Electronic Supporting Information (ESI) for

Effect of Conjugation and Aromaticity of 3,6 Di-substituted Carbazole On Triplet Energy

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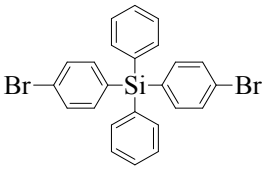
Contents

I. General methods

Proton and carbon nuclear magnetic resonance spectroscopy (^{1}H NMR and ^{13}C NMR spectra) were obtained on a Bruker AVANCE III 400 MHz FT-NMR spectrometer using deuterated chloroformas the solvent with tetramethylsilane (TMS) as internal standard. Matrix-assisted laser desorption/ionization time of flight (MALDI-TOF) measurements were carried out with a Bruker Microflex series spectrometer in order to measure the molecular masses. 2,5-dihydroxybenzoic acid (DHB) was used as matrix.

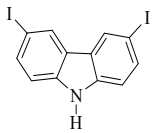
II. Synthesis procedures

Bis(4-bromophenyl)diphenylsilane, (1), Known compound.



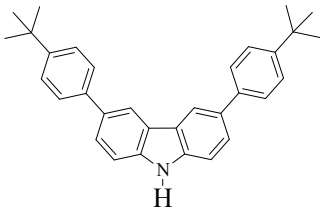
Compound **1** was prepared according to modified procedure from the literature.[20] 1,4-Dibromobenzene (4.20 g, 17.8 mmol) was dissolved in 15mL dry THF under nitrogen atmosphere. The solution was cooled to -78 °C. 9.6 mL of n-BuLi (2.0 M in cyclohexane) was added dropwise and stir for 1 h. Dichlorodiphenylsilane (1.68 mL, 8 mmol) was added slowly at -78 °C. The mixture was stirred overnight while allowing the temperature to rise to room temperature. The reaction was then quenched with water and extracted with chloroform. The organic layer was dried over anhydrous sodium sulfate. After the solvent was evaporated, the crude product was purified by recrystallization from ethanol to afford white solid (2.54 g, 64.3 %). **Melting point = 160-162 °C**. ^{1}HNMR ($CDCl_3$, 400 MHz): δ (ppm) = 7.57-7.52 (m, 8H), 7.48-7.38 (m, 10H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) = 137.93, 136.32, 134.98, 133.36, 131.14, 129.88, 128.02, 124.82.

3,6-Diiodocarbazole, (2), Known compound.



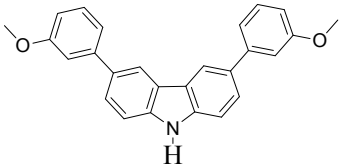
Carbazole (8.36 g, 50 mmol) was dissolved in boiling acetic acid (200 mL). To the solution, potassium iodide (10.8 g, 50 mmol) was added. The solution was cooled and potassium iodate (21.5 g, 50 mmol) was added. Solution was refluxed at 80 ºC for 1 h. The solution was decanted from undissolved potassium iodate and it was allowed to cool to room temperature. The crude product obtained was filtered and recrystallized from dichloromethane to give brown solid (13.97 g, 66.7%). **Melting point = 208 - 210 °C.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) = 8.36 (s, 2H), 8.14 (br, s, 1H), 7.71 (dd, 2H, J=8.50, 1.65 Hz), 7.24 (d, 2H, J=8.56 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) = 138.53, 134.83, 129.40, 124.58, 112.70, 82.44.

3,6-bis(4-(tert-butyl)phenyl)-9H-carbazole, (3), Known compound.



Compound **3** was prepared using Suzuki coupling reaction. 4-*Tert*-butylphenylboronic acid (1.1 g, 6.2 mmol) and compound **4** (1.25 g, 3 mmol) were dissolved in 25 ml toluene in a round bottom flask under nitrogen. A solution of potassium carbonate (2M, 1.7 ml) was added to the solution. tetrakis(triphenyl-phosphine)palladium(0) (0.14 g, 0.12 mmol) was added. The reaction mixture was reflux for 24 h under nitrogen. After cooling to room temperature, the reaction mixture was evaporated to remove solvent and extracted with chloroform and water. The organic layer was removed under reduced pressure, and the residue was subjected to a column chromatography using hexane/ethyl acetate as the eluent to obtain white solid (yield 85.6%, 1.11 g). **Melting point , decompose > 200 °C** ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.34 (d, *J*=1.71 Hz, 2H), 8.13 (s, 1H), 7.66 – 7.73 (m, 6H), 7.49 – 7.56 (m, 6H), 1.42 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 149.46, 139.30, 139.16, 132.99, 126.92, 125.72, 125.52, 124.04, 118.71, 110.85, 34.51, 31.44. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{32}H_{33}N$ 431.2613; Found 431.165.

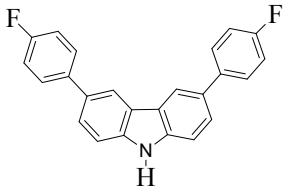
3,6-bis(3-methoxyphenyl)-9H-carbazole (4), known compound.



Compound **4** was prepared using Suzuki coupling reaction. 3-Methoxyphenylboronic acid (3.17 g, 20.9 mmol) and compound **2** (3.98 g, 9.49 mmol) were dissolved in 40 ml toluene in a round bottom flask under nitrogen. A solution of potassium carbonate (2M, 10 ml) was added to the solution. tetrakis(triphenyl-phosphine)palladium(0) (0.47 g, 0.41 mmol) was added. The reaction mixture was reflux for 24 h under nitrogen. After cooling to room temperature, the reaction mixture was evaporated to remove solvent and extracted with chloroform and water. The organic layer was removed under

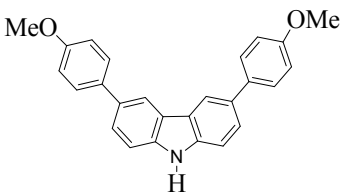
reduced pressure, and the residue was subjected to a column chromatography using hexane/ethyl acetate as the eluent to obtain white solid **6** (yield 17.4%, 0.63 g). **Melting point , decompose > 200 °C.** ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.36 (d, *J*=1.83 Hz, 2H), 8.17 (s, 1H), 7.72 (dd, *J*=8.24, 1.83 Hz, 2H), 7.53, (d, *J*=8.24 Hz, 2H), 7.38 – 7.48 (m, 2H), 7.31 – 7.37 (m, 2H), 7.24 – 7.31 (m, 2H), 6.87 – 7.00 (m, 2H), 3.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 160.07, 143.63, 139.58, 133.12, 129.83, 125.75, 124.05, 119.93, 119.04, 113.06, 112.09, 110.99, 55.44. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{26}H_{21}NO_2$ 379.1572; Found 378.868.

3,6-bis(4-fluorophenyl)-9H-carbazole, (5), known compound.



Compound **5** was prepared using Suzuki coupling reaction. 4-fluorophenylboronic acid (0.93 g, 6.7 mmol) and compound **2** (1.27 g, 3.03 mmol) were dissolved in 24 ml toluene in a round bottom flask under nitrogen. A solution of potassium carbonate (2M, 6 ml) was added to the solution. tetrakis(triphenyl-phosphine)palladium(0) (0.13 g, 0.11 mmol) was added. The reaction mixture was reflux for 24 h under nitrogen. After cooling to room temperature, the reaction mixture was evaporated to remove solvent and extracted with chloroform and water. The organic layer was removed under reduced pressure, and the residue was subjected to a column chromatography using hexane/ethyl acetate as the eluent to obtain white solid **7** (yield 30.4%, 0.33 g). **Melting point , decompose > 200 °C.** ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.29 (s, 2H), 8.17 (br. s., 1H), 7.62 – 7.72 (m, 6H), 7.53 (d, *J*=8.44 Hz, 2H), 7.19 (t, *J*=8.68 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 163.34, 160.90, 139.36, 138.15, 132.32, 128.80, 128.71, 125.58, 123.97, 118.79, 115.69, 115.48, 111.01. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{24}H_{15}F_2N$ 355.1173; Found 355.779.

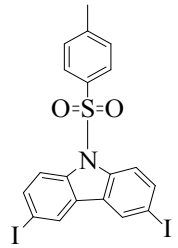
3,6-bis(4-methoxyphenyl)-9H-carbazole, (6), known compound.



