Electronic Supplementary Information (ESI)

Synthesis, Properties and Chemical Modification of a Persistent Triisopropylsilylethynyl Substituted Tri(9-anthryl)methyl Radical

Tomohiko Nishiuchi,[a,b]* Daisuke Ishii,[a] Seito Aibara,[a] Hiroyasu Sato,[c] and Takashi Kubo[a,b]*

[a] Department of Chemistry, Graduate School of Science, Osaka University, Machikaneyama 1-1, Toyonaka, Osaka 560-0043, Japan. E-mail: nishiuchit13@chem.sci.osaka-u.ac.jp

[b] Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives, (ICS-OTRI), Osaka University, Suita, Osaka 565-0871, Japan.

[c] Rigaku Corporation, 3-9-12 Matsubara, Akishima, Tokyo 196-8666, Japan

Contents

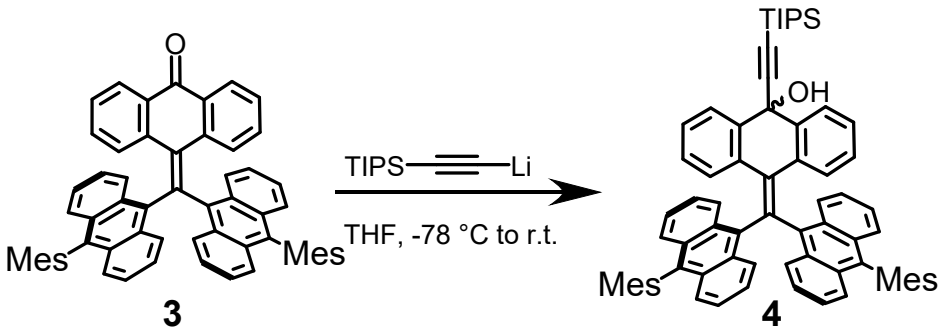
General information

All experiments with moisture- or air-sensitive compounds were performed in anhydrous solvents under nitrogen atmosphere in well-dried glassware. Dried solvents (THF and dichloromethane) were purchased from KANTO CHEMICAL. Column chromatography was performed with silica gel [Silica gel 60N (KANTO CHEMICAL)]. ^{1}H and ^{13}C NMR spectra were recorded on JEOL lambda-500 spectrometer or Bruker AVANCENEO700 spectrometer. Positive EI mass spectra were taken by using Shimadzu QP-5050. MALDI TOF MS spectra were taken by KRATOS AXIMA-PERFORMANCE (Shimazu). Dithranol was used for the matrix. APCI-MS spectra were recorded on a Bruker micrOTOF II spectrometer. Data collection for X-ray crystal analysis was performed on Rigaku XtaLAB Synaergy Custom (Detector is Hypix-6000HE. Mo-Kα (λ = 0.71069 Å)). The structure was solved with direct methods and refined with full-matrix least squares. The UV-vis spectra were recorded on JASCO V-570 spectrophotometer. IR spectra were recorded on FT/IR 6100 (Jasco) using attenuated total reflection method equipped with ZnSe prism.

Computational Methods. All DFT calculations were performed with the Gaussian 16 program. Structure optimization in both ground states were performed by (U)ωB97XD/6-31G**. TD-DFT calculations of **1** were performed by a UB3LYP/6-31G** method using optimized structures by ωB97XD/6-31G** method.

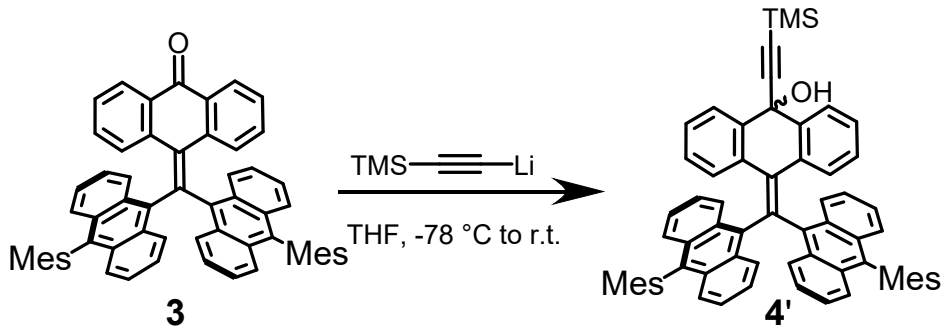
Synthesis

Synthesis of compound 4



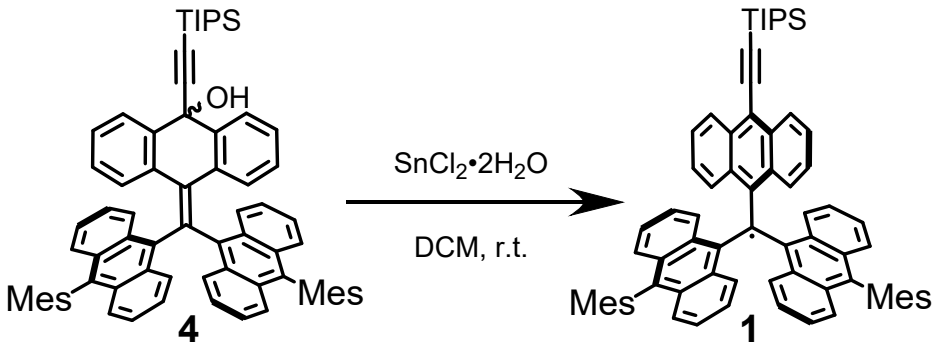
To a solution of triisopropylsilylacetylene (213 mg, 1.13 mmol) in THF (5 ml) was added *n*-BuLi (1.6 M hexane solution, 0.7 ml, 1.12 mmol) at -78 °C. After stirring for 30 min at same temperature, a solution of compound **3** (300 mg, 0.377 mmol) in THF (10 ml) was added and stirred for 1 day at room temperature. The reaction was quenched by water, extracted with dichloromethane, and washed with brine. After removal of the solvent *in vacuo*, the crude material was subjected to column chromatography on alumina (dichloromethane : hexane = 1 : 3) to afford the title compound **4** (338 mg, 0.345 mmol, 92%) as yellow solid. Mp: 186 °C (dec.). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.97-8.95 (m, 2H, aromatic proton), 8.56 (d, J = 8.0 Hz, 2H, aromatic proton), 8.28 (dd, J = 8.0 Hz, J = 1.0 Hz, 2H, aromatic proton), 7.48 (dd, J = 8.0 Hz, J = 1.0 Hz, 2H, aromatic proton), 7.45-7.42 (m, 2H, aromatic proton), 7.29-7.27 (dd, J = 7.5 Hz, J = 1.0 Hz, 2H, aromatic proton), 7.24-7.22 (m, 4H, aromatic proton), 7.14 (m, 2H, aromatic proton), 7.10-7.02 (m, 8H, aromatic proton), 6.60-6.57 (m, 2H, aromatic proton), 3.09 (s, 1H, O*H*), 2.41 (s, 6H, CH_3), 1.72 (s, 6H, CH_3), 1.43 (s, 6H, CH_3), 1.25-1.16 (m, 21H, SiC*H*(CH_3)$_2$).; ^{13}C NMR (125 MHz, CD_2Cl_2) δ 141.91, 139.34, 138.11, 138.07, 137.66, 137.64, 137.47, 137.16, 136.36, 135.19, 133.85, 131.10, 130.33, 129.90, 128.76, 128.61, 128.58, 128.54, 128.47, 128.00, 127.95, 127.80, 127.32, 126.56, 126.51, 126.00, 125.46, 125.38, 109.67, 90.94, 71.64, 21.33, 19.94, 19.73, 18.93, 11.84. HR-MS (APCI) Calcd for $C_{72}H_{68}OSi$ [(*M*+H)$^+$]: *m/z* 977.5112, Found: 977.5095.

Synthesis of compound 4'



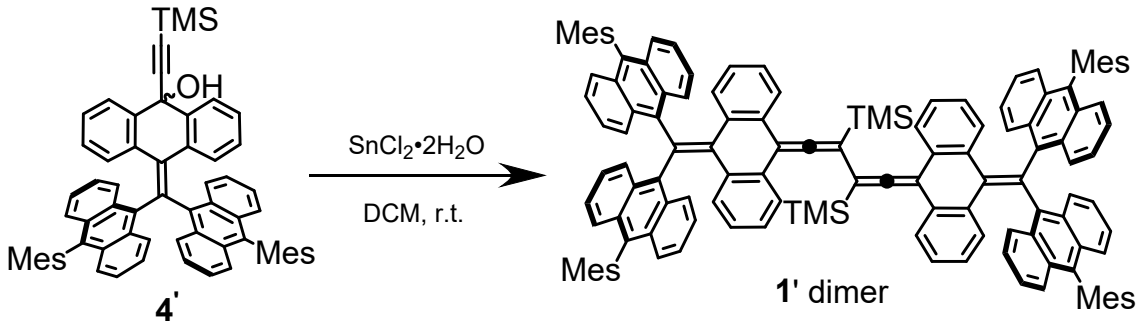
Compound **4**' was prepared from **3** and trimethylsilylacetylene by using a similar procedure to that for **4** yielding 82 % as yellow solid. Mp: 170 °C (dec.). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.89-8.87 (m, 2H, aromatic proton), 8.60 (d, *J* = 8.5 Hz, 2H, aromatic proton), 8.18 (d, *J* = 8.0 Hz, 2H, aromatic proton), 7.48 (d, *J* = 8.0 Hz, 2H, aromatic proton), 7.42-7.40 (m, 2H, aromatic proton), 7.29 (d, *J* = 8.0 Hz 2H, aromatic proton), 7.22-7.20 (m, 4H, aromatic proton), 7.15 (t, *J* = 7.5 Hz, 2H, aromatic proton), 7.11-7.05 (m, 6H, aromatic proton), 7.02 (s, 2H, aromatic proton) 6.59 (t, *J* = 7.8 Hz, 2H, aromatic proton), 3.09 (s, 1H, O*H*), 2.41 (s, 6H, C*H*$_3$), 1.72 (s, 6H, C*H*$_3$), 1.42 (s, 6H, C*H*$_3$), 0.32 (s, 9H, SiC*H*$_3$).; ^{13}C NMR (125 MHz, CD_2Cl_2) δ 141.39, 138.99, 137.91, 137.73, 137.34, 137.33, 137.16, 136.86, 135.78, 134.87, 133.10, 131.09, 129.96, 129.64, 128.40, 128.26, 128.22, 127.86, 127.81, 127.63, 127.47, 126.92, 126.28, 126.21, 125.70, 125.13, 125.04, 107.44, 93.71, 70.72, 21.01, 19.63, 19.40, –0.35. (One aromatic carbon signal is missing owing to duplicated in other carbon peaks.). HR-MS (APCI) Calcd for $C_{61}H_{47}O$ [(*M*–C_2SiMe_3)$^+$]: *m/z* 795.3621, Found: 795.3603. (Trimethylsilylethynyl unit was dissociated in the gas phase.).

Synthesis of compound 1



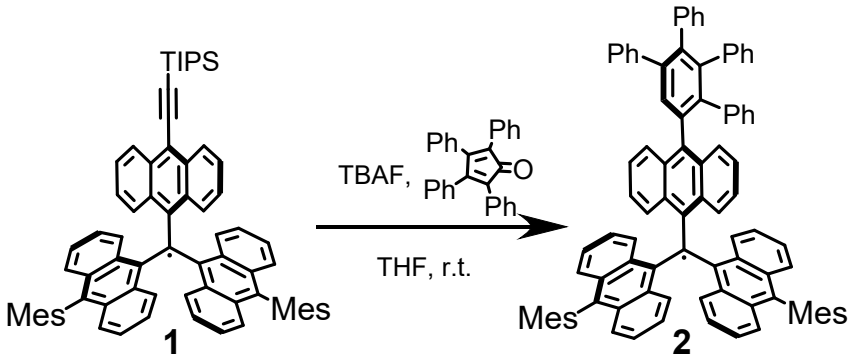
Compound **4** (335 mg, 0.343 mmol) and stannous chloride dihydrate (116 mg, 0.514 mmol) were dissolved in dichloromethane (15 ml) and stirred for 30 min at room temperature. The solution was directly subjected to column chromatography on deactivated silica gel (6% wt. water contain) (dichloromethane : hexane = 1 : 2) to afford the title compound **1** (295 mg, 0.307 mmol, 90%) as deep blue solid. Recrystallization from dichloromethane and hexane gave a red-purple crystal. Mp: > 300 °C. HR-MS (APCI) Calcd for $C_{72}H_{67}Si$ [M^+]: *m/z* 959.5007, Found: 959.5008.

Synthesis of compound 1' dimer



Compound **4'** (61.1 mg, 0.0684 mmol) and stannous chloride dihydrate (23.1 mg, 0.102 mmol) were dissolved in dichloromethane (15 ml) and stirred for 1 day at room temperature. Orange precipitation was filtered and washed with water to afford the title compound **1'** dimer (44.7 mg, 0.0255 mmol, 75%). Mp: 265 °C (dec.). ^{1}H NMR (700 MHz, CD_2Cl_2/CS_2) δ 8.80-8.79 (m, 4H, aromatic proton), 8.39 (d, J = 9.1 Hz, 4H, aromatic proton), 7.53-7.52 (m, 4H, aromatic proton), 7.39-7.38 (m, 4H, aromatic proton), 7.21 (t, J = 9.5 Hz, 8H, aromatic proton), 7.16-7.14 (m, 8H, aromatic proton), 7.00-6.97 (m, 12H, aromatic proton), 6.91-6.89 (m, 4H, aromatic proton), 6.80-6.77 (m, 4H, aromatic proton), 6.34-6.32 (m, 4H, aromatic proton) 2.43 (s, 12H, CH_3), 1.65 (s, 12H, CH_3), 1.54 (s, 12H, CH_3), 0.36 (s, 18H, SiCH_3).; ^{13}C NMR (176 MHz, CD_2Cl_2/CS_2) δ 207.74, 143.79, 139.61, 137.35 137.24, 137.08, 137.01, 135.06, 134.92, 134.28, 133.34, 131.47, 131.34, 129.97, 129.65, 129.18, 128.61, 128.56, 128.44, 127.67, 127.19, 126.65, 126.30, 126.06, 125.85, 125.79, 125.52, 125.30, 103.04, 102.78, 21.68, 20.01, 19.91, 0.30. (One aromatic carbon signal is missing owing to duplicated in other carbon peaks.). HR-MS (APCI) Calcd for $C_{66}H_{55}Si$ [(1/2M+H)$^+$]: m/z 876.4126, Found: 876.4123. (The dimer structure was dissociated into monomers in the gas phase.).

Synthesis of compound 2



To a solution of **1** (30 mg, 0.031 mmol) and tetraphenylcyclopentadienone (12 mg, 0.031 mmol) in THF (5 ml) was added TBAF (1.0 M THF solution, 0.04 ml, 0.040 mmol) at room tempareture. After stirring for 1 day, the reaction was quenched by water. Organic layer was extracted with dichloromethane and washed with brine. After removal of the solvent *in vacuo*, the crude material was subjected to column chromatography on silica gel (6% wt. water contain) (hexane : toluene = 1:1) to afford the title compound **2** (13 mg, 0.011 mmol, 37%) as blue solid. Recrystallization from chloroform and pentane gave a red-purple crystal. Mp: > 300 °C. HR-MS (APCI) Calcd for $C_{91}H_{67}$ [(M+H)$^+$]: m/z 1159.5237, Found: 1159.5232.

