0.56084000	-0.57170300
H	9.11676100	-2.12650100	-0.94622500
C	6.38696000	1.81300300	2.12447400
H	7.02453600	2.44935100	2.75048100
H	6.23170400	2.32233200	1.16769000
H	5.41079100	1.72640600	2.61286600
C	9.04566600	0.29661700	1.87857900
H	9.40298800	0.96622500	1.09090500
H	9.36866900	0.71688300	2.83957500
H	9.54759100	-0.67003600	1.75833300
C	6.87929600	-0.85196900	3.54391200
H	5.82451900	-0.94845600	3.80569100
H	7.31925600	-1.85534000	3.50653800
H	7.37477900	-0.30868100	4.35852300

E(RB3LYP) = -5978.11368657 A.U.
Zero-point correction= 1.583095 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -5976.666036

Table S11. Atomic Coordinate of ***anti*-6$_{opt}$** Calculated at the B3PW91-D3/6-31G(d) Level.



***anti*-6** (R = $SiMe_3$)

Atom	x	y	z
Si	-4.77180900	0.58789100	0.25416700
Si	-3.24313900	-0.83201800	-0.31767200
C	-4.61553600	2.46094300	0.60436200
C	-6.03197900	2.74234500	1.21348200
H	-6.01208300	2.56435400	2.29634200
H	-6.31420000	3.79665200	1.08862700
C	-7.12015600	1.84071200	0.59855000
H	-7.36982900	2.23266700	-0.39540600
H	-8.04214400	1.92106800	1.19141000
C	-6.65177500	0.35140500	0.48189100
Si	-3.32554200	2.92842800	1.94404800
Si	-4.30980500	3.46162700	-1.01346100
Si	-7.02969900	-0.65579100	2.07027100
Si	-7.52678600	-0.42591500	-1.02878800
C	-3.47532300	-2.62127700	-0.90904100
C	-3.99216200	-2.94442200	-2.18507600
C	-4.07410500	-4.28324200	-2.58768800
H	-4.48179000	-4.50625900	-3.57284900
C	-3.65569300	-5.32794800	-1.77334200
C	-3.12649300	-5.00353200	-0.52162400
H	-2.78131300	-5.80463300	0.13023300
C	-3.02439000	-3.68642600	-0.08104800
C	-2.40627200	-3.43411100	1.26766400
H	-2.19707800	-4.37360700	1.78932300
H	-3.06731500	-2.83899200	1.90586900
H	-1.45968500	-2.89016900	1.17667300
C	-4.47237900	-1.91886900	-3.17863200
H	-3.81749900	-1.89504300	-4.05894600
H	-4.50486200	-0.91689100	-2.74563000
H	-5.48143000	-2.15933600	-3.52978600
C	-3.77440100	-6.76403100	-2.20733800
H	-4.03238200	-6.84604700	-3.26799400
H	-4.55276300	-7.28401900	-1.63413800
H	-2.83669600	-7.30791000	-2.04340400
C	-1.40666800	-0.34141900	-0.26711700
C	-0.70264400	-0.16224900	-1.48274100
C	-1.35566800	-0.29240500	-2.74496000
H	-2.42030200	-0.49543100	-2.74216100
C	-0.69375800	-0.14548900	-3.93125800
H	-1.22981600	-0.24869000	-4.87106800
C	0.69460300	0.14427800	-3.93116300
H	1.23085700	0.24715900	-4.87089800
C	1.35626500	0.29160700	-2.74477800
H	2.42089700	0.49464000	-2.74182800

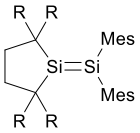
C	0.70297900	0.16189500	-1.48265200
C	1.40675200	0.34148700	-0.26694800
C	0.69841800	0.18791100	0.94934100
C	1.32923700	0.39618800	2.21192100
H	2.37272300	0.69301200	2.20322000
C	0.67516500	0.21430200	3.39871200
H	1.19639200	0.38236200	4.33721400
C	-0.67582100	-0.21285700	3.39865400
H	-1.19724200	-0.38056300	4.33711100
C	-1.32965800	-0.39517500	2.21179900
H	-2.37314500	-0.69198700	2.20299800
C	-0.69858700	-0.18738300	0.94926700
Si	3.24324000	0.83205200	-0.31727900
Si	4.77182600	-0.58784400	0.25481100
C	3.47546900	2.62115800	-0.90911400
C	4.61537400	-2.46075000	0.60562500
C	6.65176700	-0.35140000	0.48270600
C	3.99243500	2.94402000	-2.18516700
C	3.02437000	3.68648700	-0.08144200
C	6.03169800	-2.74198200	1.21509000
Si	3.32513000	-2.92770800	1.94528000
Si	4.30999000	-3.46191700	-1.01195000
C	7.11998900	-1.84072000	0.59983700
Si	7.02952000	0.65611500	2.07094100
Si	7.52699100	0.42535300	-1.02816000
C	4.07431900	4.28274100	-2.58811700
C	4.47284500	1.91824800	-3.17840400
C	3.12639500	5.00348500	-0.52235800
C	2.40617400	3.43448100	1.26729500
H	6.01168700	-2.56345500	2.29786300
H	6.31387100	-3.79636700	1.09077400
H	7.36959900	-2.23303800	-0.39399500
H	8.04196100	-1.92099300	1.19273100
H	4.48210200	4.50553100	-3.57328800
C	3.65570700	5.32762300	-1.77410200
H	3.81813800	1.89422200	-4.05884000
H	4.50523900	0.91637100	-2.74516100
H	5.48196300	2.15863700	-3.52941900
H	2.78107000	5.80472700	0.12925000
H	2.19690000	4.37410100	1.78869900
H	3.06721500	2.83956300	1.90569400
H	1.45961900	2.89047000	1.17639300
C	3.77433500	6.76360200	-2.20846400
H	4.03225100	6.84535900	-3.26915500
H	4.55271400	7.28376100	-1.63544300
H	2.83662100	7.30748800	-2.04461000
C	3.16400200	-2.57670100	-2.21681600
H	2.24126400	-2.22958400	-1.74229800
H	3.64296000	-1.70068800	-2.66499400
H	2.88411300	-3.26311200	-3.02566600
C	3.56199500	-5.17554400	-0.69666700
H	3.45701500	-5.66968200	-1.67108000
H	4.21780500	-5.80133500	-0.08186600
H	2.57152800	-5.15118800	-0.23391400
C	5.92383700	-3.86949500	-1.91342700
H	6.63924500	-4.38653800	-1.26352900
H	5.68559800	-4.54949400	-2.74111400
H	6.41621900	-2.99430300	-2.33996700

C	3.49360500	-1.80477400	3.46133100
H	2.56274700	-1.83906600	4.03789200
H	4.29903200	-2.16649900	4.11017800
H	3.69314700	-0.75875800	3.21259500
C	1.54147700	-2.93584000	1.31064300
H	0.87627200	-2.49175400	2.05937700
H	1.40895900	-2.36577600	0.38792600
H	1.20022300	-3.95998200	1.12488100
C	3.70273300	-4.64375500	2.66063400
H	3.11918700	-4.76245100	3.58296700
H	3.44032500	-5.46992100	1.99609400
H	4.76019200	-4.74415500	2.93162600
C	5.87621600	2.13872800	2.25864400
H	5.66828400	2.64390000	1.30963800
H	4.91670300	1.81471000	2.67508600
H	6.31509300	2.87197800	2.94654500
C	6.89535400	-0.39684700	3.63480500
H	5.87877400	-0.73788500	3.83567100
H	7.55296900	-1.27303100	3.59572400
H	7.21533100	0.21321300	4.48902400
C	8.82008300	1.27904200	2.13142200
H	9.05774800	2.03723400	1.37974500
H	8.98412100	1.73076100	3.11808800
H	9.53619000	0.45646300	2.02461800
C	7.26281000	2.29025100	-1.12194000
H	7.66730200	2.67458200	-2.06633100
H	6.20619100	2.56680500	-1.07695900
H	7.77451200	2.81399700	-0.30787200
C	9.39068200	0.07881900	-0.98647500
H	9.79993400	0.26876000	-1.98705100
H	9.94321200	0.70106900	-0.27895800
H	9.59463800	-0.97152600	-0.74688700
C	6.97036600	-0.39812300	-2.64282000
H	7.57969000	-1.28735700	-2.83859600
H	5.91856700	-0.69893400	-2.64334300
H	7.12391900	0.28896800	-3.48304400
C	-3.56176500	5.17529300	-0.69848200
H	-3.45639600	5.66910300	-1.67302000
H	-4.21772000	5.80134900	-0.08410200
H	-2.57146000	5.15099100	-0.23538400
C	-3.16357200	2.57603300	-2.21782300
H	-2.24095600	2.22902200	-1.74298900
H	-3.64245500	1.69990000	-2.66585400
H	-2.88347700	3.26219700	-3.02681200
C	-5.92341900	3.86908300	-1.91541000
H	-6.63896600	4.38629000	-1.26579500
H	-5.68493700	4.54890800	-2.74317100
H	-6.41573000	2.99383300	-2.34190700
C	-3.70335000	4.64470500	2.65873600
H	-3.11990300	4.76377100	3.58108500
H	-3.44092000	5.47063800	1.99391200
H	-4.76084300	4.74515100	2.92957900
C	-1.54180600	2.93650600	1.30963800
H	-0.87665600	2.49268600	2.05857800
H	-1.40915500	2.36618500	0.38710000
H	-1.20059500	3.96061400	1.12360800
C	-3.49413300	1.80600600	3.46046800
H	-2.56334400	1.84058100	4.03712600

H	-4.29966500	2.16789300	4.10909100
H	-3.69355600	0.75988300	3.21208500
C	-6.97025800	0.39712200	-2.64371000
H	-7.12357500	-0.29032100	-3.48369000
H	-7.57979900	1.28612200	-2.83986200
H	-5.91853500	0.69819800	-2.64426700
C	-9.39053800	-0.07971700	-0.98719700
H	-9.79979100	-0.27020000	-1.98766900
H	-9.94291500	-0.70174800	-0.27936300
H	-9.59468700	0.97069800	-0.74808000
C	-7.26232100	-2.29080200	-1.12193500
H	-7.66674300	-2.67552300	-2.06619800
H	-6.20566300	-2.56718000	-1.07683700
H	-7.77395400	-2.81434000	-0.30768700
C	-8.82018800	-1.27896300	2.13042100
H	-9.05756900	-2.03728400	1.37878200
H	-8.98438800	-1.73057600	3.11710800
H	-9.53638900	-0.45650200	2.02333500
C	-6.89604400	0.39745300	3.63399100
H	-5.87955700	0.73864800	3.83505000
H	-7.55376100	1.27354600	3.59460700
H	-7.21615400	-0.21250200	4.48823500
C	-5.87623600	-2.13821800	2.25847600
H	-6.31515200	-2.87140400	2.94641800
H	-5.66803800	-2.64353000	1.30960000
H	-4.91685400	-1.81399000	2.67505900

E(RB3LYP) = -5978.10979279 A.U.
Zero-point correction= 1.583234 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -5976.663305

Table S12. Atomic Coordinate of $\mathbf{7_{opt}}$ Calculated at the B3PW91-D3/6-31G(d) Level.



7 (R = $SiMe_3$)

Atom	x	y	z
Si	0.94762800	-0.00492000	-0.00021800
Si	-1.22144300	0.00570400	-0.00080900
Si	1.93199900	2.85565300	-1.12743400
Si	2.22231500	2.17074400	1.92253500
Si	2.19913700	-2.19401900	-1.92296400
Si	1.90422700	-2.87432400	1.12755200
C	2.18848000	1.44877300	0.14331300
C	3.52657700	0.72118000	-0.21891000
H	3.68916500	0.75848400	-1.30354000
H	4.38940400	1.23222400	0.23113700
C	3.51943600	-0.75656000	0.21659800
H	3.68285400	-0.79534000	1.30105300
H	4.37664400	-1.27621400	-0.23432900
C	2.17379000	-1.47085400	-0.14417900
C	3.51301800	3.88438300	-1.33118500
H	4.39629800	3.24284600	-1.43265400

H	3.69731000	4.58848000	-0.51690800
H	3.42623700	4.46467100	-2.25885500
C	0.52350200	4.01316800	-0.64459600
H	0.32092200	4.71156100	-1.46592000
H	0.77320100	4.60920900	0.23912200
H	-0.40460200	3.47847700	-0.42805000
C	1.65484700	2.17047800	-2.87156700
H	1.02795200	1.27503200	-2.89845200
H	2.61912700	1.93140100	-3.33329300
H	1.18089000	2.93503200	-3.49853000
C	3.10696300	3.84661600	2.02059700
H	3.17542600	4.12201000	3.08082800
H	2.59497900	4.66201800	1.50236000
H	4.12996700	3.78428500	1.63278600
C	0.48703600	2.36842500	2.63402800
H	0.12544000	1.40285900	3.00229800
H	-0.23809000	2.73229400	1.89877000
H	0.50155500	3.07050900	3.47674100
C	3.23523100	1.11126600	3.11687900
H	3.28672000	1.63671200	4.07896400
H	4.26475300	0.97207900	2.76693000
H	2.79739500	0.12979300	3.30153300
C	3.21974300	-1.14398800	-3.11904900
H	3.26496700	-1.66999400	-4.08114400
H	4.25102700	-1.01403300	-2.77075100
H	2.79042400	-0.15864200	-3.30311600
C	3.06905200	-3.87762000	-2.02073600
H	2.54992200	-4.68831500	-1.50219500
H	4.09261300	-3.82425400	-1.63304100
H	3.13494400	-4.15394100	-3.08088700
C	0.46140400	-2.37722700	-2.63253600
H	0.46851100	-3.08249800	-3.47268400
H	0.10894500	-1.40959200	-3.00420900
H	-0.26679000	-2.73134000	-1.89556100
C	1.63394400	-2.18578300	2.87145800
H	1.01675900	-1.28359800	2.89795100
H	2.60054700	-1.95710700	3.33358100
H	1.15140500	-2.94503900	3.49830700
C	0.48460500	-4.01883000	0.64612100
H	0.27662000	-4.71525600	1.46777000
H	0.72805300	-4.61721700	-0.23775000
H	-0.43890300	-3.47590200	0.43039600
C	3.47517300	-3.91839600	1.33115400
H	4.36475700	-3.28558300	1.43229000
H	3.65225500	-4.62432500	0.51686300
H	3.38292300	-4.49773300	2.25889000
C	-2.29904100	1.56973600	-0.06487400
C	-2.45443400	2.35455000	-1.23079600
C	-3.30797300	3.46532800	-1.21800300
H	-3.40396600	4.05790500	-2.12703400
C	-4.02304000	3.83645600	-0.08618200
C	-3.88994100	3.04155600	1.05535100
H	-4.45537800	3.30063400	1.94928000
C	-3.06046800	1.92315100	1.08302700
C	-1.73945400	2.07505100	-2.52608300
H	-2.45528000	1.88940800	-3.33601000
H	-1.08111500	1.20824700	-2.44486300
H	-1.12717800	2.93304300	-2.82212200

```
 C              -4.90244900    5.05772500   -0.07441000
 H              -5.10065300    5.42281300   -1.08730000
 H              -4.42945500    5.87487500    0.48569200
 H              -5.86541100    4.85225700    0.40725800
 C              -3.02918500    1.08960300    2.33572700
 H              -3.56296000    1.58159500    3.15525800
 H              -2.00414200    0.89994200    2.66780600
 H              -3.50174200    0.11516400    2.16403000
 C              -2.31540600   -1.54687800    0.06444400
 C              -3.08165500   -1.89209800   -1.08275600
 C              -3.92353000   -3.00117000   -1.05408500
 H              -4.49263500   -3.25409500   -1.94744900
 C              -4.06446000   -3.79432400    0.08771700
 C              -3.34416200   -3.43106500    1.21877300
 H              -3.44587600   -4.02239500    2.12799300
 C              -2.47835600   -2.32981300    1.23060800
 C              -3.04196800   -1.05940200   -2.33578700
 H              -3.58294300   -1.54509800   -3.15435100
 H              -2.01514400   -0.88251500   -2.66944700
 H              -3.50226100   -0.07917000   -2.16381400
 C              -4.95758600   -5.00560800    0.07701300
 H              -4.49428300   -5.82822500   -0.48318900
 H              -5.91854000   -4.78943500   -0.40397700
 H              -5.15911600   -5.36811200    1.09017400
 C              -1.75936600   -2.05782300    2.52526900
 H              -2.47244900   -1.86241900    3.33531700
 H              -1.09049600   -1.19928100    2.44269100
 H              -1.15755400   -2.92294000    2.82203700
---------------------------------------------------------------------
E(RB3LYP) =  -3069.46480109    A.U.
Zero-point correction=                           0.878848 (Hartree/Particle)
Sum of electronic and thermal Free Energies=       -3068.672228
```

