Supporting Information

Regioselective [2 + 2] Cycloaddition of Fullerene Dimer with Alkyne Triggered by Thermolysis of Inter-fullerene C–C Bond

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Content

1. General considerations for synthesis and characterization.

All reactions dealing with air- or moisture-sensitive compounds were carried out using standard Schlenk techniques. HPLC analyses were performed on a Shimadzu LC-10A system equipped with an SPD-M10A diode array detector and a Bucky-prep column (Nacalai Tesque Inc., 4.6 mm ID x 250 mm). Preparative HPLC was performed on a Bucky-prep column (20 mm ID x 250 mm) using toluene/2-propanol (7:3) as eluent (flow rate 8 mL/min) detected at 350 nm with a UV spectrophotometric detector, Shimadzu SPD-6A. Column chromatography was performed on silica gel 60N (Kanto Chemical, spherical and neutral, 140-325 mesh). NMR spectra were measured with a JEOL ECA-500 (500 MHz) spectrometer. Reagents and chemicals were purchased from Tokyo Chemical Industry Co., Sigma-Aldrich Co., Kanto Chemical Co., Inc., Wako Pure Chemical Industries, or other commercial suppliers and used as received.

2. Experimental procedures and spectra data for all compounds.

Synthesis of $[C_{60}(CH_2SiMe_2O^iPr)]_2$ (1). Under N_2, $C_{60}(CH_2SiMe_2O^iPr)H$ [1] (117 mg, 0.137 mmol), was dissolved in ODCB/THF (10/1 mL). Then ^{t}BuOK (1.0 M, 210 μL, 0.210 mmol) was added to the solution and the color of the solution turned to be dark green immediately. After stirring at room temperature for 15 min, I_2 (52 mg, 0.205 mmol) was added. After stirring for 1 min, the solution passed through a short silica gel column using CS_2 as the eluent. The solution was concentrated to remove most of the organic solvent and then precipitated by MeOH. After being washed by hexane (5 mL × 3) and dried under vacumn for 3 hours, the brown solid product **1** was collected, 104 mg, yield 89%. ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ = 1/2): δ 4.05-4.00 (m, OC*H*Me$_2$), 2.76 (d, ^2J = 15 Hz, CH_2), 2.64 (d, ^2J = 15 Hz, CH_2), 2.53 (d, ^2J = 15 Hz, CH_2), 2.51 (d, ^2J = 15 Hz, CH_2), 1.08 (s, OCH(CH_3)$_2$), 1.07 (s, OCH(CH_3)$_2$), 1.06 (s, OCH(CH_3)$_2$), 1.05 (s, OCH(CH_3)$_2$), 0.35 (s, SiCH_3). The ratio of the two dimer isomers (racemic and meso) is 1:2.2, which is determined by the integral ratio of the methylene signals at 2.76 and 2.64 ppm. ^{13}C NMR (125 MHz, $CDCl_3/CS_2$ = 1/2): δ 158.60, 158.52, 155.80, 155.74, 153.89, 153.74, 151.47, 151.41, 148.63, 148.35, 148.33, 147.99, 147.89, 147.81, 147.60, 147.42, 147.13, 147.03, 146.81, 146.74, 146.70, 146.67, 145.55, 145.51, 145.43, 145.40, 145.23, 144.84, 144.52, 144.50, 144.47, 144.43, 144.26, 144.21, 144.18, 144.14, 144.04, 143.84, 143.72, 143.64, 143.55, 143.27, 143.22, 143.12, 143.06, 143.01, 142.96, 142.61, 142.55, 142.51, 142.49, 142.28, 142.22, 141.95, 141.89, 141.74, 141.60, 140.88, 140.82, 139.68, 139.50, 139.24, 138.66, 138.64, 137.41, 137.33, 66.58, 66.50, 65.40, 56.06, 33.73, 33.53, 25.71, 25.69, 25.65, 1.12, 1.08, 1.04, 0.99.

Synthesis of $[C_{60}(CH_2SiMe_2C_6H_{13})]_2$ (2). Under N_2, $C_{60}(CH_2SiMe_2C_6H_{13})H$ [1] (840 mg, purity 80%, 0.765 mmol), was dissolved in ODCB/THF (80/8 mL). Then ^{t}BuOK (1.0 M, 1.15 mL, 1.15 mmol) was added to the solution and the color of the solution turned to be dark green immediately. After stirring at room temperature for 15 min, I_2 (233 mg dissolved in ODCB/THF (1/1) 1 mL, 0.917 mmol) was added. After stirring for 1 min, the solution passed through a short silica gel column using CS_2 as the eluent. The solution was concentrated to remove most of the organic solvent and then precipitated by MeOH. After being washed by hexane (10 mL × 3) and dried under vacuum for 3 hours, the brown solid product was collected, 720 mg (purity 83%), yield 86%.

The product was directly used as starting material for next step reaction. Pure compound **2** could be obtained by HPLC purification. ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ = 1/2): δ 2.79 (d, ^{2}J = 14 Hz, CH_2), 2.70 (d, ^{2}J = 14 Hz, CH_2), 2.60 (d, ^{2}J = 15 Hz, CH_2), 2.56 (d, ^{2}J = 15 Hz, CH_2), 1.39–1.17 (m, *(CH_2)$_5$*), 0.85 (t, ^{2}J = 6.3 Hz, CH_3), 0.76 (m, CH_3), 0.3 (m, SiCH_3). The ratio of the two dimer isomers (racemic and meso) is 1:2.1, which is determined by the integral ratio of the methylene signals at 2.79 and 2.70 ppm. ^{13}C NMR could not be measured because of its too low solubility.

Synthesis of 3a and 3b. Under N_2, dimer **1** (80 mg, 0.047 mmol), 4-ethynylanisole (64 μL, 0.47 mmol), was dissolved in ODCB (8 mL). After stirring at 140 °C for 2.5 hours, the solution was concentrated to remove most of the solvent. Then, MeOH was added to precipitate the crude product. After filtration, the crude product was purified by silica gel column chromatography using CH_2Cl_2/CS_2 (1/10) as the eluent. The first band is the recovered starting material, 20 mg. The second band is compound **3a**, 15 mg, 23% yield based on consumed starting material. The third band is the compound **3b**, 14 mg, 22% yield based on consumed starting material. Note: compound **3a** and **3b** can easily undergo interconversion to each other with heating or light illumination conditions. Therefore, the workup stage should be carefully done at room temperature in dark. **3a:** ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ = 1/4): δ 7.73-7.70 (m, 2H, Ar), 7.26 (s, 1H), 6.82-6.79 (m, 2H, Ar), 3.96-3.91 (m, 1H, OCH(CH_3)$_2$), 3.87-3.84 (m, 1H, OCH(CH_3)$_2$), 3.77 (s, 3H, OCH_3), 2.39 (d, 1H, ^{2}J = 14.9 Hz, CH_2), 2.21 (d, 1H, ^{2}J = 14.4 Hz, CH_2), 2.10 (d, 1H, ^{2}J = 14.3 Hz, CH_2), 1.80 (d, 1H, ^{2}J = 14.9 Hz, CH_2), 0.99-0.98 (d, 6H, ^{2}J = 6.3 Hz, OCH(CH_3)$_2$), 0.93-0.90 (doublets of doublets, 6H, OCH(CH_3)$_2$), 0.25 (s, 3H, SiCH_3), 0.22 (s, 3H, SiCH_3), 0.17 (s, 3H, SiCH_3), 0.15 (s, 3H, SiCH_3). ^{13}C NMR (125 MHz, $CDCl_3/CS_2$ = 1/4) all signals represent 1C except as being noted. δ 165.69, 160.39 (2C), 158.87, 158.82, 156.62, 155.28, 154.10, 153.79, 152.87, 151.92, 151.50, 151.46 (2C), 151.27, 149.88, 149.13, 149.10, 149.07, 148.94, 148.62, 148.51, 148.28, 148.21 (2C), 147.92, 147.67 (2C), 147.09, 147.02, 146.99, 146.80, 146.76, 146.74, 146.71, 146.67, 146.63 (3C), 146.49, 146.45, 146.36, 146.32 (2C), 146.05, 145.70, 145.62, 145.56, 145.52, 145.47, 145.45, 145.39, 145.37, 145.28 (2C), 145.21, 145.06, 144.99 (2C), 144.73, 144.60, 144.52, 144.49, 144.44, 144.37, 144.35, 144.27, 144.25 (2C), 144.21, 144.19 (2C), 144.12, 144.04, 143.93, 143.91 (2C), 143.89, 143.84, 143.81, 143.60 (2C), 143.22, 143.15, 143.04 (2C), 142.91, 142.86, 142.80, 142.76, 142.65 (2C), 142.54 (2C), 142.32, 142.22, 142.15, 141.91, 141.86, 141.64,