X-ray crystallographic data of 1 and 2

Crystal data for 1. CCDC 2123624. $C_{72}H_{67}Si$, M_W = 960.34, monoclinic, space group $P\ 2_1/n$ (no. 14), a = 15.7578(7), b = 16.3981(5), c = 22.2474(8) Å, β = 109.503(4)°, V = 5418.8(4) Å^3, Z = 4, D = 1.177 g cm^3, T = 120 K, Data collection with MoKα radiation (multi-layer mirror monochromated). 14510 measured reflection, 8404 unique reflections; structure solution by direct methods (Shelxs), refinement by fullmatrix least squares on F with anisotropic temperature factors for the non-H atoms. Final R_1 = 0.0644, wR_2 = 0.1832, GOF = 1.037.

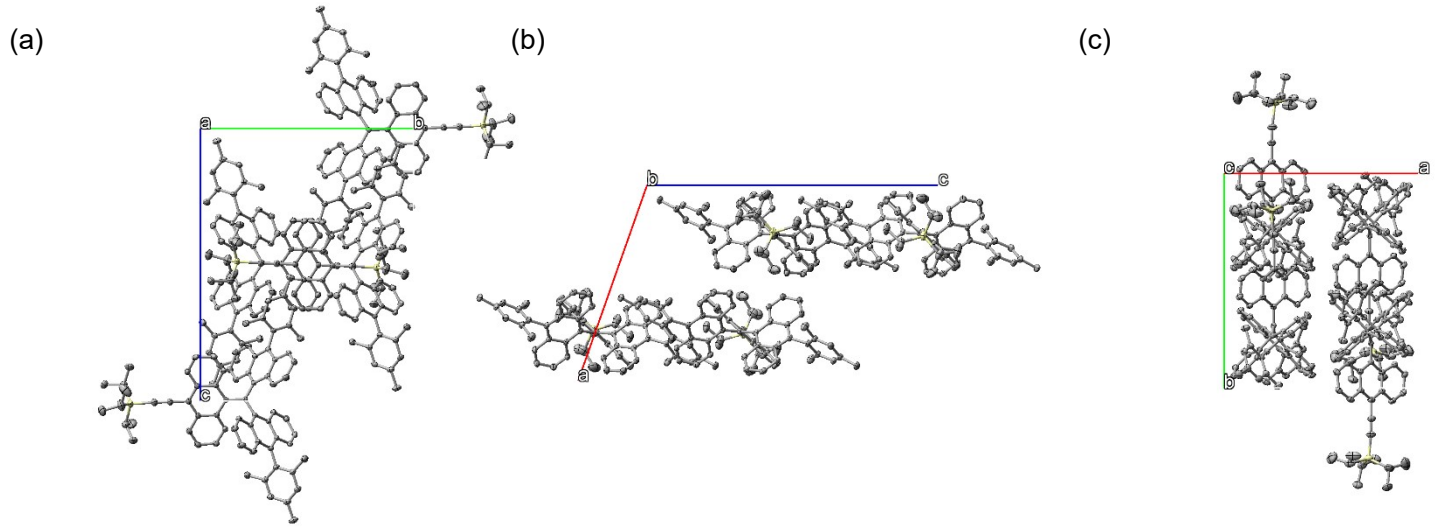


Figure S1. X-ray crystal structure of **1**. Packing structures (a) from a axis, (b) from b axis, and (c) from c axis.

Crystal data for 2. CCDC 2123625. $C_{91}H_{67}$, M_W = 1160.44, triclinic, space group P -1 (no. 2), a = 15.4442(6), b = 16.8575(5), c = 17.7961(4) Å, α = 63.340(3)°, β = 70.016(3)°, γ = 86.686(3)°, V = 3866.1(2) Å^3, Z = 2, D = 0.997 g cm^3, T = 120 K, Data collection with MoKα radiation (multi-layer mirror monochromated). 19675 measured reflection, 12823 unique reflections; structure solution by direct methods (Shelxs), refinement by fullmatrix least squares on F with anisotropic temperature factors for the non-H atoms. Final R_1 = 0.0633, wR_2 = 0.1855, GOF = 0.981.

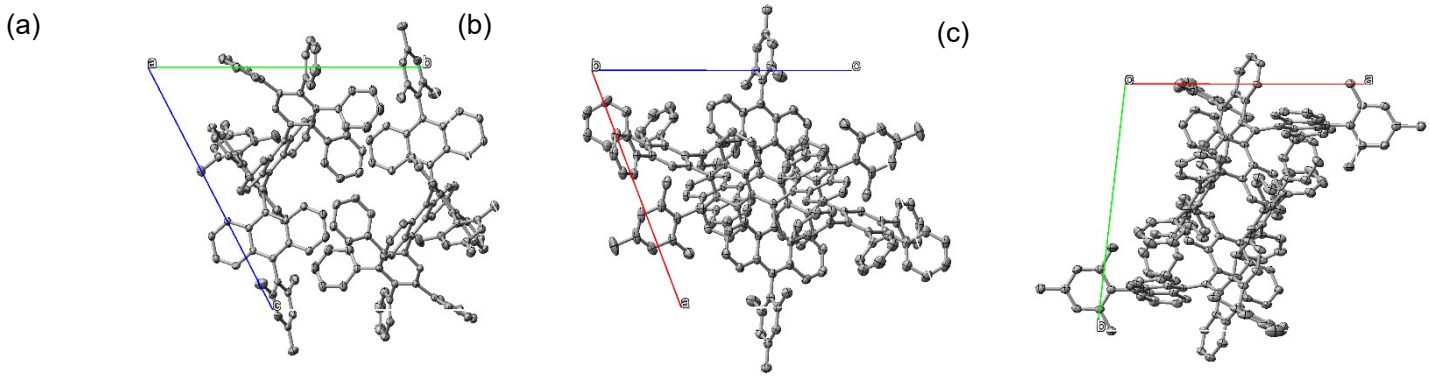


Figure S2. X-ray crystal structure of **2**. Packing structures (a) from a axis, (b) from b axis, and (c) from c axis.

Calculated spin distribution of 1’

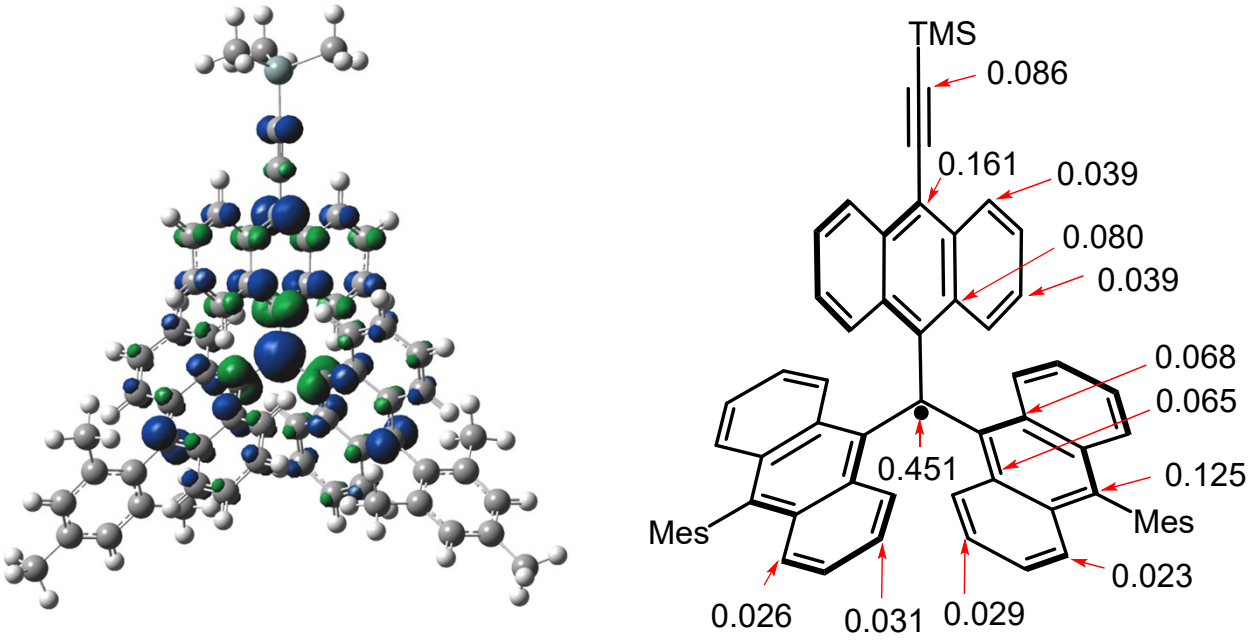
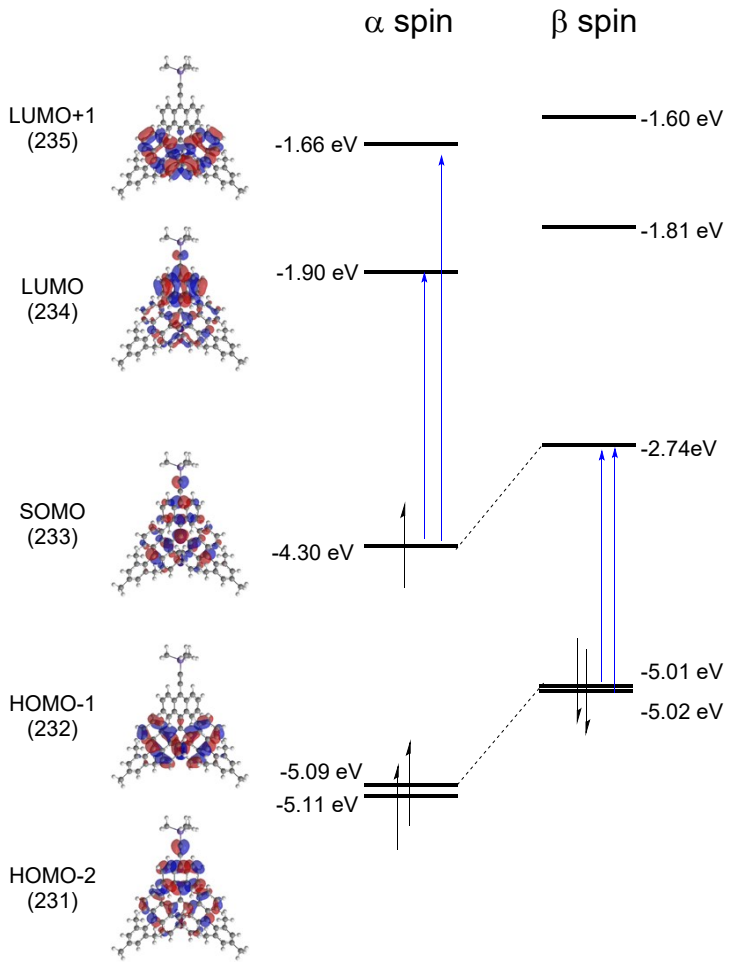


Figure S3. The calculated spin density map of **1**’ (UBLYP/6-31G**//UωB97XD/6-31G**). The blue and green surfaces represent α and β spins, respectively (left). The spin density values for α spins (right).

Frontier molecular orbitals and TD-DFT calculations of 1’



Excited State 1: 2.332-A 1.3443 eV 922.29 nm f=0.0031 <S**2>=1.110

231A -> 234A	0.13146
231A -> 236A	-0.13189
232A -> 235A	-0.12997
233A -> 234A	0.59571
230B -> 234B	0.11481
231B -> 233B	0.73557
231B -> 234B	0.11075
232B -> 235B	-0.13266

Excited State 2: 2.446-A 1.4263 eV 869.30 nm f=0.0093 <S**2>=1.246

231A -> 235A	-0.16652
232A -> 234A	-0.19264
232A -> 236A	-0.14608
233A -> 235A	0.44955
230B -> 235B	0.12496
231B -> 235B	-0.14920
232B -> 233B	0.78602
232B -> 234B	-0.21466

Excited State 3: 3.007-A 1.7335 eV 715.24 nm f=0.0090 <S**2>=2.011

231A -> 234A	-0.38265
232A -> 235A	-0.35566
233A -> 234A	0.16316
233A -> 236A	0.48439
230B -> 233B	-0.38737
231B -> 233B	-0.10534
231B -> 234B	-0.36936
232B -> 235B	-0.37154

Excited State 4: 2.074-A 1.8943 eV 654.51 nm f=0.3342 <S**2>=0.825

233A -> 234A	0.73056
233A -> 236A	-0.10861
230B -> 233B	0.15686
231B -> 233B	-0.63034
231B -> 234B	0.12358

Excited State 5: 2.359-A 1.9140 eV 647.78 nm f=0.1215 <S**2>=1.141

231A -> 235A	-0.13722
232A -> 234A	-0.13717
232A -> 236A	-0.13020
233A -> 235A	0.69173
231B -> 235B	-0.16043
232B -> 233B	-0.59614
232B -> 234B	-0.21422
232B -> 236B	-0.14557

Excited State 6: 2.753-A 2.1939 eV 565.14 nm f=0.0009 <S**2>=1.645

230A -> 236A	0.14152
231A -> 234A	0.41786
232A -> 235A	0.15594
233A -> 236A	0.53814
230B -> 233B	-0.45821
230B -> 236B	-0.15697
231B -> 234B	0.42441
232B -> 235B	0.15549

Excited State 7: 3.046-A 2.2577 eV 549.17 nm f=0.0128 <S**2>=2.070

230A -> 235A	0.15187
231A -> 235A	0.24764
232A -> 234A	0.47013
232A -> 236A	0.24176
233A -> 235A	0.55023
230B -> 235B	-0.16227
231B -> 235B	0.25260
232B -> 233B	0.11323
232B -> 234B	0.41571
232B -> 236B	0.18108

Figure S4. Frontier Molecular orbitals, energies, and transition of **1** (top). Yellow highlighted transition in TD calculated table are main contributions for the excitation (down). (UB3LYP/6-31G**// UωB97XD/6-31G**)

Cyclic voltammogram of TAntM radical

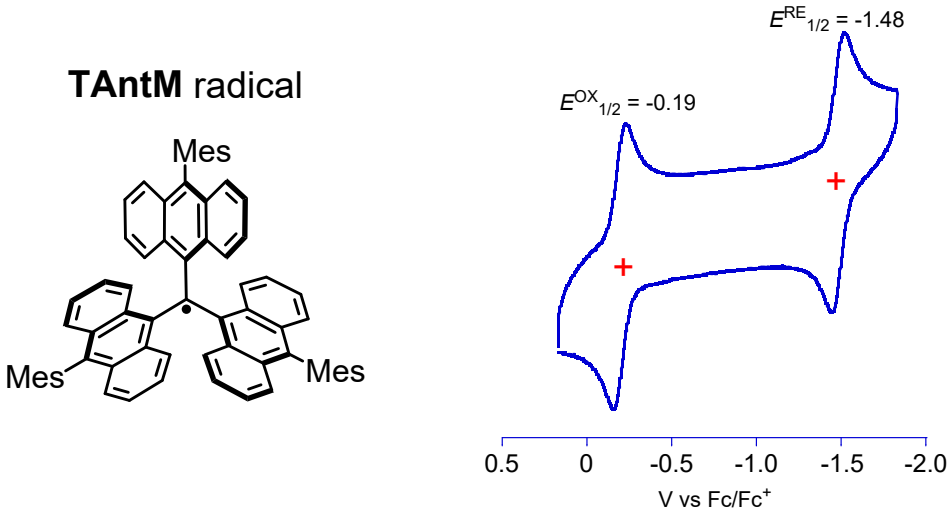


Figure S5. Cyclic voltammogram of **TAntM** radical. Measurement conditions: 0.1 M nBu$_4$NPF$_6$ in CH_2Cl_2, scan rate=100 mV s^{-1}.

