σσ* Transition in *anti,cisoid* Alternating Oligosilanes: Clear-Cut Evidence for Suppression of Conjugation Effect by a *cisoid* Turn

Supporting Information

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(1) Experimental details

General. Melting point (mp) determinations were performed by using a Yanaco MP-S3 instrument unless otherwise stated or a Seiko Instruments Inc. DSC6200 instrument. NMR spectra were measured with a JEOL EX-270 (270 MHz for ^{1}H, and 67.9 MHz for ^{13}C) spectrometer in C_6D_6. Chemical shifts are reported in δ ppm with reference relative to residual protio-solvent (*i.e.*, C_6H_6) peak. Column chromatography was performed by using Silica Gel 60 (70-230 mesh, Merck). Recycling gel permeation chromatography (GPC) was performed by using a JAI LC 908 with JAIGEL 1H,2H columns.

Materials. Diethylether and tetrahydrofuran was freshly distilled before use from sodium/benzophenone. All reactions were carried out under nitrogen, unless otherwise stated.

1,1,2,2-Tetraphenyl-1,2-disilacyclohexane. Mg (turnings, 3.69 g, 152 mmol) in THF (30 ml) was activated by dibromoethane (0.2 ml), and a solution of 1,4-dichlorobutane (8.2 ml, 75 mmol) in THF (30 ml) was added dropwise over 0.5 h. The reaction mixture was heated under reflux for 4.5 h. After cooling, THF (300 ml) was added and a solution of 1,1,2,2-tetraphenyl-1,2-dichlorodisilane (16.2 g, 37.3 mmol) in THF (80 ml) was added dropwise over 1 h at room temperature. After stirring for 15 h, the reaction mixture was quenched with 10% NH_4Claq and extracted with Et_2O. The combined extract was washed with brine and dried over $MgSO_4$. After filtration and evaporation of the solvent, the residue was recrystallized from EtOH to give 14.2 g (33.7 mmol, 90% yield) of 1,1,2,2-tetraphenyl-1,2-disilacyclohexane as a colorless crystal: ^{1}H NMR (270 MHz) δ 1.45 (m, 4H), 1.88 (m, 4H), 7.15 (m, 12H), 7.60 (dd, J = 5.7, 2.4 Hz, 8H). ^{13}C NMR (67.94 MHz) δ14.36, 26.03, 129.28, 135.04, 135.89, 136.41. ^{29}Si NMR (53.67 MHz) δ −25.17. MS(EI) *m/z* (relative intensity) 420 (M^+, 25), 149 (100).

***Cis*-1,6-Diphenyl-1,6-disilabicyclo[4.4.0]decane (1).** The silyltriflate solution was prepared as follows: To a solution of 1,1,2,2-tetraphenyl-1,2-disilacyclohexane (95.5 g, 0.227 mol) in benzene (280 ml) was added trifluoromethanesulfonic acid (40.5 ml, 0.458 mol) dropwise over

0.5 h at about 5 °C, and the mixture was stirred for 2.1 h. The Grignard reagent was prepared as follows: Mg (14.1 g, 0.582 mol) in a small amount of THF was activated by dibromoethane (0.2 ml), and 1,4-dichlorobutane (30.5 ml, 0.276 mol) was added dropwise over 0.8 h. The reaction mixture was heated under reflux for 1 h. THF was removed by vacuum pump and replaced with Et_2O (400 ml), and then the solid of Grignard reagent was crushed into pieces by spatula under a nitrogen stream. To the suspension of the Grignard reagent was added the silyltriflate solution dropwise over 2 h at 0 °C, then the mixture was stirred for a day. The reaction mixture was quenched with 10% NH_4Claq and extracted with Et_2O. The combined extract was washed with brine, and then dried over $MgSO_4$. After filtration and evaporation of the solvent, the residue was recrystallized from EtOH to give 49.3 g (0.153 mol, 67% yield) of **1** as a colorless crystals: mp 102.4 °C (DSC). ^{1}H NMR (270 MHz) δ 1.09 (m, 8H), 1.81 (m, 8H), 7.2 (m, 6H), 7.52-7.56 (m, 4H). ^{13}C NMR (67.94 MHz) δ 13.77, 26.51, 128.14, 129.04, 135.01, 137.15. ^{29}Si NMR (53.67 MHz) δ –26.22. Anal. Calcd for $C_{20}H_{26}Si_2$: C, 74.46; H, 8.12. Found: C, 74.23; H, 7.98.

1,6-Dichloro-1,6-disilabicyclo[4.4.0]decane (2). To a solution of **1** (9.85 g, 30.5 mmol) in benzene (60 ml) was added $AlCl_3$ (478 mg, 3.58 mmol), and then HCl gas was introduced into this mixture for 2.7 h at room temperature. Reaction was monitored by NMR. After completion of reaction, acetone (0.8 ml) was added and acetone/$AlCl_3$ complex was removed by filtration. Evaporation followed by bulb-to-bulb distillation (oven temperature: 120 °C / 0.4 mmHg) gave 7.05 g (29.5 mmol, 97% yield) of **2** as colorless solid. ^{1}H NMR (270 MHz) δ 0.80 (ddd, J = 15.0, 9.7, 3.0 Hz, 4H), 1.03 (ddd, *J* = 15.0, 10.0, 3.2 Hz, 4H), 1.28 (m, 4H), 1.57 (m, 4H). ^{13}C NMR (67.94 MHz) δ 18.26, 25.18.

Oligomerization of 2. To a suspension of Li (dispersion, 240 mg, 34.6 mmol) in THF (4 ml) was added a solution of **2** (956 mg, 4.00 mmol) and chlorotrimethylsilane (437 mg, 4.02 mmol) in THF (4 ml) over 3 min at 0 °C under Ar atmosphere. After stirring for a day at room temperature, 2-propanol (2.0 ml) was added to the reaction mixture to deactivate excess Li. The reaction mixture was quenched with water and neutralized with HClaq and then extracted with Et_2O (10 ml × 4) and THF (10 ml). The combined extract was washed with brine and dried over $MgSO_4$. After filtration and evaporation, the residue was subjected to column chromatography on silica gel (hexane, R_f = 0.83). The collected fraction was concentrated and recrystallized from hexane to give cyclic trimer (**7**) as colorless crystals. The mother liquor was subjected to preparative GPC (eluent: 1,2-dichloroethane) to give oligomers *C*-tetrasilane **3**, *CAC*-hexasilane **4**, *CACAC*-octasilane **5**,

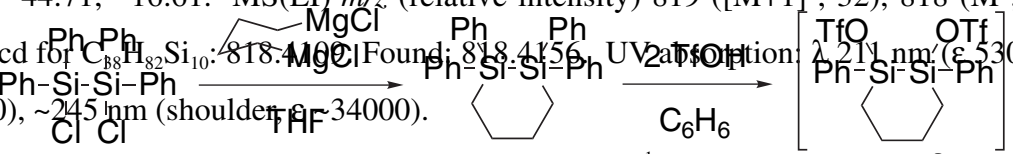
CACACAC-decasilane **6**, and the cyclic trimer.

***C*-Tetrasilane (3).** 15% yield. colorless liquid. ^{1}H NMR (270 MHz) δ 0.24 (s, 18H), 0.88 (ddd, *J* = 14.4, 8.8, 3.8 Hz, 4H), 0.96 (ddd, J = 14.4, 8.6, 3.2 Hz, 4H), 1.55-1.88 (m, 8H). ^{13}C NMR (67.94 MHz) δ –0.84, 10.73, 26.74. ^{29}Si NMR (53.67 MHz) δ –50.80, –17.11. Anal. Calcd for $C_{14}H_{34}Si_4$: C, 53.42; H, 10.89. Found: C, 53.43; H, 10.90. MS(EI) *m/z* (relative intensity) 314 (M^+, 100), 241 (81). UV absorption: λ ~210 nm (shoulder, ε ~15000).