Compound **6** was prepared using Suzuki coupling reaction. 4-methoxyphenylboronic acid (1.31 g, 8.6 mmol) and compound **2** (1.51 g, 3.6 mmol) were dissolved in 30 ml toluene in a round bottom flask

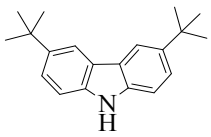
under nitrogen. A solution of potassium carbonate (2M, 3.6 ml) was added to the solution. tetrakis(triphenyl-phosphine)palladium(0) (0.17 g, 0.14 mmol) was added. The reaction mixture was reflux for 24 h under nitrogen. After cooling to room temperature, the reaction mixture was evaporated to remove solvent and extracted with chloroform and water. The organic layer was removed under reduced pressure, and the residue was subjected to a column chromatography using hexane/ethyl acetate as the eluent to obtain white solid **8** (yield 43.5%, 1.13 g). **Melting point = 198-200 °C** ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.30 (s, 2H), 8.10 (br. s., 1H), 7.60 – 7.78 (m, 6H), 7.50 (d, *J*=8.25 Hz, 2H), 6.97 – 7.09 (m, 4H), 3.90 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 158.65, 139.10, 134.74, 132.82, 128.27, 125.32, 124.05, 118.43, 114.24, 110.85, 55.40. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{26}H_{21}NO_2$ 379.1572; Found 379.511.

3,6-diiodo-9-tosyl-9H-carbazole, (8), known compound.



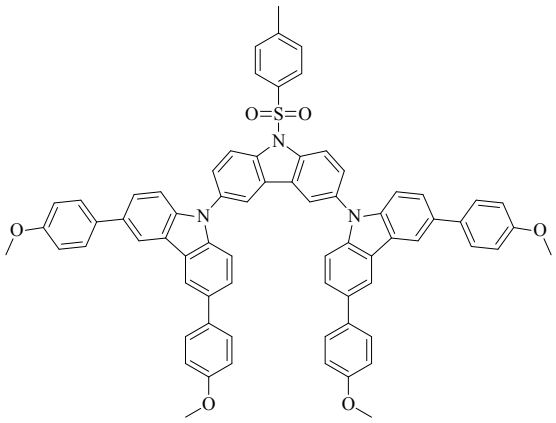
Compound **8** was prepared according to procedure from the literature. [2] To a solution of compound **2** (2.01 g, 4.8 mmol) in *N,N*-dimethylformamide (20 ml) was added sodium hydride (0.84 g, 35 mmol) at 0 ºC, and stirred for 10 mins. Subsequently, *p*-toluenesulfonyl chloride (2.9 g, 15.8 mmol) was added to this mixture and stirred at 0ºC for 4 h. the mixture was diluted with water and the precipitates were filtered. The crude product was recrystallized from dichloromethane to afford compound **8** (3.0 g, 62.4 %) as white solid. **Melting point , decompose > 250 °C** ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.20 (d, *J*=1.59 Hz, 2H), 8.10 (d, *J*=8.80 Hz, 2H), 7.80 (dd, *J*=8.74 Hz, 2H), 7.67 (d, *J*=8.44 Hz, 2H), 7.16 (d, *J*=8.07 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 145.49, 137.82, 136.55, 134.43, 129.90, 129.17, 127.19, 126.46, 116.98, 87.96, 21.56. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{19}H_{13}I_2NO_2S$ 572.8756; Found 572.885.

3,6-di-tert-butyl-9H-carbazole, (7), known compound.



In ice bath of 0 ºC, carbazole (20 mmol) was suspended in 100 ml chloroform under nitrogen. $AlCl_3$ (2.67 g, 20 mmol) was added in portions. *Tert*-butyl chloride (5.3 ml, 24 mmol) was then added drop wise. Then the mixture was stirred for 12 h. The reaction was quenched by ice water, and extracted by chloroform. The organic layer was dried with anhydrous Na_2SO_4 and the solvent was removed under reduced pressure to obtain white solid. Yield: 82.6%. **Melting point = 230-233 °C.** ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.10 (s, 2H), 7.88 (br. s., 1H), 7.49 (d, *J*=8.44 Hz, 2H), 7.36 (d, *J*=8.44 Hz, 2H), 1.48 (s, 18 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 142.24, 138.02, 123.52, 123.33, 116.18, 109.98, 34.69, 32.04. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{20}H_{25}N$ 279.1987; Found 279.235.

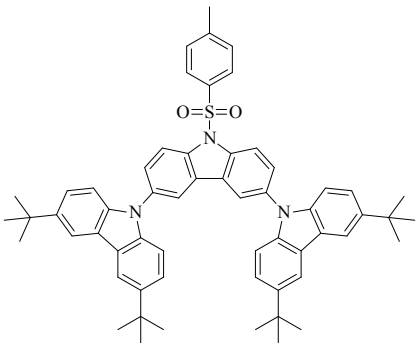
3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'-tosyl-9'H-9,3':6',9''-tercarbazole (9), New compound.



Compound **9** was prepared according to procedure from the literature. [1] A solution of compound **8** (1.16 g, 2.03 mmol) and compound **6** (1.68 g, 4.42 mmol) in *N,N*-dimethylacetamide (10 ml) was prepared. Copper oxide (0.59 g, 4.1 mmol) was added to the solution. The mixture was then refluxed for 48 h and cooled to room temperature. After cooling to room temperature, the reaction mixture was evaporated under reduced pressure to remove solvent and extracted with chloroform and water. The organic layer was evaporated under reduced pressure, and the residue was subjected to a column chromatography using hexane/ethyl acetate as the eluent to obtain white solid with (yield 49.1 %, 1.07 g). **Melting point , decompose > 300 °C**. ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.66 (d, *J*=8.80 Hz, 2H), 8.36 (d, *J*=1.35 Hz, 4H), 8.18 (d, *J*=1.83 Hz, 2H), 7.98 (d, *J*=8.44 Hz, 2H), 7.83 (dd, *J*=8.93, 2.08 Hz, 2H), 7.66 (d, *J*=8.80 Hz, 8H), 7.63 (dd, *J*=8.25, 1.83 Hz, 4H), 7.46 (d, *J*=8.56 Hz, 4H), 7.35 (d, *J*=8.07 Hz, 2H), 7.04 (d, *J*=8.80 Hz, 8H), 3.90 (s, 12H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 158.75, 140.74, 137.71, 135.05, 134.51, 134.08, 133.51, 130.17, 128.35, 128.29, 127.06, 126.82, 125.49, 125.46, 124.09, 118.88, 118.50, 116.47, 114.28, 109.87, 55.41, 21.73. HRMS (MALDI-TOF) m/z: [M]+ Calcd for

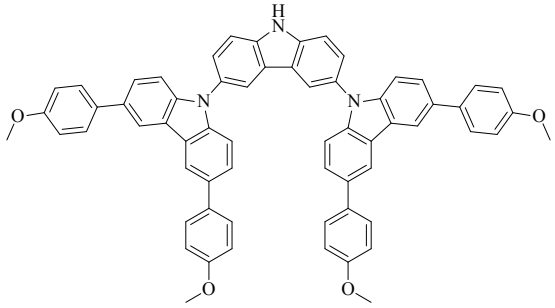
$C_{71}H_{53}N_3O_6S$ 1075.3655; Found 1075.875.

3,3'',6,6''-tetra-tert-butyl-9'-tosyl-9'H-9,3':6',9''-tercarbazole (10), Known compound.



Compound **10** was prepared according to procedure from the literature. [1] A solution of compound **8** (1.44 g, 2.51 mmol) and compound **7** (1.54 g, 5.5 mmol) in *N,N*-dimethylacetamide (10 ml) was prepared. Copper oxide (0.73 g, 5.1 mmol) was added to the solution. The mixture was then refluxed for 48 h and cooled to room temperature. After cooling to room temperature, the reaction mixture was evaporated under reduced pressure to remove solvent and extracted with chloroform and water. The organic layer was evaporated under reduced pressure, and the residue was subjected to a column chromatography using hexane/ethyl acetate as the eluent to obtain white solid with yield of 65.5% (1.44 g). **Melting point = decompose > 300 °C.** ^{1}H NMR (600M Hz, $CDCl_3$) δ [ppm]: 8.59 (d, *J*=8.80 Hz, 2H), 8.16 (d, *J*=1.65 Hz, 4H), 8.07 (d, *J*=2.02 Hz, 2H), 7.94 (d, *J*=8.25 Hz, 2H), 7.75 (dd, *J*=8.80, 2.20 Hz, 2H), 7.47 (dd, *J*=8.62, 2.02 Hz, 4H), 7.35 (d, *J*=8.25 Hz, 4H), 7.32 (d, *J*=8.25 Hz, 2H), 2.42 (s, 3H), 1.48 (s, 36H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 145.49, 143.02, 139.51, 137.38, 135.02, 134.54, 130.07, 127.09, 126.77, 123.70, 123.38, 118.50, 116.32, 108.97, 34.74, 32.00, 21.69. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{59}H_{61}N_3O_2S$ 875.4484; Found 875.756.