Stability of 1 in air-saturated solution

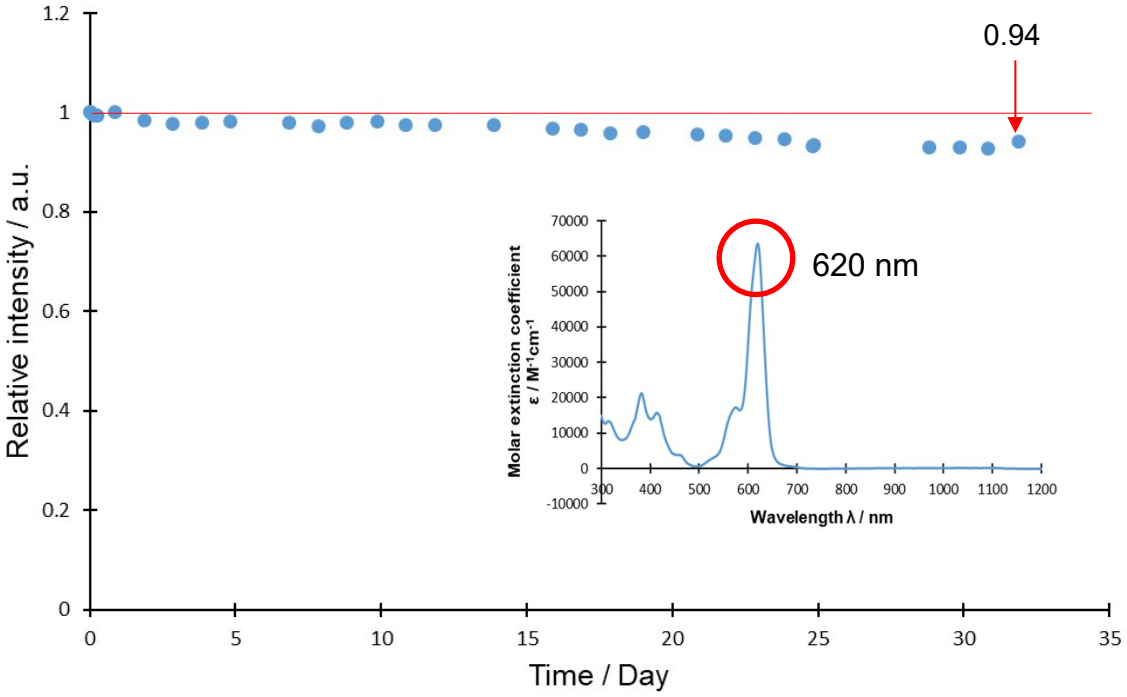


Figure S6. Decay plot of absorption intensity of **1** at 620 nm under air-saturated CH_2Cl_2 solution (1.0 x 10^{-5} M) with absence of light at room temperature. The relative intensity after 32 days from the start of measurement is 0.94.

IR spectra of 1 and 1’ dimer

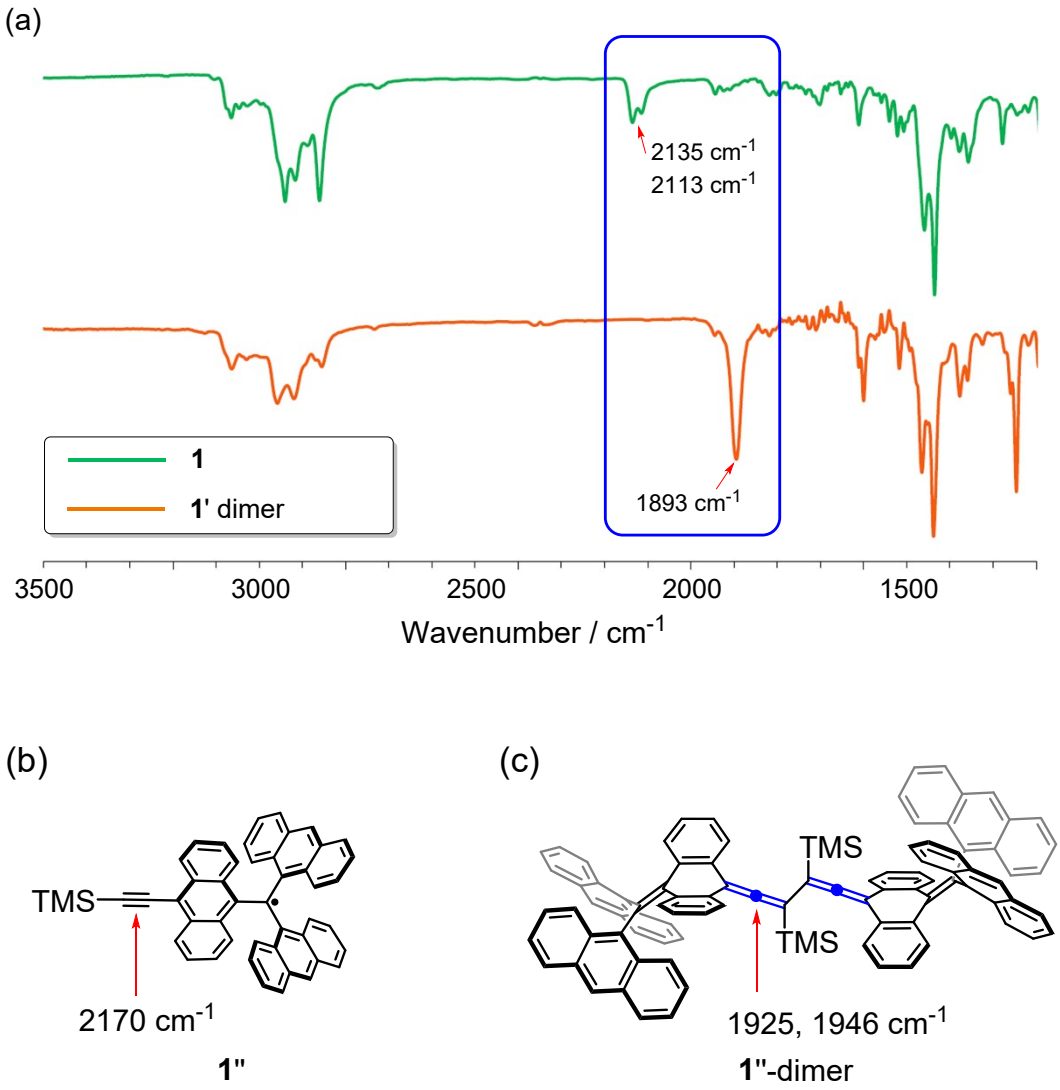


Figure S7. (a) IR spectra of **1** and **1**’ dimer. (b) Calculated frequency vibration of acetylene unit in **1**”. (c) Calculated frequency vibration of acetylene unit in **1**” dimer. Frequency vibration were computed by (U)B3LYP/6-31G*, using frequency scaling factor (0.9614). (A. P. Scott, L. Radom *J. Phys. Chem.* **1996,** *100,* 16502-16513.)

^{13}C NMR spectra of 4’ and 1’ dimer

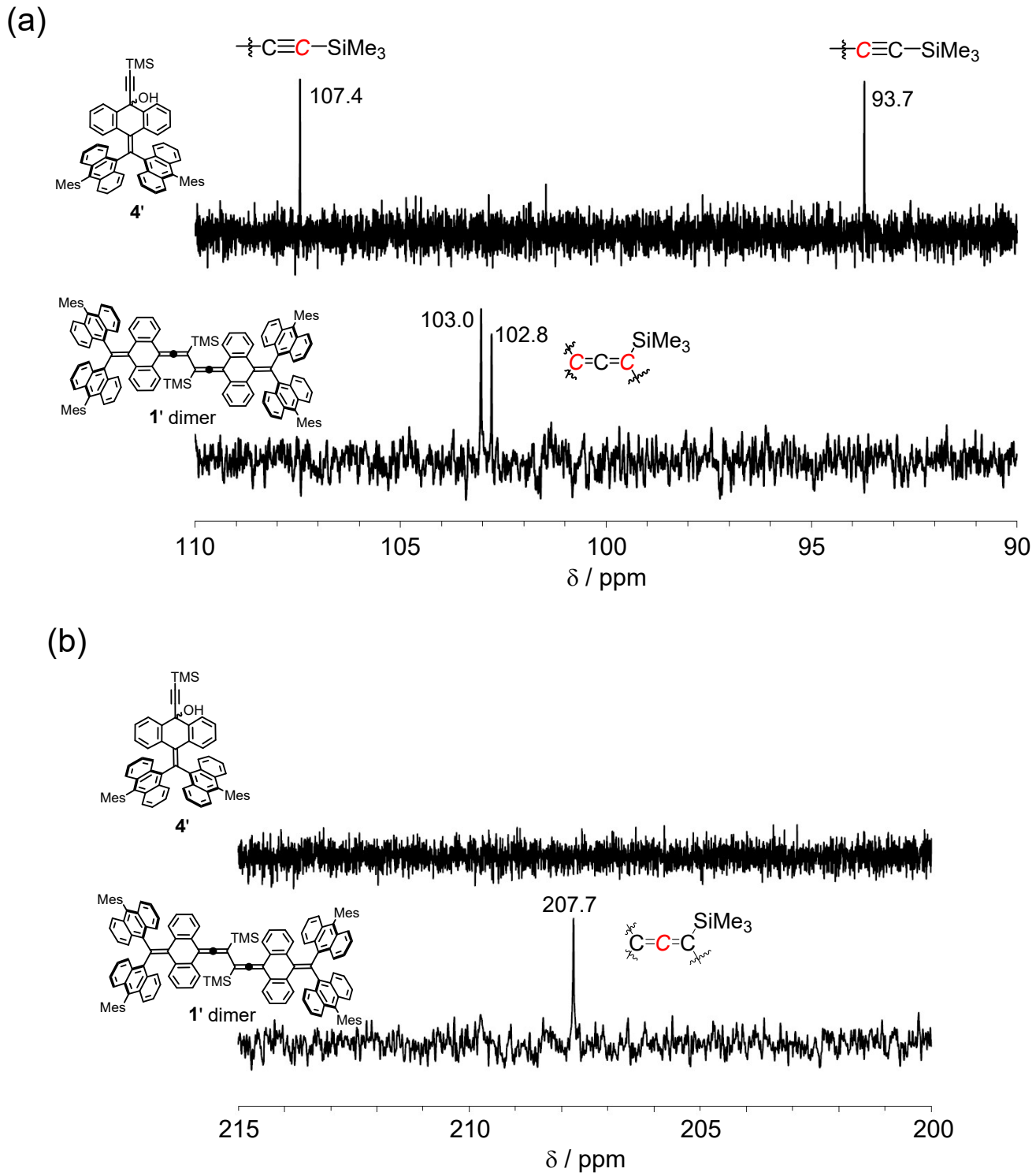


Figure S8. ^{13}C NMR spectra of **4'** and **1'** dimer. (a) Expanded chemical shift region from 90 to 110 ppm. (b) Expanded chemical shift region from 200 to 215 ppm, where a unique peak from the central carbon of the allene unit is observed at 207.7 ppm for the **1'** dimer, but no such peak is observed for the **4'**.

MS spectra of 1’ dimer

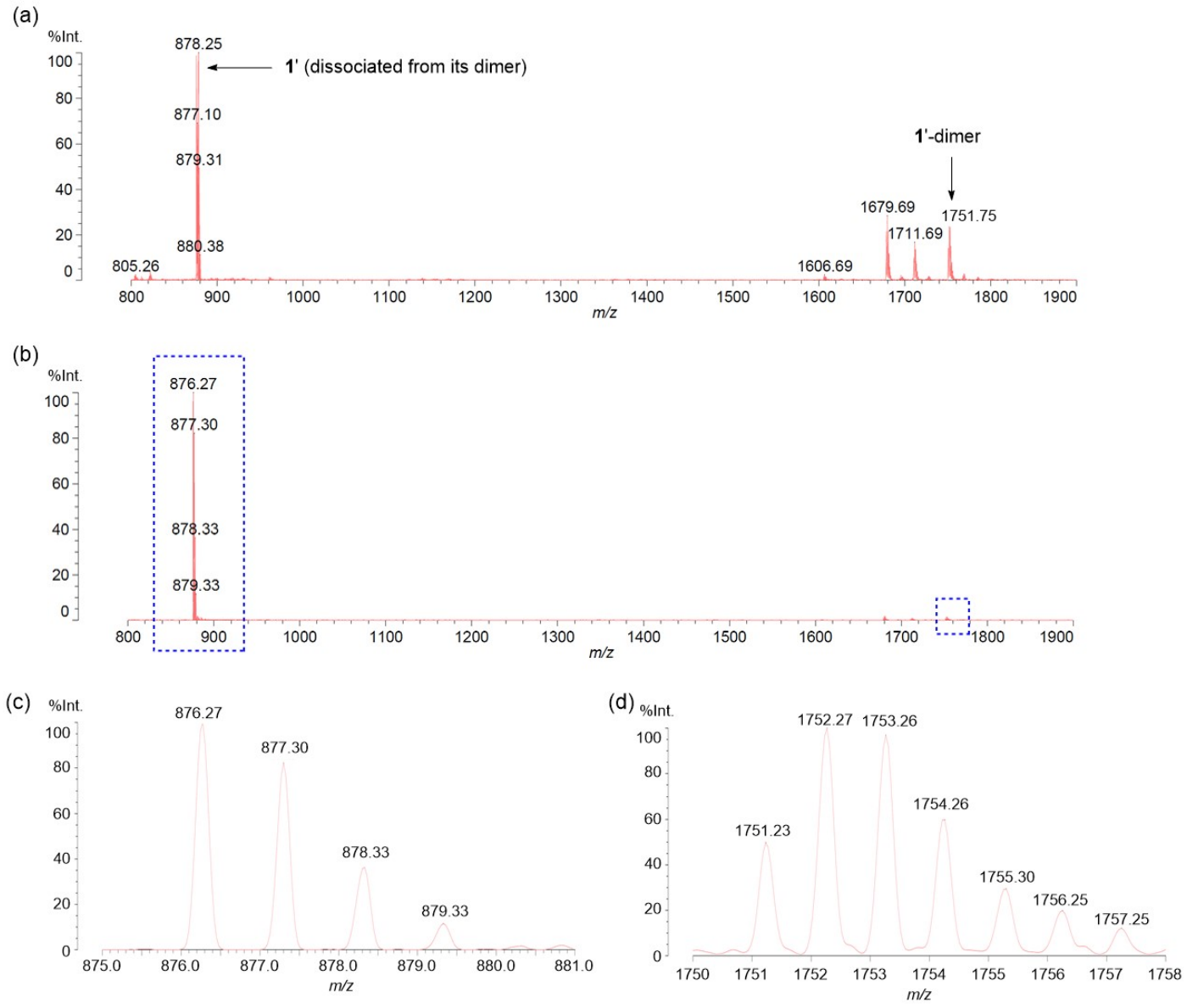


Figure S9. MALDI TOF-MS spectra of **1**' dimer. (a) Measurement with linear mode. M^+ peak of **1**’ dimer (m/z = 1751.75) as well as **1**’ (m/z = 877.10) dissociated from the dimer are observed. (b) Measurement with reflection mode. The relative intensity of **1**’ dimer is quite low compared with that of **1**’. (c) Expanded m/z region around **1**’ in (b). Due to the isotope pattern separated in each 1 Da, this MS peak is originating from dissociated from **1**’ dimer not originating from dication species of **1**’ dimer. (d) Expanded m/z region around **1**’dimer in (b).

X-ray crystallographic data of 1' dimer

Crystal data for 1. CCDC 2149932. $C_{132}H_{110}Si_2$, M_W = 1752.37, triclinic, space group *P* -1 (no. 2), *a* = 12.1360(10), *b* = 15.6410(11), *c* = 16.9992(13) Å, α = 70.519(7)°, β = 69.212(7)°, γ = 83.824(6)°, *V* = 2843.8(4) Å^3, Z = 1, *D* = 1.023g cm^3, *T* = 99 K, Data collection with CuKα radiation (multi-layer mirror monochromated). 10230 measured reflection, 3899 unique reflections; structure solution by direct methods (Shelxs), refinement by fullmatrix least squares on *F* with anisotropic temperature factors for the non-H atoms. Final R_1 = 0.0877, wR_2 = 0.2489, *GOF* = 0.925.