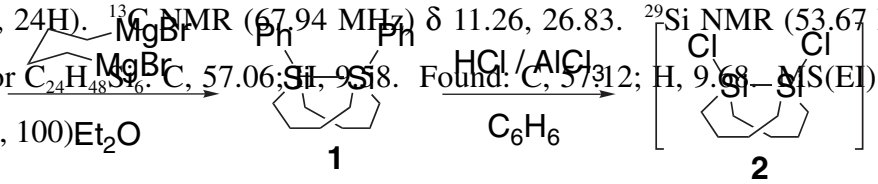
***CAC*-Hexasilane (4).** 13% yield. Colorless crystals: mp 137-140 °C. ^{1}H NMR (270 MHz) δ 0.27 (s, 18H), 0.90 (ddd, *J* = 14.3, 8.4, 3.4 Hz, 4H), 0.99 (ddd, *J* = 14.3, 8.1, 3.2 Hz, 4H), 1.09 (ddd, *J* = 14.3, 8.9, 3.0 Hz, 4H), 1.17 (ddd, *J* = 14.3, 7.8, 3.2 Hz, 4H), 1.55-1.95 (m, 16H). ^{13}C NMR (67.94 MHz) δ –0.77, 11.02, 12.73, 26.62, 26.74. ^{29}Si NMR (53.67 MHz) δ –49.79, –46.39, –16.73. Anal. Calcd for $C_{22}H_{50}Si_6$: C, 54.69; H, 10.43. Found: C, 54.95; H, 10.58. MS(EI) *m/z* (relative intensity) 482 (M^+, 100). UV absorption: λ ~210 nm (shoulder, ε ~34000), 243 nm (ε 17000).

***CACAC*-Octasilane (5).** 8% yield. Colorless crystals. ^{1}H NMR (270 MHz) δ 0.28 (s, 18H), 0.8-1.1 (m, 8H), 1.0-1.3 (m, 16H), 1.6-2.0 (m, 24H). ^{13}C NMR (67.94 MHz) δ –0.77, 11.08, 12.85, 13.12, 26.64 (x 2), 26.76. ^{29}Si NMR (53.67 MHz) δ –49.92, –45.71,–45.51,–16.66. MS(EI) *m/z* (relative intensity) 650 (M^+, 100). HRMS (EI) Calcd for $C_{30}H_{66}Si_8$: 650.3319. Found: 650.3314. UV absorption: λ = 212 nm (ε 42000), 241 nm (ε 25000).

***CACACAC*-Decasilane (6).** 5% yield. Colorless crystals. ^{1}H NMR (270 MHz) δ 0.28 (s, 18H), 0.85-1.05 (m, 8H), 1.05-1.35 (br s, 24H), 1.6-2.0 (br s, 32H). ^{13}C NMR (67.94 MHz) δ –0.77, 11.06, 12.84, 13.20 (× 2), 26.64 (× 3), 26.76. ^{29}Si NMR (53.67 MHz) δ –49.92, –45.59, –45.54, –44.71, –16.61. MS(EI) *m/z* (relative intensity) 819 ([M+1]$^+$, 32), 818 (M^+, 5). HRMS (EI) Calcd for $C_{38}H_{82}Si_{10}$: 818.4102. Found: 818.4156. UV absorption: λ 211 nm (ε 53000), 236 nm (ε 36000), ~245 nm (shoulder, ε ~34000).



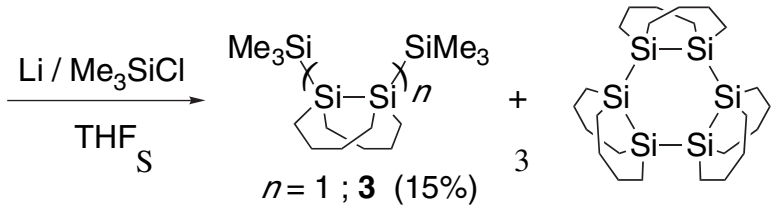
Cyclic trimer. 9% yield. Colorless crystals. ^{1}H NMR (270 MHz) δ 1.02 (br s, 24H), 1.76 (m, 24H). ^{13}C NMR (67.94 MHz) δ 11.26, 26.83. ^{29}Si NMR (53.67 MHz) δ –53.20. Anal. Calcd for $C_{24}H_{48}Si_6$: C, 57.06; H, 9.58. Found: C, 57.12; H, 9.68. MS(EI) *m/z* (relative intensity) 504 (M^+, 100)



1

overall yield 60%

2



n = 1 ; **3** (15%)
n = 2 ; **4** (13%)
n = 3 ; **5** (8%)
n = 4 ; **6** (5%)

8 (9%)

(2) X-ray crystallographic structures of 1 and 4.

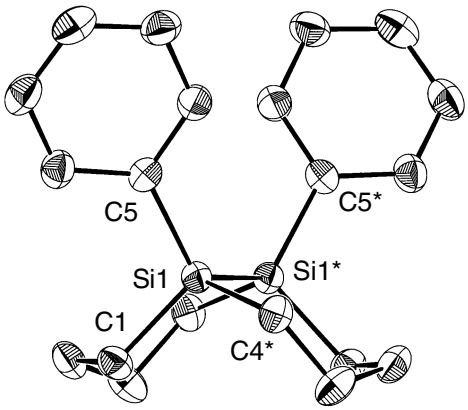


Figure S1. X-ray structure of **1** at 40% probability level. All hydrogens are omitted for clarity. Selected bond lengths (Å) and angles (deg): Si1–Si1*, 2.315(1); Si1–C1, 1.894(3); Si1–C4*, 1.882(3); Si1–C5, 1.884(3); Si1*–Si1–C1, 105.85(9); Si1*–Si1–C4*, 101.10(9); Si1*–Si1–C5, 118.82(8); C1–Si1–C4*, 109.8(1); C1–Si1–C5, 109.4(1); C4*–Si1–C5, 111.4(1); C5–Si1–Si1*–C5*, 30.7(2).

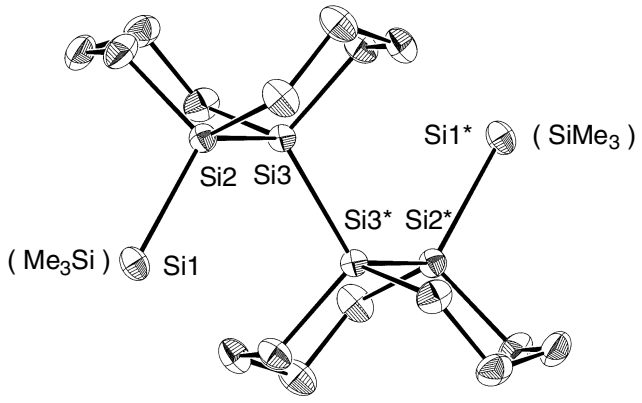


Figure S2. X-ray structure of **4** at 40% probability level. All hydrogens and methyl groups in trimethylsilyl groups are omitted for clarity. Selected bond lengths (Å) and angles (deg): Si1–Si2, 2.3410(6); Si2–Si3, 2.3232(5); Si3–Si3*, 2.3408(7); Si1–Si2–Si3, 119.72(2); Si2–Si3–Si3*, 118.89(3); Si1–Si2–Si3–Si3*, 32.91(4); Si2–Si3–Si3*–Si2*, 180.0.