Table S13. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{1}_{opt}$ Calculated at the TD-B3LYP/6-31+G(d) Level (The 164th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     3.0142 eV  411.33 nm  f=0.0139  <S**2>=0.000
    164 ->165       -0.21995
    164 ->166        0.66230

 Excited State   2:      Singlet-A     3.1324 eV  395.81 nm  f=0.0871  <S**2>=0.000
    164 ->165       -0.44875
    164 ->167        0.53400

 Excited State   3:      Singlet-A     3.4079 eV  363.82 nm  f=0.2347  <S**2>=0.000
    164 ->165        0.49059
    164 ->166        0.22218
    164 ->167        0.44616

 Excited State   4:      Singlet-A     3.7976 eV  326.48 nm  f=0.0019  <S**2>=0.000
    164 ->169        0.70465

 Excited State   5:      Singlet-A     3.9515 eV  313.77 nm  f=0.0204  <S**2>=0.000
    164 ->168        0.70055
```

```
Excited State   6:      Singlet-A     4.2055 eV  294.81 nm  f=0.0035  <S**2>=0.000
    164 ->170         0.66847

Excited State   7:      Singlet-A     4.2686 eV  290.46 nm  f=0.0064  <S**2>=0.000
    164 ->171        -0.36284
    164 ->172         0.56205
    164 ->178         0.12209

Excited State   8:      Singlet-A     4.2943 eV  288.72 nm  f=0.0045  <S**2>=0.000
    164 ->171         0.59545
    164 ->172         0.36360

Excited State   9:      Singlet-A     4.3592 eV  284.42 nm  f=0.0310  <S**2>=0.000
    161 ->165         0.12010
    163 ->165         0.68311

Excited State  10:      Singlet-A     4.4298 eV  279.89 nm  f=0.0147  <S**2>=0.000
    164 ->170        -0.17552
    164 ->172         0.16886
    164 ->174         0.35775
    164 ->175        -0.20661
    164 ->176         0.32457
    164 ->177         0.10984
    164 ->178        -0.30498
    164 ->181        -0.12038

Excited State  11:      Singlet-A     4.5062 eV  275.14 nm  f=0.0034  <S**2>=0.000
    161 ->165         0.58669
    162 ->165        -0.17742
    163 ->165        -0.11096
    164 ->173        -0.28279

Excited State  12:      Singlet-A     4.5200 eV  274.30 nm  f=0.0076  <S**2>=0.000
    161 ->165         0.27513
    162 ->165        -0.10233
    164 ->173         0.58756
    164 ->174        -0.12418
    164 ->179         0.14009

Excited State  13:      Singlet-A     4.5449 eV  272.80 nm  f=0.0043  <S**2>=0.000
    161 ->165         0.19706
    162 ->165         0.66656

Excited State  14:      Singlet-A     4.5887 eV  270.19 nm  f=0.0038  <S**2>=0.000
    164 ->175         0.57427
    164 ->176         0.31347
    164 ->178        -0.11895
    164 ->179         0.11657

Excited State  15:      Singlet-A     4.6607 eV  266.02 nm  f=0.0042  <S**2>=0.000
    164 ->173         0.11237
    164 ->174         0.56280
    164 ->175         0.26157
    164 ->176        -0.18888
    164 ->177        -0.12252
    164 ->178         0.14612
    164 ->179        -0.10866

Excited State  16:      Singlet-A     4.6965 eV  263.99 nm  f=0.0076  <S**2>=0.000
    164 ->175        -0.11841
```

```
    164 ->176        0.47021
    164 ->177       -0.31121
    164 ->178        0.36527

Excited State  17:     Singlet-A     4.7292 eV  262.17 nm  f=0.0020  <S**2>=0.000
    164 ->177        0.59738
    164 ->178        0.32423

Excited State  18:     Singlet-A     4.8300 eV  256.70 nm  f=0.0029  <S**2>=0.000
    164 ->173       -0.14849
    164 ->178        0.25059
    164 ->179        0.57099
    164 ->180       -0.14131
    164 ->188        0.10059

Excited State  19:     Singlet-A     4.8851 eV  253.80 nm  f=0.0044  <S**2>=0.000
    161 ->169       -0.23757
    162 ->167        0.56929
    163 ->166       -0.10877
    163 ->169        0.27961

Excited State  20:     Singlet-A     4.9378 eV  251.09 nm  f=0.0017  <S**2>=0.000
    164 ->175       -0.10478
    164 ->178       -0.10035
    164 ->180       -0.27746
    164 ->181        0.51677
    164 ->182        0.24943
    164 ->183        0.18565

Excited State  21:     Singlet-A     4.9447 eV  250.74 nm  f=0.0223  <S**2>=0.000
    160 ->165        0.62694
    163 ->166        0.27734

Excited State  22:     Singlet-A     4.9700 eV  249.46 nm  f=0.0303  <S**2>=0.000
    160 ->165       -0.28594
    161 ->166       -0.34693
    163 ->166        0.52498

Excited State  23:     Singlet-A     5.0199 eV  246.99 nm  f=0.0084  <S**2>=0.000
    159 ->165        0.43619
    161 ->166       -0.10227
    164 ->179        0.15233
    164 ->180        0.45303
    164 ->181        0.15443

Excited State  24:     Singlet-A     5.0232 eV  246.82 nm  f=0.0060  <S**2>=0.000
    158 ->165       -0.10446
    159 ->165        0.50971
    164 ->180       -0.40712
    164 ->181       -0.14524
    164 ->182       -0.14389

Excited State  25:     Singlet-A     5.0468 eV  245.67 nm  f=0.0040  <S**2>=0.000
    162 ->166        0.68892

Excited State  26:     Singlet-A     5.0632 eV  244.87 nm  f=0.0036  <S**2>=0.000
    164 ->178        0.13093
    164 ->179       -0.14579
    164 ->181       -0.26023
    164 ->182        0.56898
    164 ->184        0.10382
```

```
    164 ->185       -0.15406

 Excited State  27:     Singlet-A     5.0781 eV  244.16 nm  f=0.0440  <S**2>=0.000
    161 ->166       -0.34287
    161 ->167        0.35907
    163 ->166       -0.17558
    163 ->167        0.41353
    164 ->183       -0.12814

 Excited State  28:     Singlet-A     5.1029 eV  242.97 nm  f=0.1896  <S**2>=0.000
    158 ->165        0.12961
    161 ->166        0.37300
    162 ->166       -0.10437
    163 ->166        0.20096
    163 ->167        0.48989
    164 ->183        0.11684

 Excited State  29:     Singlet-A     5.1202 eV  242.15 nm  f=0.0355  <S**2>=0.000
    161 ->166       -0.11322
    164 ->179        0.15646
    164 ->181       -0.15740
    164 ->183        0.57951
    164 ->186        0.15027
    164 ->187       -0.15345

 Excited State  30:     Singlet-A     5.1597 eV  240.30 nm  f=0.0025  <S**2>=0.000
    158 ->165        0.11208
    164 ->181        0.19261
    164 ->182       -0.11940
    164 ->184        0.53629
    164 ->185       -0.22791
    164 ->186        0.17668
    164 ->187       -0.22689

 Excited State  31:     Singlet-A     5.1689 eV  239.86 nm  f=0.0731  <S**2>=0.000
    158 ->165        0.65174
    159 ->165        0.12900