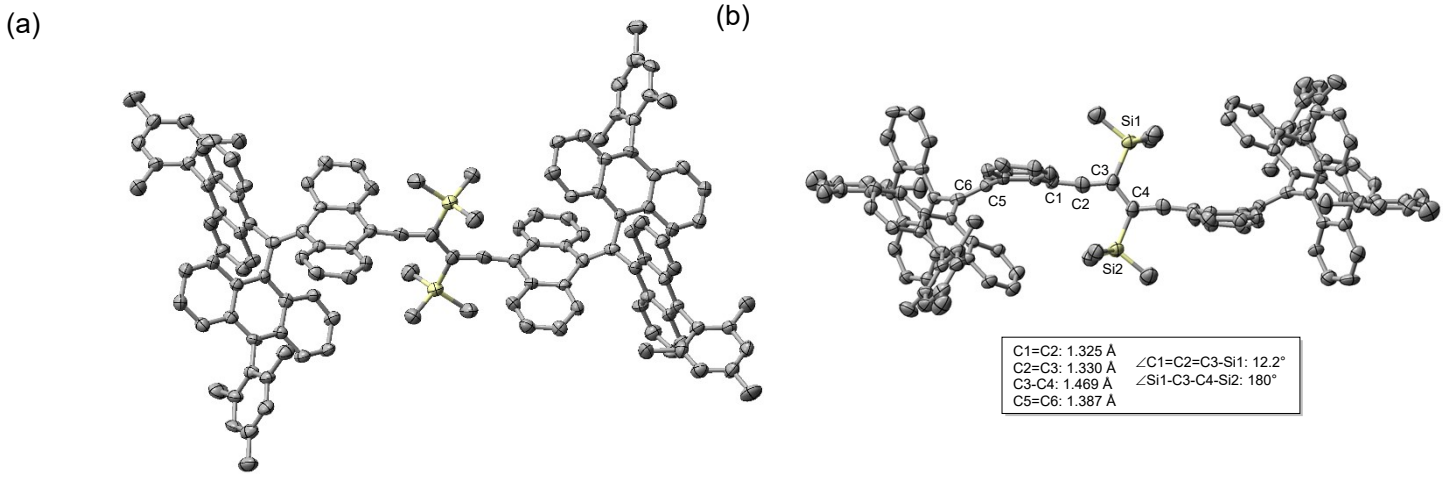


Figure S10. X-ray crystal structure of **1**' dimer. (a) Side view-1 (b) Side view-2 with bond length and dihedral angles.

Relative energy evaluation for σ-dimer structures

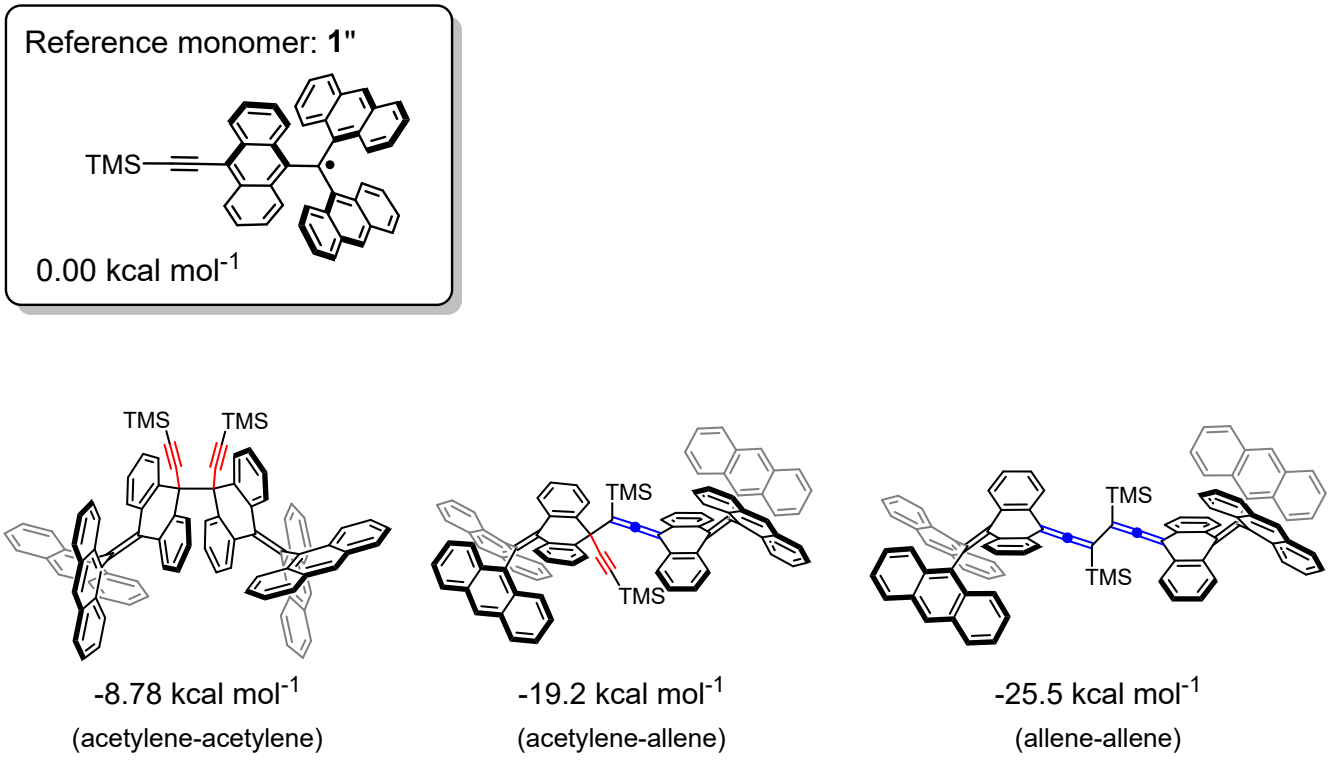


Figure S11. Quantum chemical calculations of relative energy evaluation for σ-dimer structures of **1**", acetylene-acetylene type dimer (left), acetylene-allene type dimer, (center), and allene-allene type (right) (ωB97XD/6-31G**).

UV-vis-NIR, ESR spectra, CV of 2

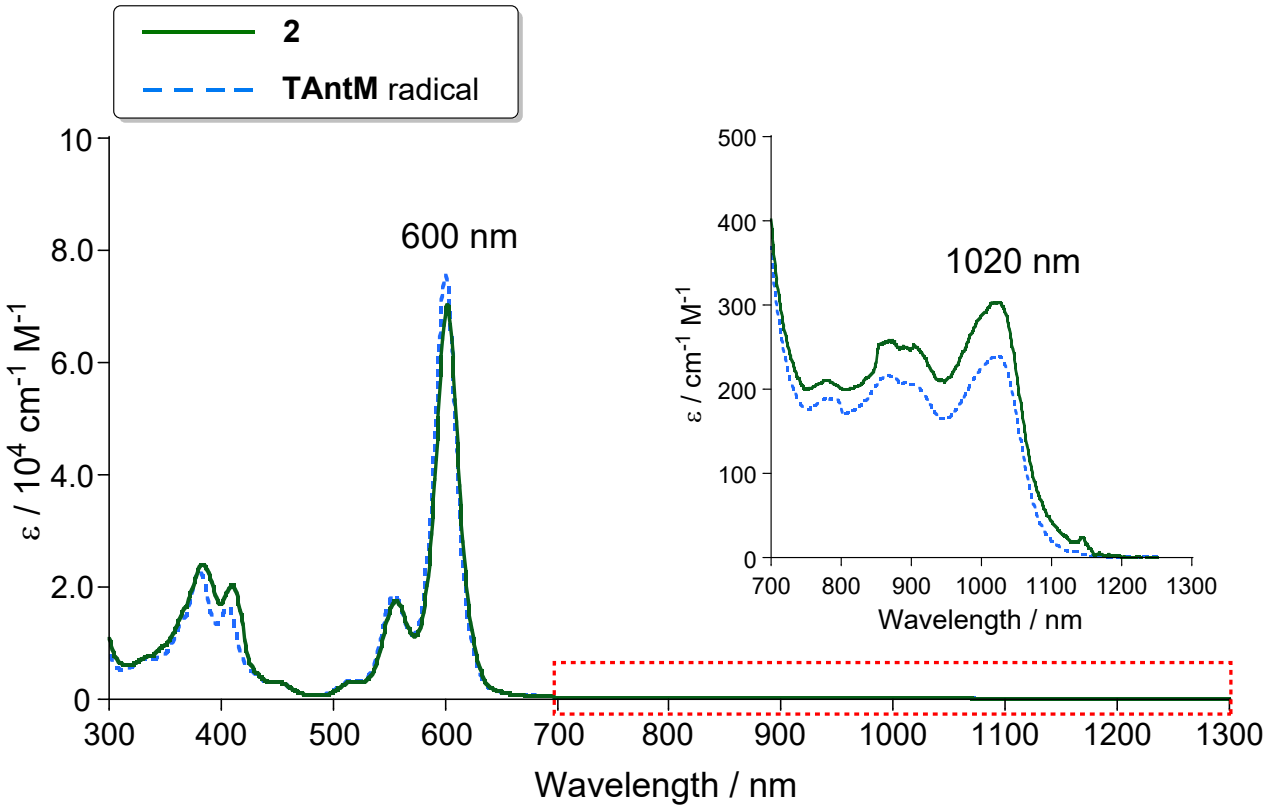


Figure S12. UV/Vis/NIRspectra of **2** (green solid) and **TAntM** radical (blue dash) in CH_2Cl_2 (inset:expansion from 700 to 1300 nm).

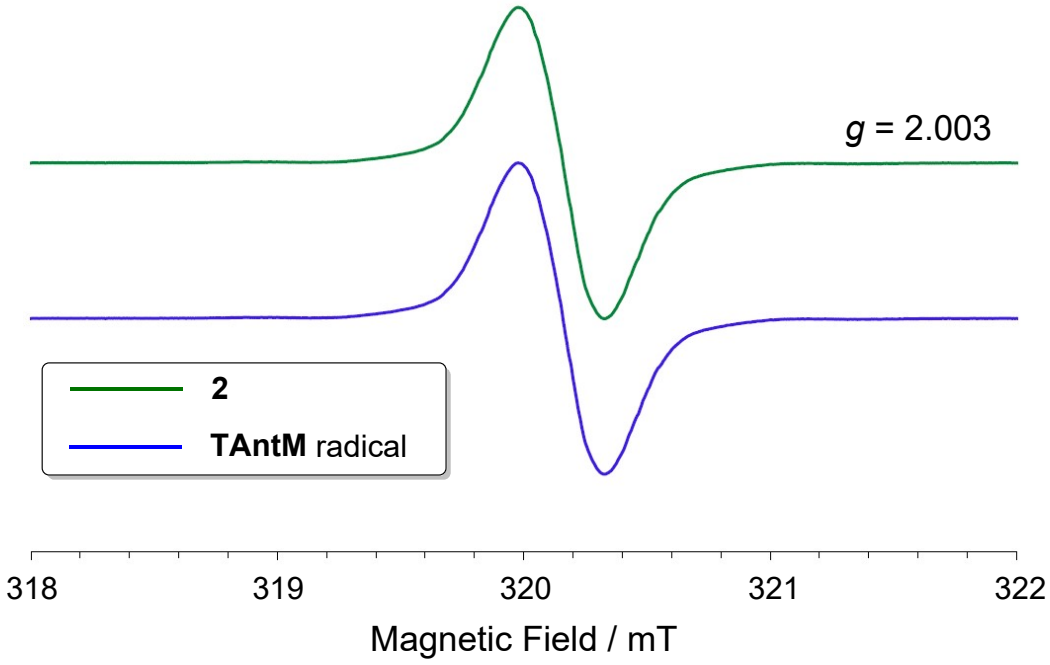


Figure S13. ESR spectra of **2** (green solid) and **TAntM** radical (blue solid) in toluene.

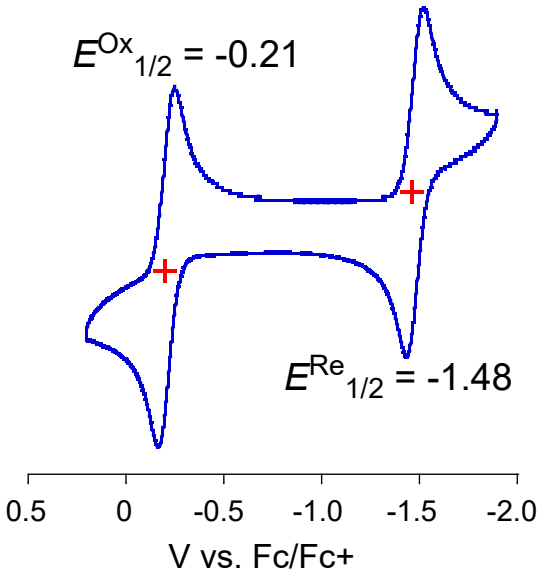


Figure S14. Cyclic voltammogram of **2**. Measurement conditions: 0.1 M nBu$_4$NPF$_6$ in CH_2Cl_2, scan rate=100 mV s^{-1}.