(3) Computational details

The starting geometries of the *A C*-alternating oligosilanes **3**-**6** were built on Spartan[1] based on the X-ray structures of **1** and **4**. A virtual octadecasilane **7** with *A,C*-alternating conformation was also built on a computer in the same manner for a more detailed investigation of the conformational effect. The permethylated oligosilanes up to n-$Si_{18}Me_{38}$ were also built on Spartan. All oligosilanes were adapted to the C_2-point group. The geometry optimization calculations were performed with an HIT HPC-PA264U computer using the Gaussian 98[2] program at the HF/3-21G(d) level, followed by the CIS calculations with the 6-31G(d) basis set. The Cartesian coordinates of the *A,C*-alternating oligosilaes **3**-**7** optimized at the HF/3-21G(d) level are shown in Table 1-5. The details of the CIS calculations are also shown. The calculated absorption maximum wavelengths in the parentheses are the scaled values (scale factor = 0.76).

[1] PC Spartan Pro Version 1.0.2; Wavefunction, Inc., Irvine, CA, 2000.
[2] Fisch, M. J., et al. Gaussian 98, revision 9.A; Gaussian Inc.; Pittsburgh, PA, 1998.

Table 1. HF/3-21(d) optimized geometry of the *C*-tetrasilane **3**.

1Si	0.353131	1.105392	-0.605758	27Si	0.105993	2.437735	1.315846
2C	2.485993	0.056956	-2.294332	28C	1.240080	1.803577	2.697435
3C	0.679873	-1.817065	-2.049139	29H	0.999946	0.782342	2.982255
4C	2.190502	-1.435210	-2.000004	30H	1.146611	2.423883	3.587146
5Si	-0.353131	-1.105392	-0.605758	31H	2.283647	1.825072	2.389977
6C	2.190502	1.028121	-1.112875	32C	0.615268	4.218702	0.904312
7H	1.925568	0.360855	-3.173257	33H	-0.013378	4.641675	0.123726
8H	0.267349	-1.464009	-2.993104	34H	1.646933	4.266131	0.562002
9H	2.612820	-1.695485	-1.033385	35H	0.528434	4.858640	1.780710
10H	2.784548	0.715300	-0.253995	36C	-1.680352	2.461272	1.949888
11H	3.537866	0.146335	-2.551376	37H	-2.354032	2.899685	1.217190
12H	0.590313	-2.902664	-2.067653	38H	-1.752723	3.055969	2.859051
13H	2.717800	-2.031302	-2.739303	39H	-2.044063	1.462728	2.179931
14H	2.541381	2.024048	-1.382866	40Si	-0.105993	-2.437735	1.315846
15C	-0.679873	1.817065	-2.049139	41C	-1.240080	-1.803577	2.697435
16H	-0.590313	2.902664	-2.067653	42H	-0.999946	-0.782342	2.982255
17H	-0.267349	1.464009	-2.993104	43H	-2.283647	-1.825072	2.389977
18C	-2.190502	-1.028121	-1.112875	44C	1.680352	-2.461272	1.949888
19H	-2.784548	-0.715300	-0.253995	45H	2.044063	-1.462728	2.179931
20H	-2.541381	-2.024048	-1.382866	46H	1.752723	-3.055969	2.859051
21C	-2.485993	-0.056956	-2.294332	47H	-1.146611	-2.423883	3.587146
22H	-3.537866	-0.146335	-2.551376	48H	2.354032	-2.899685	1.217190
23H	-1.925568	-0.360855	-3.173257	49C	-0.615268	-4.218702	0.904312
24C	-2.190502	1.435210	-2.000004	50H	0.013378	-4.641675	0.123726
25H	-2.717800	2.031302	-2.739303	51H	-1.646933	-4.266131	0.562002
26H	-2.612820	1.695485	-1.033385	52H	-0.528434	-4.858640	1.780710

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Summary of CIS calculation output for **3**.
(HOMO = 87, LUMO = 88)

(a) Excitation energies (not scaled) and oscillator strengths:

Excited State 1: Singlet-B 6.9137 eV 179.33 (235.96) nm f=0.0444
86(B) -> 91(A) 0.15524
87(A) -> 88(B) 0.64516
87(A) -> 96(B) 0.10448
This state for optimization and/or second-order correction.
Total Energy, E(CIS) = -1705.45159086
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 7.2458 eV 171.11 (225.15) nm f=0.0496
86(B) -> 90(B) -0.20660
87(A) -> 89(A) 0.61932

Excited State 3: Singlet-A 7.7218 eV 160.56 (211.27) nm f=0.0121
84(A) -> 91(A) 0.12263
85(A) -> 91(A) 0.15096
86(B) -> 88(B) 0.56509
87(A) -> 91(A) 0.30558

Excited State 4: Singlet-B 7.8431 eV 158.08 (208.00) nm f=0.5921
85(A) -> 90(B) -0.15162
86(B) -> 89(A) 0.49267
87(A) -> 90(B) -0.38512

Excited State 5: Singlet-B 8.3838 eV 147.89 nm (194.59) f=0.1516
84(A) -> 88(B) -0.12364
85(A) -> 88(B) -0.20679
85(A) -> 90(B) -0.11022
86(B) -> 89(A) 0.33584
86(B) -> 91(A) -0.19610
87(A) -> 88(B) 0.10079
87(A) -> 90(B) 0.45319

(b) Orbital symmetries and eigenvalues (Hartree) of ten high energy occupied orbitals and ten low energy unoccupied orbitals:

occ. eigenvalues:
#78 -0.45232(B), #79 -0.42768(B), #80 -0.42606(A), #81 -0.42419(A), #82 -0.42176(B)
#83 -0.40790(B), #84 -0.38365(A), #85 -0.36574(A), #86 -0.34059(B), #87 -0.31957(A)

virt. eigenvalues:
#88 0.14653(B), #89 0.14989(A), #90 0.17489(B), #91 0.18085(A), #92 0.18358(A)
#93 0.21333(B), #94 0.21544(A), #95 0.22320(B), #96 0.23756(B), #97 0.23768(A)

Table 2. HF/3-21(d) optimized geometry of the *CAC*-hexasilane **4**.