 Excited State  32:     Singlet-A     5.1869 eV  239.03 nm  f=0.0031  <S**2>=0.000
    164 ->182        0.16310
    164 ->184        0.21295
    164 ->185        0.59113
    164 ->187       -0.13271
    164 ->188       -0.12751
```

Table S14. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of ***anti*-2$_{opt}$** Calculated at the TD-B3LYP/6-31+G(d) Level (The 306th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     2.7444 eV  451.77 nm  f=0.0515  <S**2>=0.000
    305 -> 307       0.16430
    306 -> 307       0.48263
    306 -> 308       0.35805
    306 -> 309      -0.30998

 Excited State   2:     Singlet-A     2.9047 eV  426.83 nm  f=0.0197  <S**2>=0.000
    305 -> 307      -0.19930
    305 -> 308      -0.37413
```

```
    305 -> 309       0.21946
    306 -> 307      -0.26934
    306 -> 308       0.37911
    306 -> 309      -0.18700

Excited State   3:     Singlet-A     2.9899 eV  414.68 nm  f=0.2463  <S**2>=0.000
    305 -> 307       0.39816
    305 -> 308       0.16608
    305 -> 309      -0.28118
    306 -> 307      -0.35343
    306 -> 308       0.30353

Excited State   4:     Singlet-A     3.1104 eV  398.61 nm  f=0.0410  <S**2>=0.000
    305 -> 307      -0.37819
    305 -> 308       0.41580
    305 -> 309      -0.11425
    305 -> 310       0.17360
    306 -> 309      -0.27136
    306 -> 310       0.20679
    306 -> 311      -0.10598

Excited State   5:     Singlet-A     3.1986 eV  387.62 nm  f=0.0271  <S**2>=0.000
    305 -> 309       0.17020
    305 -> 310       0.17722
    305 -> 311      -0.19643
    306 -> 307       0.20895
    306 -> 308       0.16997
    306 -> 309       0.41770
    306 -> 310       0.35238
    306 -> 311      -0.12806

Excited State   6:     Singlet-A     3.2387 eV  382.82 nm  f=0.0029  <S**2>=0.000
    305 -> 307      -0.10943
    305 -> 309      -0.17417
    305 -> 310      -0.20661
    305 -> 311      -0.32761
    306 -> 310       0.15360
    306 -> 311       0.51760

Excited State   7:     Singlet-A     3.3968 eV  365.00 nm  f=0.0482  <S**2>=0.000
    305 -> 307       0.30824
    305 -> 308      -0.11614
    305 -> 309       0.10900
    305 -> 310       0.12707
    305 -> 311      -0.15922
    306 -> 308      -0.31256
    306 -> 309      -0.31907
    306 -> 310       0.35001

Excited State   8:     Singlet-A     3.4560 eV  358.75 nm  f=0.2869  <S**2>=0.000
    305 -> 307       0.13032
    305 -> 308       0.35934
    305 -> 309       0.51946
    305 -> 310      -0.11202
    306 -> 307      -0.11570
    306 -> 310      -0.12102
    306 -> 311       0.15471

Excited State   9:     Singlet-A     3.7055 eV  334.59 nm  f=0.0060  <S**2>=0.000
    305 -> 310       0.22683
    305 -> 311       0.50062
```

```
    306 -> 310       0.21198
    306 -> 311       0.36836

Excited State  10:     Singlet-A     3.7493 eV  330.69 nm  f=0.0017  <S**2>=0.000
    305 -> 310       0.41981
    305 -> 311      -0.17358
    305 -> 313       0.16204
    305 -> 314      -0.12891
    306 -> 310      -0.24998
    306 -> 311       0.13020
    306 -> 312       0.18155
    306 -> 313      -0.32945
    306 -> 315      -0.10619

Excited State  11:     Singlet-A     3.7596 eV  329.78 nm  f=0.0014  <S**2>=0.000
    305 -> 310       0.35887
    305 -> 311      -0.15468
    305 -> 312       0.10258
    305 -> 313      -0.19627
    305 -> 314       0.13495
    306 -> 310      -0.21435
    306 -> 311       0.10892
    306 -> 312      -0.21283
    306 -> 313       0.39175
    306 -> 314      -0.10481

Excited State  12:     Singlet-A     3.7834 eV  327.71 nm  f=0.0012  <S**2>=0.000
    305 -> 313       0.15030
    305 -> 314       0.19055
    305 -> 315       0.21211
    306 -> 314       0.50389
    306 -> 315       0.34818

Excited State  13:     Singlet-A     3.9118 eV  316.95 nm  f=0.0491  <S**2>=0.000
    305 -> 314       0.11338
    305 -> 315      -0.13197
    306 -> 312       0.57810
    306 -> 313       0.33425

Excited State  14:     Singlet-A     3.9773 eV  311.73 nm  f=0.0007  <S**2>=0.000
    305 -> 312      -0.29727
    305 -> 313      -0.22531
    306 -> 312       0.10756
    306 -> 313      -0.19901
    306 -> 314      -0.30646
    306 -> 315       0.44923

Excited State  15:     Singlet-A     4.0501 eV  306.12 nm  f=0.0003  <S**2>=0.000
    305 -> 312      -0.30847
    305 -> 313       0.46131
    305 -> 314      -0.20581
    306 -> 312      -0.15493
    306 -> 313       0.23780
    306 -> 314      -0.21124

Excited State  16:     Singlet-A     4.0822 eV  303.72 nm  f=0.0054  <S**2>=0.000
    304 -> 307       0.66760
    304 -> 308      -0.16595

Excited State  17:     Singlet-A     4.1230 eV  300.71 nm  f=0.0020  <S**2>=0.000
    305 -> 313       0.17440
```

```
    305 -> 314       0.34033
    305 -> 315       0.25410
    306 -> 314      -0.20616
    306 -> 315      -0.12138
    306 -> 316      -0.24812
    306 -> 317       0.22710
    306 -> 318      -0.11015
    306 -> 321       0.18095
    306 -> 323       0.11225

Excited State  18:     Singlet-A     4.1464 eV  299.02 nm  f=0.0051  <S**2>=0.000
    305 -> 312      -0.29842
    306 -> 314       0.10170
    306 -> 315      -0.15253
    306 -> 316       0.36442
    306 -> 317       0.36413
    306 -> 321       0.17558

Excited State  19:     Singlet-A     4.1562 eV  298.31 nm  f=0.0012  <S**2>=0.000
    305 -> 312      -0.29614
    305 -> 314       0.37461
    305 -> 315       0.10106
    306 -> 315      -0.28765
    306 -> 316       0.10352
    306 -> 317      -0.32018
    306 -> 321      -0.14744

Excited State  20:     Singlet-A     4.1912 eV  295.82 nm  f=0.0014  <S**2>=0.000
    305 -> 312       0.26631
    305 -> 313       0.19964
    305 -> 314       0.11919
    305 -> 315       0.14652
    305 -> 317       0.19142
    305 -> 318      -0.12421
    305 -> 321       0.10944
    306 -> 314      -0.15562
    306 -> 315       0.10287
    306 -> 316       0.46191

Excited State  21:     Singlet-A     4.2028 eV  295.00 nm  f=0.0533  <S**2>=0.000
    304 -> 308       0.39787
    305 -> 313      -0.16778
    305 -> 314      -0.20254
    305 -> 315       0.27376
    306 -> 317      -0.13211
    306 -> 318      -0.34084

Excited State  22:     Singlet-A     4.2212 eV  293.72 nm  f=0.0828  <S**2>=0.000
    304 -> 307       0.12675
    304 -> 308       0.49558
    305 -> 313       0.10545
    305 -> 314       0.13874
    305 -> 315      -0.32118
    306 -> 318       0.19118
    306 -> 320      -0.13388

Excited State  23:     Singlet-A     4.2511 eV  291.65 nm  f=0.0067  <S**2>=0.000
    304 -> 308       0.15502
    305 -> 315       0.30203
    305 -> 316      -0.17019
    305 -> 319      -0.13328
```

```
    306 -> 317       0.27385
    306 -> 318       0.29625
    306 -> 320       0.26659
    306 -> 321      -0.17543

Excited State  24:     Singlet-A     4.2810 eV  289.61 nm  f=0.0014  <S**2>=0.000
    305 -> 317      -0.39677
    305 -> 321      -0.14983
    306 -> 316       0.16538
    306 -> 319       0.45017

Excited State  25:     Singlet-A     4.3224 eV  286.84 nm  f=0.0017  <S**2>=0.000
    305 -> 315       0.12736
    305 -> 316       0.37358
    306 -> 317       0.14018
    306 -> 320      -0.34723
    306 -> 321      -0.35082
    306 -> 323      -0.13966

Excited State  26:     Singlet-A     4.3333 eV  286.12 nm  f=0.0051  <S**2>=0.000
    305 -> 314       0.11636
    305 -> 315      -0.10172
    305 -> 318      -0.20220
    305 -> 321       0.29787
    305 -> 323       0.18158
    306 -> 316      -0.14802
    306 -> 317       0.13100
    306 -> 318      -0.21514
    306 -> 319       0.31614
    306 -> 320       0.13142

Excited State  27:     Singlet-A     4.3530 eV  284.82 nm  f=0.0037  <S**2>=0.000
    305 -> 314      -0.10417
    305 -> 315       0.17238
    305 -> 317       0.11984
    305 -> 321       0.18085
    305 -> 324       0.11838
    306 -> 318       0.35116
    306 -> 319       0.17712
    306 -> 320      -0.32126
    306 -> 321       0.15735
    306 -> 323       0.12065

Excited State  28:     Singlet-A     4.3889 eV  282.50 nm  f=0.0012  <S**2>=0.000
    300 -> 307       0.39924
    300 -> 308       0.19303
    301 -> 307       0.11736
    302 -> 307       0.48475
    302 -> 308       0.13404

Excited State  29:     Singlet-A     4.4249 eV  280.20 nm  f=0.0010  <S**2>=0.000
    305 -> 316       0.50927
    306 -> 317      -0.14040
    306 -> 318       0.18176
    306 -> 320       0.30467
    306 -> 321       0.17895
    306 -> 323      -0.10220

Excited State  30:     Singlet-A     4.4407 eV  279.20 nm  f=0.0166  <S**2>=0.000
    300 -> 307       0.31486
    300 -> 308      -0.29917
```

```
    302 -> 307      -0.26732
    302 -> 308       0.44540

 Excited State  31:     Singlet-A     4.4679 eV  277.50 nm  f=0.0013  <S**2>=0.000
    305 -> 317       0.44924
    305 -> 318       0.28271
    305 -> 321      -0.12219
    305 -> 326       0.12374
    306 -> 319       0.33537
    306 -> 325       0.10855

 Excited State  32:     Singlet-A     4.4710 eV  277.31 nm  f=0.0003  <S**2>=0.000
    305 -> 317      -0.18013
    305 -> 318       0.46540
    305 -> 320      -0.17810
    306 -> 322       0.33646
    306 -> 324       0.16987
```

Table S15. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of ***syn*-2$_{opt}$** Calculated at the TD-B3LYP/6-31+G(d) Level (The 306th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     2.5404 eV  488.05 nm  f=0.2522  <S**2>=0.000
    305 -> 307       0.11982
    306 -> 307       0.66541
    306 -> 309       0.17699

 Excited State   2:     Singlet-A     2.7518 eV  450.55 nm  f=0.0680  <S**2>=0.000
    305 -> 307       0.64086
    305 -> 309       0.20078
    306 -> 307      -0.11768
    306 -> 308      -0.12111

 Excited State   3:     Singlet-A     3.0537 eV  406.02 nm  f=0.0498  <S**2>=0.000
    305 -> 308      -0.18055
    305 -> 311       0.20336
    306 -> 308       0.51958
    306 -> 310       0.26447
    306 -> 311      -0.25015

 Excited State   4:     Singlet-A     3.1010 eV  399.82 nm  f=0.0268  <S**2>=0.000
    305 -> 308      -0.10713
    305 -> 310      -0.30433
    306 -> 307      -0.11648
    306 -> 309       0.51059
    306 -> 310      -0.23633
    306 -> 311      -0.21677

 Excited State   5:     Singlet-A     3.1943 eV  388.14 nm  f=0.0106  <S**2>=0.000
    305 -> 308       0.21038
    305 -> 309      -0.24305
    305 -> 310       0.22527
    305 -> 311       0.14367
    306 -> 308      -0.20027
    306 -> 309       0.36368
    306 -> 310       0.36620

 Excited State   6:     Singlet-A     3.3190 eV  373.56 nm  f=0.0338  <S**2>=0.000
```

```
    305 -> 308       0.11289
    305 -> 309       0.42711
    305 -> 310       0.16956
    306 -> 308       0.28407
    306 -> 309       0.21973
    306 -> 311       0.35777

Excited State   7:     Singlet-A     3.4447 eV  359.93 nm  f=0.2225  <S**2>=0.000
    305 -> 307       0.12081
    305 -> 308       0.59414
    306 -> 308       0.20044
    306 -> 310      -0.15381
    306 -> 311      -0.18958

Excited State   8:     Singlet-A     3.4756 eV  356.73 nm  f=0.1705  <S**2>=0.000
    305 -> 307      -0.20825
    305 -> 308       0.14393
    305 -> 309       0.42283
    305 -> 310      -0.11447
    305 -> 311       0.14914
    306 -> 308      -0.20385
    306 -> 310       0.27365
    306 -> 311      -0.26832

Excited State   9:     Singlet-A     3.6044 eV  343.98 nm  f=0.0080  <S**2>=0.000
    305 -> 310      -0.12371
    305 -> 312      -0.27495
    306 -> 312       0.60715
    306 -> 313       0.10530

Excited State  10:     Singlet-A     3.6754 eV  337.33 nm  f=0.0104  <S**2>=0.000
    305 -> 310       0.50846
    305 -> 311       0.15068
    306 -> 310      -0.31375
    306 -> 311      -0.26416
    306 -> 312       0.17011

Excited State  11:     Singlet-A     3.7385 eV  331.64 nm  f=0.0073  <S**2>=0.000
    305 -> 310      -0.14286
    305 -> 311       0.56727
    305 -> 315      -0.10928
    306 -> 310      -0.17124
    306 -> 311       0.22422
    306 -> 315      -0.16675

Excited State  12:     Singlet-A     3.7568 eV  330.03 nm  f=0.0027  <S**2>=0.000
    305 -> 311       0.19060
    305 -> 314      -0.16314
    305 -> 315       0.30325
    306 -> 314      -0.25820
    306 -> 315       0.49749

Excited State  13:     Singlet-A     3.8098 eV  325.44 nm  f=0.0387  <S**2>=0.000
    305 -> 314       0.14270
    306 -> 312      -0.10463
    306 -> 313       0.66468

Excited State  14:     Singlet-A     3.9096 eV  317.13 nm  f=0.0269  <S**2>=0.000
    305 -> 313       0.37519
    306 -> 314       0.52673
    306 -> 315       0.24932
```

```
Excited State  15:      Singlet-A     3.9973 eV  310.17 nm  f=0.0010  <S**2>=0.000
    305 -> 312       0.61737
    306 -> 312       0.27268
    306 -> 315      -0.11154

Excited State  16:      Singlet-A     4.0370 eV  307.12 nm  f=0.0077  <S**2>=0.000
    305 -> 313      -0.12118
    305 -> 314      -0.18373
    306 -> 316       0.59506
    306 -> 318      -0.12987
    306 -> 328       0.10684

Excited State  17:      Singlet-A     4.0797 eV  303.90 nm  f=0.0219  <S**2>=0.000
    304 -> 307      -0.20892
    305 -> 313       0.21380
    305 -> 315       0.37001
    306 -> 315      -0.26819
    306 -> 317       0.40461

Excited State  18:      Singlet-A     4.0893 eV  303.19 nm  f=0.0014  <S**2>=0.000
    305 -> 313       0.44313
    305 -> 314       0.17078
    305 -> 315      -0.28572
    306 -> 314      -0.32648
    306 -> 316       0.19203

Excited State  19:      Singlet-A     4.0996 eV  302.43 nm  f=0.0469  <S**2>=0.000
    304 -> 307       0.37162
    305 -> 313       0.25484
    305 -> 314      -0.16319
    305 -> 315       0.23098
    306 -> 315      -0.23609
    306 -> 317      -0.31346

Excited State  20:      Singlet-A     4.1290 eV  300.28 nm  f=0.0104  <S**2>=0.000
    305 -> 316       0.26176
    305 -> 328       0.10950
    306 -> 316       0.15324
    306 -> 317       0.13728
    306 -> 318       0.38701
    306 -> 319      -0.17465
    306 -> 321      -0.11735
    306 -> 324       0.31846

Excited State  21:      Singlet-A     4.1404 eV  299.45 nm  f=0.0345  <S**2>=0.000
    304 -> 307       0.51005
    305 -> 315      -0.10211
    306 -> 317       0.41397

Excited State  22:      Singlet-A     4.1630 eV  297.82 nm  f=0.0025  <S**2>=0.000
    305 -> 314      -0.40139
    305 -> 315      -0.18900
    306 -> 318       0.25282
    306 -> 319       0.42352

Excited State  23:      Singlet-A     4.2281 eV  293.24 nm  f=0.0066  <S**2>=0.000
    305 -> 314       0.13032
    305 -> 316      -0.14214
    305 -> 317       0.35994
    306 -> 318       0.17229
```

```
    306 -> 320       0.48207

Excited State  24:     Singlet-A     4.2516 eV  291.62 nm  f=0.0057  <S**2>=0.000
    300 -> 307      -0.11803
    301 -> 307      -0.13337
    305 -> 314       0.28898
    305 -> 315       0.14663
    305 -> 316      -0.18823
    305 -> 317      -0.16156
    306 -> 313      -0.11495
    306 -> 316       0.14472
    306 -> 319       0.36699
    306 -> 320      -0.12399
    306 -> 324       0.24190

Excited State  25:     Singlet-A     4.2702 eV  290.35 nm  f=0.0036  <S**2>=0.000
    300 -> 307       0.19018
    301 -> 307       0.12340
    305 -> 314      -0.20024
    305 -> 315      -0.13358
    305 -> 316      -0.22613
    305 -> 319       0.10596
    305 -> 324      -0.12356
    306 -> 318      -0.29125
    306 -> 320       0.13721
    306 -> 324       0.34837
    306 -> 328      -0.10616

Excited State  26:     Singlet-A     4.2755 eV  289.99 nm  f=0.0081  <S**2>=0.000
    300 -> 307       0.35948
    301 -> 307       0.36130
    302 -> 307       0.11703
    303 -> 307      -0.28409
    305 -> 314       0.18113
    306 -> 318       0.11182
    306 -> 320      -0.15794

Excited State  27:     Singlet-A     4.3035 eV  288.10 nm  f=0.0015  <S**2>=0.000
    303 -> 307      -0.11180
    305 -> 318       0.17071
    305 -> 321      -0.13272
    305 -> 324       0.32924
    305 -> 325       0.11781
    306 -> 316      -0.17132
    306 -> 319       0.11824
    306 -> 321      -0.16530
    306 -> 322       0.17192
    306 -> 324       0.10312
    306 -> 325       0.19543
    306 -> 328       0.22435

Excited State  28:     Singlet-A     4.3122 eV  287.52 nm  f=0.0011  <S**2>=0.000
    300 -> 307      -0.18206
    301 -> 307      -0.19097
    302 -> 307       0.56374
    303 -> 307      -0.28190

Excited State  29:     Singlet-A     4.3540 eV  284.76 nm  f=0.0002  <S**2>=0.000
    305 -> 316       0.51038
    306 -> 318      -0.31295
    306 -> 319       0.27715
```