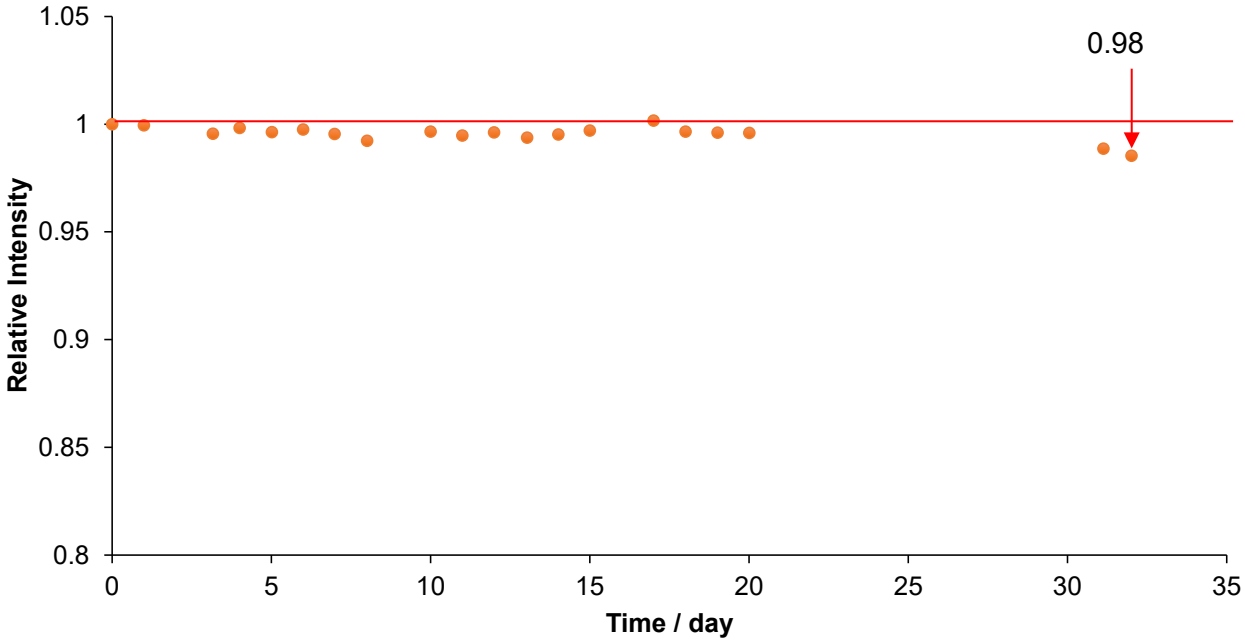
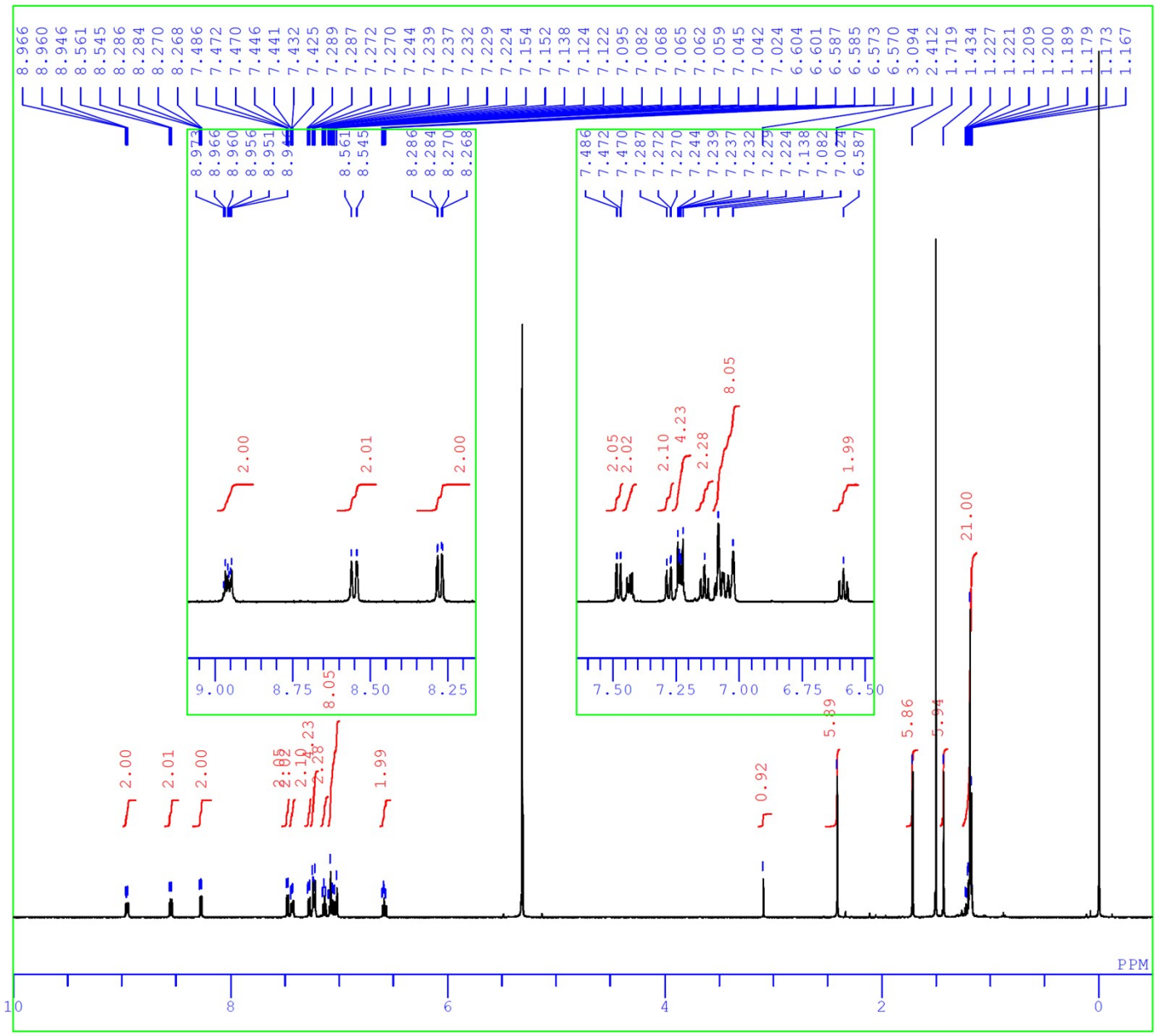


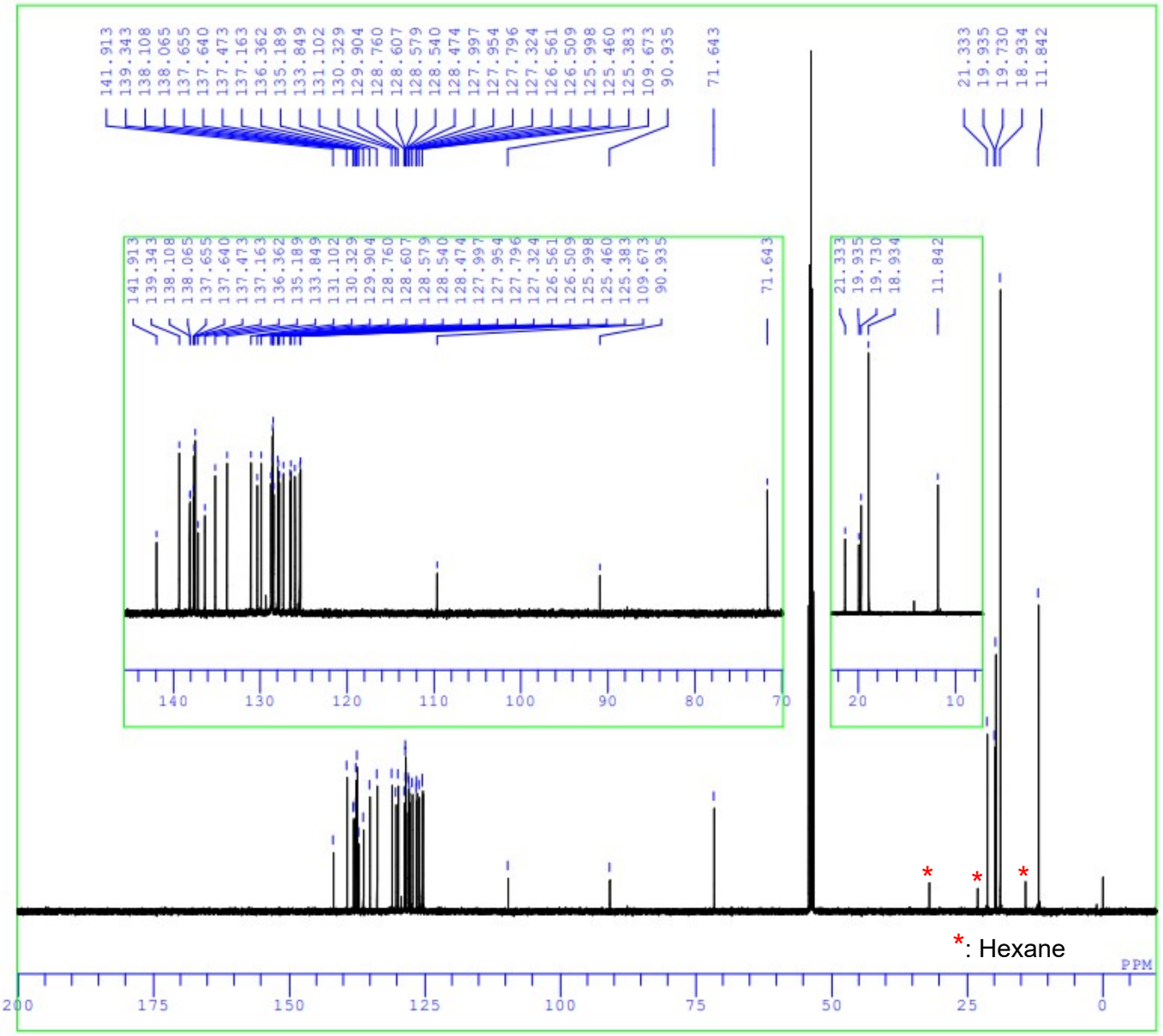
Figure S15. Decay plot of absorption intensity of **2** at 600 nm under air-saturated CH_2Cl_2 solution (1.0 x 10^{-5} M) with absence of light at room temperature. The relative intensity after 32 days from the start of measurement is 0.98.

NMR spectra

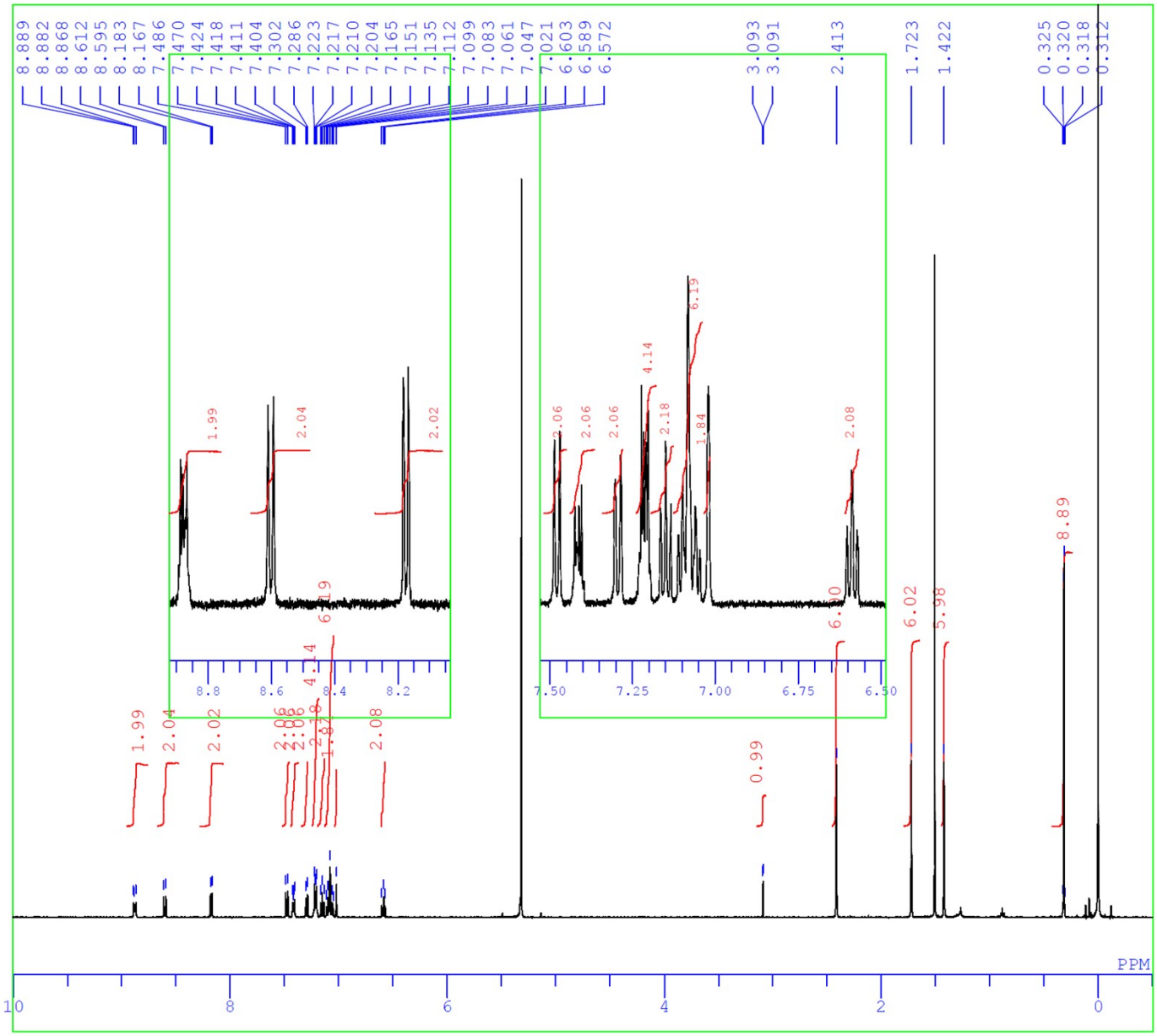
^{1}H NMR (500 MHz) of compound **4** (CD_2Cl_2)



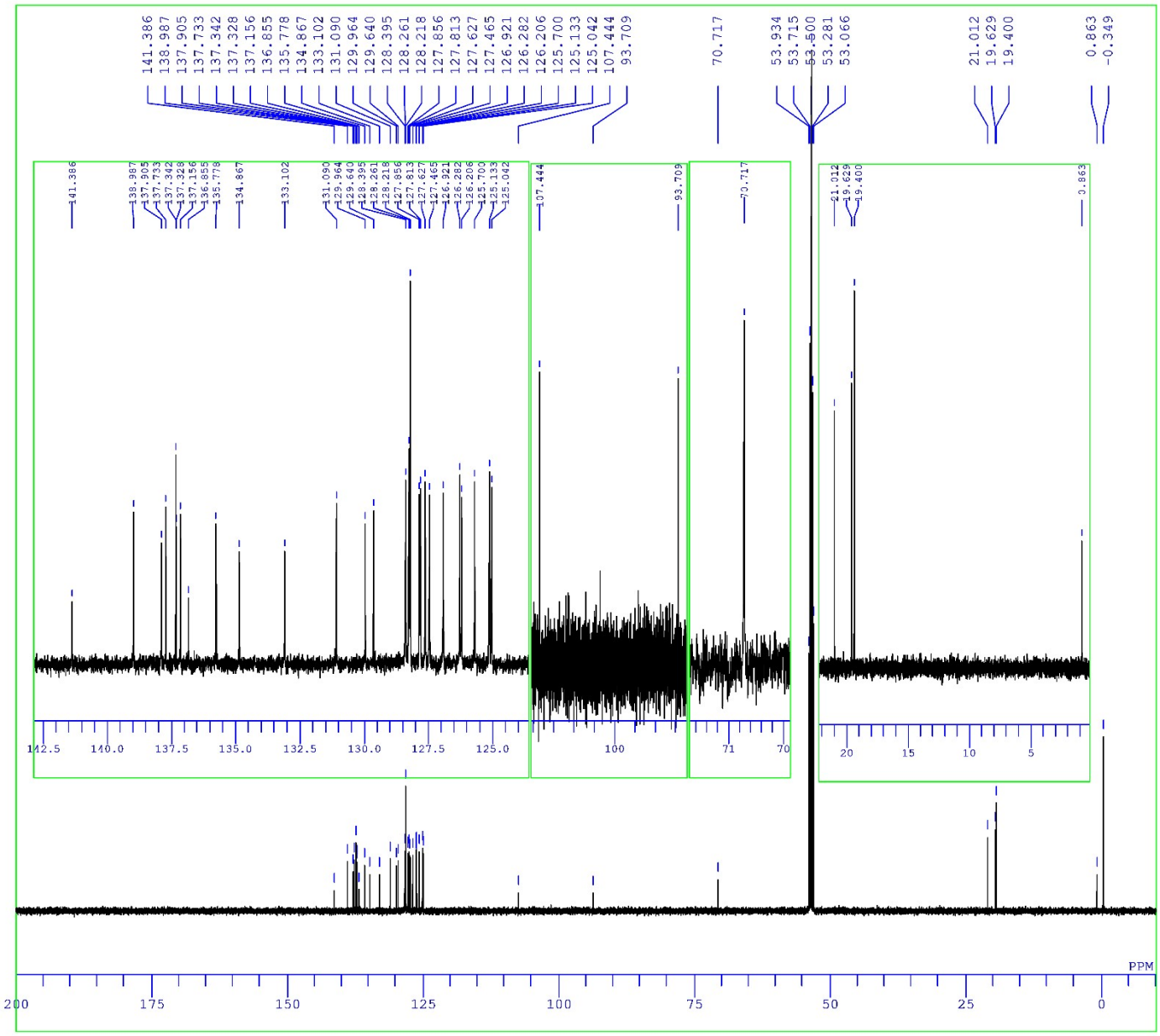
^{13}C NMR (125 MHz) of compound **4** (CD_2Cl_2)