1Si	0.487256	3.036777	0.248485	40Si	-0.906638	-0.749964	0.164261
2C	1.676740	2.805186	2.893731	41Si	-0.487256	-3.036777	0.248485
3C	2.064510	0.523687	1.668476	42C	-1.900036	-0.514517	-1.447867
4C	1.605484	1.259986	2.963844	43H	-2.359000	0.472651	-1.460610
5Si	0.906638	0.749964	0.164261	44H	-1.212037	-0.541799	-2.293088
6C	0.511614	3.472122	2.104980	45C	-3.008293	-1.581562	-1.687469
7H	2.631153	3.098332	2.467192	46H	-3.717104	-1.573980	-0.864857
8H	3.056252	0.887766	1.402619	47H	-3.563466	-1.298593	-2.577483
9H	0.592787	0.967629	3.222529	48C	-2.064510	-3.743179	-0.571144
10H	-0.431051	3.169268	2.561009	49H	-2.892776	-3.677493	0.132756
11H	1.661495	3.187382	3.910665	50H	-1.926528	-4.804415	-0.775870
12H	2.182253	-0.535782	1.892022	51C	-2.483606	-3.024726	-1.887917
13H	2.240927	0.933126	3.782031	52H	-3.272094	-3.604904	-2.358694
14H	0.579019	4.553140	2.226608	53H	-1.652423	-3.005333	-2.587402
15C	2.064510	3.743179	-0.571144	54C	-2.064510	-0.523687	1.668476
16H	1.926528	4.804415	-0.775870	55H	-2.182253	0.535782	1.892022
17H	2.892776	3.677493	0.132756	56H	-3.056252	-0.887766	1.402619
18C	1.900036	0.514517	-1.447867	57C	-0.511614	-3.472122	2.104980
19H	1.212037	0.541799	-2.293088	58H	0.431051	-3.169268	2.561009
20H	2.359000	-0.472651	-1.460610	59H	-0.579019	-4.553140	2.226608
21C	3.008293	1.581562	-1.687469	60C	-1.605484	-1.259986	2.963844
22H	3.563466	1.298593	-2.577483	61H	-0.592787	-0.967629	3.222529
23H	3.717104	1.573980	-0.864857	62H	-2.240927	-0.933126	3.782031
24C	2.483606	3.024726	-1.887917	63C	-1.676740	-2.805186	2.893731
25H	3.272094	3.604904	-2.358694	64H	-1.661495	-3.187382	3.910665
26H	1.652423	3.005333	-2.587402	65H	-2.631153	-3.098332	2.467192
27Si	-1.427255	3.959076	-0.758023	66S	1.427255	-3.959076	-0.758023
28C	-2.993974	3.345090	0.115949	67C	2.993974	-3.345090	0.115949
29H	-3.092679	2.264055	0.064923	68H	3.092679	-2.264055	0.064923
30H	-3.883041	3.779578	-0.337913	69H	2.990676	-3.627447	1.166937
31H	-2.990676	3.627447	1.166937	70C	1.540600	-3.552251	-2.605703
32C	-1.353921	5.846602	-0.573203	71H	1.562215	-2.480980	-2.788374
33H	-0.477118	6.261410	-1.065718	72H	2.447169	-3.978075	-3.032752
34H	-1.317495	6.140897	0.473577	73H	3.883041	-3.779578	-0.337913
35H	-2.232265	6.312577	-1.016609	74H	0.695801	-3.966270	-3.151685
36C	-1.540600	3.552251	-2.605703	75C	1.353921	-5.846602	-0.573203
37H	-0.695801	3.966270	-3.151685	76H	2.232265	-6.312577	-1.016609
38H	-2.447169	3.978075	-3.032752	77H	0.477118	-6.261410	-1.065718
39H	-1.562215	2.480980	-2.788374	78H	1.317495	-6.140897	0.473577

CIS calculation output for **4**.
(HOMO = 133, LUMO = 134)

(a) Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 6.6864 eV 185.43 (243.99) nm f=0.0045
131(A) ->139(A) -0.11150
132(B) ->134(B) -0.10478
132(B) ->136(B) -0.21102
133(A) ->135(A) 0.58973
133(A) ->137(A) -0.10902
This state for optimization and/or second-order correction.
Total Energy, E(CIS) = -2595.58698932
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-B 6.7434 eV 183.86 (241.92) nm f=0.3751
132(B) ->135(A) -0.12843
132(B) ->137(A) 0.14522
133(A) ->134(B) 0.60851

Excited State 3: Singlet-B 7.1520 eV 173.36 (228.10) nm f=0.0726
131(A) ->134(B) -0.11866
131(A) ->136(B) -0.12927
132(B) ->135(A) -0.38351
132(B) ->139(A) -0.10925
133(A) ->134(B) -0.12232
133(A) ->136(B) 0.45323

Excited State 4: Singlet-A 7.3584 eV 168.49 (221.70) nm f=0.0146
130(B) ->134(B) -0.10603
131(A) ->137(A) -0.19899
132(B) ->134(B) 0.39483
132(B) ->138(B) 0.19326
133(A) ->135(A) 0.12067
133(A) ->137(A) 0.39787

Excited State 5: Singlet-A 7.6184 eV 162.74 (214.14) nm f=0.0001
129(A) ->139(A) -0.12401
130(B) ->134(B) 0.10600
131(A) ->135(A) 0.45680
132(B) ->136(B) 0.34418
133(A) ->139(A) -0.23868

(b) Orbital symmetries and eigenvalues (Hartree) of ten high energy occupied orbitals and ten low energy unoccupied orbitals:

occ. eigenvalues:
#124 -0.42270(A), #125 -0.41420(A), #126 -0.40697(B), #127 -0.38830(A), #128 -0.37857(B)
#129 -0.36726(A), #130 -0.36265(B), #131 -0.33794(A), #132 -0.33368(B), #133 -0.30764(A)

virt. eigenvalues:
#134 0.13527(B), #135 0.14015(A), #136 0.15809(B), #137 0.16030(A), #138 0.17884(B)
#139 0.18176(A), #140 0.18587(A), #141 0.20087(B), #142 0.20710(B), #143 0.21501(A)

Table 3. HF/3-21(d) optimized geometry of the *CACAC*-octasilane **5**.

1Si	3.359054	3.286815	0.687262	43H	3.233294	0.156039	-2.035263
2C	1.286753	5.281243	1.129991	44H	2.671887	-1.064530	-0.924961
3C	0.185514	2.928760	1.460434	45C	2.015242	-1.378148	-2.961372
4C	0.097936	4.342627	0.809234	46H	1.696882	-0.789521	-3.816417
5Si	1.564606	1.806570	0.758425	47H	2.920766	-1.897375	-3.262723
6C	2.580733	4.987690	0.315645	48C	-0.525473	-1.904137	-2.640496
7H	1.498068	5.236740	2.193997	49H	-0.706358	-1.400385	-3.589211
8H	0.350357	3.055393	2.529844	50H	-1.210090	-2.751074	-2.614062
9H	0.002418	4.254143	-0.268312	51C	0.936387	-2.442477	-2.646973
10H	2.341917	5.052797	-0.745982	52H	1.007056	-3.223498	-3.398693
11H	0.975404	6.300440	0.918343	53H	1.169950	-2.907163	-1.694306
12H	-0.781284	2.438034	1.360999	54C	0.525473	1.904137	-2.640496
13H	-0.810704	4.821881	1.162475	55H	1.210090	2.751074	-2.614062
14H	3.307871	5.774476	0.516222	56H	0.706358	1.400385	-3.589211
15C	3.940297	3.260058	2.509409	57C	-2.365343	0.443492	-1.766869
16H	4.898939	3.770723	2.595112	58H	-2.671887	1.064530	-0.924961
17H	3.239512	3.831289	3.116375	59H	-3.233294	-0.156039	-2.035263
18C	2.075574	0.514960	2.065997	60C	-0.936387	2.442477	-2.646973
19H	2.790309	-0.175204	1.616940	61H	-1.169950	2.907163	-1.694306
20H	1.214197	-0.084824	2.354226	62H	-1.007056	3.223498	-3.398693
21C	2.718746	1.113447	3.351447	63C	-2.015242	1.378148	-2.961372
22H	2.884581	0.302626	4.055354	64H	-2.920766	1.897375	-3.262723
23H	2.027092	1.801261	3.828662	65H	-1.696882	0.789521	-3.816417
24C	4.070044	1.834531	3.123225	66Si	-1.564606	-1.806570	0.758425
25H	4.570364	1.919184	4.083686	67Si	-3.359054	-3.286815	0.687262
26H	4.702750	1.211131	2.497384	68C	-2.075574	-0.514960	2.065997
27Si	5.189176	2.931813	-0.746140	69H	-1.214197	0.084824	2.354226
28C	4.650601	3.091518	-2.557352	70H	-2.790309	0.175204	1.616940
29H	3.886249	2.366195	-2.822943	71C	-3.940297	-3.260058	2.509409
30H	5.496854	2.938885	-3.225036	72H	-3.239512	-3.831289	3.116375
31H	4.249180	4.082956	-2.757914	73H	-4.898939	-3.770723	2.595112
32C	6.486511	4.274018	-0.402351	74C	-2.718746	-1.113447	3.351447
33H	6.846207	4.227216	0.623221	75H	-2.884581	-0.302626	4.055354
34H	6.079804	5.269615	-0.566860	76H	-2.027092	-1.801261	3.828662
35H	7.346916	4.156485	-1.058969	77C	-4.070044	-1.834531	3.123225
36C	6.007098	1.243034	-0.479187	78H	-4.570364	-1.919184	4.083686
37H	6.404934	1.155014	0.529390	79H	-4.702750	-1.211131	2.497384
38H	6.837030	1.110278	-1.171414	80C	-0.185514	-2.928760	1.460434
39H	5.312834	0.421661	-0.635909	81H	0.781284	-2.438034	1.360999
40Si	0.936387	0.694453	-1.217970	82H	-0.350357	-3.055393	2.529844
41Si	-0.936387	-0.694453	-1.217970	83C	-2.580733	-4.987690	0.315645
42C	2.365343	-0.443492	-1.766869	84H	-2.341917	-5.052797	-0.745982