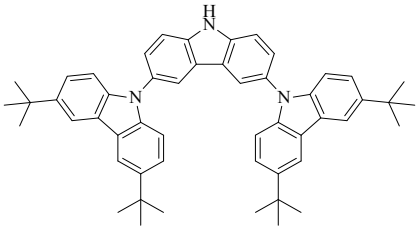
3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-9,3':6',9''-tercarbazole (11), New compound.



Compound **11** was prepared according to the procedure from the literature. [1] To a solution of compound **9** (1.04 g, 0.965 mmol) in 9 ml tetrahydrofuran were added dimethyl sulfoxide (2.45 ml) and water (1.0

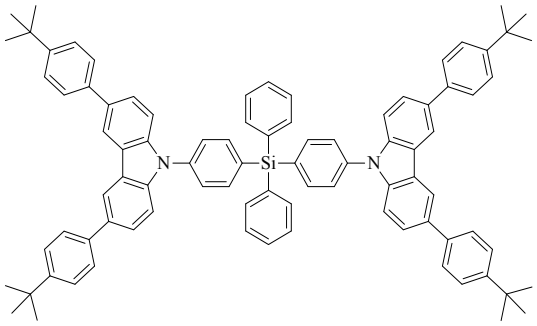
ml), and the mixture was stirred for 10 mins. Subsequently, potassium hydroxide (1.36 g, 0.024 mol) was added to this mixture, and the reaction mixture was refluxed for 4 hours, cooled to room temperature and diluted with water. After neutralization with HCl solution, the crude product was filtered and recrystallized from dichloromethane-hexane (1:1) to give compound **11** as white solid (yield 99.4 %, 0.884 g). **Melting point , decompose > 300 °C,** ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.62 (br. s., 1H), 8.25 – 8.44 (m, 6H), 7.40 – 7.82 (m, 20H), 7.04 (d, *J*=8.80 Hz, 8H), 3.89 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 158.66, 146.60, 141.42, 139.33, 134.73, 130.06, 128.30, 126.11, 125.35, 123.82, 120.44, 119.70, 118.41, 114.25, 112.13, 110.03, 55.40. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{64}H_{47}N_3O_4$ 921.3567; Found 921.795.

3,3'',6,6''-tetra-tert-butyl-9'H-9,3':6',9''-tercarbazole (12), Known compound.



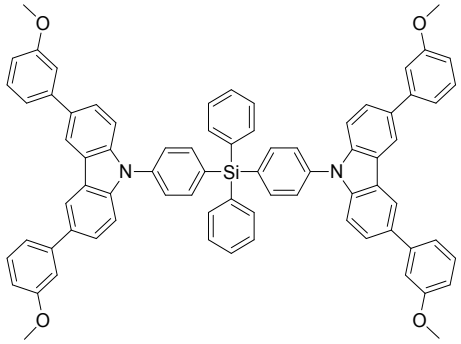
Compound **12** was prepared according to the procedure from the literature. [1] To a solution of compound **10** (1.39 g, 1.59 mmol) in 10 ml tetrahydrofuran were added dimethyl sulfoxide (4.8 ml) and water (1.6 ml), and the mixture was stirred for 10 mins. Subsequently, potassium hydroxide (1.59 g, 0.03 mol) was added to this mixture, and the reaction mixture was refluxed for 4 hours, cooled to room temperature and diluted with water. After neutralization with HCl solution, the crude product was filtered and recrystallized from dichloromethane-hexane (1:1) to give compound **12** as white solid (yield 99.5%, 1.14 g). **Melting point , decompose > 300 °C.** ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.52 (br. s., 1H), 8.18 (d, *J*=1.65 Hz, 6H), 7.70 (d, *J*=8.16 Hz, 2H), 7.63 (dd, *J*=8.48, 1.88 Hz, 2H), 7.47 (dd, *J*=8.57, 1.65 Hz, 4H), 7.33 (d, *J*=8.07 Hz, 4H), 1.48 (s, 36H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 142.50, 140.19, 139.07, 125.97, 124.11, 123.54, 123.07, 119.43, 116.18, 111.84, 109.11, 102.16, 34.73, 32.05 HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{52}H_{55}N_3$ 721.4396; Found 721.654.

Bis(4-(3,6-bis(4-(tert-butyl)phenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane, P1, New compound.



Compound **1** (0.25 g, 0.51 mmol), carbazole **3** (0.48 g, 1.12 mmol), copper powder (0.13 g, 2.05 mmol), and 18-Crown-6 (0.013 g, 0.049 mmol) and K_2CO_3 (0.55 g, 4.0 mmol) were dissolved in 4 ml anhydrous *o*-dichlorobenzene under nitrogen atmosphere. The reaction mixture was refluxed for 72 h at 180 ºC. After cooling to room temperature, the mixture was diluted in dichloromethane and filtered through silica gel. The filtrate was evaporated under reduced pressure to give crude product, which purified through column chromatography to give white powdery product (yield 20.1 %, 0.123g). **Melting point , decompose > 300 °C.** ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm]: 8.41 (d, *J*=1.47 Hz, 4H), 7.95 (d, *J*=8.31 Hz, 4H), 7.46 – 7.80 (m, 38H), 1.42 (s, 36H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 149.63, 140.32, 139.26, 138.98, 137.99, 136.48, 133.71, 133.55, 133.23, 130.09, 128.24, 126.95, 126.11, 125.77, 125.61, 124.25, 118.71, 110.25, 34.52, 31.43. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{88}H_{82}N_2Si$ 1194.6247; Found 1195.097.

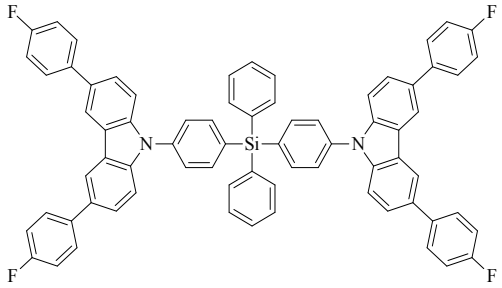
Bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane, P2. New compound.



Compound **1** (0.20 g, 0.404 mmol), carbazole **4** (0.33 g, 0.86 mmol), copper powder (0.10 g, 1.57 mmol), and 18-Crown-6 (0.011 g, 0.042 mmol) and K_2CO_3 (0.44 g, 3.2 mmol) were dissolved in 4 ml anhydrous *o*-dichlorobenzene under nitrogen atmosphere. The reaction mixture was refluxed for 72 h at 180 ºC. After cooling to room temperature, the mixture was diluted in dichloromethane and filtered through silica gel. The filtrate was evaporated under reduced pressure to give crude product, which purified through column chromatography to give white powdery product (yield 27.7%, 0.122 g). **Melting point ,**

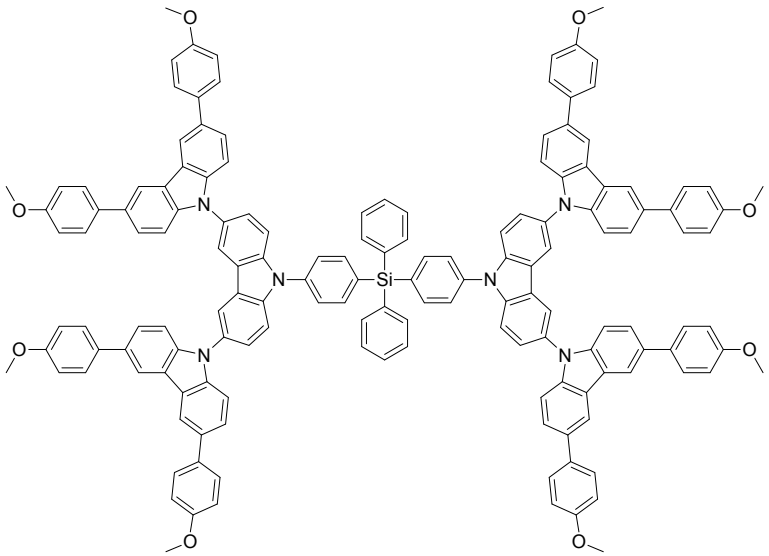
decompose > 300 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.43 (d, *J*=1.47 Hz, 4H), 7.96 (d, *J*=8.25 Hz, 4H), 7.79 (dd, *J*=7.98, 1.56 Hz, 4H), 7.75 (d, *J*=8.25 Hz, 4H), 7.72 (dd, *J*=8.53, 1.47 Hz, 4H), 7.64 (d, *J*=8.44, 4H), 7.51 – 7.60 (m, 6H), 7.40 – 7.46 (m, 4H), 7.35 (d, *J*=8.07 Hz, 4H), 7.29 – 7.31 (m, 4H), 6.94 (dd, *J*=8.25, 1.83 Hz, 4H), 3.94 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 160.06, 143.37, 140.58, 139.15, 138.03, 136.47, 133.76, 133.48, 133.39, 130.13, 129.81, 128.26, 126.13, 125.75, 124.20, 119.88, 118.97, 113.12, 112.07, 110.32, 55.39. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{76}H_{58}N_2O_4Si$ 1090.4166; Found 1091.070.

Bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl), P3. New compound.



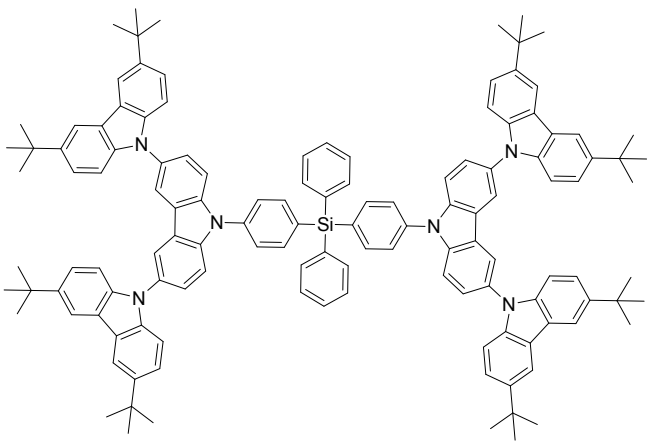
Compound **1** (0.20 g, 0.40 mmol), carbazole **5** (0.31 g, 0.87 mmol), copper powder (0.10 g, 1.57 mmol), and 18-Crown-6 (0.011 g, 0.042 mmol) and K_2CO_3 (0.44 g, 3.2 mmol) were dissolved in 4 ml anhydrous *o*-dichlorobenzene under nitrogen atmosphere. The reaction mixture was refluxed for 72 h at 180 ºC. After cooling to room temperature, the mixture was diluted in dichloromethane and filtered through silica gel. The filtrate was evaporated under reduced pressure to give crude product, which purified through column chromatography to give white powdery product (yield 16.9%, 0.072 g). **Melting point , decompose > 300 °C.** ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.33 – 8.38 (m, 4H), 7.97 (d, *J*=8.25 Hz, 2H), 7.41 – 7.84 (m, 32H), 7.15 – 7.24 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 163.03, 161.37, 140.81, 140.44, 139.11, 138.06, 137.95, 136.47, 133.02, 131.19, 130.02, 128.85, 128.81, 128.76, 128.28, 126.13, 125.65, 125.61, 124.19, 118.86, 118.81, 118.75, 115.72, 115.58, 115.55, 110.45, 110.41, 110.27. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{72}H_{46}F_4N_2Si$ 1042.3366; Found 1042.574.

Diphenylbis(4-(3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane, P4. New compound.



Compound **1** (0.22 g, 0.45 mmol), carbazole **11** (0.89 g, 0.97 mmol), copper powder (0.11 g, 1.73 mmol), and 18-Crown-6 (0.012 g, 0.045 mmol) and K_2CO_3 (0.49 g, 3.5 mmol) were dissolved in 4 ml anhydrous *o*-dichlorobenzene under nitrogen atmosphere. The reaction mixture was refluxed for 72 h at 180 ºC. After cooling to room temperature, the mixture was diluted in dichloromethane and filtered through silica gel. The filtrate was evaporated under reduced pressure to give crude product, which purified through column chromatography to give white powdery product (yield 43.3%, 0.41 g). **Melting point , decompose > 300 °C.** ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.31 – 8.43 (m, 12H), 7.60 – 7.88 (m, 44H), 7.58 – 7.40 (m, 14H), 7.04 (d, *J*=8.62 Hz, 16H), 3.90 (s, 24H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 158.67, 141.38, 141.35, 140.77, 136.45, 136.37, 134.73, 133.11, 131.39, 130.34, 130.31, 128.30, 128.25, 127.28, 126.14, 125.37, 123.98, 123.85, 119.59, 118.43, 114.25, 111.41, 110.03, 55.40. . HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{152}H_{110}N_6O_8Si$ 2174.8154; Found 2175.097.

Diphenylbis(4-(3,3'',6,6''-tetra-tert-butyl-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane, P5. New compound.



Compound **1** (0.28 g, 0.57 mmol), carbazole **10** (0.87 g, 1.20 mmol), copper powder (0.14 g, 2.20 mmol), and 18-Crown-6 (0.015 g, 0.057 mmol) and K_2CO_3 (0.61 g, 4.4 mmol) were dissolved in 4.5 ml anhydrous *o*-dichlorobenzene under nitrogen atmosphere. The reaction mixture was refluxed for 72 h at 180 ºC. After cooling to room temperature, the mixture was diluted in dichloromethane and filtered through silica gel. The filtrate was evaporated under reduced pressure to give crude product, which purified through column chromatography to give white powdery product (yield 17.9%, 0.178 g). **Melting point , decompose > 300 °C.** ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm]: 8.27 (d, *J*=1.83 Hz, 4H), 8.18 (d, *J*=1.65 Hz, 8H), 8.06 (d, *J*=8.25 Hz, 4H), 7.88 (d, *J*=8.25 Hz, 4H), 7.82 – 7.84 (m, 4H), 7.79 (d, *J*=8.80 Hz, 4H), 7.65 (dd, *J*=8.71, 1.93 Hz, 4H), 7.59 – 7.60 (m, 2H), 7.58 (d, *J*=7.34 Hz, 4H), 7.48 (dd, *J*=8.62, 1.83 Hz, 8H), 7.36 (d, *J*=8.26 Hz, 8H), 1.48 (s, 24H). ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]: 142.59, 140.11, 138.87, 138.25, 136.49, 133.27, 131.11, 130.25, 128.34, 128.10, 126.42, 125.99, 124.20, 123.57, 123.13, 119.34, 116.23, 111.27, 109.06, 34.73, 32.04. HRMS (MALDI-TOF) m/z: [M]+ Calcd for $C_{128}H_{126}N_6Si$ 1774.9813; Found 1776.242.

III. Copies of 1H and 13C NMR for synthesized compounds

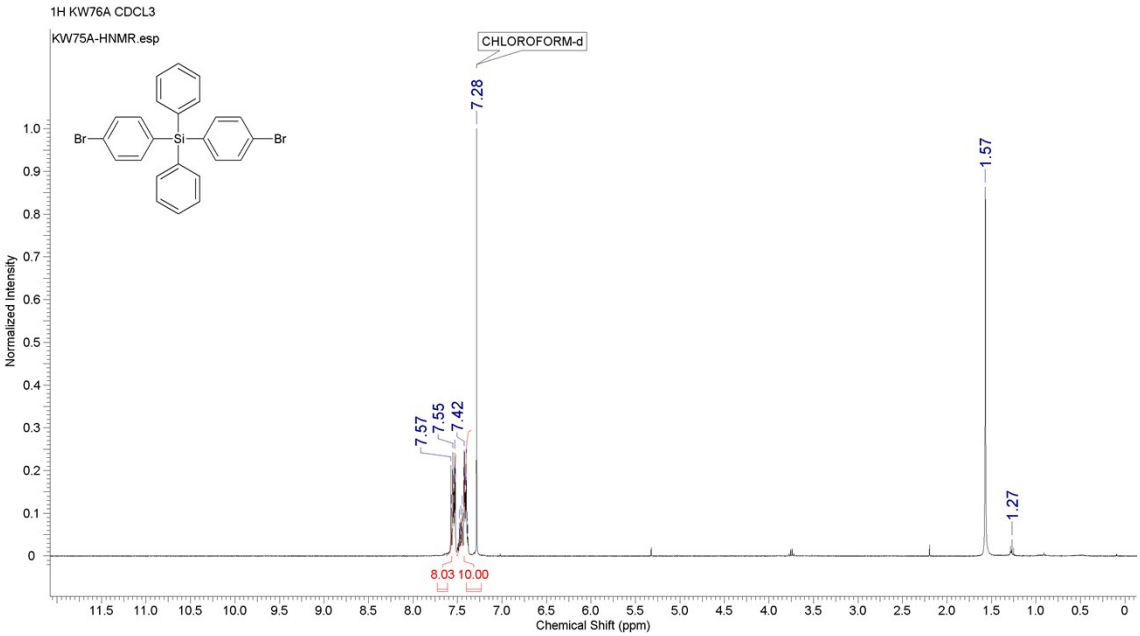


Fig. S1.[1]H NMR spectrum (400 MHz) for *bis(4-bromophenyl)diphenylsilane* (Compound **1**) in $CDCl_3$.