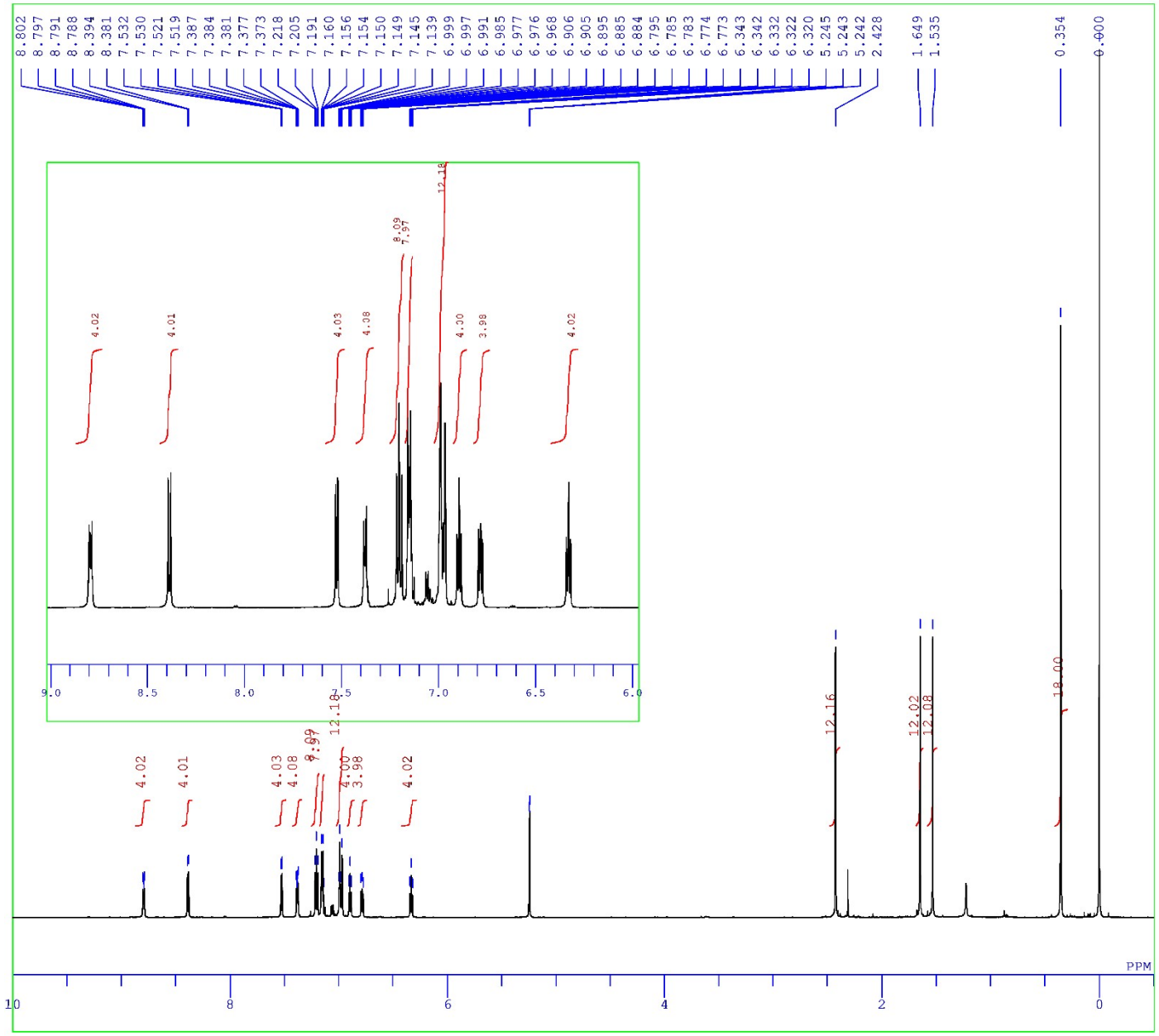
^{1}H NMR (500 MHz) of compound **4'** (CD_2Cl_2)



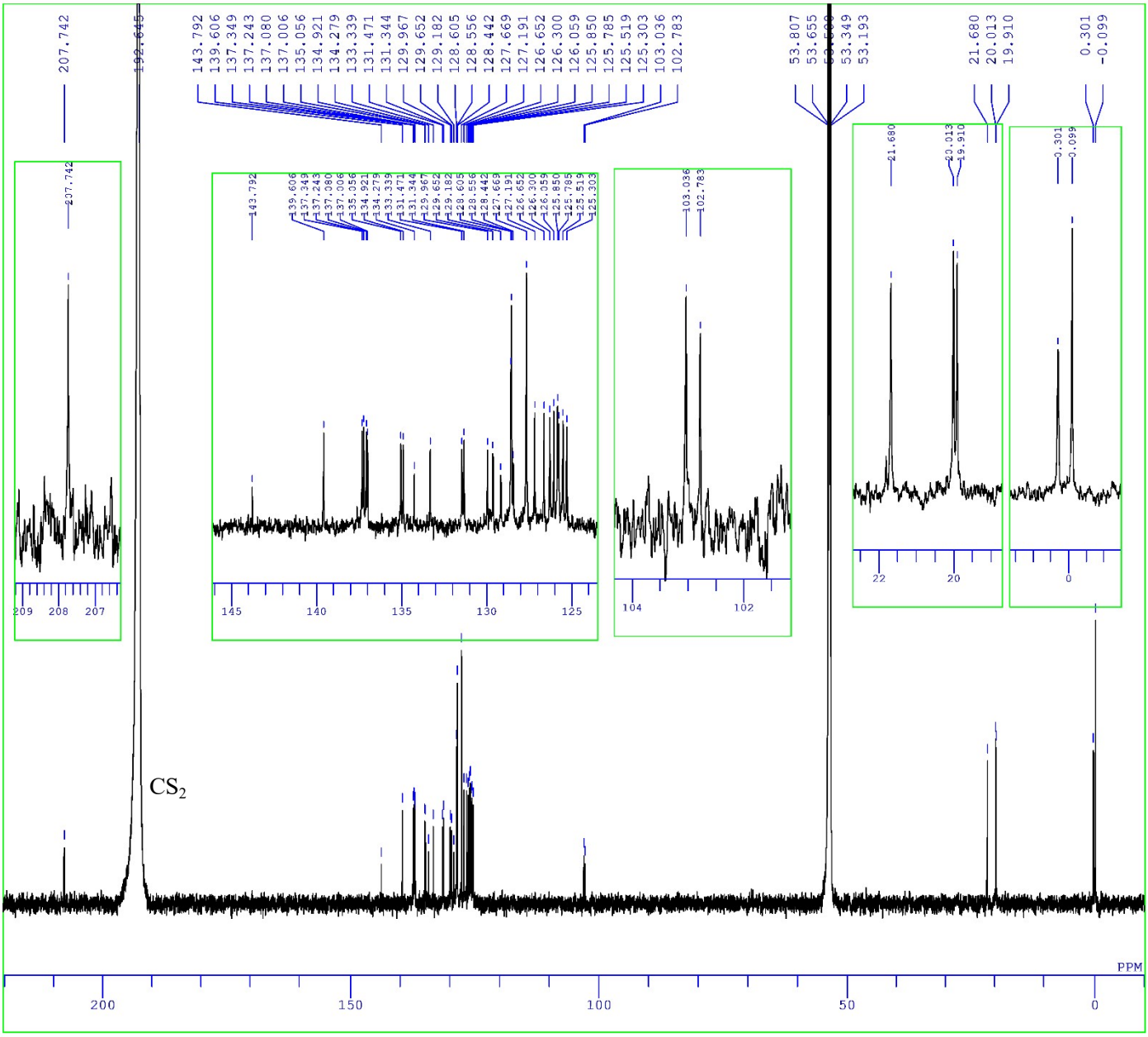
^{13}C NMR (125 MHz) of compound **4'** (CD_2Cl_2)



^{1}H NMR (700 MHz) of compound **1'** dimer (CD_2Cl_2/CS_2).



^{13}C NMR (175 MHz) of compound **1'** dimer (CD_2Cl_2/CS_2)



Calculated Cartesian coordination

Table S1. Cartesian Coordinates of **1'** ($C_{66}H_{55}Si$, total 122 atoms) (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.379275	-0.003823	0.004101
2	6	0	0.402506	-1.245537	0.144445
3	6	0	0.121727	-2.393733	-0.651814
4	6	0	-0.984423	-2.461990	-1.557176
5	6	0	-1.218200	-3.563667	-2.328245
6	6	0	-0.350766	-4.683642	-2.270245
7	6	0	0.746159	-4.644587	-1.463279
8	6	0	1.031368	-3.503805	-0.647035
9	6	0	2.217061	-3.453723	0.107158
10	6	0	3.227860	-4.545700	-0.011507
11	6	0	3.202469	-5.638029	0.867372
12	6	0	4.163620	-6.638546	0.729416
13	6	0	5.147868	-6.576526	-0.255092
14	6	0	2.147895	-5.724019	1.941264
15	6	0	6.199884	-7.650701	-0.366432
16	6	0	0.388972	1.245548	-0.141065
17	6	0	1.517835	1.282219	-1.008731
18	6	0	1.756609	0.268504	-1.989385
19	6	0	2.870650	0.280030	-2.777762
20	6	0	3.831302	1.316316	-2.649415
21	6	0	3.612764	2.337499	-1.773654
22	6	0	2.439764	2.374762	-0.954070
23	6	0	2.184286	3.469541	-0.111637
24	6	0	3.186888	4.569329	0.004403
25	6	0	4.173223	4.490866	1.000343
26	6	0	5.115484	5.512854	1.097858
27	6	0	5.099221	6.608756	0.236421
28	6	0	4.206298	3.319264	1.949655
29	6	0	6.108269	7.719481	0.381693
30	6	0	-1.832325	-0.011466	0.008777
31	6	0	-2.570666	0.754651	-0.953083
32	6	0	-1.934037	1.458063	-2.019753
33	6	0	-2.647220	2.190719	-2.926698
34	6	0	-4.058253	2.259212	-2.843222
35	6	0	-4.713758	1.553991	-1.876337
36	6	0	-4.000089	0.767177	-0.925307
37	6	0	-4.695485	-0.027369	0.017371
38	6	0	1.536212	-1.271507	1.006094
39	6	0	1.771348	-0.255065	1.984865
40	6	0	2.889292	-0.256665	2.767763
41	6	0	3.857973	-1.284953	2.635511
42	6	0	3.643753	-2.308505	1.761484
43	6	0	2.467217	-2.356169	0.947537
44	6	0	4.206765	-4.463687	-1.014558
45	6	0	5.151671	-5.482445	-1.119119
46	6	0	4.224087	-3.295821	-1.968896
47	6	0	-2.556358	-0.785629	0.974976
48	6	0	-1.905795	-1.481872	2.037953
49	6	0	-2.605476	-2.222731	2.948732
50	6	0	-4.016100	-2.307322	2.873168
51	6	0	-4.684866	-1.609234	1.910248
52	6	0	-3.985695	-0.814143	0.955527
53	6	0	0.101640	2.391187	0.656669
54	6	0	-1.000845	2.449633	1.567116
55	6	0	-1.240634	3.549095	2.339538
56	6	0	-0.383170	4.676508	2.277885
57	6	0	0.710345	4.647120	1.465878
58	6	0	1.001603	3.509132	0.647931
59	6	0	3.152449	5.660608	-0.875571
60	6	0	4.111138	6.664342	-0.744733
61	6	0	2.095834	5.737832	-1.948124
62	1	0	-1.657439	-1.621201	-1.641018
63	1	0	-2.073472	-3.577312	-2.996097
64	1	0	-0.552194	-5.558823	-2.879431
65	1	0	1.433513	-5.482918	-1.428853
66	1	0	4.142136	-7.488188	1.408301
67	1	0	2.222262	-4.877777	2.632235
68	1	0	2.247213	-6.646199	2.518579
69	1	0	1.142301	-5.695572	1.509430
70	1	0	5.833523	-8.608459	0.012670
71	1	0	7.090928	-7.386031	0.213722
72	1	0	6.515069	-7.793514	-1.403710
73	1	0	1.025931	-0.516749	-2.127115
74	1	0	3.015224	-0.502970	-3.515368
75	1	0	4.723761	1.307144	-3.266796
76	1	0	4.322735	3.153306	-1.691249
77	1	0	5.883294	5.451261	1.865974
78	1	0	3.296497	3.286347	2.558849
79	1	0	5.065470	3.382484	2.621720
80	1	0	4.258452	2.368137	1.410407
81	1	0	7.063495	7.343113	0.757812
82	1	0	5.753821	8.479017	1.087427
83	1	0	6.291729	8.218945	-0.573409
84	1	0	-0.860261	1.405940	-2.124879
85	1	0	-2.126118	2.712912	-3.722478
86	1	0	-4.617033	2.851601	-3.560521
87	1	0	-5.796588	1.568284	-1.819180
88	1	0	1.034877	0.524204	2.125642
89	1	0	3.030917	0.528116	3.504049
90	1	0	4.753280	-1.267855	3.248593
91	1	0	4.360048	-3.118442	1.676177
92	1	0	5.909872	-5.421324	-1.896772
93	1	0	3.311399	-3.274163	-2.574285
94	1	0	5.080965	-3.353330	-2.644392
95	1	0	4.269349	-2.342156	-1.433547
96	1	0	-0.832148	-1.417468	2.137189
97	1	0	-2.074003	-2.739075	3.741458
98	1	0	-4.564008	-2.906328	3.593348
99	1	0	-5.767670	-1.635689	1.858688
100	1	0	-1.666162	1.603008	1.653712
101	1	0	-2.092959	3.555209	3.011257
102	1	0	-0.589373	5.549764	2.888241
103	1	0	1.390284	5.491333	1.428470
104	1	0	4.086415	7.510090	-1.428374
105	1	0	2.177040	4.893134	-2.640247
106	1	0	2.185647	6.661609	-2.524440
107	1	0	1.091223	5.699491	-1.514816
108	6	0	-6.119234	-0.033804	0.020402
109	6	0	-7.337929	-0.035372	0.018917
110	14	0	-9.176420	-0.018094	-0.009334
111	6	0	-9.729920	1.076927	-1.433539
112	1	0	-9.360878	2.099470	-1.309498
113	1	0	-9.356906	0.696854	-2.389277
114	1	0	-10.822837	1.117006	-1.489261
115	6	0	-9.794007	-1.775774	-0.257618
116	1	0	-9.424701	-2.192707	-1.199121
117	1	0	-9.460764	-2.429877	0.553579
118	1	0	-10.888634	-1.799531	-0.282611
119	6	0	-9.802033	0.668789	1.624491
120	1	0	-9.468840	0.053139	2.465222
121	1	0	-9.437457	1.687124	1.788072
122	1	0	-10.896838	0.694577	1.637441