85H	-3.307871	-5.774476	0.516222	95H	-4.249180	-4.082956	-2.757914
86C	-1.286753	-5.281243	1.129991	96C	-6.007098	-1.243034	-0.479187
87H	-0.975404	-6.300440	0.918343	97H	-5.312834	-0.421661	-0.635909
88H	-1.498068	-5.236740	2.193997	98H	-6.837030	-1.110278	-1.171414
89C	-0.097936	-4.342627	0.809234	99H	-5.496854	-2.938885	-3.225036
90H	-0.002418	-4.254143	-0.268312	100H	-6.404934	-1.155014	0.529390
91H	0.810704	-4.821881	1.162475	101C	-6.486511	-4.274018	-0.402351
92Si	-5.189176	-2.931813	-0.746140	102H	-6.846207	-4.227216	0.623221
93C	-4.650601	-3.091518	-2.557352	103H	-6.079804	-5.269615	-0.566860
94H	-3.886249	-2.366195	-2.822943	104H	-7.346916	-4.156485	-1.058969

CIS calculation output for **5**.
(HOMO = 179, LUMO = 180)

(a) Excitation energies and oscillator strengths:

Excited State 1: Singlet-B 6.6012 eV 187.82 (247.13) nm f=0.1225
176(A) ->181(B) -0.13378
176(A) ->184(B) -0.10563
178(B) ->183(A) -0.21698
179(A) ->181(B) 0.54566
179(A) ->182(B) 0.15797
179(A) ->184(B) 0.14014
This state for optimization and/or second-order correction.
Total Energy, E(CIS) = -3485.71699279
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 6.6809 eV 185.58 (244.19) nm f=0.0844
178(B) ->182(B) -0.31921
179(A) ->180(A) 0.54102

Excited State 3: Singlet-B 6.7741 eV 183.03 (240.83) nm f=0.6389
178(B) ->180(A) -0.39982
178(B) ->183(A) -0.10133
179(A) ->181(B) -0.16096
179(A) ->182(B) 0.42902

Excited State 4: Singlet-A 6.9592 eV 178.16 (234.42) nm f=0.0981
176(A) ->180(A) 0.11072
177(B) ->181(B) 0.10805
178(B) ->181(B) -0.33622
178(B) ->182(B) -0.15778
178(B) ->184(B) 0.11083
179(A) ->180(A) -0.17571
179(A) ->183(A) 0.41100
179(A) ->185(A) -0.11825

Excited State 5: Singlet-B 7.2816 eV 170.27 (224.04) nm f=0.0323
175(A) ->181(B) 0.14874
176(A) ->181(B) -0.19297
176(A) ->182(B) -0.17507
176(A) ->184(B) 0.11637
177(B) ->180(A) 0.12831
177(B) ->183(A) 0.12800
178(B) ->183(A) 0.35013
179(A) ->184(B) 0.34887
179(A) ->186(B) 0.11990

(b) Orbital symmetries and eigenvalues (Hartree) of ten high energy occupied orbitals and ten low energy unoccupied orbitals:

occ. eigenvalues:
#170 -0.39077(A), #171 -0.38270(B), #172 -0.37710(A), #173 -0.36802(A), #174 -0.36298(B)
#175 -0.36270(A), #176 -0.33706(A), #177 -0.33693(B), #178 -0.32081(B), #179 -0.30278(A)

virt. eigenvalues:
#180 0.13193(A), #181 0.13548(B), #182 0.14602(B), #183 0.14936(A), #184 0.16418(B)
#185 0.16668(A), #186 0.18064(B), #187 0.18202(A), #188 0.18719(A), #189 0.19475(B)

Table 4. HF/3-21(d) optimized geometry of the *CACACAC*-decasilane **6**.

1Si	-3.381855	5.510111	0.625438	42C	-2.910348	1.983372	-2.237544
2C	-3.329497	5.024499	3.494015	43H	-3.746536	2.669470	-2.359689
3C	-1.422097	3.583663	2.424681	44H	-2.046160	2.472519	-2.687389
4C	-2.633700	3.644332	3.404071	45C	-3.208657	0.684035	-3.040562
5Si	-1.878518	3.734095	0.574524	46H	-4.063312	0.168014	-2.613699
6C	-4.276402	5.350771	2.302112	47H	-3.490407	0.966500	-4.051128
7H	-2.573964	5.797981	3.592029	48C	-1.772406	-1.147361	-1.850325
8H	-0.735648	4.389885	2.680843	49H	-2.704763	-1.647569	-1.591272
9H	-3.372447	2.896635	3.133571	50H	-1.061900	-1.938667	-2.084488
10H	-5.031206	4.566949	2.237080	51C	-2.016404	-0.298310	-3.133389
11H	-3.914789	5.045440	4.409168	52H	-2.205950	-0.978354	-3.959048
12H	-0.877546	2.657474	2.600404	53H	-1.121687	0.259768	-3.390697
13H	-2.278843	3.384017	4.397258	54C	-4.156825	1.008672	0.437029
14H	-4.810820	6.275101	2.521201	55H	-4.832331	1.827531	0.681605
15C	-2.191759	7.005716	0.702217	56H	-4.683328	0.390990	-0.289508
16H	-2.752016	7.927297	0.547521	57C	-1.670760	-1.086277	1.259388
17H	-1.768926	7.074868	1.703325	58H	-1.241472	-0.575288	2.121565
18C	-0.390730	4.412381	-0.408435	59H	-1.245294	-2.087909	1.256768
19H	-0.639558	4.404487	-1.469952	60C	-3.919881	0.155922	1.719004
20H	0.466752	3.752117	-0.292792	61H	-3.350279	0.723635	2.447907
21C	0.037749	5.858054	-0.020074	62H	-4.885237	-0.050627	2.172351
22H	0.940708	6.102796	-0.572530	63C	-3.208657	-1.196504	1.473164
23H	0.298402	5.899307	1.033276	64H	-3.386367	-1.830728	2.337200
24C	-1.019140	6.949027	-0.321204	65H	-3.669908	-1.692928	0.624753
25H	-0.515870	7.911685	-0.319510	66Si	1.165540	0.160680	-0.329316
26H	-1.403605	6.801407	-1.326674	67Si	2.572706	-1.698846	-0.381895
27Si	-4.966885	5.833588	-1.081579	68C	1.670760	1.086277	1.259388
28C	-6.235842	4.424478	-1.083875	69H	1.245294	2.087909	1.256768
29H	-5.773068	3.456547	-1.256389	70H	1.241472	0.575288	2.121565
30H	-6.979660	4.578526	-1.863787	71C	4.156825	-1.008672	0.437029
31H	-6.763055	4.373922	-0.133184	72H	4.683328	-0.390990	-0.289508
32C	-5.894153	7.453042	-0.734439	73H	4.832331	-1.827531	0.681605
33H	-5.219221	8.306167	-0.732082	74C	3.208657	1.196504	1.473164
34H	-6.395821	7.423392	0.230513	75H	3.386367	1.830728	2.337200
35H	-6.651933	7.634523	-1.494767	76H	3.669908	1.692928	0.624753
36C	-4.173399	5.968428	-2.797542	77C	3.919881	-0.155922	1.719004
37H	-3.504866	6.824626	-2.854286	78H	4.885237	0.050627	2.172351
38H	-4.939610	6.100051	-3.559903	79H	3.350279	-0.723635	2.447907
39H	-3.600800	5.081479	-3.055725	80C	1.772406	1.147361	-1.850325
40Si	-2.572706	1.698846	-0.381895	81H	1.061900	1.938667	-2.084488
41Si	-1.165540	-0.160680	-0.329316	82H	2.704763	1.647569	-1.591272