```
    306 -> 320       0.14553

 Excited State  30:     Singlet-A     4.3650 eV  284.04 nm  f=0.0096  <S**2>=0.000
    300 -> 307       0.47300
    300 -> 308       0.10504
    301 -> 307      -0.32224
    301 -> 308      -0.13021
    302 -> 307       0.17840
    303 -> 307       0.25672

 Excited State  31:     Singlet-A     4.3833 eV  282.85 nm  f=0.0023  <S**2>=0.000
    300 -> 307      -0.10916
    301 -> 307       0.36180
    302 -> 307       0.31759
    303 -> 307       0.45861
    303 -> 308       0.12929

 Excited State  32:     Singlet-A     4.3903 eV  282.40 nm  f=0.0047  <S**2>=0.000
    305 -> 316       0.13553
    305 -> 317      -0.28202
    305 -> 318       0.26532
    305 -> 319       0.38593
    306 -> 321       0.24635
    306 -> 322       0.20063
```

Table S16. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of ***anti*-3$_{opt}$** Calculated at the TD-B3LYP/6-31+G(d) Level (The 327th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:     Singlet-A     2.4662 eV  502.73 nm  f=0.0286  <S**2>=0.000
    326 -> 328       0.10437
    327 -> 328       0.68108

 Excited State   2:     Singlet-A     2.4975 eV  496.42 nm  f=0.0085  <S**2>=0.000
    326 -> 328       0.67896
    327 -> 328      -0.10019

 Excited State   3:     Singlet-A     3.1027 eV  399.60 nm  f=0.3132  <S**2>=0.000
    325 -> 328       0.11736
    326 -> 330       0.13023
    326 -> 331       0.23860
    326 -> 332      -0.14639
    327 -> 328      -0.11133
    327 -> 329       0.45082
    327 -> 330      -0.25070
    327 -> 331      -0.25303
    327 -> 332      -0.18735

 Excited State   4:     Singlet-A     3.1360 eV  395.36 nm  f=0.0185  <S**2>=0.000
    326 -> 329       0.37502
    326 -> 330      -0.13548
    326 -> 331      -0.13208
    326 -> 332      -0.35169
    327 -> 329       0.13475
    327 -> 330       0.15302
    327 -> 331       0.29121
    327 -> 332      -0.22826
```

```
Excited State   5:      Singlet-A     3.1880 eV  388.91 nm  f=0.0114  <S**2>=0.000
    326 -> 329      -0.39373
    326 -> 331      -0.14090
    327 -> 329       0.43028
    327 -> 330       0.30086
    327 -> 331       0.16611

Excited State   6:      Singlet-A     3.2257 eV  384.37 nm  f=0.0026  <S**2>=0.000
    326 -> 330       0.54179
    326 -> 332      -0.10998
    327 -> 330       0.39595
    327 -> 332      -0.11033

Excited State   7:      Singlet-A     3.3279 eV  372.56 nm  f=0.6866  <S**2>=0.000
    325 -> 328       0.31052
    326 -> 329       0.16530
    326 -> 330       0.30996
    326 -> 331      -0.24867
    326 -> 332       0.18320
    327 -> 329       0.13145
    327 -> 330      -0.20005
    327 -> 331       0.25740
    327 -> 332       0.22626

Excited State   8:      Singlet-A     3.3814 eV  366.67 nm  f=0.0327  <S**2>=0.000
    326 -> 329       0.38056
    326 -> 330      -0.12195
    326 -> 331       0.10498
    326 -> 332       0.29529
    327 -> 329       0.17733
    327 -> 330       0.30254
    327 -> 331      -0.24457
    327 -> 332       0.20076

Excited State   9:      Singlet-A     3.5702 eV  347.28 nm  f=0.6171  <S**2>=0.000
    325 -> 328       0.60921
    326 -> 329      -0.11893
    326 -> 330      -0.19312
    327 -> 329      -0.14171
    327 -> 330       0.13273

Excited State  10:      Singlet-A     3.7644 eV  329.36 nm  f=0.0280  <S**2>=0.000
    325 -> 329      -0.24771
    326 -> 332       0.10141
    326 -> 333      -0.12226
    327 -> 333       0.59518

Excited State  11:      Singlet-A     3.7758 eV  328.37 nm  f=0.0286  <S**2>=0.000
    325 -> 329       0.57540
    326 -> 333       0.24110
    327 -> 333       0.25063

Excited State  12:      Singlet-A     3.7907 eV  327.08 nm  f=0.0284  <S**2>=0.000
    325 -> 329      -0.29921
    325 -> 330      -0.11040
    326 -> 331       0.15256
    326 -> 333       0.50862
    327 -> 331       0.10974
    327 -> 332       0.17641
    327 -> 337       0.11815
```

```
Excited State  13:      Singlet-A     3.8122 eV  325.23 nm  f=0.0007  <S**2>=0.000
    326 -> 336      -0.32020
    326 -> 337       0.25618
    327 -> 336       0.46545
    327 -> 337      -0.28469

Excited State  14:      Singlet-A     3.8181 eV  324.73 nm  f=0.0100  <S**2>=0.000
    325 -> 330       0.41151
    326 -> 332      -0.23719
    326 -> 336       0.14048
    326 -> 337       0.24573
    327 -> 331      -0.14334
    327 -> 332       0.28152
    327 -> 336       0.15978
    327 -> 337       0.19038

Excited State  15:      Singlet-A     3.8195 eV  324.61 nm  f=0.0053  <S**2>=0.000
    325 -> 330      -0.22175
    326 -> 331      -0.17081
    326 -> 332       0.21918
    326 -> 335       0.11317
    326 -> 336       0.23999
    326 -> 337       0.30055
    327 -> 332      -0.28204
    327 -> 336       0.14411
    327 -> 337       0.28396

Excited State  16:      Singlet-A     3.8212 eV  324.46 nm  f=0.0200  <S**2>=0.000
    325 -> 330       0.49471
    326 -> 331       0.11491
    326 -> 332       0.29674
    326 -> 333       0.14149
    327 -> 331       0.14703
    327 -> 332      -0.29301

Excited State  17:      Singlet-A     3.8325 eV  323.51 nm  f=0.0034  <S**2>=0.000
    326 -> 331       0.48633
    326 -> 333      -0.26510
    326 -> 336       0.12049
    327 -> 331       0.34121
    327 -> 332       0.10661

Excited State  18:      Singlet-A     3.9676 eV  312.49 nm  f=0.0035  <S**2>=0.000
    326 -> 335       0.36606
    327 -> 334       0.56442
    327 -> 335      -0.13342

Excited State  19:      Singlet-A     3.9752 eV  311.89 nm  f=0.0315  <S**2>=0.000
    326 -> 334       0.51852
    326 -> 335       0.13355
    327 -> 335       0.43235

Excited State  20:      Singlet-A     4.1926 eV  295.72 nm  f=0.0007  <S**2>=0.000
    326 -> 334      -0.28914
    326 -> 335      -0.24796
    326 -> 339       0.14931
    327 -> 334       0.25379
    327 -> 335       0.34999
    327 -> 336      -0.14237
    327 -> 337      -0.11473
    327 -> 338       0.10946
```

```
    327 -> 339      -0.21884

Excited State  21:     Singlet-A     4.2012 eV  295.12 nm  f=0.0010  <S**2>=0.000
    326 -> 334      -0.28484
    326 -> 335       0.39044
    326 -> 336      -0.13459
    326 -> 337      -0.12338
    326 -> 339       0.11696
    326 -> 341       0.13285
    327 -> 334      -0.20128
    327 -> 335       0.25870
    327 -> 338      -0.15049
    327 -> 339       0.15043
    327 -> 341       0.11078

Excited State  22:     Singlet-A     4.2273 eV  293.30 nm  f=0.0010  <S**2>=0.000
    326 -> 335      -0.20669
    326 -> 336      -0.14940
    326 -> 337      -0.26361
    326 -> 338       0.14226
    326 -> 341       0.12079
    327 -> 335       0.18003
    327 -> 336       0.17800
    327 -> 337       0.34056
    327 -> 338      -0.31730
    327 -> 341      -0.13923

Excited State  23:     Singlet-A     4.2430 eV  292.21 nm  f=0.0051  <S**2>=0.000
    326 -> 333       0.11218
    326 -> 337      -0.16804
    326 -> 338       0.28845
    326 -> 339       0.30993
    326 -> 341      -0.12899
    326 -> 342       0.10727
    327 -> 336       0.13746
    327 -> 338       0.29910
    327 -> 339       0.26770

Excited State  24:     Singlet-A     4.2511 eV  291.65 nm  f=0.0010  <S**2>=0.000
    326 -> 336       0.45786
    326 -> 337      -0.25833
    327 -> 336       0.28036
    327 -> 337      -0.26775
    327 -> 338      -0.14043

Excited State  25:     Singlet-A     4.2584 eV  291.16 nm  f=0.0011  <S**2>=0.000
    326 -> 337       0.23987
    326 -> 338       0.34524
    326 -> 341       0.11957
    327 -> 336      -0.21001
    327 -> 337      -0.20287
    327 -> 338      -0.28626
    327 -> 339       0.16112
    327 -> 341      -0.25635

Excited State  26:     Singlet-A     4.2933 eV  288.78 nm  f=0.0185  <S**2>=0.000
    321 -> 328       0.37883
    321 -> 330       0.11095
    326 -> 342      -0.29481
    327 -> 339      -0.11722
    327 -> 340       0.37786
```

```
    327 -> 342       0.20942

 Excited State  27:     Singlet-A     4.2968 eV  288.55 nm  f=0.0044  <S**2>=0.000
    321 -> 328      -0.11362
    322 -> 328       0.36836
    322 -> 329      -0.10005
    326 -> 340       0.36165
    326 -> 342      -0.11965
    327 -> 340       0.18570
    327 -> 342      -0.28464

 Excited State  28:     Singlet-A     4.3054 eV  287.97 nm  f=0.0001  <S**2>=0.000
    321 -> 328      -0.33698
    321 -> 330      -0.10750
    322 -> 328       0.36747
    326 -> 340      -0.27018
    327 -> 339      -0.10104
    327 -> 342       0.31219

 Excited State  29:     Singlet-A     4.3071 eV  287.86 nm  f=0.0028  <S**2>=0.000
    321 -> 328       0.41861
    322 -> 328       0.39385
    326 -> 340      -0.10740
    326 -> 342       0.19089
    327 -> 340      -0.24823

 Excited State  30:     Singlet-A     4.3295 eV  286.37 nm  f=0.0013  <S**2>=0.000
    321 -> 328       0.10398
    322 -> 328      -0.10059
    323 -> 328       0.66159
    323 -> 330       0.14899

 Excited State  31:     Singlet-A     4.3381 eV  285.80 nm  f=0.0001  <S**2>=0.000
    324 -> 328      -0.19726
    326 -> 335      -0.19644
    326 -> 339       0.11025
    326 -> 340      -0.11186
    326 -> 343       0.17463
    327 -> 334       0.18579
    327 -> 338      -0.12963
    327 -> 339       0.34838
    327 -> 340       0.14934
    327 -> 341       0.34333

 Excited State  32:     Singlet-A     4.3404 eV  285.65 nm  f=0.0011  <S**2>=0.000
    322 -> 328       0.13781
    324 -> 328       0.62724
    324 -> 329      -0.12592
    327 -> 339       0.11854
    327 -> 341       0.11877
```

Table S17. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of ***syn*-3$_{opt}$** Calculated at the TD-B3LYP/6-31+G(d) Level (The 327th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:     Singlet-A     2.4872 eV  498.48 nm  f=0.0467  <S**2>=0.000
    326 -> 328      -0.22923
    327 -> 328       0.63372
```

```
    327 -> 330       0.15996

Excited State   2:     Singlet-A     2.5163 eV  492.73 nm  f=0.0167  <S**2>=0.000
    326 -> 328       0.63327
    326 -> 330       0.16784
    327 -> 328       0.23110

Excited State   3:     Singlet-A     3.0562 eV  405.69 nm  f=0.0525  <S**2>=0.000
    325 -> 328       0.11722
    326 -> 329      -0.23174
    326 -> 330      -0.14970
    326 -> 332       0.23373
    327 -> 329       0.45693
    327 -> 330      -0.27982
    327 -> 331      -0.22038

Excited State   4:     Singlet-A     3.0794 eV  402.62 nm  f=0.1199  <S**2>=0.000
    326 -> 331       0.11914
    326 -> 332       0.15342
    327 -> 329       0.33487
    327 -> 330       0.46623
    327 -> 331       0.31020

Excited State   5:     Singlet-A     3.0855 eV  401.83 nm  f=0.0725  <S**2>=0.000
    326 -> 329       0.48655
    326 -> 330       0.11923
    326 -> 332      -0.25022
    327 -> 329       0.39739
    327 -> 332       0.10106

Excited State   6:     Singlet-A     3.1454 eV  394.17 nm  f=0.0076  <S**2>=0.000
    326 -> 328      -0.17261
    326 -> 329      -0.18726
    326 -> 330       0.62670
    327 -> 330      -0.15731

Excited State   7:     Singlet-A     3.3175 eV  373.73 nm  f=0.2987  <S**2>=0.000
    325 -> 328       0.31189
    326 -> 330      -0.11270
    326 -> 331       0.11366
    326 -> 332      -0.26006
    327 -> 328       0.10251
    327 -> 330      -0.24599
    327 -> 331       0.46268

Excited State   8:     Singlet-A     3.3995 eV  364.71 nm  f=0.2719  <S**2>=0.000
    326 -> 329       0.35683
    326 -> 331       0.11928
    326 -> 332       0.45237
    327 -> 330      -0.20517
    327 -> 331       0.21234
    327 -> 332      -0.18936

Excited State   9:     Singlet-A     3.5577 eV  348.50 nm  f=0.4919  <S**2>=0.000
    325 -> 328       0.60475
    326 -> 329       0.12947
    326 -> 330       0.10257
    326 -> 332       0.11165
    327 -> 330       0.18840
    327 -> 331      -0.16842
```

```
Excited State  10:      Singlet-A     3.6893 eV  336.07 nm  f=0.0079  <S**2>=0.000
    326 -> 334       0.19277
    327 -> 333       0.17259
    327 -> 334       0.62651
    327 -> 335      -0.16596

Excited State  11:      Singlet-A     3.7085 eV  334.32 nm  f=0.0286  <S**2>=0.000
    325 -> 329       0.61132
    327 -> 333       0.29476

Excited State  12:      Singlet-A     3.7118 eV  334.03 nm  f=0.0021  <S**2>=0.000
    325 -> 329      -0.32488
    327 -> 333       0.54888
    327 -> 334      -0.17461
    327 -> 337      -0.11337