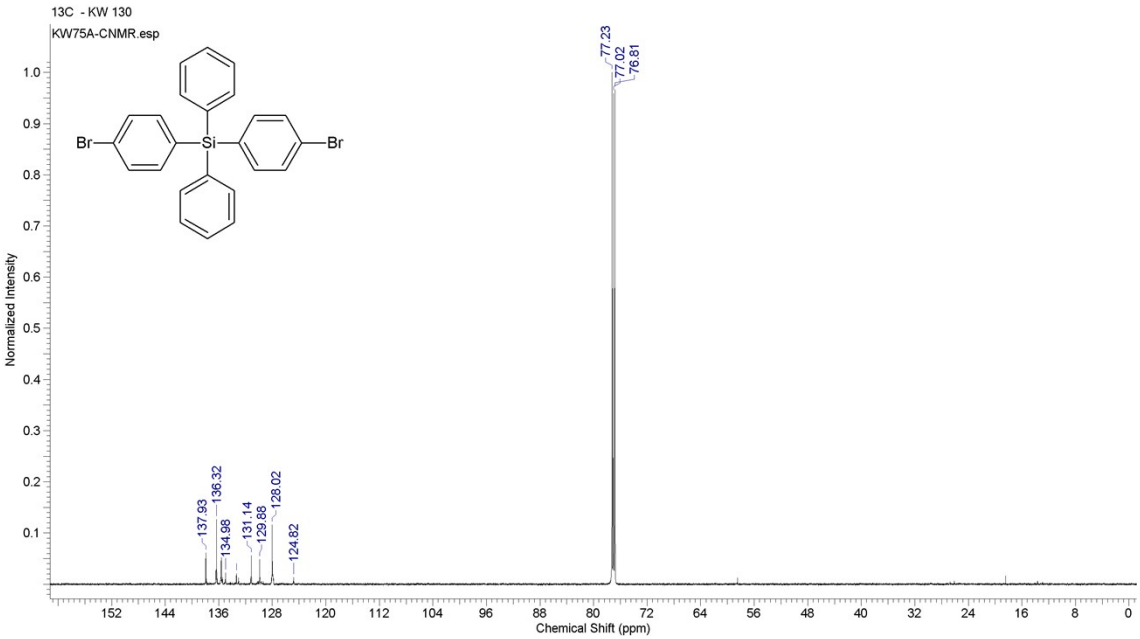


Fig. S2. [13]C NMR spectrum (100 MHz) for *bis(4-bromophenyl)diphenylsilane* (Compound **1**) in $CDCl_3$.

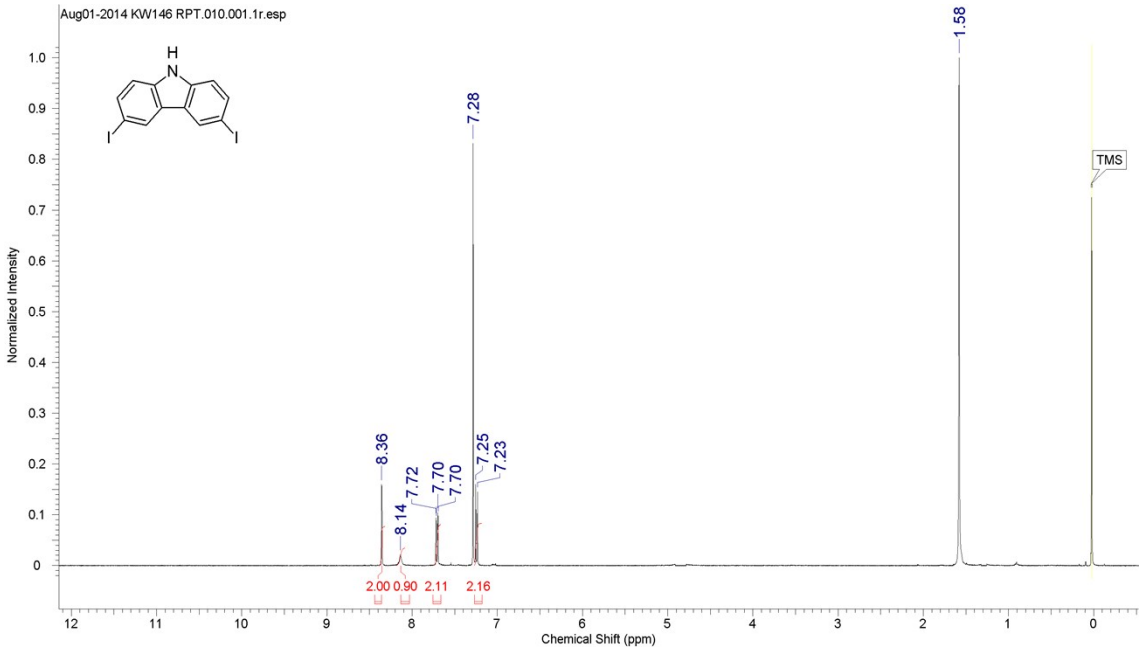


Fig. S3. ^{1}H NMR spectrum (400 MHz) for *3,6-diiodocarbazole* (Compound **2**) in $CDCl_3$.

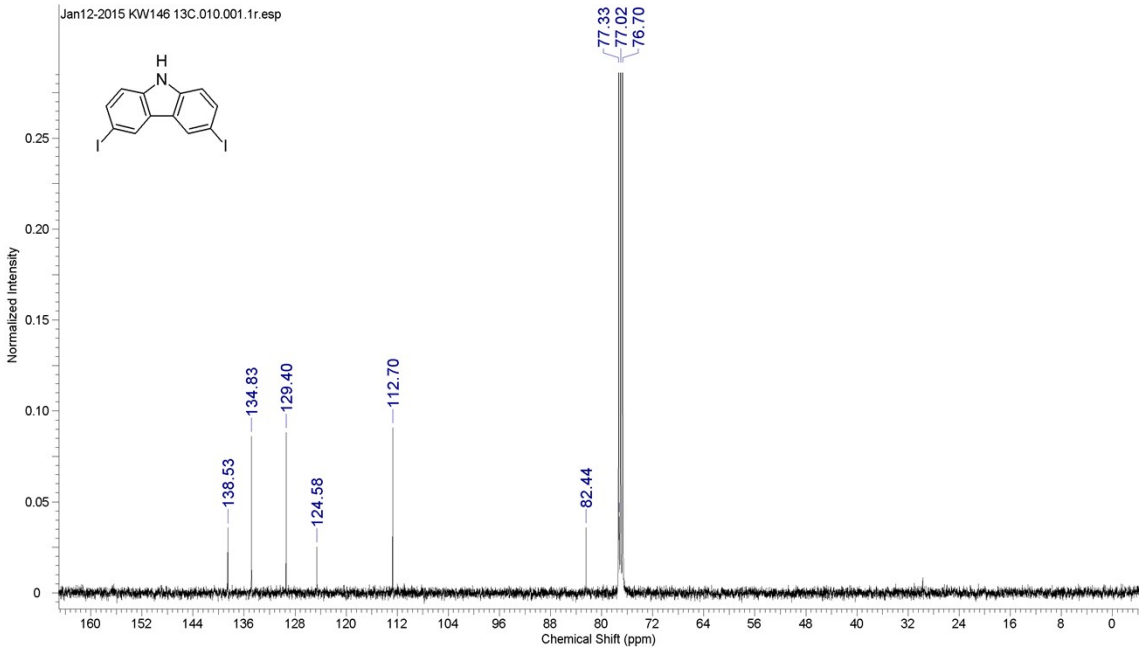


Fig. S4. ^{13}C NMR spectrum (100 MHz) for *3,6-diiodocarbazole* (Compound **2**) in $CDCl_3$.