83C	2.910348	-1.983372	-2.237544	107C	1.422097	-3.583663	2.424681
84H	2.046160	-2.472519	-2.687389	108H	0.877546	-2.657474	2.600404
85H	3.746536	-2.669470	-2.359689	109H	0.735648	-4.389885	2.680843
86C	3.208657	-0.684035	-3.040562	110C	4.276402	-5.350771	2.302112
87H	3.490407	-0.966500	-4.051128	111H	5.031206	-4.566949	2.237080
88H	4.063312	-0.168014	-2.613699	112H	4.810820	-6.275101	2.521201
89C	2.016404	0.298310	-3.133389	113C	2.633700	-3.644332	3.404071
90H	1.121687	-0.259768	-3.390697	114H	2.278843	-3.384017	4.397258
91H	2.205950	0.978354	-3.959048	115H	3.372447	-2.896635	3.133571
92Si	1.878518	-3.734095	0.574524	116C	3.329497	-5.024499	3.494015
93Si	3.381855	-5.510111	0.625438	117H	3.914789	-5.045440	4.409168
94Si	4.966885	-5.833588	-1.081579	118H	2.573964	-5.797981	3.592029
95C	0.390730	-4.412381	-0.408435	119C	6.235842	-4.424478	-1.083875
96H	-0.466752	-3.752117	-0.292792	120H	6.979660	-4.578526	-1.863787
97H	0.639558	-4.404487	-1.469952	121H	6.763055	-4.373922	-0.133184
98C	-0.037749	-5.858054	-0.020074	122H	5.773068	-3.456547	-1.256389
99H	-0.298402	-5.899307	1.033276	123C	4.173399	-5.968428	-2.797542
100H	-0.940708	-6.102796	-0.572530	124H	3.600800	-5.081479	-3.055725
101C	2.191759	-7.005716	0.702217	125H	3.504866	-6.824626	-2.854286
102H	1.768926	-7.074868	1.703325	126H	4.939610	-6.100051	-3.559903
103H	2.752016	-7.927297	0.547521	127C	5.894153	-7.453042	-0.734439
104C	1.019140	-6.949027	-0.321204	128H	5.219221	-8.306167	-0.732082
105H	0.515870	-7.911685	-0.319510	129H	6.395821	-7.423392	0.230513
106H	1.403605	-6.801407	-1.326674	130H	6.651933	-7.634523	-1.494767

CIS calculation output for **6**.
(HOMO = 225, LUMO = 226)
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 6.5843 eV 188.30 (247.77) nm f=0.0244
223(A) ->227(A) 0.12313
223(A) ->231(A) 0.16165
224(B) ->228(B) 0.25213
225(A) ->227(A) 0.44669
225(A) ->229(A) 0.26337
225(A) ->231(A) 0.14676
This state for optimization and/or second-order correction.
Total Energy, E(CIS) = -4375.84443517
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-B 6.6174 eV 187.36 (246.53) nm f=0.2006
223(A) ->226(B) 0.11702
223(A) ->230(B) -0.17749
224(B) ->229(A) 0.27406
225(A) ->226(B) 0.45671
225(A) ->228(B) 0.24916

Excited State 3: Singlet-A 6.7162 eV 184.60 (242.90) nm f=0.0079
223(A) ->229(A) -0.18014
224(B) ->226(B) 0.34862
224(B) ->230(B) 0.23854
225(A) ->227(A) -0.24808
225(A) ->229(A) 0.33614

Excited State 4: Singlet-B 6.7514 eV 183.64 (241.64) nm f=1.1346
223(A) ->226(B) 0.15067
223(A) ->230(B) 0.10118
224(B) ->227(A) 0.38588
224(B) ->229(A) -0.19163
225(A) ->226(B) -0.18439
225(A) ->228(B) 0.32524
225(A) ->230(B) -0.15709

Excited State 5: Singlet-B 6.9017 eV 179.64 (236.37) nm f=0.2491
223(A) ->226(B) -0.28129
224(B) ->227(A) 0.10866
224(B) ->229(A) 0.26239
224(B) ->231(A) -0.10086
225(A) ->226(B) -0.22009
225(A) ->228(B) 0.16176
225(A) ->230(B) 0.33895

(b) Orbital symmetries and eigenvalues (Hartree) of ten high energy occupied orbitals and ten low energy unoccupied orbitals:

occ. eigenvalues:
#216 -0.37628(B), #217 -0.36850(A), #218 -0.36506(B), #219 -0.36302(B), #220 -0.36075(A)
#221 -0.33743(B), #222 -0.33653(A), #223 -0.32862(A), #224 -0.31294(B), #225 -0.30031(A)

virt. eigenvalues:
#226 0.13117(B), #227 0.13213(A), #228 0.14083(B), #229 0.14266(A), #230 0.15219(B)
#231 0.15643(A), #232 0.16790(A), #233 0.17112(B), #234 0.18181(A), #235 0.18205(B)

Table 5. HF/3-21(d) optimized geometry of the *CA* alt.-octadecasilane **7**.