Excited State  13:      Singlet-A     3.7425 eV  331.29 nm  f=0.0144  <S**2>=0.000
    326 -> 333       0.66325

Excited State  14:      Singlet-A     3.8148 eV  325.01 nm  f=0.0001  <S**2>=0.000
    326 -> 332       0.23331
    327 -> 332       0.65241

Excited State  15:      Singlet-A     3.8351 eV  323.29 nm  f=0.0008  <S**2>=0.000
    326 -> 331       0.66495
    327 -> 331      -0.20435

Excited State  16:      Singlet-A     3.8381 eV  323.04 nm  f=0.1729  <S**2>=0.000
    325 -> 330       0.68747

Excited State  17:      Singlet-A     3.8623 eV  321.01 nm  f=0.0020  <S**2>=0.000
    326 -> 336       0.41942
    326 -> 337       0.48839
    327 -> 336      -0.15423
    327 -> 337      -0.17569

Excited State  18:      Singlet-A     3.9742 eV  311.98 nm  f=0.0259  <S**2>=0.000
    326 -> 336       0.10482
    327 -> 334       0.14921
    327 -> 335       0.59339
    327 -> 336       0.24599
    327 -> 337      -0.15202

Excited State  19:      Singlet-A     4.0087 eV  309.29 nm  f=0.0114  <S**2>=0.000
    326 -> 333       0.10289
    326 -> 334       0.12242
    326 -> 335       0.55911
    326 -> 336      -0.20467
    326 -> 337       0.23565
    327 -> 336       0.14003
    327 -> 337      -0.13135

Excited State  20:      Singlet-A     4.1631 eV  297.82 nm  f=0.0005  <S**2>=0.000
    326 -> 334       0.66276
    327 -> 334      -0.19952

Excited State  21:      Singlet-A     4.1783 eV  296.73 nm  f=0.0028  <S**2>=0.000
    326 -> 335      -0.13418
    326 -> 336       0.12580
    327 -> 335      -0.23953
    327 -> 336       0.40571
```

```
    327 -> 337      -0.28882
    327 -> 338      -0.29974
    327 -> 339       0.18228

Excited State  22:     Singlet-A     4.2034 eV  294.96 nm  f=0.0028  <S**2>=0.000
    321 -> 328       0.47795
    321 -> 330      -0.17978
    322 -> 328       0.40994
    322 -> 330      -0.12985
    324 -> 328       0.18954

Excited State  23:     Singlet-A     4.2178 eV  293.96 nm  f=0.0007  <S**2>=0.000
    326 -> 335       0.28904
    326 -> 336       0.36580
    326 -> 337      -0.29831
    326 -> 338       0.33904
    327 -> 336      -0.10571
    327 -> 337       0.11401
    327 -> 338      -0.16848

Excited State  24:     Singlet-A     4.2362 eV  292.68 nm  f=0.0022  <S**2>=0.000
    326 -> 337       0.12907
    327 -> 333       0.13190
    327 -> 336       0.12326
    327 -> 337       0.33488
    327 -> 339       0.47655
    327 -> 340       0.11586
    327 -> 341      -0.20110

Excited State  25:     Singlet-A     4.2503 eV  291.71 nm  f=0.0003  <S**2>=0.000
    321 -> 328      -0.11750
    322 -> 328      -0.14022
    324 -> 328       0.64423
    324 -> 330      -0.18553

Excited State  26:     Singlet-A     4.2660 eV  290.63 nm  f=0.0003  <S**2>=0.000
    326 -> 337       0.17257
    326 -> 341       0.11287
    327 -> 336       0.35215
    327 -> 337       0.39198
    327 -> 339      -0.35027
    327 -> 341       0.13007

Excited State  27:     Singlet-A     4.2797 eV  289.70 nm  f=0.0067  <S**2>=0.000
    326 -> 335      -0.12348
    326 -> 336      -0.19970
    326 -> 338       0.29023
    326 -> 339       0.44476
    326 -> 340      -0.12040
    326 -> 341       0.24266
    327 -> 338      -0.13045
    327 -> 341      -0.17550

Excited State  28:     Singlet-A     4.2916 eV  288.90 nm  f=0.0046  <S**2>=0.000
    326 -> 338       0.14830
    327 -> 336       0.14331
    327 -> 337      -0.10494
    327 -> 338       0.33194
    327 -> 340       0.45948
    327 -> 342       0.23828
```

```
 Excited State  29:      Singlet-A     4.3400 eV  285.68 nm  f=0.0040  <S**2>=0.000
    326 -> 338      -0.20363
    326 -> 340      -0.37429
    326 -> 342       0.38264
    327 -> 340       0.23524
    327 -> 341       0.10204
    327 -> 342      -0.15642

 Excited State  30:      Singlet-A     4.3473 eV  285.20 nm  f=0.0097  <S**2>=0.000
    326 -> 336       0.13628
    326 -> 340      -0.20682
    326 -> 342       0.11720
    327 -> 335      -0.13560
    327 -> 336       0.17153
    327 -> 338       0.36413
    327 -> 340      -0.30927
    327 -> 341      -0.21166
    327 -> 342      -0.10608
    327 -> 344       0.10812
    327 -> 345      -0.13961

 Excited State  31:      Singlet-A     4.3559 eV  284.64 nm  f=0.0040  <S**2>=0.000
    321 -> 328      -0.37358
    322 -> 328       0.38196
    323 -> 328       0.38502

 Excited State  32:      Singlet-A     4.3791 eV  283.13 nm  f=0.0010  <S**2>=0.000
    321 -> 328       0.18542
    321 -> 329      -0.15699
    322 -> 328      -0.28653
    322 -> 329       0.22503
    323 -> 328       0.52060
```

Table S18. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{4}_{\mathbf{opt}}$ Calculated at the TD-B3LYP/6-31+G(d) Level (The 189th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     1.8427 eV  672.83 nm  f=0.0252  <S**2>=0.000
    189 ->190        0.70469

 Excited State   2:      Singlet-A     2.9087 eV  426.25 nm  f=0.1061  <S**2>=0.000
    188 ->190       -0.12080
    189 ->191        0.63315
    189 ->193        0.21586
    189 ->197        0.12296

 Excited State   3:      Singlet-A     3.0611 eV  405.03 nm  f=0.1495  <S**2>=0.000
    188 ->190        0.68509
    189 ->193        0.10596

 Excited State   4:      Singlet-A     3.2718 eV  378.95 nm  f=0.0062  <S**2>=0.000
    189 ->192        0.69939

 Excited State   5:      Singlet-A     3.5104 eV  353.19 nm  f=0.0286  <S**2>=0.000
    189 ->191       -0.10513
    189 ->193        0.58177
    189 ->194        0.14553
    189 ->195       -0.24065
    189 ->197       -0.19412
```

```
    189 ->200       -0.10339

Excited State   6:     Singlet-A     3.6334 eV  341.23 nm  f=0.0016  <S**2>=0.000
    189 ->195        0.54046
    189 ->196       -0.22371
    189 ->197       -0.30651
    189 ->199        0.14843
    189 ->200       -0.14753

Excited State   7:     Singlet-A     3.7330 eV  332.13 nm  f=0.1625  <S**2>=0.000
    188 ->191        0.17068
    189 ->191        0.21183
    189 ->193       -0.24828
    189 ->194        0.44468
    189 ->195       -0.17090
    189 ->196       -0.25743
    189 ->197       -0.17501

Excited State   8:     Singlet-A     3.7802 eV  327.98 nm  f=0.0230  <S**2>=0.000
    189 ->194        0.49404
    189 ->195        0.29043
    189 ->196        0.36698

Excited State   9:     Singlet-A     3.7920 eV  326.97 nm  f=0.0412  <S**2>=0.000
    188 ->191        0.16304
    189 ->191        0.11786
    189 ->194       -0.14838
    189 ->195       -0.10943
    189 ->196        0.48417
    189 ->197       -0.36906
    189 ->199        0.12033
    189 ->200       -0.13682

Excited State  10:     Singlet-A     3.8052 eV  325.83 nm  f=0.0244  <S**2>=0.000
    185 ->190        0.42520
    186 ->190       -0.23192
    187 ->190        0.20305
    188 ->191        0.19577
    188 ->192        0.38535

Excited State  11:     Singlet-A     3.9013 eV  317.80 nm  f=0.0174  <S**2>=0.000
    185 ->190       -0.19072
    186 ->190       -0.27274
    187 ->190        0.56752
    188 ->191       -0.20884
    188 ->192       -0.10055

Excited State  12:     Singlet-A     3.9184 eV  316.41 nm  f=0.0022  <S**2>=0.000
    185 ->190        0.17603
    186 ->190        0.54688
    187 ->190        0.24550
    188 ->191       -0.27794
    188 ->192        0.16251

Excited State  13:     Singlet-A     3.9298 eV  315.50 nm  f=0.0282  <S**2>=0.000
    185 ->190       -0.14513
    186 ->190        0.25629
    187 ->190        0.26977
    188 ->191        0.51768
    188 ->192       -0.17429
    189 ->197        0.11347
```

```
Excited State  14:      Singlet-A     4.0615 eV  305.27 nm  f=0.0067  <S**2>=0.000
    189 ->198        0.69344

Excited State  15:      Singlet-A     4.1134 eV  301.42 nm  f=0.0008  <S**2>=0.000
    189 ->197        0.35602
    189 ->199        0.50818
    189 ->200       -0.32426

Excited State  16:      Singlet-A     4.1422 eV  299.32 nm  f=0.0040  <S**2>=0.000
    189 ->199        0.40870
    189 ->200        0.54876
    189 ->203        0.10316

Excited State  17:      Singlet-A     4.3325 eV  286.18 nm  f=0.0004  <S**2>=0.000
    189 ->201        0.48300
    189 ->202        0.25877
    189 ->203       -0.33244
    189 ->205       -0.14564
    189 ->206       -0.17945

Excited State  18:      Singlet-A     4.3891 eV  282.48 nm  f=0.0007  <S**2>=0.000
    182 ->190        0.59829
    183 ->190       -0.15248
    184 ->190       -0.20484
    188 ->196        0.22696

Excited State  19:      Singlet-A     4.4284 eV  279.98 nm  f=0.0018  <S**2>=0.000
    189 ->200       -0.10394
    189 ->201        0.46070
    189 ->202       -0.37565
    189 ->203        0.34168

Excited State  20:      Singlet-A     4.4561 eV  278.24 nm  f=0.0013  <S**2>=0.000
    189 ->202        0.48753
    189 ->203        0.43982
    189 ->204        0.18194
    189 ->205       -0.12026

Excited State  21:      Singlet-A     4.4817 eV  276.65 nm  f=0.0070  <S**2>=0.000
    188 ->193        0.53716
    189 ->202       -0.13588
    189 ->204        0.40957

Excited State  22:      Singlet-A     4.4840 eV  276.50 nm  f=0.0010  <S**2>=0.000
    188 ->193       -0.42824
    189 ->203       -0.12155
    189 ->204        0.52200

Excited State  23:      Singlet-A     4.5001 eV  275.51 nm  f=0.0006  <S**2>=0.000
    189 ->201        0.16100
    189 ->202        0.11021
    189 ->204        0.12656
    189 ->205        0.64815

Excited State  24:      Singlet-A     4.5497 eV  272.51 nm  f=0.0090  <S**2>=0.000
    183 ->190       -0.45780
    184 ->190        0.50864
    189 ->206        0.11389

Excited State  25:      Singlet-A     4.5555 eV  272.17 nm  f=0.0006  <S**2>=0.000
```

```
    184 ->190       -0.18571
    189 ->203       -0.16021
    189 ->206        0.58132
    189 ->210       -0.18948

Excited State  26:     Singlet-A     4.5679 eV  271.43 nm  f=0.0051  <S**2>=0.000
    182 ->190        0.24696
    183 ->190        0.50631
    184 ->190        0.38786
    189 ->206        0.12722

Excited State  27:     Singlet-A     4.6984 eV  263.89 nm  f=0.0636  <S**2>=0.000
    185 ->190        0.12915
    187 ->191       -0.23133
    188 ->192       -0.16672
    188 ->194       -0.25477
    188 ->195        0.49298
    189 ->208        0.13851

Excited State  28:     Singlet-A     4.7253 eV  262.38 nm  f=0.0409  <S**2>=0.000
    187 ->191        0.10113
    188 ->194        0.11842
    188 ->195       -0.20464
    188 ->197       -0.12415
    189 ->205        0.12957
    189 ->207        0.32565
    189 ->208        0.42170
    189 ->211       -0.12712
    189 ->214        0.12598

Excited State  29:     Singlet-A     4.7425 eV  261.43 nm  f=0.0325  <S**2>=0.000
    186 ->191        0.10996
    186 ->195        0.17841
    187 ->191        0.51105
    187 ->193        0.11310
    188 ->194       -0.18676
    188 ->195        0.20334
    188 ->196        0.14942
    188 ->197        0.12599

Excited State  30:     Singlet-A     4.7566 eV  260.66 nm  f=0.0635  <S**2>=0.000
    181 ->190       -0.14587
    187 ->191       -0.21994
    188 ->192        0.10705
    188 ->195       -0.21718
    188 ->196        0.37978
    188 ->197        0.32502
    188 ->199       -0.15574
    188 ->200        0.14302
    189 ->207        0.12283

Excited State  31:     Singlet-A     4.7802 eV  259.37 nm  f=0.4387  <S**2>=0.000
    185 ->190       -0.26046
    188 ->192        0.29132
    188 ->195        0.13275
    188 ->196       -0.15797
    189 ->207        0.46981
    189 ->209       -0.12589

Excited State  32:     Singlet-A     4.7872 eV  258.99 nm  f=0.5093  <S**2>=0.000
    185 ->190       -0.27383
```

```
    188 ->192        0.30772
    188 ->195        0.11970
    189 ->207       -0.34065
    189 ->208        0.35486
```

Table S19. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{5_{opt}}$ Calculated at the TD-B3LYP/6-31+G(d) Level (The 189th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     1.8061 eV  686.47 nm  f=0.0710  <S**2>=0.000
    189 ->190        0.70441

 Excited State   2:      Singlet-A     2.9112 eV  425.89 nm  f=0.1115  <S**2>=0.000
    188 ->190       -0.15882
    189 ->191        0.63103
    189 ->192        0.13578
    189 ->193       -0.18202

 Excited State   3:      Singlet-A     3.1107 eV  398.57 nm  f=0.0952  <S**2>=0.000
    188 ->190        0.67655
    189 ->191        0.11588
    189 ->193       -0.11039