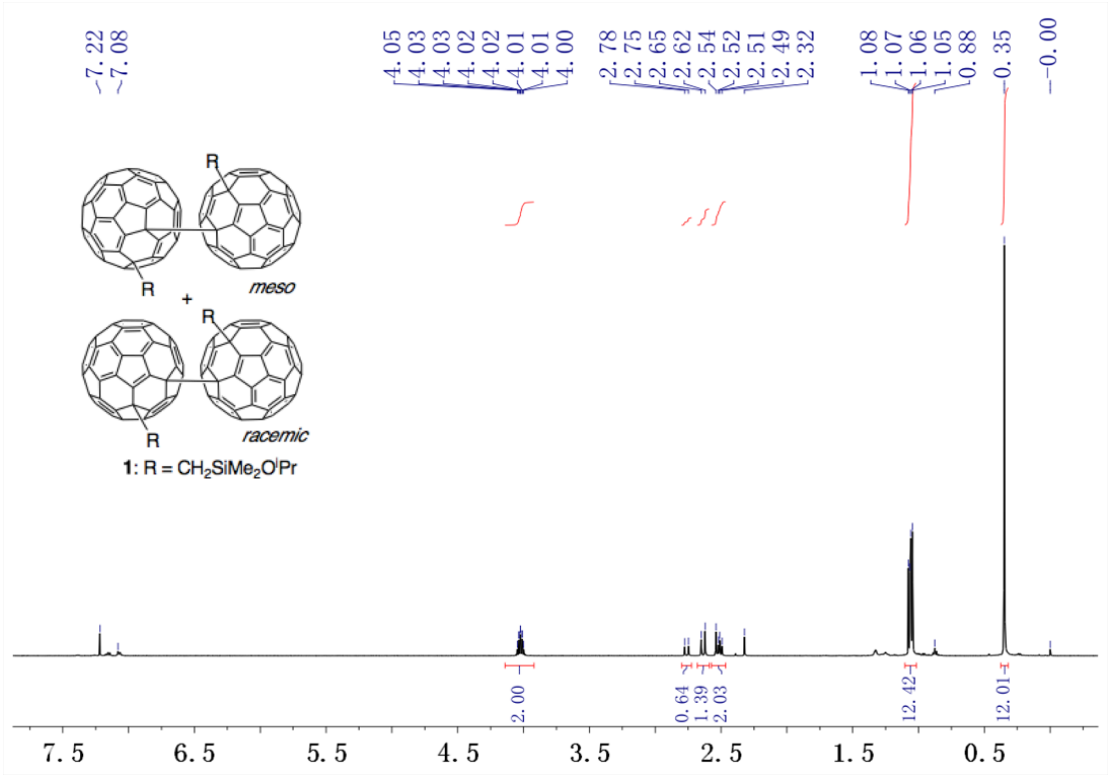
141.57 (2C), 141.47, 141.19, 140.90, 140.85, 140.69, 140.51, 139.98, 139.51, 138.94, 138.26, 137.92, 137.87, 136.84, 133.88, 129.91, 127.07 (2C, Ar), 124.80, 113.91 (2C, Ar), 75.22 (sp^3, C_{60}), 66.89 (sp^3, C_{60}), 65.88 (sp^3, C_{60}, pivot), 65.31 (O*C*H(CH_3)$_2$), 65.18 (O*C*H(CH_3)$_2$), 63.59 (sp^3, C_{60}, pivot), 57.68 (sp^3, C_{60}*C*H_2), 55.96 (sp^3, C_{60}*C*H_2), 54.87 (O*C*H_3), 33.39 (*C*H_2), 30.81 (*C*H_2), 25.65 (OCH(*C*H_3)$_2$), 25.58 (OCH(*C*H_3)$_2$), 25.55 (OCH(*C*H_3)$_2$), 25.48 (OCH(*C*H_3)$_2$), 1.49 (Si*C*H_3), 1.08 (Si*C*H_3), 0.99 (Si*C*H_3), 0.88 (Si*C*H_3). **3b:** ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ = 1/4): δ 7.80-7.78 (m, 2H, Ar), 7.30 (s, 1H), 6.84-6.82 (m, 2H, Ar), 4.00-3.95 (m, 1H, OC*H*(CH_3)$_2$), 3.84-3.80 (m, 1H, OC*H*(CH_3)$_2$), 3.74 (s, 3H, OC*H*$_3$), 2.31 (d, 1H, ^2J = 14.9 Hz, C*H*$_2$), 2.22 (d, 1H, ^2J = 14.9 Hz, C*H*$_2$), 2.15 (d, 1H, ^2J = 14.3 Hz, C*H*$_2$), 1.83 (d, 1H, ^2J = 14.3 Hz, C*H*$_2$), 1.05-1.02 (doublets of doublets, 6H, OCH(C*H*$_3$)$_2$), 0.92-0.90 (doublets of doublets, 6H, OCH(C*H*$_3$)$_2$), 0.27 (s, 6H, SiC*H*$_3$), 0.14 (s, 3H, SiC*H*$_3$), 0.13 (s, 3H, SiC*H*$_3$). ^{13}C NMR (125 MHz, $CDCl_3/CS_2$ = 1/4) all signals represent 1C except as being noted. δ 165.73, 160.40, 159.00, 158.41, 156.78, 156.06, 154.47, 154.12, 153.30, 151.87, 151.84, 151.24, 151.07, 150.82, 149.93, 149.23, 149.21, 149.13, 148.98, 148.63, 148.37, 148.31, 147.78, 147.76, 147.54, 147.49, 147.36, 147.14, 147.06, 147.02, 146.88, 146.80 (2C), 146.73 (3C), 146.65, 146.54, 146.51 (2C), 146.50, 146.45, 146.43, 145.97, 145.90, 145.75, 145.64, 145.54, 145.40 (2C), 145.37, 145.31, 145.28, 145.20, 145.09, 145.07, 145.02, 145.00, 144.92, 144.86 (2C), 144.58, 144.49 (2C), 144.40 (2C), 144.34 (2C), 144.32, 144.30, 144.28, 144.26, 144.24, 144.22, 144.02, 143.98, 143.90, 143.81, 143.78, 143.76, 143.66, 143.45, 143.30 (2C), 143.22, 143.04, 143.01 (2C), 142.91, 142.66 (2C), 142.60, 142.57, 142.49 (2C), 142.27, 142.11, 141.98, 141.97, 141.87, 141.83, 141.74, 141.70, 141.50, 141.29, 141.12, 140.71, 140.59, 140.21, 139.76, 139.08, 138.65, 138.05, 137.98, 137.72, 134.10, 130.34, 127.16 (2C, Ar), 125.04, 114.23 (2C, Ar), 75.36 (sp^3, C_{60}), 67.06 (sp^3, C_{60}), 65.73 (sp^3, C_{60}, pivot), 65.39 (O*C*H(CH_3)$_2$), 65.16 (O*C*H(CH_3)$_2$), 63.75 (sp^3, C_{60}, pivot), 57.48 (sp^3, C_{60}*C*H_2), 56.00 (sp^3, C_{60}*C*H_2), 54.90 (O*C*H_3), 33.94 (*C*H_2), 31.03 (*C*H_2), 25.76 (OCH(*C*H_3)$_2$), 25.67 (OCH(*C*H_3)$_2$), 25.52 (OCH(*C*H_3)$_2$), 25.49 (OCH(*C*H_3)$_2$), 1.31 (Si*C*H_3), 1.08 (Si*C*H_3), 0.89 (Si*C*H_3), 0.74 (Si*C*H_3).