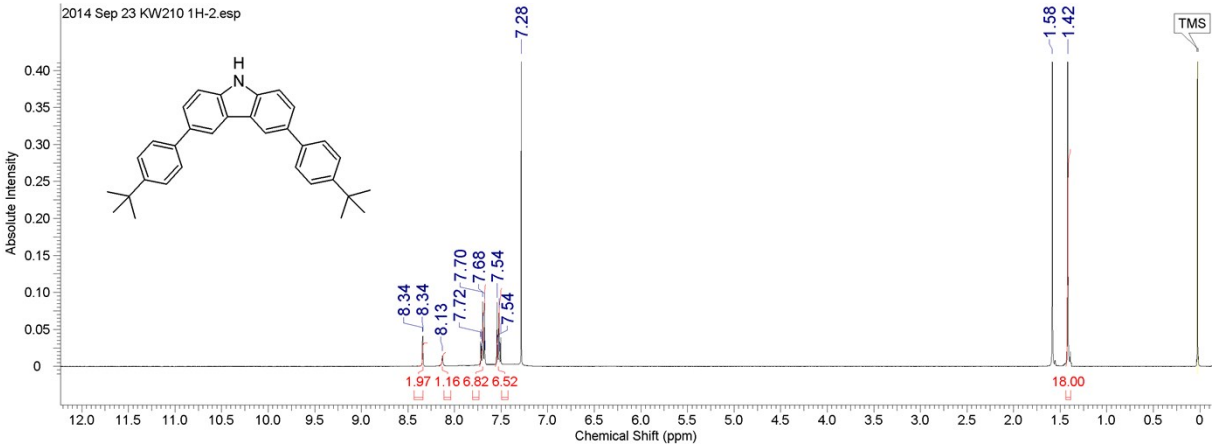


Figure S5. ^{1}H NMR spectrum (400 MHz) for *3,6-bis(4-(tert-butyl)phenyl)-9H-carbazole* (Compound **3**) in $CDCl_3$.

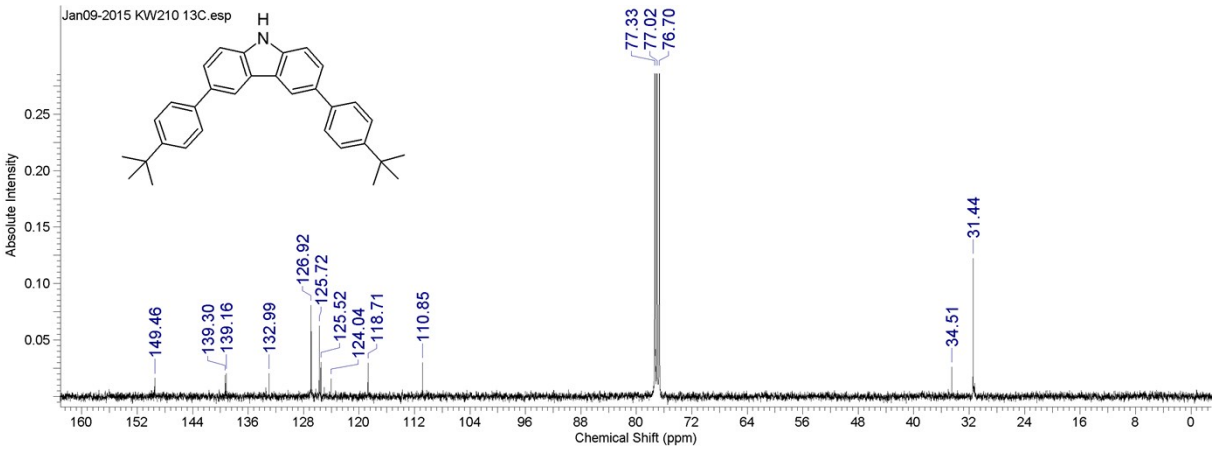


Figure S6. ^{13}C NMR spectrum (100 MHz) for *3,6-bis(4-(tert-butyl)phenyl)-9H-carbazole* (Compound **3**) in $CDCl_3$.

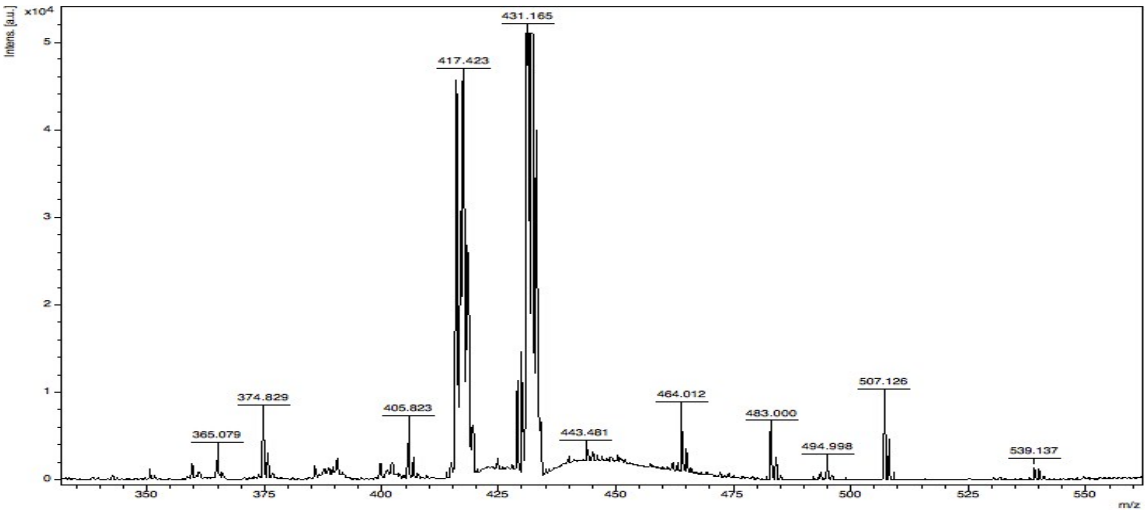


Figure S7. MALDI-TOF MS spectrum for *3,6-bis(4-(tert-butyl)phenyl)-9H-carbazole* (Compound **3**) in $CDCl_3$.

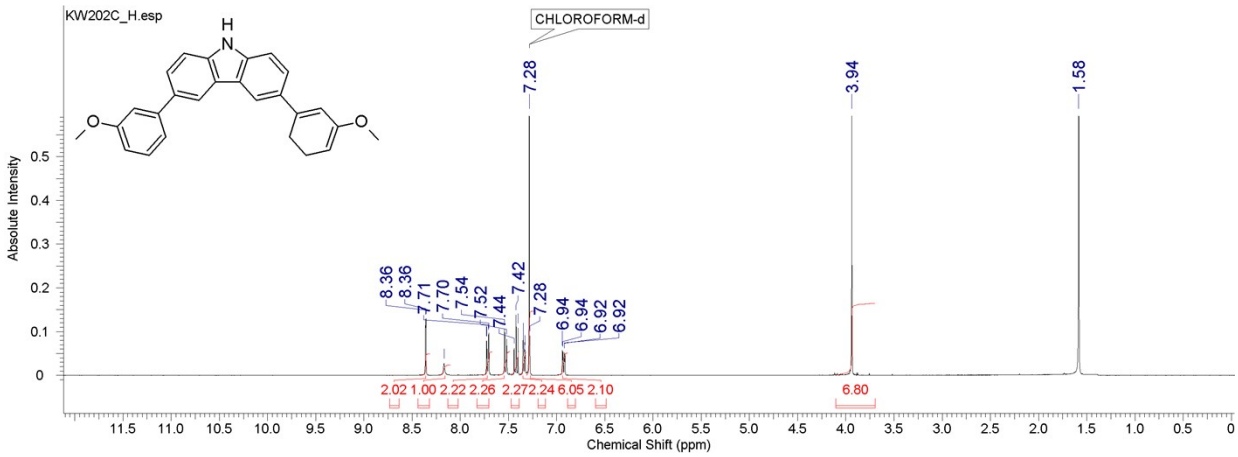


Figure S8. ^{1}H NMR spectrum (400 MHz) for *3,6-bis(3-methoxyphenyl)-9H-carbazole* (Compound **4**) in $CDCl_3$.

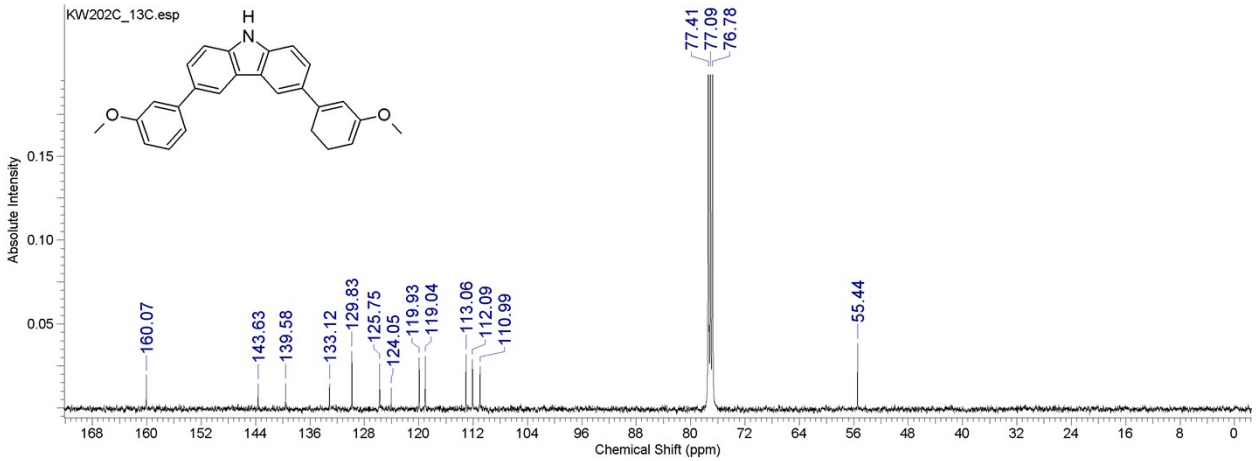


Figure S9. ^{13}C NMR spectrum (100 MHz) for *3,6-bis(3-methoxyphenyl)-9H-carbazole* (Compound **4**) in $CDCl_3$.