 Excited State   4:      Singlet-A     3.3704 eV  367.86 nm  f=0.0271  <S**2>=0.000
    189 ->191       -0.12303
    189 ->192        0.68240

 Excited State   5:      Singlet-A     3.5190 eV  352.32 nm  f=0.0036  <S**2>=0.000
    181 ->190        0.10029
    184 ->190        0.36691
    186 ->190        0.36695
    187 ->190        0.45030

 Excited State   6:      Singlet-A     3.5608 eV  348.20 nm  f=0.0339  <S**2>=0.000
    189 ->191        0.16839
    189 ->193        0.64105
    189 ->194        0.12416

 Excited State   7:      Singlet-A     3.6974 eV  335.33 nm  f=0.0226  <S**2>=0.000
    189 ->194        0.67324

 Excited State   8:      Singlet-A     3.7223 eV  333.08 nm  f=0.0078  <S**2>=0.000
    184 ->190       -0.11469
    186 ->190       -0.46626
    187 ->190        0.49151
    189 ->194        0.10688

 Excited State   9:      Singlet-A     3.8207 eV  324.51 nm  f=0.0355  <S**2>=0.000
    184 ->190        0.28718
    185 ->190        0.44489
    186 ->190       -0.28940
    188 ->192        0.23778
    189 ->195        0.13705
    189 ->197       -0.11092

 Excited State  10:      Singlet-A     3.8566 eV  321.49 nm  f=0.0150  <S**2>=0.000
    182 ->190       -0.10365
    184 ->190        0.36971
```

```
    185 ->190       -0.15579
    186 ->190       -0.20654
    187 ->190       -0.14889
    188 ->192       -0.10170
    189 ->195       -0.33509
    189 ->196        0.15522
    189 ->197        0.23670
    189 ->199       -0.11309

Excited State  11:     Singlet-A     3.8704 eV  320.34 nm  f=0.0701  <S**2>=0.000
    184 ->190       -0.25792
    185 ->190        0.34966
    186 ->190        0.12112
    187 ->190        0.10372
    188 ->191       -0.13528
    188 ->192        0.21201
    189 ->195       -0.32218
    189 ->196        0.17794
    189 ->197        0.19653

Excited State  12:     Singlet-A     3.9383 eV  314.82 nm  f=0.0116  <S**2>=0.000
    188 ->191        0.48994
    189 ->196        0.44874
    189 ->197       -0.15665

Excited State  13:     Singlet-A     3.9705 eV  312.26 nm  f=0.0222  <S**2>=0.000
    188 ->191       -0.42915
    189 ->195        0.24947
    189 ->196        0.46914
    189 ->197       -0.11509

Excited State  14:     Singlet-A     4.0542 eV  305.81 nm  f=0.1074  <S**2>=0.000
    188 ->191        0.17993
    189 ->191        0.11112
    189 ->195        0.41915
    189 ->197        0.46052
    189 ->199       -0.11688
    189 ->200        0.12436

Excited State  15:     Singlet-A     4.1841 eV  296.32 nm  f=0.0003  <S**2>=0.000
    181 ->190        0.33229
    182 ->190        0.32566
    183 ->190        0.50573

Excited State  16:     Singlet-A     4.2380 eV  292.55 nm  f=0.0061  <S**2>=0.000
    189 ->197        0.12578
    189 ->198        0.68302

Excited State  17:     Singlet-A     4.3319 eV  286.21 nm  f=0.0056  <S**2>=0.000
    181 ->190        0.10233
    182 ->190       -0.19961
    189 ->197       -0.28930
    189 ->198        0.11068
    189 ->199       -0.38014
    189 ->200        0.43056

Excited State  18:     Singlet-A     4.3497 eV  285.04 nm  f=0.0088  <S**2>=0.000
    181 ->190       -0.11463
    182 ->190        0.55233
    183 ->190       -0.28573
    184 ->190        0.17616
```

```
    189 ->199       -0.16781
    189 ->200        0.15463

Excited State  19:     Singlet-A     4.3710 eV  283.65 nm  f=0.0012  <S**2>=0.000
    181 ->190        0.35387
    183 ->190       -0.23451
    189 ->199        0.42393
    189 ->200        0.34200

Excited State  20:     Singlet-A     4.3753 eV  283.37 nm  f=0.0102  <S**2>=0.000
    181 ->190        0.44719
    183 ->190       -0.29431
    184 ->190       -0.10802
    189 ->199       -0.27702
    189 ->200       -0.33532

Excited State  21:     Singlet-A     4.5581 eV  272.01 nm  f=0.0056  <S**2>=0.000
    189 ->201        0.60561
    189 ->202       -0.15583
    189 ->205        0.15001
    189 ->206        0.22368

Excited State  22:     Singlet-A     4.5699 eV  271.31 nm  f=0.0607  <S**2>=0.000
    180 ->190       -0.14183
    187 ->191        0.66504

Excited State  23:     Singlet-A     4.5970 eV  269.70 nm  f=0.0447  <S**2>=0.000
    180 ->190       -0.13241
    186 ->191        0.65507
    187 ->194        0.12332

Excited State  24:     Singlet-A     4.6391 eV  267.26 nm  f=0.0038  <S**2>=0.000
    179 ->190       -0.10701
    180 ->190        0.38056
    186 ->191        0.10748
    187 ->191        0.10491
    189 ->201        0.16702
    189 ->202        0.41904
    189 ->203       -0.28742
    189 ->204       -0.10512

Excited State  25:     Singlet-A     4.6443 eV  266.96 nm  f=0.0094  <S**2>=0.000
    179 ->190       -0.14154
    180 ->190        0.49246
    186 ->191        0.10540
    187 ->191        0.10810
    189 ->202       -0.38856
    189 ->203        0.21005

Excited State  26:     Singlet-A     4.6765 eV  265.12 nm  f=0.0020  <S**2>=0.000
    189 ->202        0.32395
    189 ->203        0.58862
    189 ->204       -0.17608

Excited State  27:     Singlet-A     4.7034 eV  263.61 nm  f=0.0715  <S**2>=0.000
    188 ->192        0.26260
    188 ->193       -0.30007
    189 ->202        0.14146
    189 ->204        0.51622

Excited State  28:     Singlet-A     4.7125 eV  263.10 nm  f=0.0636  <S**2>=0.000
```

```
    180 ->190        0.10717
    188 ->192       -0.29331
    188 ->193        0.47000
    189 ->204        0.36426

 Excited State  29:      Singlet-A     4.7581 eV  260.58 nm  f=0.0136  <S**2>=0.000
    189 ->205        0.54110
    189 ->206       -0.38083
    189 ->213        0.11025

 Excited State  30:      Singlet-A     4.7642 eV  260.24 nm  f=0.0022  <S**2>=0.000
    189 ->201       -0.28568
    189 ->204       -0.15773
    189 ->205        0.37978
    189 ->206        0.45289
    189 ->213       -0.10467

 Excited State  31:      Singlet-A     4.8098 eV  257.77 nm  f=0.0253  <S**2>=0.000
    179 ->190        0.64082
    180 ->190        0.18025
    188 ->193       -0.12335

 Excited State  32:      Singlet-A     4.8347 eV  256.45 nm  f=0.5903  <S**2>=0.000
    179 ->190       -0.13988
    185 ->190        0.25840
    185 ->191        0.36072
    188 ->192       -0.35262
    188 ->193       -0.34454
```

Table S20. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of ***syn*-6$_{opt}$** Calculated at the TD-B3LYP/6-31+G(d) Level (The 331th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     1.7258 eV  718.42 nm  f=0.1077  <S**2>=0.000
    331 -> 332       0.70423

 Excited State   2:      Singlet-A     1.7785 eV  697.12 nm  f=0.0029  <S**2>=0.000
    330 -> 332       0.70496

 Excited State   3:      Singlet-A     2.8514 eV  434.82 nm  f=0.2018  <S**2>=0.000
    329 -> 332       0.43032
    330 -> 333       0.32999
    331 -> 334       0.41727

 Excited State   4:      Singlet-A     2.8886 eV  429.22 nm  f=0.1181  <S**2>=0.000
    330 -> 334       0.38055
    330 -> 336       0.14264
    330 -> 342       0.11781
    331 -> 333       0.51479
    331 -> 337      -0.16759

 Excited State   5:      Singlet-A     2.9418 eV  421.46 nm  f=0.1072  <S**2>=0.000
    329 -> 332       0.54210
    330 -> 333      -0.23985
    330 -> 337       0.14395
    331 -> 334      -0.27314
    331 -> 336      -0.13660
```

```
    331 -> 342      -0.10666

Excited State   6:     Singlet-A     3.1305 eV  396.05 nm  f=0.0019  <S**2>=0.000
    330 -> 333       0.49392
    331 -> 334      -0.44359
    331 -> 335       0.22028

Excited State   7:     Singlet-A     3.1396 eV  394.91 nm  f=0.0003  <S**2>=0.000
    330 -> 334       0.54188
    330 -> 335      -0.14290
    331 -> 333      -0.42436

Excited State   8:     Singlet-A     3.2583 eV  380.52 nm  f=0.0069  <S**2>=0.000
    330 -> 333      -0.18715
    331 -> 334       0.12940
    331 -> 335       0.66024

Excited State   9:     Singlet-A     3.3149 eV  374.02 nm  f=0.0000  <S**2>=0.000
    330 -> 335       0.68595
    331 -> 333      -0.11962

Excited State  10:     Singlet-A     3.4682 eV  357.49 nm  f=0.0404  <S**2>=0.000
    330 -> 337      -0.18583
    330 -> 339       0.11609
    331 -> 336       0.59105
    331 -> 342      -0.21176
    331 -> 345      -0.12603

Excited State  11:     Singlet-A     3.5077 eV  353.46 nm  f=0.0176  <S**2>=0.000
    330 -> 336       0.49285
    330 -> 340      -0.13681
    330 -> 342      -0.18183
    331 -> 337      -0.32472
    331 -> 339       0.22867

Excited State  12:     Singlet-A     3.5866 eV  345.69 nm  f=0.0003  <S**2>=0.000
    330 -> 337       0.31513
    330 -> 339      -0.26324
    330 -> 341       0.11199
    331 -> 336       0.10047
    331 -> 340       0.50753
    331 -> 342      -0.13643
    331 -> 345      -0.10164

Excited State  13:     Singlet-A     3.5985 eV  344.54 nm  f=0.0037  <S**2>=0.000
    330 -> 336       0.30102
    330 -> 340       0.38959
    330 -> 342      -0.19139
    330 -> 345      -0.13065
    331 -> 337       0.31100
    331 -> 339      -0.23873
    331 -> 341       0.12489
    331 -> 354      -0.10817

Excited State  14:     Singlet-A     3.6960 eV  335.45 nm  f=0.0880  <S**2>=0.000
    324 -> 332       0.14006
    327 -> 332      -0.10960
    329 -> 334      -0.14600
    330 -> 333       0.15102
    330 -> 337       0.12523
    330 -> 339       0.25846
```

```
    331 -> 334       0.10965
    331 -> 336      -0.16104
    331 -> 338       0.42418
    331 -> 342      -0.23260
    331 -> 345      -0.11576

Excited State  15:     Singlet-A     3.7143 eV  333.80 nm  f=0.1309  <S**2>=0.000
    326 -> 332      -0.15404
    328 -> 332      -0.13803
    329 -> 333      -0.16440
    330 -> 334       0.16511
    330 -> 336      -0.10543
    330 -> 338       0.29018
    330 -> 340      -0.10357
    330 -> 342      -0.13776
    331 -> 333       0.12768
    331 -> 337       0.27099
    331 -> 339       0.39216

Excited State  16:     Singlet-A     3.7298 eV  332.42 nm  f=0.0339  <S**2>=0.000
    324 -> 332       0.33334
    325 -> 332      -0.31264
    327 -> 332      -0.29508
    329 -> 334      -0.18309
    329 -> 335       0.31401
    331 -> 338      -0.19593

Excited State  17:     Singlet-A     3.7401 eV  331.50 nm  f=0.0179  <S**2>=0.000
    326 -> 332       0.38826
    328 -> 332       0.53084
    330 -> 338       0.15544
    331 -> 339       0.11025

Excited State  18:     Singlet-A     3.7689 eV  328.97 nm  f=0.0891  <S**2>=0.000
    325 -> 332      -0.10649
    330 -> 333      -0.12458
    330 -> 337      -0.16591
    330 -> 339      -0.11581
    330 -> 341       0.27261
    331 -> 334      -0.10756
    331 -> 338       0.41837
    331 -> 340       0.15294
    331 -> 342       0.27485
    331 -> 345       0.14946

Excited State  19:     Singlet-A     3.7754 eV  328.40 nm  f=0.0201  <S**2>=0.000
    330 -> 336      -0.19558
    330 -> 338       0.36396
    330 -> 340       0.18460
    331 -> 337      -0.32426
    331 -> 341       0.39277

Excited State  20:     Singlet-A     3.8042 eV  325.91 nm  f=0.0027  <S**2>=0.000
    330 -> 337       0.52694
    331 -> 336       0.26359
    331 -> 340      -0.20897
    331 -> 342       0.25598

Excited State  21:     Singlet-A     3.8112 eV  325.32 nm  f=0.0121  <S**2>=0.000
    326 -> 332      -0.17384
    328 -> 332       0.22090
```

```
    330 -> 340      -0.10575
    330 -> 342      -0.18373
    331 -> 339      -0.16809
    331 -> 343       0.45691
    331 -> 344      -0.30712

Excited State  22:     Singlet-A     3.8185 eV  324.70 nm  f=0.0008  <S**2>=0.000
    324 -> 332       0.16865
    325 -> 332      -0.23141
    327 -> 332       0.60820
    329 -> 334      -0.10966

Excited State  23:     Singlet-A     3.8185 eV  324.69 nm  f=0.0115  <S**2>=0.000
    326 -> 332       0.38627
    327 -> 332      -0.12993
    328 -> 332      -0.31932
    330 -> 336       0.15843
    330 -> 338       0.14918
    330 -> 340      -0.16184
    330 -> 342       0.11953
    331 -> 337       0.15896
    331 -> 343       0.23368
    331 -> 344      -0.18166

Excited State  24:     Singlet-A     3.8241 eV  324.22 nm  f=0.0424  <S**2>=0.000
    326 -> 332       0.36071
    328 -> 332      -0.18070
    329 -> 333      -0.18747
    330 -> 336      -0.22013
    330 -> 338      -0.17885
    330 -> 340       0.11680
    330 -> 342      -0.27603
    330 -> 345      -0.14986
    331 -> 337      -0.18564
    331 -> 341      -0.15863
    331 -> 354      -0.11718

Excited State  25:     Singlet-A     3.8593 eV  321.26 nm  f=0.0082  <S**2>=0.000
    324 -> 332      -0.10363
    325 -> 332      -0.22638
    330 -> 339      -0.31427
    330 -> 343       0.41929
    330 -> 344      -0.29697
    331 -> 340      -0.19264
    331 -> 342      -0.12355

Excited State  26:     Singlet-A     3.8632 eV  320.94 nm  f=0.0079  <S**2>=0.000
    324 -> 332       0.33064
    325 -> 332       0.51788
    329 -> 334      -0.15010
    329 -> 335       0.13790
    330 -> 339      -0.15088
    330 -> 343       0.14598
    330 -> 344      -0.11922

Excited State  27:     Singlet-A     3.9061 eV  317.41 nm  f=0.0658  <S**2>=0.000
    329 -> 333       0.63043
    331 -> 339       0.12417
    331 -> 341      -0.11785
    331 -> 343       0.12648
```

```
 Excited State  28:      Singlet-A     3.9321 eV  315.31 nm  f=0.0143  <S**2>=0.000
    324 -> 332       0.19109
    329 -> 334       0.62226
    329 -> 335       0.20919

 Excited State  29:      Singlet-A     3.9480 eV  314.04 nm  f=0.0061  <S**2>=0.000
    330 -> 338      -0.21573
    330 -> 340       0.38981
    330 -> 342       0.15234
    330 -> 345       0.12806
    331 -> 339       0.38592
    331 -> 343       0.26777
    331 -> 344      -0.11723

 Excited State  30:      Singlet-A     3.9609 eV  313.02 nm  f=0.0001  <S**2>=0.000
    330 -> 339       0.36821
    330 -> 341      -0.21253
    330 -> 343       0.37985
    330 -> 344      -0.14284
    331 -> 340       0.33709
    331 -> 342       0.16739

 Excited State  31:      Singlet-A     3.9641 eV  312.77 nm  f=0.0097  <S**2>=0.000
    330 -> 338      -0.36159
    330 -> 340      -0.24837
    330 -> 342      -0.19727
    331 -> 341       0.46635

 Excited State  32:      Singlet-A     3.9787 eV  311.62 nm  f=0.0001  <S**2>=0.000
    330 -> 339       0.21285
    330 -> 341       0.50195
    330 -> 344      -0.14323
    331 -> 338      -0.24800
    331 -> 342      -0.13927
    331 -> 345       0.28197
```