Synthesis of 4a and 4b. Under N_2, dimer **2** (600 mg, purity 83%, 0.284 mmol), PhC≡CCOOEt (560 μL, 2.84 mmol), was dissolved in ODCB (30 mL). After stirring at 140 °C for 8 hours, MeOH was added to precipitate the crude product. After filtration, the crude product was purified

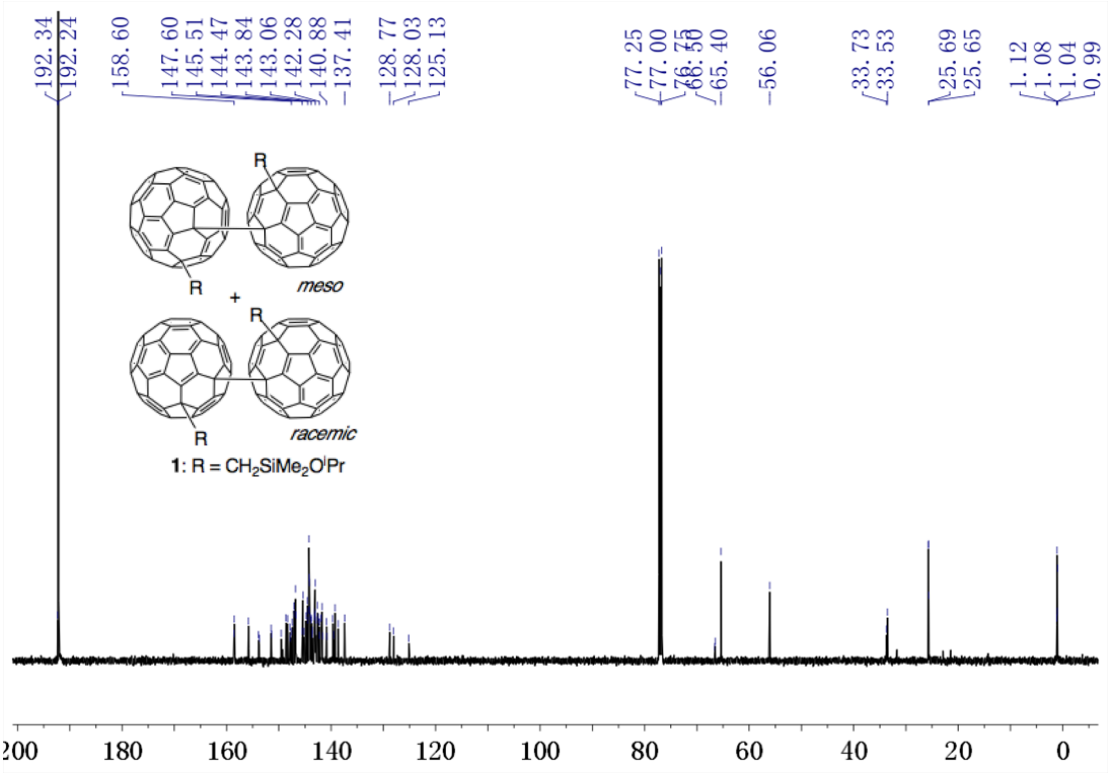
by silica gel column chromatography using CS_2 as the eluent. The mixture of **4a** and **4b** was obtained, 205 mg, yield 31%. ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ = 1/1): δ 8.44-8.41 (m, 2H, Ph), 7.47-7.42 (m, 3H, Ph), 4.38-4.35 (m, 2H, OCH_2CH_3), 2.42-1.81 (m, 4H, $C_{60}CH_2Si$), 1.73-0.51 (m, 26H, Si-hexyl and OCH_2CH_3), 0.21 (s, Si-Me), 0.18 (s, Si-Me), 0.15 (s, Si-Me), 0.14 (s, Si-Me), 0.10 (s, Si-Me), 0.09 (s, Si-Me), 0.06 (s, Si-Me), 0.05 (s, Si-Me).