Table S2. Cartesian Coordinates of **1**'' ($C_{48}H_{35}Si$, total 84atoms) (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.322674	0.000209	0.000788
2	6	0	2.065337	-1.271729	0.002889
3	6	0	1.704853	-2.318193	-0.898436
4	6	0	0.696584	-2.172547	-1.903788
5	6	0	0.376302	-3.193747	-2.751475
6	6	0	1.046634	-4.443163	-2.675036
7	6	0	2.050430	-4.610886	-1.770269
8	6	0	2.424002	-3.558576	-0.878308
9	6	0	3.504283	-3.718901	-0.012680
10	6	0	2.060867	1.274664	-0.005409
11	6	0	3.149579	1.480982	-0.904334
12	6	0	3.511664	0.540602	-1.920337
13	6	0	4.556606	0.769146	-2.768902
14	6	0	5.319467	1.963579	-2.681730
15	6	0	4.978292	2.911736	-1.765605
16	6	0	3.879831	2.714243	-0.873056
17	6	0	3.491540	3.726708	0.002392
18	6	0	-0.139345	-0.002639	0.004852
19	6	0	-0.874454	0.856640	-0.874058
20	6	0	-0.237698	1.655364	-1.873208
21	6	0	-0.948813	2.476382	-2.701804
22	6	0	-2.359293	2.548920	-2.603847
23	6	0	-3.015755	1.756249	-1.708835
24	6	0	-2.304349	0.872802	-0.844093
25	6	0	-3.002352	-0.011776	0.010323
26	6	0	3.159484	-1.474412	0.896027
27	6	0	3.523719	-0.532920	1.910239
28	6	0	4.573831	-0.758026	2.753328
29	6	0	5.340261	-1.949859	2.662025
30	6	0	4.997512	-2.899052	1.747563
31	6	0	3.893734	-2.705187	0.860799
32	6	0	-0.865700	-0.865142	0.887845
33	6	0	-0.219930	-1.658467	1.885484
34	6	0	-0.922627	-2.482052	2.718712
35	6	0	-2.333098	-2.562702	2.627280
36	6	0	-2.997950	-1.775768	1.733405
37	6	0	-2.295537	-0.890200	0.863663
38	6	0	1.701516	2.320007	0.897665
39	6	0	0.698942	2.171027	1.908188
40	6	0	0.379648	3.191191	2.757502
41	6	0	1.045400	4.442833	2.677548
42	6	0	2.043894	4.613896	1.767544
43	6	0	2.416349	3.562806	0.873687
44	6	0	-4.426821	-0.017006	0.010441
45	6	0	-5.645324	-0.019243	0.007491
46	14	0	-7.483927	-0.000890	-0.004764
47	6	0	-8.051417	1.616554	-0.776395
48	6	0	-8.099815	-1.458801	-1.018542
49	6	0	-8.097964	-0.132037	1.766828
50	1	0	0.179998	-1.229203	-2.009906
51	1	0	-0.394816	-3.043868	-3.500138
52	1	0	0.771590	-5.247459	-3.349544
53	1	0	2.597544	-5.547749	-1.714456
54	1	0	4.055194	-4.656219	-0.018332
55	1	0	2.939630	-0.369295	-2.033102
56	1	0	4.800047	0.031501	-3.526722
57	1	0	6.153342	2.124002	-3.357338
58	1	0	5.528511	3.846267	-1.701830
59	1	0	4.039323	4.665871	0.005121
60	1	0	0.834517	1.603416	-1.991685
61	1	0	-0.426783	3.067762	-3.446934
62	1	0	-2.916063	3.213973	-3.256039
63	1	0	-4.098174	1.772222	-1.645044
64	1	0	2.949220	0.375040	2.026077
65	1	0	4.818732	-0.019639	3.509954
66	1	0	6.178180	-2.107547	3.333259
67	1	0	5.550537	-3.831716	1.680802
68	1	0	0.852449	-1.599900	1.999379
69	1	0	-0.393941	-3.068896	3.462728
70	1	0	-2.883209	-3.229063	3.283771
71	1	0	-4.080535	-1.797082	1.675126
72	1	0	0.186057	1.225964	2.016963
73	1	0	-0.387067	3.038766	3.510165
74	1	0	0.771199	5.246228	3.353473
75	1	0	2.587546	5.552596	1.708846
76	1	0	-7.685536	2.474588	-0.204790
77	1	0	-7.683839	1.713070	-1.802466
78	1	0	-9.144878	1.669544	-0.803678
79	1	0	-7.737189	-1.402467	-2.049080
80	1	0	-7.758535	-2.407265	-0.593442
81	1	0	-9.194590	-1.474231	-1.044913
82	1	0	-7.756821	-1.060219	2.234995
83	1	0	-7.734016	0.703592	2.371728
84	1	0	-9.192611	-0.121181	1.797570

Table S3. Cartesian Coordinates of **1**'' dimer (acetylene-acetylene) ($C_{96}H_{70}Si_2$, total 168 atoms) (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.175725	2.607849	0.928419	57	6	0	-2.314216	4.618498	-1.874196
2	6	0	-0.704927	1.842471	2.019439	58	6	0	-1.147561	4.920949	-1.125083
3	6	0	0.377250	0.775360	1.886431	59	6	0	-4.448714	5.337376	-2.902883
4	6	0	1.147561	0.840189	0.578988	60	6	0	-4.679316	4.076588	-3.360686
5	6	0	0.649672	1.589575	-0.491610	61	6	0	-3.736172	3.047038	-3.088196
6	6	0	-0.300037	2.700675	-0.271307	62	6	0	-2.600994	3.306109	-2.378741
7	6	0	-0.101296	3.861900	-0.968494	63	6	0	4.679316	-4.076588	-3.360686
8	6	0	2.301673	0.078171	0.394482	64	6	0	3.736172	-3.047038	-3.088196
9	6	0	2.849480	-0.087508	-0.870411	65	6	0	2.600994	-3.306109	-2.378741
10	6	0	2.224804	0.489878	-1.971679	66	6	0	2.314216	-4.618498	-1.874196
11	6	0	1.145176	1.336202	-1.775757	67	6	0	3.274666	-5.648307	-2.146599
12	6	0	-2.340691	3.366162	1.121057	68	6	0	4.448714	-5.337376	-2.902883
13	6	0	-2.966711	3.444780	2.355217	69	6	0	1.147561	-4.920949	-1.125083
14	6	0	-2.413512	2.802954	3.456519	70	6	0	0.972390	-6.222709	-0.610199
15	6	0	-1.293104	2.008465	3.276506	71	6	0	1.938486	-7.244769	-0.897361
16	6	0	1.317244	0.901535	2.995829	72	6	0	3.057562	-6.937384	-1.665199
17	6	0	2.159117	1.031438	3.860827	73	6	0	-0.124194	-6.573960	0.240002
18	6	0	1.175725	-2.607849	0.928419	74	6	0	-0.269762	-7.838442	0.725932
19	6	0	0.704927	-1.842471	2.019439	75	6	0	0.671830	-8.856735	0.406137
20	6	0	-0.377250	-0.775360	1.886431	76	6	0	1.745153	-8.563321	-0.377001
21	6	0	-1.147561	-0.840189	0.578988	77	6	0	-3.418450	-3.880293	1.498281
22	6	0	-0.649672	-1.589575	-0.491610	78	6	0	-4.702845	-4.160826	0.957636
23	6	0	0.300037	-2.700675	-0.271307	79	6	0	-4.819115	-4.475088	-0.361138
24	6	0	0.101296	-3.861900	-0.968494	80	6	0	-3.675638	-4.503330	-1.221374
25	6	0	-2.301673	-0.078171	0.394482	81	6	0	-2.378988	-4.184739	-0.696460
26	6	0	-2.849480	0.087508	-0.870411	82	6	0	-2.308080	-3.899575	0.708810
27	6	0	-2.224804	-0.489878	-1.971679	83	6	0	-3.813748	-4.839571	-2.565079
28	6	0	-1.145176	-1.336202	-1.775757	84	6	0	-2.720820	-4.842823	-3.425965
29	6	0	2.340691	-3.366162	1.121057	85	6	0	-1.423734	-4.484452	-2.927655
30	6	0	2.966711	-3.444780	2.355217	86	6	0	-1.251152	-4.169608	-1.561462
31	6	0	2.413512	-2.802954	3.456519	87	6	0	-2.882738	-5.164709	-4.810379
32	6	0	1.293104	-2.008465	3.276506	88	6	0	-1.834156	-5.099234	-5.675301
33	6	0	-1.317244	-0.901535	2.995829	89	6	0	-0.557537	-4.688185	-5.201329
34	6	0	-2.159117	-1.031438	3.860827	90	6	0	-0.362799	-4.391607	-3.885040
35	6	0	1.834156	5.099234	-5.675301	91	14	0	3.577871	0.954783	5.021800
36	6	0	0.557537	4.688185	-5.201329	92	6	0	3.063427	-0.066149	6.514812
37	6	0	0.362799	4.391607	-3.885040	93	6	0	4.064723	2.690650	5.554055
38	6	0	1.423734	4.484452	-2.927655	94	6	0	4.984265	0.122389	4.094719
39	6	0	2.720820	4.842823	-3.425965	95	14	0	-3.577871	-0.954783	5.021800
40	6	0	2.882738	5.164709	-4.810379	96	6	0	-3.063427	0.066149	6.514812
41	6	0	1.251152	4.169608	-1.561462	97	6	0	-4.984265	-0.122389	4.094719
42	6	0	2.378988	4.184739	-0.696460	98	6	0	-4.064723	-2.690650	5.554055
43	6	0	3.675638	4.503330	-1.221374	99	1	0	2.768818	-0.397944	1.248142
44	6	0	3.813748	4.839571	-2.565079	100	1	0	3.732726	-0.705125	-0.996225
45	6	0	2.308080	3.899575	0.708810	101	1	0	2.599344	0.315485	-2.975488
46	6	0	3.418450	3.880293	1.498281	102	1	0	0.690634	1.833381	-2.624409
47	6	0	4.702845	4.160826	0.957636	103	1	0	-2.776899	3.902193	0.294980
48	6	0	4.819115	4.475088	-0.361138	104	1	0	-3.869617	4.038270	2.456826
49	6	0	0.269762	7.838442	0.725932	105	1	0	-2.856872	2.906139	4.441972
50	6	0	-0.671830	8.856735	0.406137	106	1	0	-0.865866	1.485133	4.123119
51	6	0	-1.745153	8.563321	-0.377001	107	1	0	-2.768818	0.397944	1.248142
52	6	0	-1.938486	7.244769	-0.897361	108	1	0	-3.732726	0.705125	-0.996225
53	6	0	-0.972390	6.222709	-0.610199	109	1	0	-2.599344	-0.315485	-2.975488
54	6	0	0.124194	6.573960	0.240002	110	1	0	-0.690634	-1.833381	-2.624409
55	6	0	-3.057562	6.937384	-1.665199	111	1	0	2.776899	-3.902193	0.294980
56	6	0	-3.274666	5.648307	-2.146599	112	1	0	3.869617	-4.038270	2.456826

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
113	1	0	2.856872	-2.906139	4.441972
114	1	0	0.865866	-1.485133	4.123119
115	1	0	1.968768	5.341456	-6.724565
116	1	0	-0.270901	4.603261	-5.897422
117	1	0	-0.614223	4.062424	-3.563882
118	1	0	3.871359	5.452969	-5.156819
119	1	0	4.797634	5.093888	-2.952024
120	1	0	1.350285	3.693822	1.167632
121	1	0	3.310974	3.640697	2.551449
122	1	0	5.578214	4.135357	1.598893
123	1	0	5.788095	4.709883	-0.792891
124	1	0	1.110899	8.070903	1.371003
125	1	0	-0.535096	9.859228	0.798659
126	1	0	-2.482894	9.323678	-0.617406
127	1	0	0.843413	5.817013	0.515904
128	1	0	-3.784912	7.715907	-1.882524
129	1	0	-5.157877	6.136797	-3.098630
130	1	0	-5.575536	3.851698	-3.929566
131	1	0	-3.921867	2.040221	-3.450240
132	1	0	-1.906587	2.499400	-2.178107
133	1	0	5.575536	-3.851698	-3.929566
134	1	0	3.921867	-2.040221	-3.450240
135	1	0	1.906587	-2.499400	-2.178107
136	1	0	5.157877	-6.136797	-3.098630
137	1	0	3.784912	-7.715907	-1.882524
138	1	0	-0.843413	-5.817013	0.515904
139	1	0	-1.110899	-8.070903	1.371003
140	1	0	0.535096	-9.859228	0.798659
141	1	0	2.482894	-9.323678	-0.617406
142	1	0	-3.310974	-3.640697	2.551449
143	1	0	-5.578214	-4.135357	1.598893
144	1	0	-5.788095	-4.709883	-0.792891
145	1	0	-1.350285	-3.693822	1.167632
146	1	0	-4.797634	-5.093888	-2.952024
147	1	0	-3.871359	-5.452969	-5.156819
148	1	0	-1.968768	-5.341456	-6.724565
149	1	0	0.270901	-4.603261	-5.897422
150	1	0	0.614223	-4.062424	-3.563882
151	1	0	2.230730	0.404860	7.045722
152	1	0	3.894556	-0.178024	7.218845
153	1	0	2.742842	-1.067000	6.209318
154	1	0	4.885403	2.655952	6.278345
155	1	0	4.399613	3.287183	4.699726
156	1	0	3.224333	3.212905	6.020733
157	1	0	4.674003	-0.867407	3.744806
158	1	0	5.266195	0.711887	3.216665
159	1	0	5.870211	0.004006	4.727179
160	1	0	-3.894556	0.178024	7.218845
161	1	0	-2.230730	-0.404860	7.045722
162	1	0	-2.742842	1.067000	6.209318
163	1	0	-4.674003	0.867407	3.744806
164	1	0	-5.870211	-0.004006	4.727179
165	1	0	-5.266195	-0.711887	3.216665
166	1	0	-4.399613	-3.287183	4.699726
167	1	0	-3.224333	-3.212905	6.020733
168	1	0	-4.885403	-2.655952	6.278345

Table S4. Cartesian Coordinates of **1**'' dimer (acetylene-allene) ($C_{96}H_{70}Si_2$, total 168 atoms) (ωB97XD/6-31G**).