1Si	-0.996487	-2.924509	0.385792
2C	-2.116259	-2.495222	3.043285
3C	-2.111560	-0.178672	1.830933
4C	-1.785557	-0.985696	3.122834
5Si	-1.017676	-0.591546	0.317892
6C	-1.080977	-3.339758	2.245165
7H	-3.108173	-2.621146	2.619976
8H	-3.152495	-0.363282	1.568265
9H	-0.738445	-0.869960	3.383886
10H	-0.097493	-3.183370	2.689101
11H	-2.160787	-2.882718	4.057349
12H	-2.042709	0.884279	2.056780
13H	-2.358255	-0.559995	3.941967
14H	-1.311140	-4.394594	2.380882
15C	-2.674946	-3.342712	-0.429096
16H	-2.717486	-4.405682	-0.661251
17H	-3.468372	-3.161188	0.294867
18C	-1.974633	-0.178103	-1.279004
19H	-1.318077	-0.330387	-2.136051
20H	-2.246140	0.875581	-1.287906
21C	-3.260956	-1.027602	-1.493005
22H	-3.781558	-0.641228	-2.364868
23H	-3.934947	-0.905139	-0.650578
24C	-3.001453	-2.535923	-1.720998
25H	-3.891738	-2.964565	-2.172478
26H	-2.201674	-2.648015	-2.446155
27Si	1.017676	0.591546	0.317892
28Si	0.996487	2.924509	0.385792
29C	1.974633	0.178103	-1.279004
30H	2.246140	-0.875581	-1.287906
31H	1.318077	0.330387	-2.136051
32C	3.260956	1.027602	-1.493005
33H	3.934947	0.905139	-0.650578
34H	3.781558	0.641228	-2.364868
35C	2.674946	3.342712	-0.429096
36H	3.468372	3.161188	0.294867
37H	2.717486	4.405682	-0.661251
38C	3.001453	2.535923	-1.720998
39H	3.891738	2.964565	-2.172478
40H	2.201674	2.648015	-2.446155
41C	2.111560	0.178672	1.830933
42H	2.042709	-0.884279	2.056780
43H	3.152495	0.363282	1.568265
44C	1.080977	3.339758	2.245165
45H	0.097493	3.183370	2.689101
46H	1.311140	4.394594	2.380882
47C	1.785557	0.985696	3.122834
48H	0.738445	0.869960	3.383886
49H	2.358255	0.559995	3.941967
50C	2.116259	2.495222	3.043285
51H	2.160787	2.882718	4.057349
52H	3.108173	2.621146	2.619976
53Si	-0.797653	4.104825	-0.578180
54Si	-0.743813	6.437684	-0.624922
55C	-2.396235	3.692010	0.376260
56H	-2.641918	2.639178	0.252708
57H	-2.221965	3.840702	1.442227
58C	-2.607262	6.860880	-0.693332
59H	-2.967047	6.684375	-1.706265
60H	-2.751203	7.923583	-0.504367
61C	-3.629403	4.545368	-0.039884
62H	-4.500940	4.158671	0.481008
63H	-3.825504	4.427300	-1.101290
64C	-3.505367	6.052230	0.289438
65H	-4.502569	6.482774	0.269957
66H	-3.141240	6.159658	1.306305
67C	-1.045830	3.693176	-2.428875
68H	-0.876148	2.630773	-2.596458
69H	-2.087766	3.875826	-2.689003
70C	0.053407	6.857163	-2.305589
71H	1.130939	6.705731	-2.236446
72H	-0.091356	7.911819	-2.531495
73C	-0.482704	6.012007	-3.497301
74H	-0.046108	6.401131	-4.412945
75H	-1.557483	6.135331	-3.590079
76C	-0.149863	4.503172	-3.412644
77H	0.896624	4.389599	-3.148048
78H	-0.266578	4.078079	-4.405535
79Si	0.386015	7.619580	1.068251
80Si	0.319407	9.951558	1.058197
81Si	0.124060	11.128100	-0.971126
82C	2.246165	7.206368	0.992839

83H	2.404479	6.155743	1.227623
84H	2.600325	7.346641	-0.028761
85C	3.131648	8.068801	1.938974
86H	2.796633	7.961589	2.966228
87H	4.145610	7.680327	1.901818
88C	1.925343	10.387445	2.000377
89H	1.759249	10.225682	3.064712
90H	2.142318	11.448989	1.887587
91C	3.182768	9.572151	1.575251
92H	4.050075	10.006062	2.064772
93H	3.349347	9.668315	0.507075
94C	-0.276782	7.224404	2.817557
95H	-0.509386	6.163356	2.893197
96H	0.516516	7.410513	3.540501
97C	-1.177743	10.385832	2.157430
98H	-2.095161	10.233720	1.588489
99H	-1.151557	11.442776	2.416225
100C	-1.530112	8.042530	3.249531
101H	-1.900854	7.627263	4.182395
102H	-2.325356	7.924871	2.520299
103C	-1.272357	9.552643	3.468454
104H	-2.089173	9.949512	4.064901
105H	-0.369191	9.678334	4.057854
106C	-1.571914	10.747265	-1.757511
107H	-2.347110	10.891597	-1.004469
108H	-1.622862	9.699784	-2.048567
109C	1.521042	10.732271	-2.214540
110H	1.746862	9.667448	-2.195340
111H	1.162142	10.945897	-3.220725
112Si	0.797653	-4.104825	-0.578180
113C	0.149863	-4.503172	-3.412644
114C	-0.053407	-6.857163	-2.305589
115C	0.482704	-6.012007	-3.497301
116Si	0.743813	-6.437684	-0.624922
117C	1.045830	-3.693176	-2.428875
118H	-0.896624	-4.389599	-3.148048
119H	-1.130939	-6.705731	-2.236446
120H	1.557483	-6.135331	-3.590079
121H	2.087766	-3.875826	-2.689003
122H	0.266578	-4.078079	-4.405535
123H	0.091356	-7.911819	-2.531495
124H	0.046108	-6.401131	-4.412945
125H	0.876148	-2.630773	-2.596458
126C	2.396235	-3.692010	0.376260
127H	2.221965	-3.840702	1.442227
128H	2.641918	-2.639178	0.252708
129C	2.607262	-6.860880	-0.693332
130H	2.967047	-6.684375	-1.706265
131H	2.751203	-7.923583	-0.504367
132C	3.505367	-6.052230	0.289438
133H	4.502569	-6.482774	0.269957
134H	3.141240	-6.159658	1.306305
135C	3.629403	-4.545368	-0.039884
136H	4.500940	-4.158671	0.481008
137H	3.825504	-4.427300	-1.101290
138Si	-0.386015	-7.619580	1.068251
139C	-2.246165	-7.206368	0.992839
140H	-2.404479	-6.155743	1.227623
141C	0.276782	-7.224404	2.817557
142H	-0.516516	-7.410513	3.540501
143H	0.509386	-6.163356	2.893197
144Si	0.215157	13.453384	-0.918586
145Si	-0.630361	14.682690	0.899464
146C	-0.745832	13.902023	-2.510556
147H	-0.117535	13.698715	-3.376407
148H	-0.945116	14.973059	-2.527818
149C	2.056221	13.880781	-1.172942
150H	2.596579	13.726716	-0.238803
151H	2.156154	14.938737	-1.415296
152C	-1.925343	11.625262	-2.993844
153H	-1.173553	11.499734	-3.767315
154H	-2.861200	11.262219	-3.409559
155C	-2.089174	13.134774	-2.690055
156H	-2.633393	13.584865	-3.515432
157H	-2.711154	13.252657	-1.806973
158C	2.750264	13.043551	-2.286922
159H	3.760489	13.421681	-2.417255
160H	2.240611	13.189190	-3.234424
161C	2.843161	11.527171	-1.988776
162H	3.193229	11.391287	-0.970502
163H	3.605851	11.105564	-2.637368
164C	0.396878	14.353803	2.459120
165H	0.380589	13.306269	2.747513
166H	0.016791	14.933397	3.298679
167H	1.436221	14.638688	2.307656
168C	-2.452829	14.301333	1.253900