3. NMR spectra of all compounds

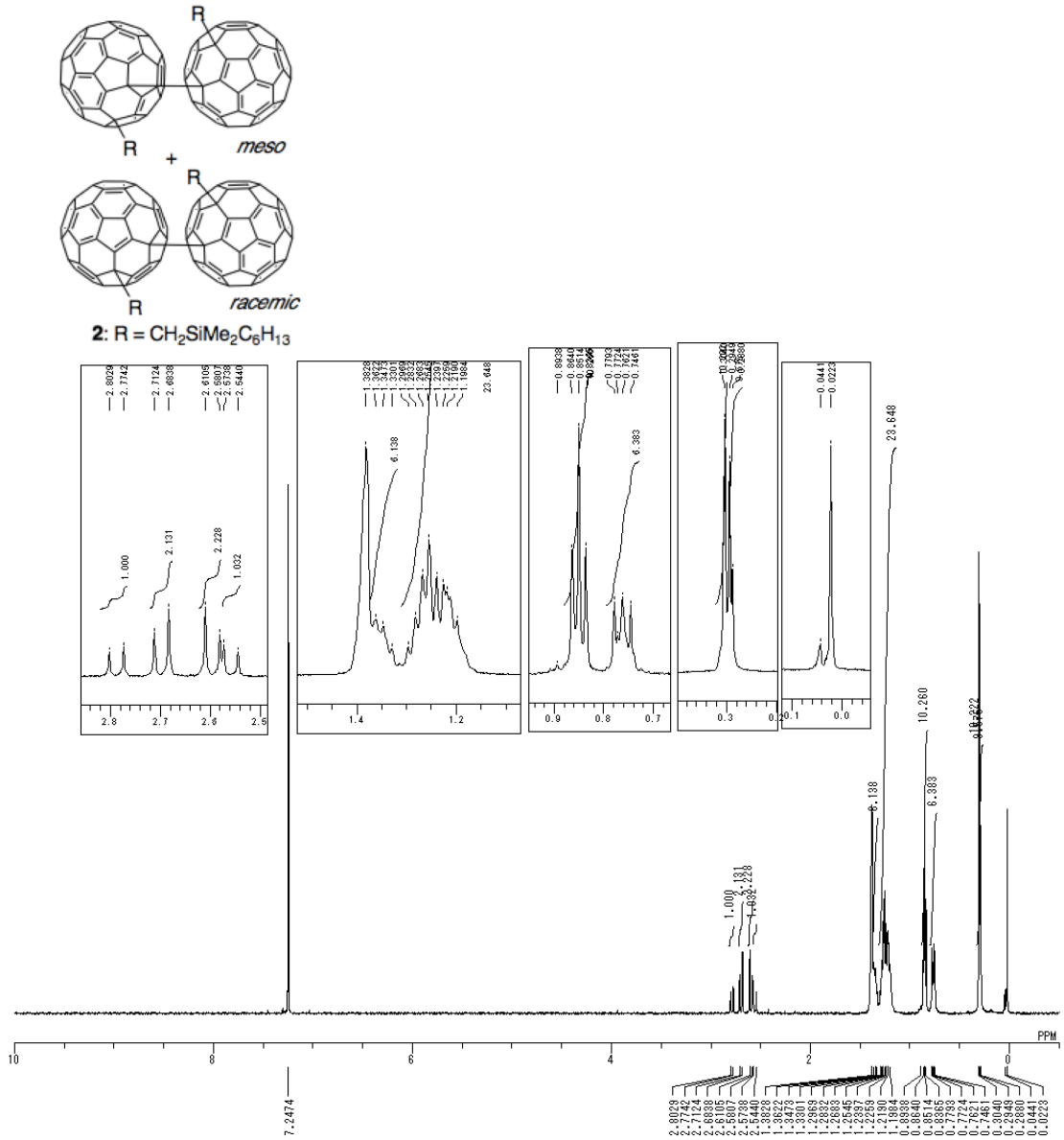
^{1}H NMR for compound 1



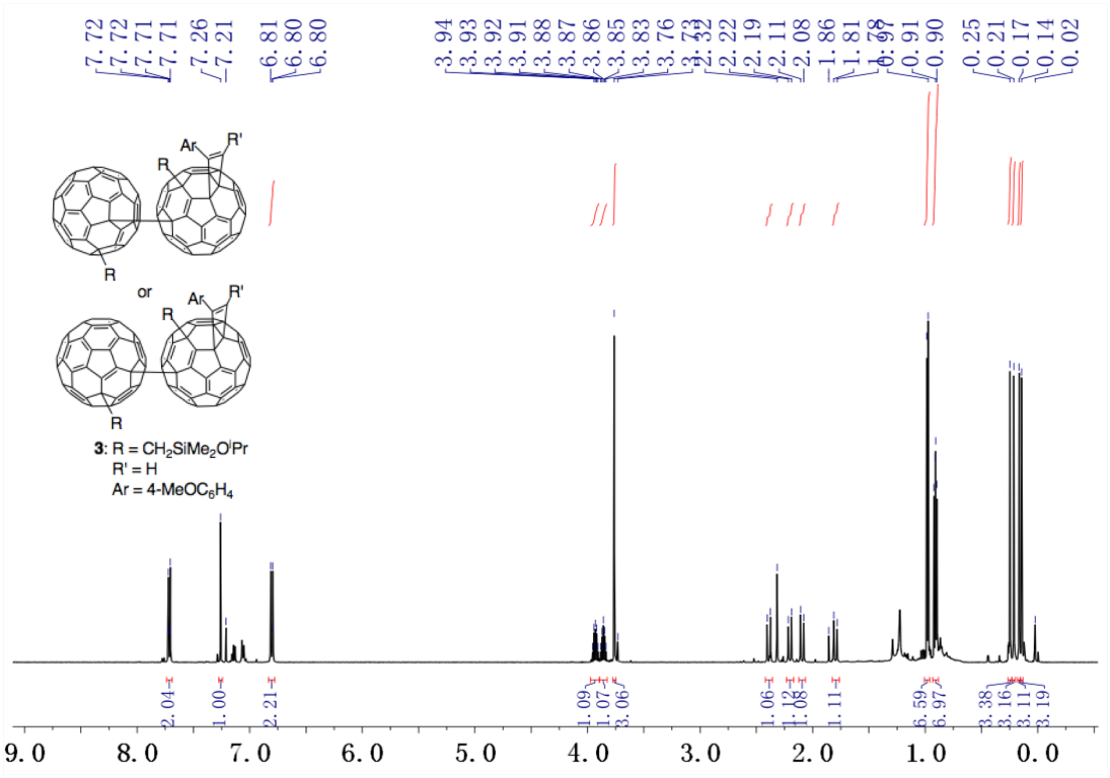
^{13}C NMR for compound 1



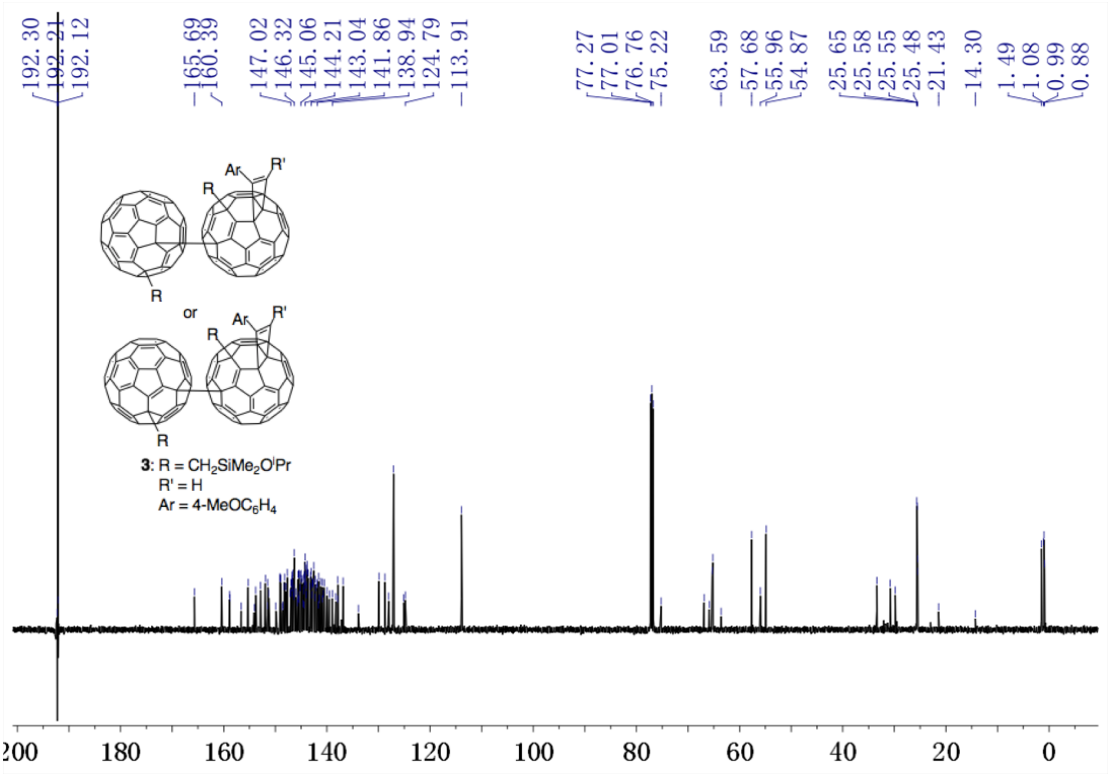
^{1}H NMR for compound 2