Table S21. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of ***anti*-6$_{opt}$** Calculated at the TD-B3LYP/6-31+G(d) Level (The 331th orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     1.7273 eV  717.81 nm  f=0.0974  <S**2>=0.000
    331 -> 332       0.70431

 Excited State   2:      Singlet-A     1.7775 eV  697.51 nm  f=0.0000  <S**2>=0.000
    330 -> 332       0.70507

 Excited State   3:      Singlet-A     2.8566 eV  434.03 nm  f=0.3173  <S**2>=0.000
    329 -> 332       0.44622
    330 -> 333       0.31317
    331 -> 334       0.41560

 Excited State   4:      Singlet-A     2.8915 eV  428.79 nm  f=0.0118  <S**2>=0.000
    330 -> 334       0.40683
    330 -> 336      -0.13528
    330 -> 342      -0.10234
    331 -> 333       0.49889
    331 -> 337      -0.15615
    331 -> 341      -0.10149
```

```
Excited State   5:      Singlet-A     2.9396 eV  421.77 nm  f=0.1241  <S**2>=0.000
    329 -> 332       0.53021
    330 -> 333      -0.23181
    330 -> 337       0.14020
    331 -> 334      -0.30193
    331 -> 336       0.13061

Excited State   6:      Singlet-A     3.1394 eV  394.92 nm  f=0.0002  <S**2>=0.000
    330 -> 334       0.50830
    331 -> 333      -0.44432
    331 -> 335      -0.18661

Excited State   7:      Singlet-A     3.1448 eV  394.25 nm  f=0.0009  <S**2>=0.000
    330 -> 333       0.53692
    330 -> 335       0.12060
    331 -> 334      -0.43451

Excited State   8:      Singlet-A     3.2611 eV  380.19 nm  f=0.0020  <S**2>=0.000
    330 -> 334       0.15302
    331 -> 333      -0.11775
    331 -> 335       0.66967

Excited State   9:      Singlet-A     3.3163 eV  373.87 nm  f=0.0101  <S**2>=0.000
    330 -> 335       0.69015

Excited State  10:      Singlet-A     3.4705 eV  357.25 nm  f=0.0556  <S**2>=0.000
    330 -> 333       0.10761
    330 -> 337       0.18526
    331 -> 336       0.58709
    331 -> 342      -0.22595
    331 -> 346       0.10971

Excited State  11:      Singlet-A     3.5080 eV  353.43 nm  f=0.0003  <S**2>=0.000
    330 -> 336       0.50033
    330 -> 339      -0.16077
    330 -> 342      -0.18752
    331 -> 337       0.32997
    331 -> 338       0.12067
    331 -> 341      -0.17091

Excited State  12:      Singlet-A     3.5865 eV  345.70 nm  f=0.0070  <S**2>=0.000
    330 -> 337      -0.30807
    330 -> 341       0.26593
    331 -> 336       0.10138
    331 -> 339       0.47606
    331 -> 340      -0.20786
    331 -> 342      -0.13511

Excited State  13:      Singlet-A     3.5986 eV  344.54 nm  f=0.0001  <S**2>=0.000
    330 -> 336       0.29497
    330 -> 339       0.34733
    330 -> 340      -0.20155
    330 -> 342      -0.19842
    330 -> 346       0.10828
    331 -> 337      -0.31662
    331 -> 341       0.25260

Excited State  14:      Singlet-A     3.7104 eV  334.15 nm  f=0.0091  <S**2>=0.000
    324 -> 332       0.19899
    325 -> 332       0.11591
```

```
    327 -> 332      -0.14033
    329 -> 333      -0.20124
    329 -> 335      -0.13306
    330 -> 334      -0.12336
    330 -> 339      -0.19826
    330 -> 340      -0.17758
    331 -> 337      -0.27060
    331 -> 338       0.37092
    331 -> 341      -0.20224

Excited State  15:     Singlet-A     3.7194 eV  333.34 nm  f=0.2663  <S**2>=0.000
    326 -> 332       0.18328
    328 -> 332      -0.14670
    329 -> 334       0.12849
    330 -> 333       0.15310
    330 -> 337       0.17261
    330 -> 338      -0.24163
    330 -> 341       0.14523
    331 -> 334       0.13185
    331 -> 336       0.15675
    331 -> 339       0.23561
    331 -> 340       0.28036
    331 -> 342       0.26937

Excited State  16:     Singlet-A     3.7381 eV  331.68 nm  f=0.0221  <S**2>=0.000
    324 -> 332      -0.31125
    325 -> 332      -0.25072
    327 -> 332       0.25158
    329 -> 333       0.16072
    329 -> 335       0.29977
    330 -> 340      -0.14372
    331 -> 337      -0.12555
    331 -> 338       0.32367

Excited State  17:     Singlet-A     3.7477 eV  330.83 nm  f=0.0145  <S**2>=0.000
    326 -> 332      -0.39380
    328 -> 332       0.48054
    330 -> 338      -0.21126
    331 -> 340       0.19436

Excited State  18:     Singlet-A     3.7586 eV  329.87 nm  f=0.0131  <S**2>=0.000
    325 -> 332       0.12335
    329 -> 335      -0.10854
    330 -> 334       0.12564
    330 -> 339       0.10283
    330 -> 340      -0.18447
    330 -> 342       0.10458
    330 -> 346      -0.10289
    331 -> 337       0.25144
    331 -> 338       0.35770
    331 -> 341       0.38636

Excited State  19:     Singlet-A     3.7800 eV  328.00 nm  f=0.1235  <S**2>=0.000
    328 -> 332       0.19482
    329 -> 334       0.11602
    330 -> 338       0.38877
    330 -> 341       0.13996
    331 -> 336       0.13234
    331 -> 340      -0.20965
    331 -> 342       0.37130
    331 -> 343       0.15210
```

```
Excited State  20:     Singlet-A     3.7972 eV  326.51 nm  f=0.0356  <S**2>=0.000
    330 -> 337       0.52120
    330 -> 338       0.14151
    330 -> 341       0.17375
    331 -> 336      -0.24065
    331 -> 339       0.18022
    331 -> 340      -0.20956
    331 -> 342      -0.15185

Excited State  21:     Singlet-A     3.8042 eV  325.91 nm  f=0.0096  <S**2>=0.000
    329 -> 333       0.10131
    330 -> 336       0.34777
    330 -> 339      -0.13103
    330 -> 340       0.17645
    330 -> 342       0.35286
    330 -> 346      -0.12280
    331 -> 337      -0.30321

Excited State  22:     Singlet-A     3.8165 eV  324.86 nm  f=0.0143  <S**2>=0.000
    326 -> 332      -0.17472
    328 -> 332      -0.24303
    330 -> 341      -0.21054
    331 -> 339       0.19642
    331 -> 343       0.42319
    331 -> 346       0.29789

Excited State  23:     Singlet-A     3.8280 eV  323.89 nm  f=0.0086  <S**2>=0.000
    326 -> 332       0.50585
    328 -> 332       0.37598
    329 -> 334      -0.13065
    330 -> 341      -0.12269
    331 -> 343       0.17317
    331 -> 346       0.13390

Excited State  24:     Singlet-A     3.8281 eV  323.88 nm  f=0.0010  <S**2>=0.000
    324 -> 332       0.19511
    325 -> 332       0.17642
    327 -> 332       0.62315
    329 -> 333      -0.10782
    329 -> 335      -0.10573

Excited State  25:     Singlet-A     3.8555 eV  321.57 nm  f=0.0007  <S**2>=0.000
    330 -> 339       0.36058
    330 -> 342       0.24112
    330 -> 343       0.41121
    330 -> 346       0.23334
    331 -> 338       0.12974
    331 -> 341      -0.21185

Excited State  26:     Singlet-A     3.8786 eV  319.66 nm  f=0.0043  <S**2>=0.000
    324 -> 332      -0.30577
    325 -> 332       0.59659
    329 -> 333       0.11746
    329 -> 335       0.12662

Excited State  27:     Singlet-A     3.8943 eV  318.37 nm  f=0.0910  <S**2>=0.000
    329 -> 334       0.65402
    330 -> 341      -0.15049

Excited State  28:     Singlet-A     3.9170 eV  316.53 nm  f=0.0005  <S**2>=0.000
```

```
    324 -> 332       0.19265
    329 -> 333       0.60298
    329 -> 335      -0.19569
    331 -> 341      -0.16733

 Excited State  29:     Singlet-A     3.9450 eV  314.29 nm  f=0.0011  <S**2>=0.000
    330 -> 338       0.32628
    330 -> 341      -0.33918
    331 -> 339       0.34009
    331 -> 340       0.21529
    331 -> 343      -0.24063
    331 -> 346      -0.18889

 Excited State  30:     Singlet-A     3.9600 eV  313.09 nm  f=0.0003  <S**2>=0.000
    330 -> 339       0.36980
    330 -> 340       0.11946
    330 -> 343      -0.36335
    330 -> 346      -0.25051
    331 -> 338       0.16435
    331 -> 341      -0.28543
    331 -> 345       0.12963

 Excited State  31:     Singlet-A     3.9635 eV  312.82 nm  f=0.0001  <S**2>=0.000
    330 -> 338       0.26534
    330 -> 341       0.34617
    330 -> 348      -0.12441
    331 -> 340       0.40442
    331 -> 342      -0.26063
    331 -> 343       0.17226

 Excited State  32:     Singlet-A     3.9821 eV  311.35 nm  f=0.0018  <S**2>=0.000
    330 -> 340       0.50759
    330 -> 342      -0.27761
    331 -> 338       0.20159
    331 -> 341       0.17570
    331 -> 344      -0.15449
    331 -> 348      -0.16808
```

Table S22. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{7_{opt}}$ Calculated at the TD-B3LYP/6-31+G(d) Level (The 331th Orbital is Highest Occupied π(Si=Si) Orbital Shown in Figure 3 in the Main Text)

```
Excited State   1:      Singlet-A     2.8505 eV  434.96 nm  f=0.0824  <S**2>=0.000
    175 ->176        0.63897
    175 ->180        0.13392
    175 ->181        0.24525

 Excited State   2:     Singlet-A     3.0855 eV  401.83 nm  f=0.0168  <S**2>=0.000
    175 ->177        0.70471

 Excited State   3:     Singlet-A     3.5227 eV  351.96 nm  f=0.0011  <S**2>=0.000
    175 ->178        0.61004
    175 ->179       -0.35405

 Excited State   4:     Singlet-A     3.6053 eV  343.89 nm  f=0.0074  <S**2>=0.000
    175 ->180        0.67552
    175 ->181       -0.17850

 Excited State   5:     Singlet-A     3.7058 eV  334.57 nm  f=0.0028  <S**2>=0.000
```

```
    175 ->178        0.35309
    175 ->179        0.60782

Excited State   6:     Singlet-A     3.7859 eV  327.49 nm  f=0.2669  <S**2>=0.000
    175 ->176       -0.27773
    175 ->180        0.11580
    175 ->181        0.60891
    175 ->190        0.12321

Excited State   7:     Singlet-A     4.0111 eV  309.10 nm  f=0.0005  <S**2>=0.000
    175 ->182        0.53717
    175 ->183       -0.44697

Excited State   8:     Singlet-A     4.0369 eV  307.13 nm  f=0.0098  <S**2>=0.000
    175 ->182        0.45199
    175 ->183        0.53567

Excited State   9:     Singlet-A     4.0617 eV  305.25 nm  f=0.0040  <S**2>=0.000
    175 ->184        0.69721

Excited State  10:     Singlet-A     4.2492 eV  291.78 nm  f=0.0003  <S**2>=0.000
    175 ->186        0.67386
    175 ->191        0.12647
    175 ->192        0.10654

Excited State  11:     Singlet-A     4.3322 eV  286.19 nm  f=0.0069  <S**2>=0.000
    175 ->181       -0.12843
    175 ->185        0.47347
    175 ->188       -0.15277
    175 ->190        0.39733
    175 ->194        0.15209
    175 ->195       -0.11247
    175 ->196        0.13981