169H	-2.616814	13.249988	1.475158	202H	2.347110	-10.891597	-1.004469
170H	-3.080636	14.564992	0.405618	203Si	-0.215157	-13.453384	-0.918586
171H	-2.800619	14.876958	2.110226	204Si	0.630361	-14.682690	0.899464
172C	-0.487016	16.529791	0.486058	205C	0.745832	-13.902023	-2.510556
173H	0.546054	16.814857	0.298474	206H	0.117535	-13.698715	-3.376407
174H	-0.852932	17.139358	1.310549	207H	0.945116	-14.973059	-2.527818
175H	-1.068302	16.786917	-0.396749	208C	-2.056221	-13.880781	-1.172942
176Si	-0.319407	-9.951558	1.058197	209H	-2.596579	-13.726716	-0.238803
177Si	-0.124060	-11.128100	-0.971126	210H	-2.156154	-14.938737	-1.415296
178C	-1.925343	-10.387445	2.000377	211C	1.925343	-11.625262	-2.993844
179H	-1.759249	-10.225682	3.064712	212H	2.861200	-11.262219	-3.409559
180H	-2.142318	-11.448989	1.887587	213H	1.173553	-11.499734	-3.767315
181C	1.177743	-10.385832	2.157430	214C	2.089174	-13.134774	-2.690055
182H	2.095161	-10.233720	1.588489	215H	2.711154	-13.252657	-1.806973
183H	1.151557	-11.442776	2.416225	216H	2.633393	-13.584865	-3.515432
184C	-3.182768	-9.572151	1.575251	217C	-0.396878	-14.353803	2.459120
185H	-4.050075	-10.006062	2.064772	218H	-1.436221	-14.638688	2.307656
186H	-3.349347	-9.668315	0.507075	219H	-0.380589	-13.306269	2.747513
187H	-2.600325	-7.346641	-0.028761	220H	-0.016791	-14.933397	3.298679
188C	-3.131648	-8.068801	1.938974	221C	2.452829	-14.301333	1.253900
189H	-2.796633	-7.961589	2.966228	222H	2.800619	-14.876958	2.110226
190H	-4.145610	-7.680327	1.901818	223H	2.616814	-13.249988	1.475158
191C	1.530112	-8.042530	3.249531	224H	3.080636	-14.564992	0.405618
192H	1.900854	-7.627263	4.182395	225C	0.487016	-16.529791	0.486058
193H	2.325356	-7.924871	2.520299	226H	0.852932	-17.139358	1.310549
194C	1.272357	-9.552643	3.468454	227H	1.068302	-16.786917	-0.396749
195H	2.089173	-9.949512	4.064901	228H	-0.546054	-16.814857	0.298474
196H	0.369191	-9.678334	4.057854	229C	-2.843161	-11.527171	-1.988776
197C	-1.521042	-10.732271	-2.214540	230H	-3.193229	-11.391287	-0.970502
198H	-1.746862	-9.667448	-2.195340	231H	-3.605851	-11.105564	-2.637368
199H	-1.162142	-10.945897	-3.220725	232C	-2.750264	-13.043551	-2.286922
200C	1.571914	-10.747265	-1.757511	233H	-3.760489	-13.421681	-2.417255
201H	1.622862	-9.699784	-2.048567	234H	-2.240611	-13.189190	-3.234424

CIS calculation output for **7**.
(HOMO = 409, LUMO = 410)

Excited State 1: Singlet-B 6.5768 eV 188.52 (248.05) nm f=0.0206
405(A) -> 419(B) -0.15170
406(B) -> 416(A) 0.19972
407(A) -> 414(B) -0.19266
408(B) -> 412(A) 0.24766
408(B) -> 416(A) -0.17188
409(A) -> 410(B) 0.37434
409(A) -> 417(B) 0.11040
This state for optimization and/or second-order correction.
Total Energy, E(CIS) = -7936.35203218
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 6.5777 eV 188.49 (248.02) nm f=0.0050
405(A) -> 418(A) -0.10803
406(B) -> 413(B) 0.10422
406(B) -> 417(B) 0.13564
407(A) -> 415(A) -0.25125
408(B) -> 413(B) -0.25484
408(B) -> 414(B) 0.15045
409(A) -> 411(A) 0.38890

Excited State 3: Singlet-A 6.5908 eV 188.11 (247.52) nm f=0.0435
406(B) -> 410(B) -0.14165
407(A) -> 411(A) -0.14428
407(A) -> 418(A) 0.11606
408(B) -> 410(B) 0.21519
408(B) -> 417(B) 0.14596
408(B) -> 419(B) 0.12583
409(A) -> 412(A) 0.19916
409(A) -> 415(A) 0.17694
409(A) -> 416(A) -0.26248

Excited State 4: Singlet-B 6.6021 eV 187.79 (247.10) nm f=0.1588
405(A) -> 413(B) -0.10560
406(B) -> 415(A) -0.12275
407(A) -> 413(B) -0.17549
407(A) -> 417(B) 0.18390
408(B) -> 411(A) -0.27447
408(B) -> 415(A) -0.25695
409(A) -> 410(B) 0.12419
409(A) -> 413(B) 0.23319
409(A) -> 414(B) -0.17645

Excited State 5: Singlet-A 6.6431 eV 186.64 (245.58) nm f=0.0130
404(B) -> 413(B) 0.10924
406(B) -> 413(B) 0.11220
406(B) -> 417(B) -0.10662
407(A) -> 411(A) 0.21928
407(A) -> 415(A) 0.10315
408(B) -> 410(B) 0.22431
408(B) -> 413(B) 0.17611

408(B) -> 417(B) -0.15696
409(A) -> 412(A) 0.20800
409(A) -> 415(A) -0.24461

Excited State 6: Singlet-B 6.6798 eV 185.61 (244.23) nm f=2.1395
403(A) -> 413(B) 0.10847
404(B) -> 411(A) -0.13200
405(A) -> 410(B) -0.15751
406(B) -> 411(A) -0.18851
407(A) -> 410(B) -0.19920
407(A) -> 413(B) -0.11057
408(B) -> 412(A) 0.18905
408(B) -> 415(A) -0.15626
409(A) -> 414(B) 0.16931
409(A) -> 417(B) -0.16396
409(A) -> 419(B) 0.21360
409(A) -> 420(B) -0.17832

Excited State 7: Singlet-B 6.7287 eV 184.26 (242.45) nm f=2.0054
405(A) -> 410(B) -0.11605
406(B) -> 412(A) -0.25178
406(B) -> 418(A) -0.11360
407(A) -> 410(B) 0.16431
407(A) -> 414(B) 0.23274
407(A) -> 417(B) -0.15688
408(B) -> 412(A) -0.18991
408(B) -> 416(A) -0.21829
408(B) -> 418(A) -0.11633
409(A) -> 414(B) -0.14133
409(A) -> 419(B) 0.11307

Excited State 8: Singlet-A 6.7435 eV 183.86 (241.92) nm f=0.0971
405(A) -> 412(A) 0.14619
406(B) -> 410(B) 0.20857
406(B) -> 414(B) 0.15074
406(B) -> 417(B) -0.11037
407(A) -> 412(A) -0.27010
407(A) -> 416(A) -0.13164
407(A) -> 418(A) -0.11310
408(B) -> 414(B) 0.25089
408(B) -> 417(B) -0.10219
408(B) -> 419(B) -0.12057
409(A) -> 416(A) 0.19518

(b) Orbital symmetries and eigenvalues (Hartree) of ten high energy occupied orbitals and ten low energy unoccupied orbitals:

occ. eigenvalues:
#400 -0.35924(B), #401 -0.33687(A), #402 -0.33677(B), #403 -0.33408(A), #404 -0.33200(B),
#405 -0.32556(A), #406 -0.31683(B), #407 -0.30828(A), #408 -0.30141(B), #409 -0.29695(A)

virt. eigenvalues:
#410 0.12978(B), #411 0.13000(A), #412 0.13216(A), #413 0.13268(B), #414 0.13569(B),
#415 0.14009(A), #416 0.14408(A), #417 0.14442(B), #418 0.15032(A), #419 0.15148(B)