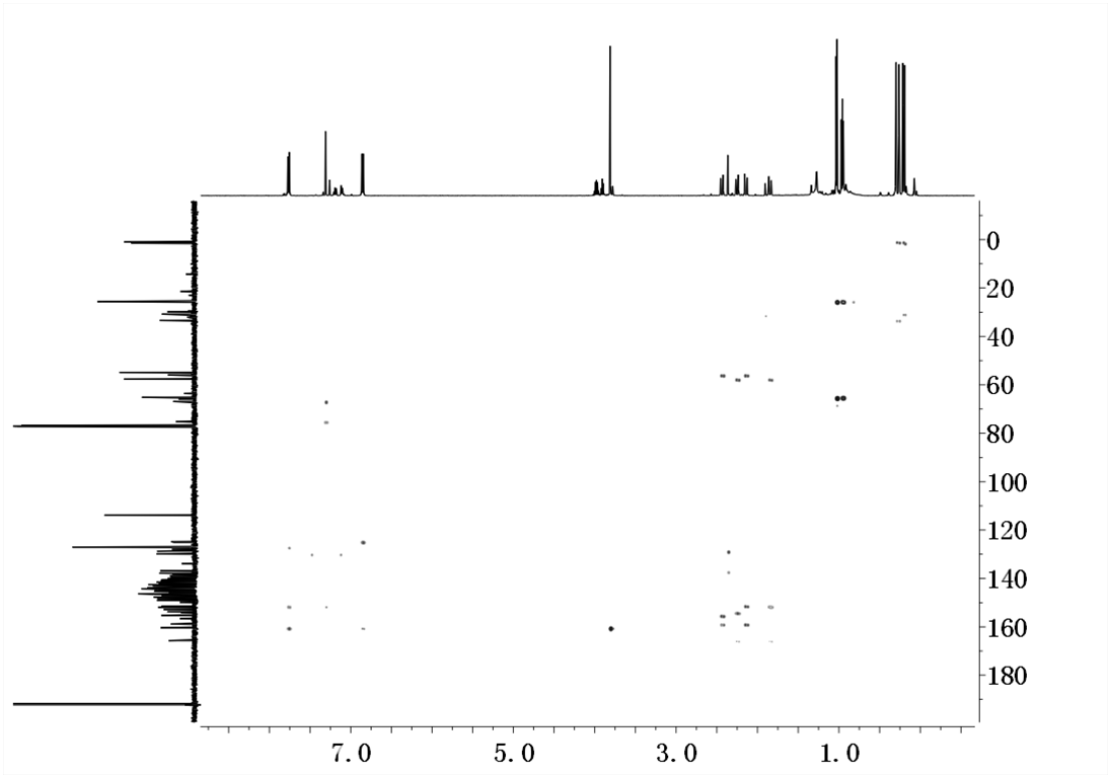
^{1}H NMR for compound 3a

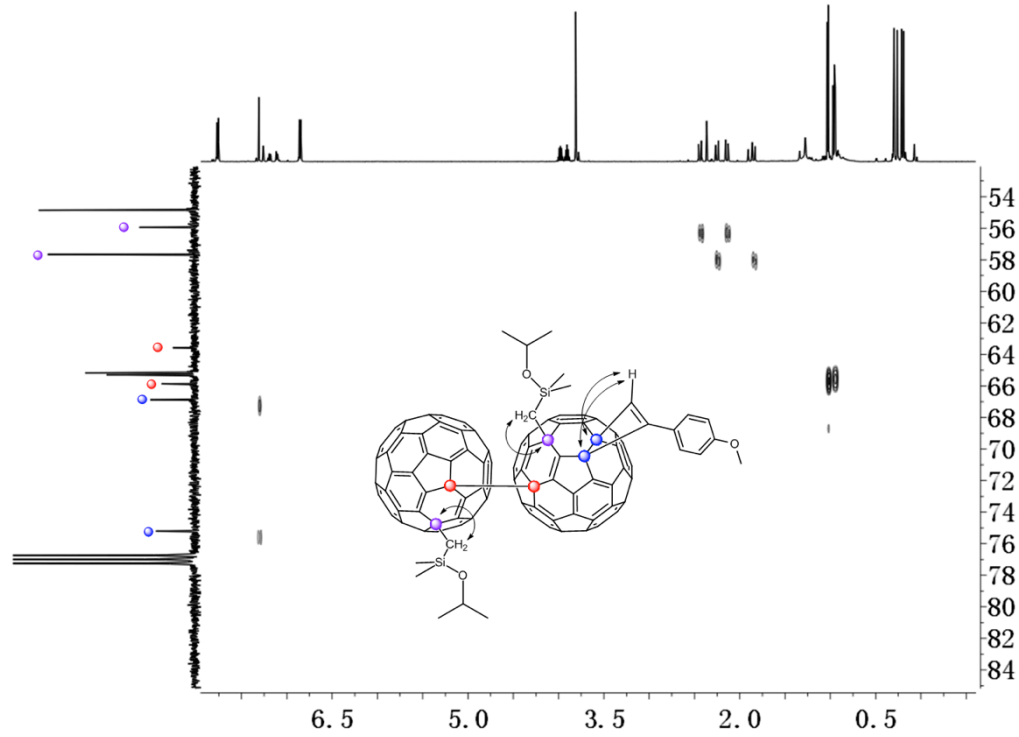


^{13}C NMR for compound 3a

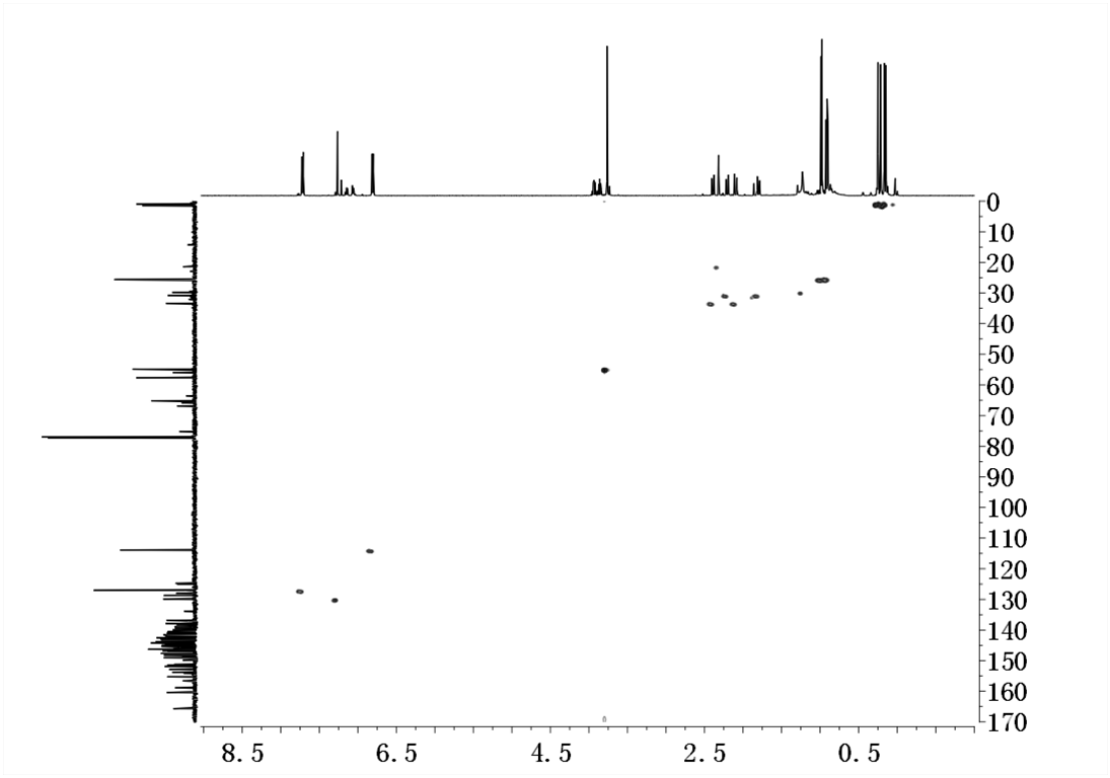


HMBC spectrum for compound 3a