Excited State  12:     Singlet-A     4.4056 eV  281.42 nm  f=0.0001  <S**2>=0.000
    175 ->181        0.10057
    175 ->185        0.51753
    175 ->188        0.17293
    175 ->190       -0.33435
    175 ->194       -0.18610
    175 ->195        0.12079
    175 ->196       -0.14981

Excited State  13:     Singlet-A     4.4237 eV  280.27 nm  f=0.0010  <S**2>=0.000
    175 ->187        0.69844

Excited State  14:     Singlet-A     4.4553 eV  278.29 nm  f=0.0004  <S**2>=0.000
    175 ->188        0.66270
    175 ->190        0.18690

Excited State  15:     Singlet-A     4.4890 eV  276.20 nm  f=0.0017  <S**2>=0.000
    175 ->189        0.70244

Excited State  16:     Singlet-A     4.6071 eV  269.11 nm  f=0.0027  <S**2>=0.000
    175 ->186       -0.15189
    175 ->191        0.64311
    175 ->192        0.18955

Excited State  17:     Singlet-A     4.6737 eV  265.28 nm  f=0.0004  <S**2>=0.000
    171 ->178        0.11526
    172 ->177       -0.15336
```

```
    173 ->176       -0.13501
    173 ->180        0.13428
    174 ->176        0.63871

Excited State  18:     Singlet-A     4.7375 eV  261.71 nm  f=0.0207  <S**2>=0.000
    171 ->176        0.48070
    171 ->180       -0.11265
    172 ->176       -0.32870
    173 ->177        0.10331
    173 ->178       -0.14019
    174 ->177        0.21578
    175 ->192        0.21275

Excited State  19:     Singlet-A     4.7423 eV  261.44 nm  f=0.0046  <S**2>=0.000
    171 ->176       -0.16068
    172 ->176        0.10733
    175 ->191       -0.21402
    175 ->192        0.62215

Excited State  20:     Singlet-A     4.7688 eV  259.99 nm  f=0.0342  <S**2>=0.000
    171 ->176        0.44914
    172 ->176        0.49866
    173 ->178        0.11426

Excited State  21:     Singlet-A     4.7756 eV  259.62 nm  f=0.0005  <S**2>=0.000
    173 ->176        0.37933
    175 ->190       -0.34193
    175 ->194        0.38921
    175 ->195       -0.20525
    175 ->196        0.15056

Excited State  22:     Singlet-A     4.7836 eV  259.19 nm  f=0.0056  <S**2>=0.000
    173 ->176        0.54258
    174 ->176        0.15277
    175 ->190        0.19544
    175 ->194       -0.29202
    175 ->195        0.12934
    175 ->196       -0.10985

Excited State  23:     Singlet-A     4.8449 eV  255.91 nm  f=0.0020  <S**2>=0.000
    175 ->193        0.69465

Excited State  24:     Singlet-A     4.8613 eV  255.04 nm  f=0.0001  <S**2>=0.000
    175 ->194        0.38405
    175 ->195        0.57029
    175 ->196       -0.11935

Excited State  25:     Singlet-A     4.9386 eV  251.05 nm  f=0.0080  <S**2>=0.000
    175 ->198        0.66980
    175 ->200       -0.13191

Excited State  26:     Singlet-A     4.9483 eV  250.56 nm  f=0.0004  <S**2>=0.000
    175 ->194       -0.18781
    175 ->195        0.25718
    175 ->196        0.61430

Excited State  27:     Singlet-A     4.9885 eV  248.54 nm  f=0.0117  <S**2>=0.000
    171 ->176       -0.13979
    171 ->180       -0.10576
    172 ->176        0.33166
    173 ->178       -0.18288
```

```
    173 ->179       0.11172
    174 ->177       0.53196

Excited State  28:     Singlet-A     5.0343 eV  246.28 nm  f=0.0032  <S**2>=0.000
    171 ->178      -0.10591
    172 ->177       0.28018
    174 ->176       0.11837
    175 ->197       0.59464

Excited State  29:     Singlet-A     5.0437 eV  245.82 nm  f=0.0035  <S**2>=0.000
    171 ->178      -0.18288
    171 ->179       0.11070
    172 ->177       0.45556
    173 ->176      -0.10315
    173 ->180      -0.16046
    173 ->181       0.13227
    174 ->176       0.18741
    175 ->197      -0.36078

Excited State  30:     Singlet-A     5.0498 eV  245.52 nm  f=0.0033  <S**2>=0.000
    175 ->199       0.69072

Excited State  31:     Singlet-A     5.1312 eV  241.63 nm  f=0.0005  <S**2>=0.000
    175 ->192      -0.10766
    175 ->198       0.13111
    175 ->200       0.67064

Excited State  32:     Singlet-A     5.2190 eV  237.56 nm  f=0.0004  <S**2>=0.000
    175 ->196       0.10909
    175 ->201       0.68080
```

Table. S23. Selected Structural Parameters of Disilenes $\mathbf{1_{opt}}$-$\mathbf{7_{opt}}$.

Compound	Distance	Bent Angle θ/deg		Twist Angle	Dihedral	Dihedral
	d(Si=Si)/Å	$R^H{}_2Si$	*Si*ArMes	τ/deg	Angle δ_{Ar}/deg	Angle δ_{Mes}/deg
$\mathbf{1_{opt}}$	2.189	14.0	28.4	1.9	83.2	88.5
***anti*-$\mathbf{2_{opt}}$**	2.191	17.0	32.2	7.3	82.4	85.1
(Si8=Si9)						
(Si10=Si11)	2.191	16.1	30.9	0.5	88.8	86.9
***syn*-2opt**	2.183	14.1	26.6	2.4	80.4	89.6
(Si8=Si9)						
(Si10=Si11)	2.189	15.3	29.4	11.2	64.1	82.8
***anti*-$\mathbf{3_{opt}}$**	2.192	14.6	29.8	2.2	83.7	88.4
(Si1=Si2)						
(Si90=Si91)	2.192	14.7	30.0	1.7	84.9	88.2
***syn*-3opt**	2.193	14.7	31.7	0.9	86.4	84.4
(Si1=Si2)						
(Si90=Si91)	2.199	16.9	34.5	12.6	79.2	83.8
$\mathbf{4_{opt}}$	2.164	0.7	0.1	0.2	73.0	70.7
$\mathbf{5_{opt}}$	2.174	14.4	18.5	12.0	59.7	73.6
***syn*-$\mathbf{6_{opt}}$**	2.165	3.5	1.5	3.9	70.5	71.0
***anti*-$\mathbf{6_{opt}}$**	2.163	1.7	0.1	1.3	71.7	70.0
$\mathbf{7_{opt}}$	2.169	0.0	0.0	8.0	-	70.9, 70.8

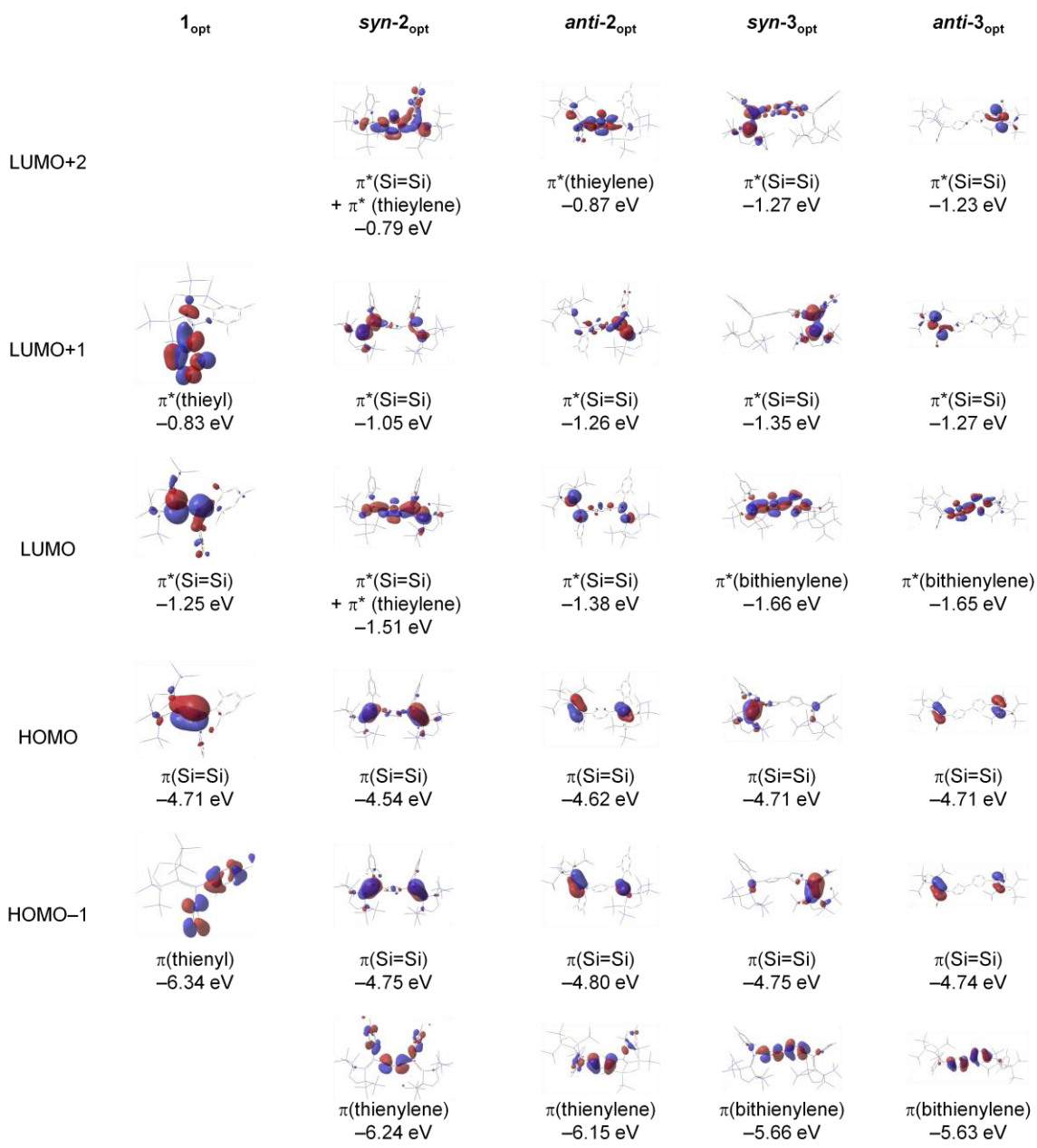


Figure S50. Frontier Kohn-Sham orbitals and their energy levels of **1$_{opt}$-3$_{opt}$** at the B3LYP/6-31+G(d)//B3PW91-D3/6-31G(d) level of theory (isosuface value = 0.04).

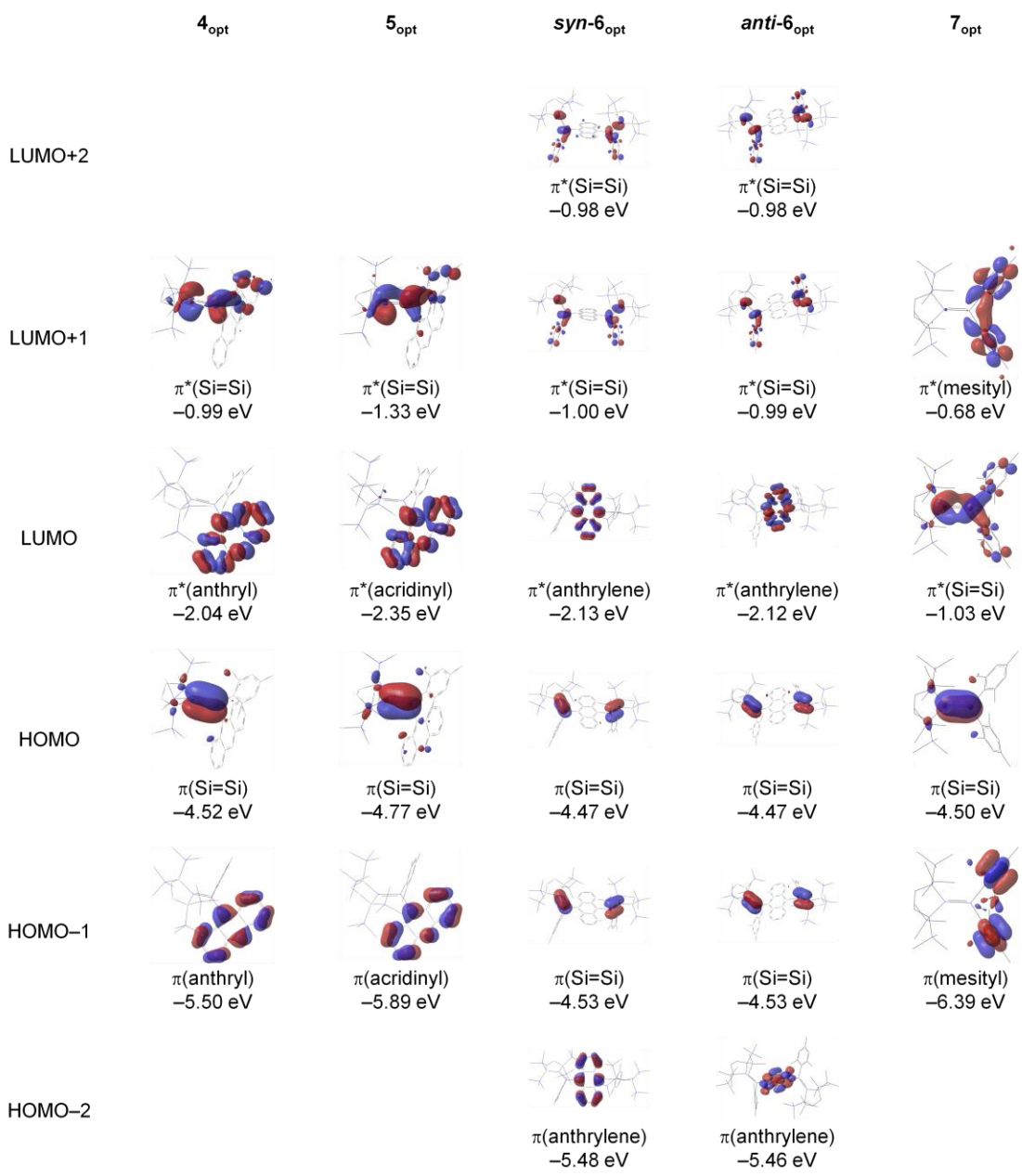


Figure S51. Frontier Kohn-Sham orbitals and their energy levels of **4$_{opt}$-7$_{opt}$** at the B3LYP/6-31+G(d)//B3PW91-D3/6-31G(d) level of theory (isosuface value = 0.04).