Center Number	Atomic Numbe	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.668842	1.523500	0.263677
2	6	0	-2.346758	1.146878	0.589599
3	6	0	-1.807198	-0.151197	0.121426
4	6	0	-2.398387	-0.677593	-1.122883
5	6	0	-3.727400	-0.337343	-1.399060
6	6	0	-4.498424	0.491786	-0.432729
7	6	0	-5.800389	0.197019	-0.167377
8	6	0	-1.653317	-1.413179	-2.047517
9	6	0	-2.224898	-1.812861	-3.246270
10	6	0	-3.541535	-1.458607	-3.539215
11	6	0	-4.280640	-0.720557	-2.626667
12	6	0	-4.098862	2.796240	0.659103
13	6	0	-3.262439	3.660077	1.354000
14	6	0	-1.963629	3.278239	1.671792
15	6	0	-1.511228	2.028270	1.280444
16	6	0	-0.782087	-0.740049	0.700580
17	6	0	0.291263	-1.283075	1.202751
18	6	0	3.870833	-1.930857	0.069575
19	6	0	2.463666	-1.927604	0.065242
20	6	0	1.675078	-0.781304	0.716980
21	6	0	2.443925	-0.212182	1.916387
22	6	0	3.840485	-0.299819	1.949577
23	6	0	4.568670	-0.798806	0.754295
24	6	0	5.674306	-0.156257	0.297564
25	6	0	1.769390	0.382411	2.981721
26	6	0	2.460787	0.828244	4.100941
27	6	0	3.841152	0.667179	4.169948
28	6	0	4.523197	0.109895	3.098096
29	6	0	4.519942	-2.996305	-0.565494
30	6	0	3.813724	-4.003912	-1.208774
31	6	0	2.427012	-3.969578	-1.240565
32	6	0	1.764269	-2.929570	-0.604689
33	6	0	1.467951	0.231527	-0.335053
34	6	0	1.194808	0.986312	-1.247363
35	6	0	10.082417	1.663424	2.433045
36	6	0	9.499893	0.373073	2.309734
37	6	0	8.240680	0.224497	1.809489
38	6	0	7.453289	1.335419	1.379592
39	6	0	8.014120	2.637808	1.601545
40	6	0	9.348629	2.760810	2.100876
41	6	0	6.156380	1.190917	0.827080
42	6	0	5.360204	2.356334	0.681248
43	6	0	5.914756	3.652678	0.963435
44	6	0	7.240811	3.768140	1.362168
45	6	0	3.983068	2.328213	0.302208
46	6	0	3.216786	3.451830	0.252836
47	6	0	3.779308	4.730057	0.517574
48	6	0	5.095626	4.821015	0.846894
49	6	0	5.027266	1.453769	-3.637349
50	6	0	5.985646	1.262473	-4.671092
51	6	0	7.052765	0.444215	-4.460535
52	6	0	7.233991	-0.222064	-3.208306
53	6	0	6.302478	0.011993	-2.142722
54	6	0	5.181796	0.857103	-2.421164
55	6	0	8.293874	-1.103978	-3.013138
56	6	0	8.418514	-1.826901	-1.831076
57	6	0	7.488789	-1.605772	-0.760709
58	6	0	6.483626	-0.621006	-0.892247
59	6	0	9.453564	-2.804110	-1.675894
60	6	0	9.538366	-3.572224	-0.556525
61	6	0	8.576175	-3.412313	0.480890
62	6	0	7.601815	-2.465616	0.383877
63	6	0	-8.079066	4.622200	-1.605070
64	6	0	-7.058238	3.795269	-2.152593
65	6	0	-6.628507	2.684103	-1.491111
66	6	0	-7.178570	2.301940	-0.220029
67	6	0	-8.197061	3.150315	0.328591
68	6	0	-8.626838	4.304143	-0.401191
69	6	0	-6.754337	1.152423	0.492396
70	6	0	-7.305585	0.887156	1.765132
71	6	0	-8.325113	1.743767	2.301024
72	6	0	-8.754663	2.845021	1.566680
73	6	0	-6.868813	-0.201553	2.584274
74	6	0	-7.417482	-0.437601	3.809051
75	6	0	-8.448411	0.398743	4.320743
76	6	0	-8.882441	1.459562	3.587277
77	6	0	-4.076981	-3.314749	1.625872
78	6	0	-4.606183	-4.612018	1.383261
79	6	0	-5.676119	-4.750539	0.556010
80	6	0	-6.276947	-3.615545	-0.076482
81	6	0	-5.735592	-2.303031	0.139086
82	6	0	-4.606856	-2.214449	1.022348
83	6	0	-7.391886	-3.779135	-0.891536
84	6	0	-7.989330	-2.694244	-1.524517
85	6	0	-7.453568	-1.376896	-1.331679
86	6	0	-6.339015	-1.178582	-0.483901
87	6	0	-9.118511	-2.883552	-2.381630
88	6	0	-9.679688	-1.838026	-3.047751
89	6	0	-9.126752	-0.536400	-2.900457
90	6	0	-8.060587	-0.317898	-2.079298
91	14	0	0.085292	-2.667522	2.495833
92	6	0	1.727354	-3.129940	3.284159
93	6	0	-0.626516	-4.177711	1.622251
94	6	0	-1.110789	-2.009881	3.792424
95	14	0	0.693583	1.957902	-2.731411
96	6	0	1.038584	0.866779	-4.222033
97	6	0	1.697202	3.547528	-2.829752
98	6	0	-1.133902	2.370862	-2.608215
99	1	0	-0.610426	-1.625596	-1.836132
100	1	0	-1.637355	-2.376934	-3.963731
101	1	0	-3.987112	-1.745206	-4.486059
102	1	0	-5.297612	-0.430565	-2.867403
103	1	0	-5.090983	3.136323	0.410994
104	1	0	-3.630142	4.641665	1.634892
105	1	0	-1.300659	3.955982	2.199906
106	1	0	-0.483313	1.735227	1.467249
107	1	0	0.689602	0.476876	2.943836
108	1	0	1.918996	1.283564	4.923569
109	1	0	4.387893	0.983448	5.052046
110	1	0	5.600996	-0.000937	3.142306
111	1	0	5.594704	-3.061969	-0.553898
112	1	0	4.357712	-4.813211	-1.684667

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
113	1	0	1.861728	-4.743954	-1.748839
114	1	0	0.681290	-2.895930	-0.620068
115	1	0	11.091817	1.769047	2.817099
116	1	0	10.056159	-0.503404	2.626784
117	1	0	7.809662	-0.760971	1.771560
118	1	0	9.755937	3.760117	2.226817
119	1	0	7.665914	4.754387	1.531705
120	1	0	3.513497	1.387463	0.073225
121	1	0	2.165389	3.355749	0.003694
122	1	0	3.161011	5.619753	0.454686
123	1	0	5.552457	5.784924	1.053134
124	1	0	4.156566	2.073893	-3.825006
125	1	0	5.850957	1.756012	-5.628131
126	1	0	7.781239	0.266929	-5.246715
127	1	0	4.420759	0.988985	-1.666018
128	1	0	9.014420	-1.258968	-3.812435
129	1	0	10.162440	-2.930524	-2.489362
130	1	0	10.319881	-4.318241	-0.456994
131	1	0	8.615893	-4.056650	1.353338
132	1	0	6.860387	-2.381423	1.171812
133	1	0	-8.410434	5.501549	-2.147470
134	1	0	-6.613412	4.055789	-3.107646
135	1	0	-5.838960	2.080269	-1.922819
136	1	0	-9.403314	4.925367	0.036352
137	1	0	-9.533032	3.486346	1.973025
138	1	0	-6.076213	-0.843888	2.232113
139	1	0	-7.059101	-1.271281	4.404321
140	1	0	-8.875865	0.192452	5.296643
141	1	0	-9.658713	2.117931	3.966925
142	1	0	-3.236917	-3.199098	2.301724
143	1	0	-4.157684	-5.476743	1.861327
144	1	0	-6.104441	-5.729492	0.359965
145	1	0	-4.167506	-1.247771	1.231738
146	1	0	-7.800127	-4.775585	-1.042121
147	1	0	-9.511648	-3.890004	-2.494969
148	1	0	-10.533897	-1.992790	-3.698876
149	1	0	-9.555073	0.294393	-3.452193
150	1	0	-7.658036	0.680269	-2.007396
151	1	0	2.133364	-2.319384	3.895074
152	1	0	1.588002	-4.007241	3.925577
153	1	0	2.471074	-3.385890	2.523355
154	1	0	0.157853	-4.697789	1.064027
155	1	0	-1.048912	-4.884946	2.344612
156	1	0	-1.417015	-3.899723	0.918493
157	1	0	-0.619629	-1.250555	4.409384
158	1	0	-1.464424	-2.804696	4.457202
159	1	0	-1.982477	-1.540522	3.324615
160	1	0	0.802473	1.388110	-5.155700
161	1	0	2.089587	0.562882	-4.253141
162	1	0	0.424952	-0.038350	-4.174949
163	1	0	1.607089	3.986875	-3.829153
164	1	0	1.334245	4.286788	-2.108938
165	1	0	2.757480	3.381263	-2.619019
166	1	0	-1.748562	1.468830	-2.677504
167	1	0	-1.424432	3.044388	-3.421915
168	1	0	-1.367324	2.862456	-1.658434

Table S5. Cartesian Coordinates of **1**'' dimer (allene-allene) ($C_{96}H_{70}Si_2$, total 168 atoms) (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomi Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.744103	1.373763	-1.311851
2	6	0	-3.764106	2.379399	-1.246922
3	6	0	-2.364811	1.930075	-1.080209
4	6	0	-2.045320	0.644787	-1.751672
5	6	0	-3.037202	-0.352154	-1.825993
6	6	0	-4.316356	-0.039300	-1.103380
7	6	0	-4.930063	-0.842051	-0.190442
8	6	0	-0.801401	0.462046	-2.354265
9	6	0	-0.513203	-0.705516	-3.042970
10	6	0	-1.495474	-1.680486	-3.155789
11	6	0	-2.740426	-1.503467	-2.561692
12	6	0	-6.077134	1.731532	-1.510173
13	6	0	-6.439653	3.069048	-1.607946
14	6	0	-5.470289	4.064273	-1.504475
15	6	0	-4.136009	3.719660	-1.329902
16	6	0	-1.416388	2.566782	-0.421816
17	6	0	-0.341068	3.057913	0.138881
18	6	0	5.121322	1.938062	-0.286023
19	6	0	4.170379	2.967654	-0.453296
20	6	0	2.944700	2.705439	-1.239550
21	6	0	3.074704	1.703089	-2.317814
22	6	0	3.990683	0.660722	-2.115481
23	6	0	4.753418	0.595151	-0.838693
24	6	0	4.927883	-0.591376	-0.198831
25	6	0	2.334236	1.767304	-3.498145
26	6	0	2.504012	0.805649	-4.484865
27	6	0	3.433801	-0.217007	-4.302879
28	6	0	4.173813	-0.283395	-3.129980
29	6	0	6.285294	2.242107	0.429639
30	6	0	6.489029	3.500622	0.981468
31	6	0	5.533273	4.498761	0.831505
32	6	0	4.384246	4.229083	0.104492
33	6	0	1.795660	3.297760	-0.982857
34	6	0	0.621696	3.818879	-0.745736
35	6	0	-9.898173	-1.989330	1.119507
36	6	0	-8.963732	-2.511168	0.185288
37	6	0	-7.713358	-1.980427	0.071751
38	6	0	-7.268305	-0.885238	0.878003
39	6	0	-8.232186	-0.354465	1.803977
40	6	0	-9.534925	-0.937619	1.901188
41	6	0	-5.976101	-0.306457	0.774224
42	6	0	-5.663249	0.797692	1.616348
43	6	0	-6.649448	1.331604	2.513308
44	6	0	-7.904744	0.742383	2.590358
45	6	0	-4.386536	1.445830	1.636777
46	6	0	-4.131232	2.532118	2.416562
47	6	0	-5.127639	3.069630	3.273864
48	6	0	-6.347073	2.471127	3.324582
49	6	0	-2.394841	-2.063769	3.071277
50	6	0	-1.884753	-3.387747	3.156859
51	6	0	-2.269596	-4.317654	2.240467
52	6	0	-3.164110	-3.981378	1.176458
53	6	0	-3.663256	-2.639927	1.066786
54	6	0	-3.251147	-1.708185	2.072000
55	6	0	-3.539025	-4.934466	0.233007
56	6	0	-4.358540	-4.602013	-0.840026
57	6	0	-4.815453	-3.250864	-0.992794
58	6	0	-4.478336	-2.273969	-0.029208
59	6	0	-4.723182	-5.586996	-1.813817
60	6	0	-5.479802	-5.263780	-2.896419
61	6	0	-5.909662	-3.917913	-3.077755
62	6	0	-5.587597	-2.955564	-2.169453
63	6	0	-0.125637	-1.816443	0.148399
64	6	0	0.620091	-0.608495	0.212348
65	6	0	1.962224	-0.589858	-0.011116
66	6	0	2.694421	-1.782689	-0.322757
67	6	0	1.926399	-2.995647	-0.409905
68	6	0	0.516245	-2.972832	-0.157815
69	6	0	4.098062	-1.817146	-0.528338
70	6	0	4.699711	-3.035151	-0.926375
71	6	0	3.919154	-4.235524	-1.014547
72	6	0	2.557413	-4.191094	-0.732217
73	6	0	6.072594	-3.131730	-1.313358
74	6	0	6.634647	-4.313462	-1.696704
75	6	0	5.865478	-5.508231	-1.726744
76	6	0	4.544331	-5.461710	-1.401438
77	6	0	9.217771	-0.580654	-0.717790
78	6	0	10.081825	-0.993968	0.335630
79	6	0	9.558866	-1.295128	1.554717
80	6	0	8.151020	-1.211522	1.800947
81	6	0	7.266783	-0.840945	0.733450
82	6	0	7.870519	-0.511053	-0.527532
83	6	0	7.633828	-1.472160	3.066385
84	6	0	6.274028	-1.335050	3.331505
85	6	0	5.379078	-0.974653	2.269848
86	6	0	5.871729	-0.778561	0.961090
87	6	0	5.756950	-1.537488	4.649683
88	6	0	4.433568	-1.365844	4.918688
89	6	0	3.546855	-0.972282	3.878013
90	6	0	4.002417	-0.786827	2.607499
91	14	0	0.024755	2.857314	1.996430
92	6	0	-0.883383	1.352825	2.685654
93	6	0	1.866673	2.644591	2.281396
94	6	0	-0.546103	4.452877	2.821748
95	14	0	0.076122	5.389043	-1.649626
96	6	0	-0.900856	4.868879	-3.171037
97	6	0	1.611861	6.344775	-2.158725
98	6	0	-0.993043	6.393424	-0.472244
99	1	0	-0.053811	1.244324	-2.271294
100	1	0	0.468882	-0.842467	-3.483609
101	1	0	-1.300934	-2.592122	-3.711483
102	1	0	-3.484137	-2.270190	-2.701731
103	1	0	-6.833548	0.955095	-1.564021
104	1	0	-7.480506	3.335660	-1.759031
105	1	0	-5.753569	5.109736	-1.571545
106	1	0	-3.373421	4.489630	-1.262304
107	1	0	1.629462	2.582063	-3.637030
108	1	0	1.923964	0.862105	-5.400351
109	1	0	3.587923	-0.959436	-5.078974
110	1	0	4.900419	-1.077257	-2.995568
111	1	0	7.056959	1.500231	0.554686
112	1	0	7.406454	3.697457	1.526519

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
113	1	0	5.690683	5.483771	1.258837
114	1	0	3.635311	4.999955	-0.051786
115	1	0	-10.888896	-2.424531	1.200256
116	1	0	-9.245746	-3.344961	-0.449981
117	1	0	-7.045499	-2.412355	-0.650063
118	1	0	-10.230602	-0.511014	2.618367
119	1	0	-8.645179	1.149586	3.274572
120	1	0	-3.593574	1.068427	1.008592
121	1	0	-3.147970	2.988218	2.380151
122	1	0	-4.907822	3.938032	3.886158
123	1	0	-7.125232	2.847566	3.982550
124	1	0	-2.095107	-1.321916	3.804482
125	1	0	-1.193621	-3.650702	3.950716
126	1	0	-1.895121	-5.336099	2.292572
127	1	0	-3.621490	-0.696427	2.040296
128	1	0	-3.173067	-5.953797	0.329672
129	1	0	-4.372000	-6.604517	-1.667037
130	1	0	-5.747833	-6.018715	-3.628095
131	1	0	-6.490669	-3.654954	-3.955818
132	1	0	-5.896059	-1.930605	-2.343970
133	1	0	-1.196697	-1.799881	0.312648
134	1	0	0.102582	0.322548	0.405681
135	1	0	2.478881	0.358624	0.033515
136	1	0	-0.035753	-3.905924	-0.228714
137	1	0	1.971491	-5.105831	-0.780925
138	1	0	6.678931	-2.240321	-1.326991
139	1	0	7.679978	-4.338543	-1.988046
140	1	0	6.328536	-6.443617	-2.023952
141	1	0	3.930909	-6.357659	-1.440897
142	1	0	9.638796	-0.311861	-1.681329
143	1	0	11.151494	-1.053865	0.163853
144	1	0	10.203957	-1.595945	2.375492
145	1	0	7.233528	-0.171168	-1.336807
146	1	0	8.307743	-1.764048	3.868196
147	1	0	6.451317	-1.821878	5.435331
148	1	0	4.053004	-1.516311	5.923873
149	1	0	2.495790	-0.812708	4.097743
150	1	0	3.310959	-0.473945	1.840453
151	1	0	-0.176736	0.533495	2.850077
152	1	0	-1.371180	1.581793	3.638275
153	1	0	-1.651658	0.979606	2.004018
154	1	0	2.058710	2.532942	3.354429
155	1	0	2.450525	3.496003	1.922594
156	1	0	2.251466	1.747778	1.787695
157	1	0	0.027785	5.302944	2.438321
158	1	0	-0.396122	4.409787	3.905583
159	1	0	-1.604106	4.658422	2.631732
160	1	0	-0.245468	4.364706	-3.888895
161	1	0	-1.705888	4.173419	-2.916637
162	1	0	-1.344208	5.735086	-3.673486
163	1	0	2.309781	5.697429	-2.699486
164	1	0	1.355903	7.185398	-2.811491
165	1	0	2.136165	6.745626	-1.285476
166	1	0	-0.397619	6.787952	0.357276
167	1	0	-1.787631	5.775156	-0.042706
168	1	0	-1.460055	7.241068	-0.983826