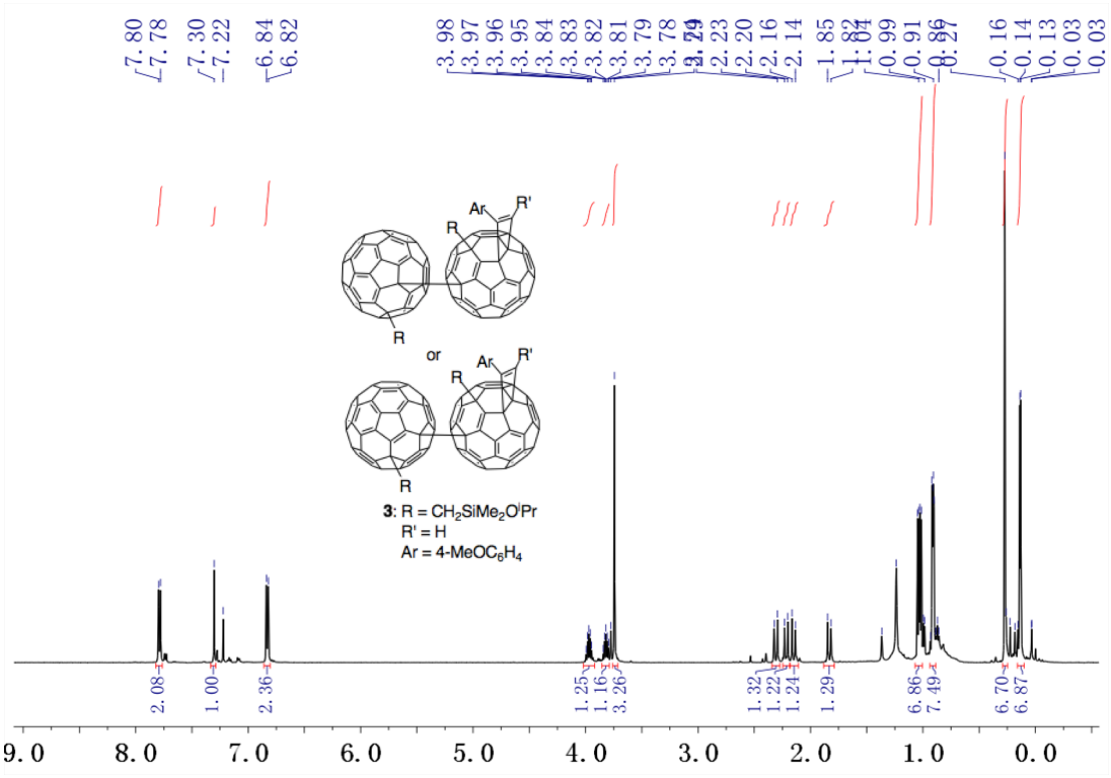




HMQC spectrum for compound 3a



^{1}H NMR for compound 3b



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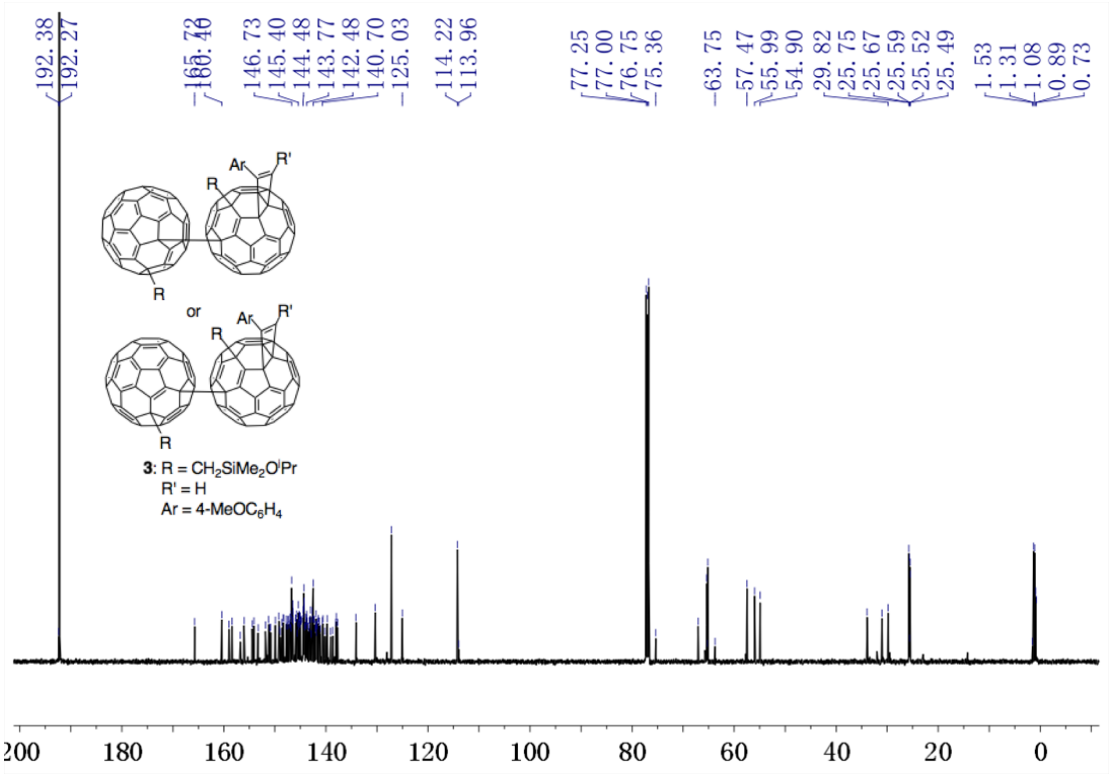
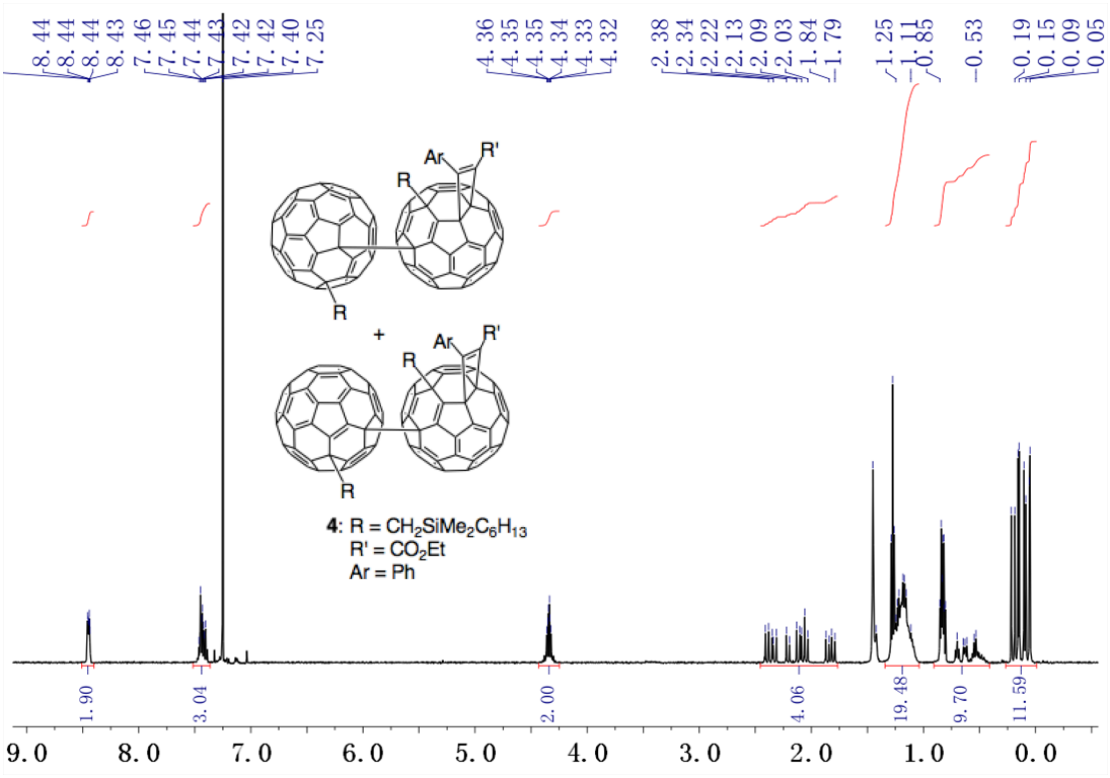