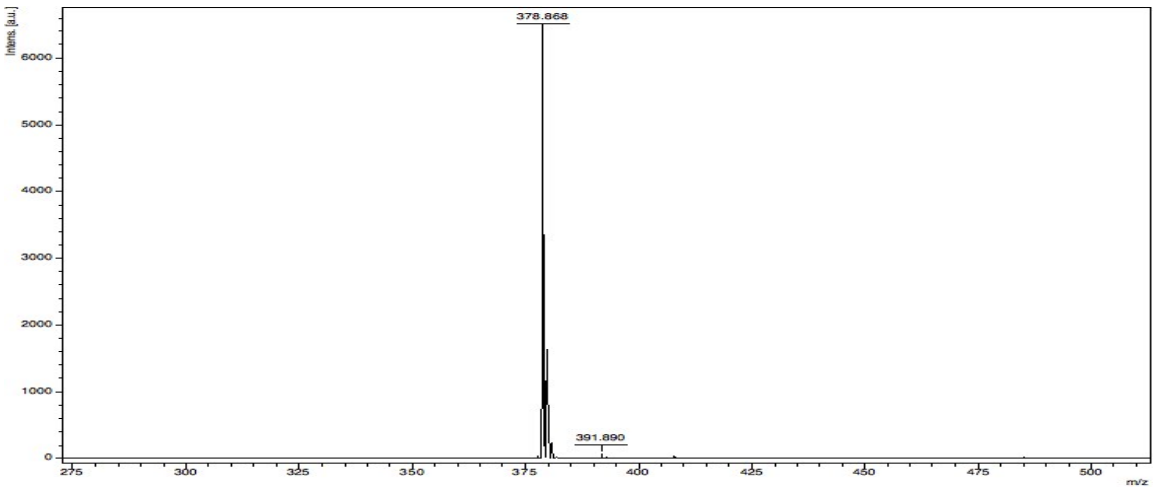


Figure S10. MALDI-TOF MS spectrum for *3,6-bis(3-methoxyphenyl)-9H-carbazole* (Compound **4**) in $CDCl_3$.

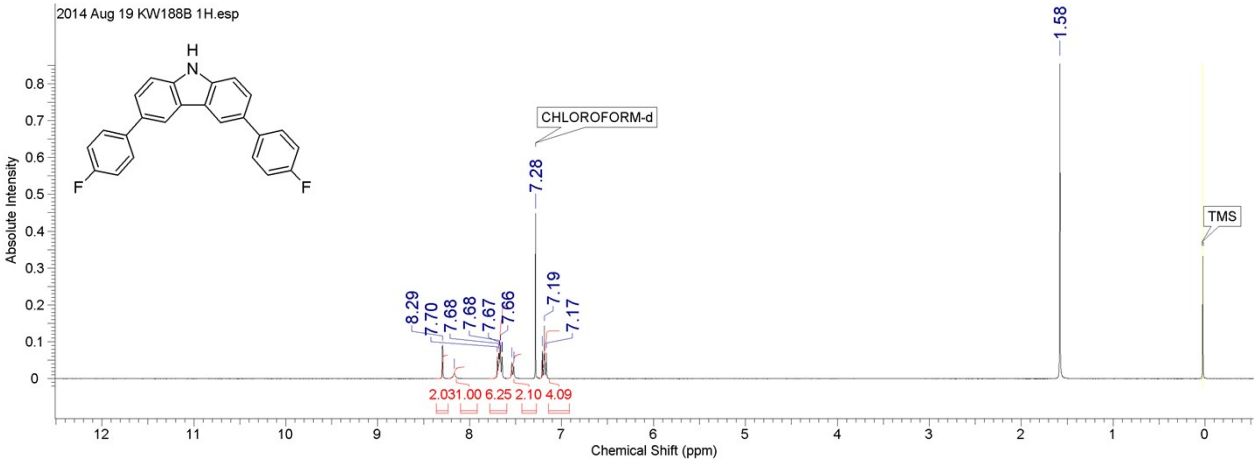


Figure S11. ^{1}H NMR spectrum (400 MHz) for *3,6-bis(4-fluorophenyl)-9H-carbazole* (Compound **5**) in $CDCl_3$.

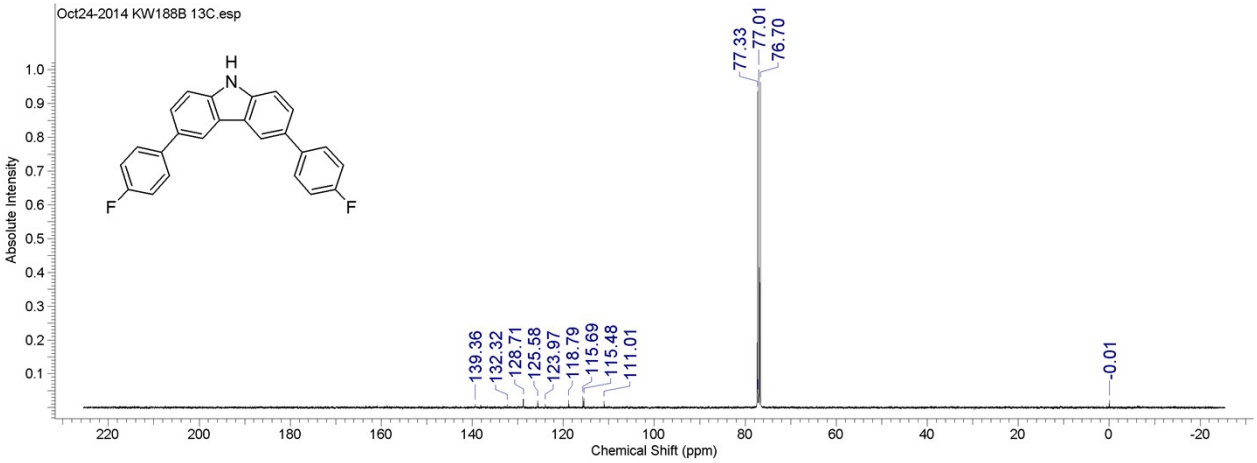


Figure S12. ^{13}C NMR spectrum (100 MHz) for *3,6-bis(4-fluorophenyl)-9H-carbazole* (Compound **5**) in $CDCl_3$.

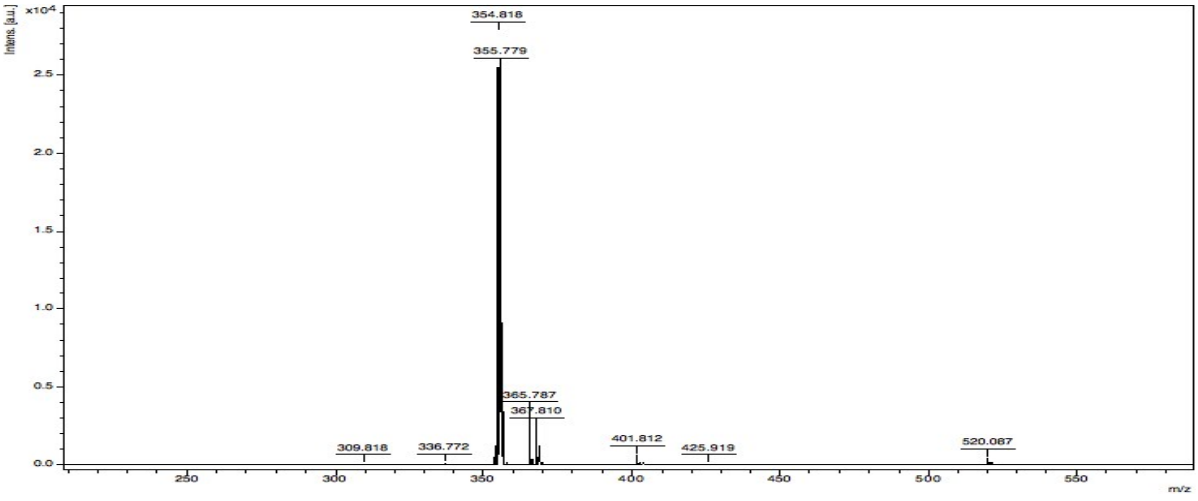


Figure S13. MALDI-TOF MS spectrum for *3,6-bis(4-fluorophenyl)-9H-carbazole* (Compound **5**) in $CDCl_3$