^{1}H NMR for compound 4a and 4b



4. X-ray crystallographic analysis of 4a·4b mixture crystal.

Single crystals of **4a**·**4b** suitable for X-ray analysis were obtained by slow diffusion of EtOH into a solution of **4a**·**4b** in CS_2. The data sets were collected on a RIGAKU R-AXIS RAPID imaging plate diffractometer using CuKα (graphite monochromated, l = 1.5418Å) radiation. The structures of **4a**·**4b** were solved by the directed method (SIR97).[2] The positional and thermal parameters of non-hydrogen atoms were refined anisotropically on F^2 by the full-matrix least-squares method using SHELXL-97.[3] Hydrogen atoms were placed at calculated positions and refined with a riding mode on their corresponding carbon atoms.

Table S1. Crystal data and structure analysis results for compounds **4a**·**4b**

	4a·**4b**·2.5CS_2
formula	$C_{151.5}H_{52}O_2S_5Si_2$
crystal system	triclinic
space group	*P*-1
R (*I*>2σ(*I*)), *R* (all data)	0.0999, 0.1829
wR	0.3182
GOF on F^2	0.977
a, Å	9.962
b, Å	18.792
c, Å	25.713
α, deg	108.23
β, deg	94.9
γ, deg	91.61
V, Å ^{3}	4547.7
Z	2
T, K	123(2)
crystal size, mm	0.1, 0.1, 0.05
D_{calcd}, g/cm^{-3}	1.557
$2\theta_{min}$, $2\theta_{max}$, deg	1.62, 25.35
no. refl. measured (*I*>2σ(*I*))	16275
no. parameters	1398

5. Optimized geometries, spin density distribution, and Cartesian coordinates for 59π-electron and 57π-electron fullerene radicals.

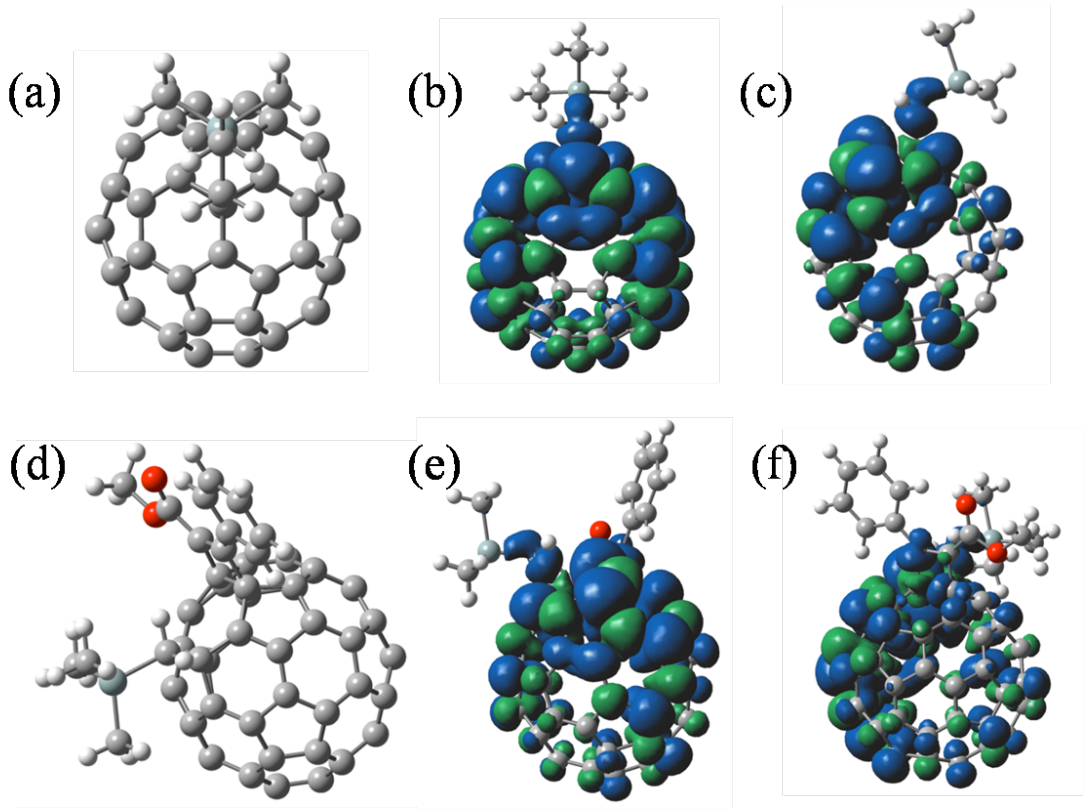


Figure S1. Optimized structures for 59π-electron (**a**) and 57π-electron (**d**) fullerene radicals at UB3LYP/6-31G level. Spin density distribution for 59π-electron (**b, c**) and 57π-electron (**e, f**) fullerene radicals.

Table S2. Cartesian coordinates for **5**9π-electron and 57π-electron fullerene radicals

59π-electron radicals:

1	C	-0.787553	-1.824196	-2.605833
2	C	0.545603	-2.416350	-2.608530
3	C	1.643228	-1.663909	-3.036770
4	C	1.455632	-0.285997	-3.484371
5	C	0.179606	0.282270	-3.475174
6	C	-0.964979	-0.499392	-3.022747
7	C	0.662542	-3.265849	-1.427203
8	C	2.903642	-1.731930	-2.310047
9	C	2.605736	0.494900	-3.040530
10	C	-0.008005	1.660709	-3.030482
11	C	-1.865172	0.384492	-2.299803
12	C	-1.488821	-2.297562	-1.429113

13	C	1.101846	2.412296	-2.609782
14	C	2.428373	1.815443	-2.610026
15	C	0.991800	3.262753	-1.429813
16	C	3.143724	2.298528	-1.430403
17	C	1.871778	-3.330256	-0.728167
18	C	3.497449	-0.396757	-2.310202
19	C	2.254416	3.195516	-0.700618
20	C	4.178960	0.064201	-1.179950
21	C	3.016834	-2.547615	-1.178665
22	C	-1.265182	1.735978	-2.313493
23	C	-2.557967	-0.074319	-1.190241
24	C	1.871722	-3.329491	0.731724
25	C	-2.334310	-1.421857	-0.729512
26	C	-0.597613	-3.191569	-0.696729
27	C	-2.962214	0.839225	-0.000587
28	C	-2.334382	-1.421097	0.730751
29	C	-0.597668	-3.190842	0.699957
30	C	3.996411	1.441238	-0.730553
31	C	-1.366471	2.536997	-1.166002
32	C	3.725085	-2.064015	0.001185
33	C	-2.558051	-0.073063	1.190048
34	C	-1.488932	-2.296067	1.431338
35	C	0.662431	-3.264353	1.430600
36	C	0.545403	-2.413622	2.611031
37	C	3.016739	-2.546378	1.181488
38	C	4.291679	-0.784476	0.000536
39	C	4.178865	0.065434	1.180125
40	C	-0.787755	-1.821467	2.607610
41	C	-0.965207	-0.496223	3.023120
42	C	0.179345	0.285909	3.474827
43	C	-1.865341	0.386903	2.299191
44	C	-0.211993	3.325354	-0.727867
45	C	3.497269	-0.394340	2.310808
46	C	-2.076968	2.084157	-0.001201
47	C	-1.366565	2.538223	1.163184
48	C	2.903463	-1.729511	2.312009
49	C	3.996355	1.442001	0.729280
50	C	3.143620	2.300023	1.428172
51	C	1.642995	-1.660734	3.038565
52	C	1.455367	-0.282351	3.484706
53	C	-1.265357	1.738402	2.311514
54	C	-0.008233	1.663881	3.028679
55	C	2.605505	0.498080	3.040138
56	C	-0.212048	3.326118	0.724310

57	C	2.254365	3.196250	0.697384
58	C	2.428176	1.818174	2.608244
59	C	0.991692	3.264254	1.426413
60	C	1.101650	2.415027	2.607276
61	C	-4.472814	1.272597	-0.000945
62	H	-4.629264	1.914874	0.877262
63	H	-4.629175	1.913845	-0.879899
64	C	-5.917165	-1.127151	-1.571117
65	H	-5.829851	-0.517561	-2.477570
66	H	-5.092466	-1.845970	-1.564985
67	H	-6.857168	-1.688674	-1.630662
68	C	-5.922816	-1.116191	1.578820
69	H	-5.093804	-1.830049	1.583864
70	H	-5.846107	-0.499679	2.481559
71	H	-6.859863	-1.682944	1.635220
72	C	-7.510660	1.051057	-0.006787
73	H	-8.404664	0.416721	-0.006297
74	H	-7.554536	1.696482	0.878136
75	H	-7.551036	1.690208	-0.896418
76	Si	-5.921889	-0.028001	0.000084

57π-electron radicals:

1	Si	-3.681303	3.992417	0.130223
2	C	-1.372888	1.404811	1.027279
3	C	0.051096	2.298383	-2.140612
4	C	-0.153459	1.062024	-2.905370
5	C	-0.998513	0.071476	-2.349272
6	C	1.452535	2.667092	-2.274594
7	C	-1.755646	0.271812	-1.182621
8	C	-0.627426	-1.343507	-2.458514
9	O	-5.390227	-2.120208	2.272957
10	C	-1.879931	-1.116400	1.082852
11	C	2.212332	-0.884493	3.369998
12	C	-0.821926	-2.093209	1.596633
13	C	3.209421	-3.290108	-0.322346
14	C	0.580351	-1.709278	-3.055463
15	C	3.267573	-2.505724	2.023035
16	C	-0.090682	-1.483966	2.678886
17	C	0.489562	0.873228	3.135300
18	C	2.781921	-2.370661	-2.579691
19	C	1.380223	-2.749613	-2.445258
20	C	-0.356008	2.371281	1.384328
21	C	4.941747	0.819878	-1.086219

22	C	4.729516	-0.414680	-1.836957
23	C	1.446031	3.435809	0.059501
24	C	-0.197694	-3.031150	0.792764
25	C	-1.804187	1.614263	-0.452994
26	C	-2.057764	-1.076004	-0.529152
27	C	2.139370	3.240002	-1.198795
28	C	4.826964	-1.683517	0.286674
29	C	-0.353711	-2.992669	-0.685823
30	C	2.110176	1.669102	-3.108813
31	C	4.134526	1.866150	-1.702050
32	C	1.862987	-3.640273	-0.189903
33	C	1.216327	-1.881438	2.987312
34	C	-1.420237	0.203065	1.701918
35	C	0.923927	-3.365777	-1.270266
36	C	3.977788	1.120079	2.355825
37	C	-0.626177	2.508181	-0.946734
38	C	0.102060	3.042285	0.175455
39	C	3.677850	-2.635246	-1.541397
40	C	-1.133076	-2.023206	-1.295776
41	C	1.941587	2.526925	2.306218
42	C	1.111255	0.672478	-3.486704
43	C	1.854944	0.464020	3.445245
44	C	3.482793	-1.270263	2.772808
45	C	1.171456	-3.431207	1.076354
46	C	1.477569	-0.680552	-3.578890
47	C	2.838425	-1.088790	-3.283001
48	C	2.755266	1.488938	2.929035
49	C	4.347542	-0.288862	2.273560
50	C	5.034778	-0.500695	1.005173
51	C	3.421661	1.275719	-2.831443
52	C	3.925784	-2.705205	0.806436
53	C	3.659760	2.781250	0.547645
54	C	0.542093	2.135652	2.433483
55	C	3.507032	2.827552	-0.904687
56	C	1.865298	-2.880461	2.162908
57	C	-4.606803	-1.744897	-1.196771
58	C	-3.531779	-1.495620	-0.251143
59	C	4.437740	1.779462	1.138355
60	C	3.796615	-0.132813	-2.917667
61	C	5.091435	0.777299	0.303505
62	C	4.673969	-1.640906	-1.162975
63	C	-3.221850	2.263964	-0.639054
64	C	2.384362	3.158960	1.142013
65	C	-3.354711	-1.515739	1.107186

66	C	-0.459242	-0.076799	2.745988
67	C	-4.187535	-1.797595	2.263925
68	O	-3.463338	-1.655624	3.427416
69	C	-4.178380	-1.906032	4.685823
70	C	-5.901849	-2.126151	-0.770129
71	C	-6.909236	-2.359608	-1.706728
72	C	-6.654075	-2.220148	-3.077051
73	C	-5.377175	-1.843181	-3.511734
74	C	-4.363533	-1.607551	-2.583337
75	C	-2.595356	5.413920	-0.561814
76	C	-5.496086	4.282651	-0.428849
77	C	-3.624655	3.974515	2.047112
78	H	-3.402166	2.349514	-1.719881
79	H	-3.967331	1.550592	-0.260880
80	H	-5.027904	-1.225899	4.777303
81	H	-4.536603	-2.937290	4.715442
82	H	-3.439972	-1.722667	5.463486
83	H	-6.101359	-2.234845	0.289420
84	H	-7.897006	-2.652296	-1.365720
85	H	-7.442408	-2.404361	-3.800036
86	H	-5.172005	-1.734928	-4.571701
87	H	-3.380165	-1.318039	-2.931682
88	H	-2.558484	5.382307	-1.656660
89	H	-3.021103	6.380174	-0.265752
90	H	-1.568898	5.365039	-0.186988
91	H	-5.868101	5.237774	-0.040167
92	H	-5.572673	4.310214	-1.522008
93	H	-6.156303	3.488444	-0.061665
94	H	-4.199319	3.131813	2.447958
95	H	-2.601141	3.897943	2.426172
96	H	-4.064649	4.899931	2.437658

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