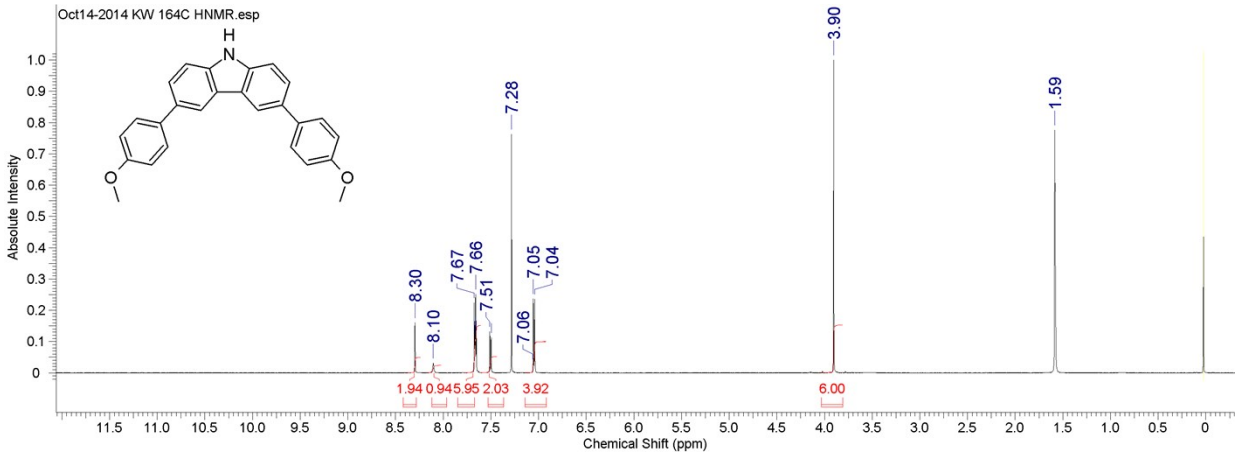


Figure S14. ^{1}H NMR spectrum (600 MHz) for *3,6-bis(4-methoxyphenyl)-9H-carbazole* (Compound **6**) in $CDCl_3$.

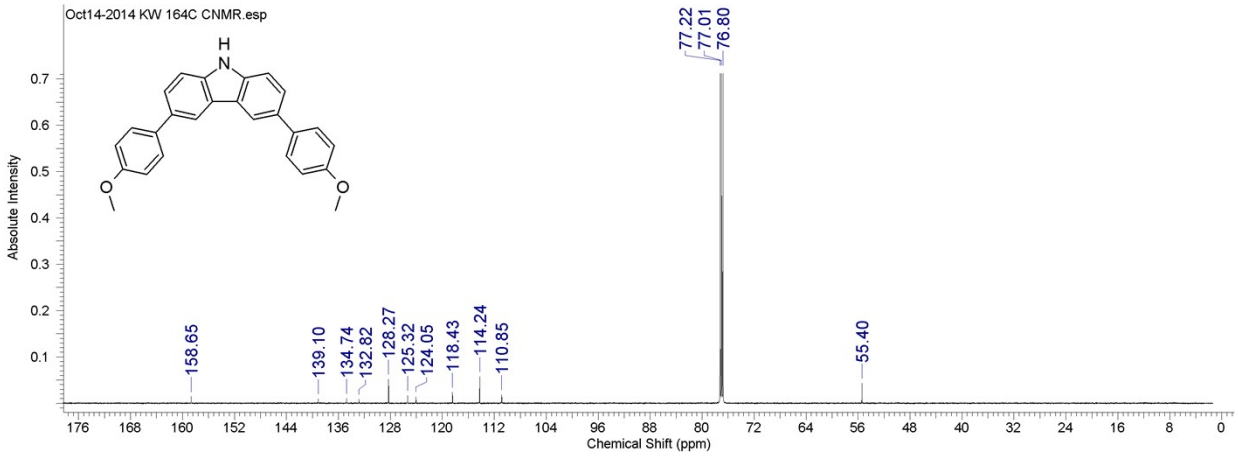


Figure S15. ^{13}C NMR spectrum (100 MHz) for *3,6-bis(4-methoxyphenyl)-9H-carbazole* (Compound **6**) in $CDCl_3$.

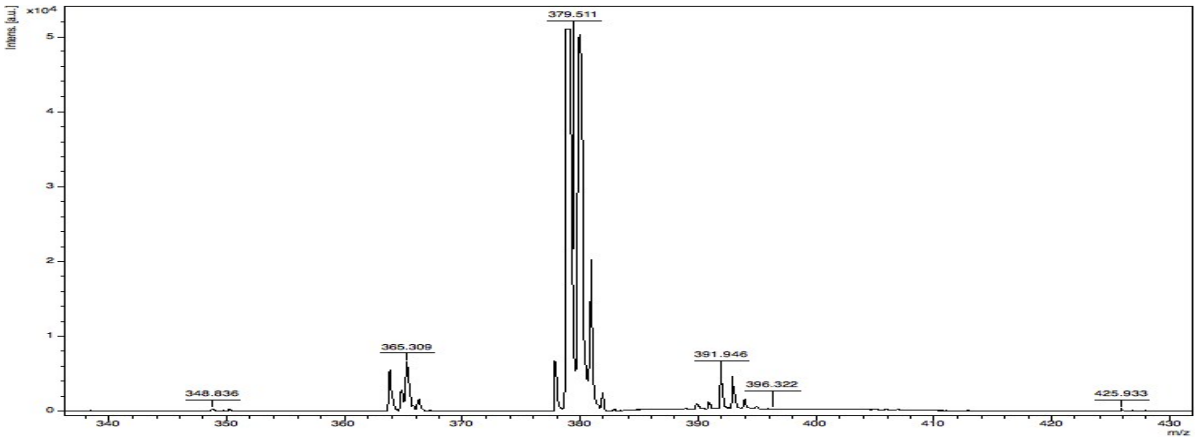


Figure S16. MALDI-TOF MS spectrum for *3,6-bis(4-methoxyphenyl)-9H-carbazole* (Compound **6**) in $CDCl_3$.

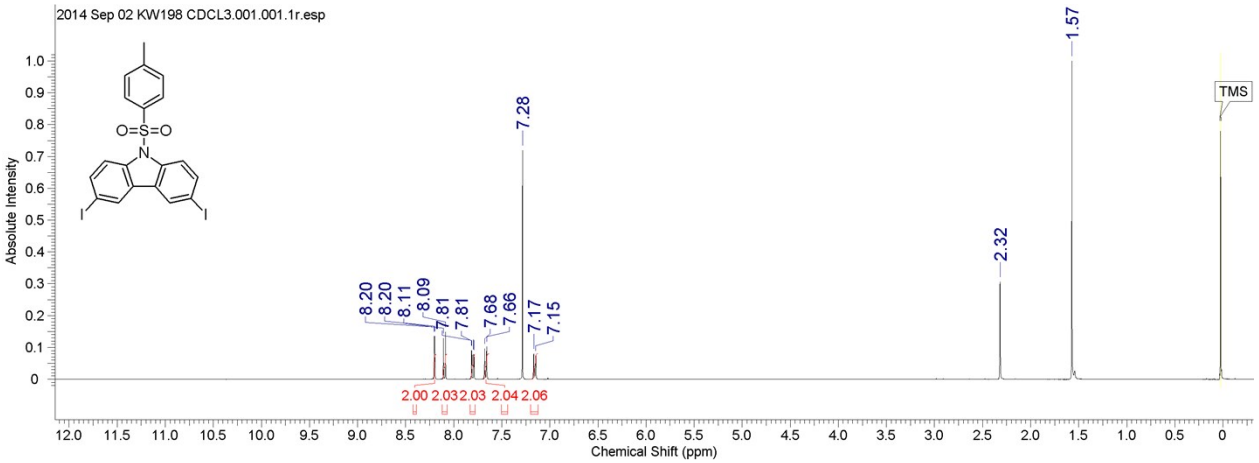


Figure S17. ^{1}H NMR spectrum (400 MHz) for *3,6-diiodo-9-tosyl-9H-carbazole* (Compound **8**) in $CDCl_3$.

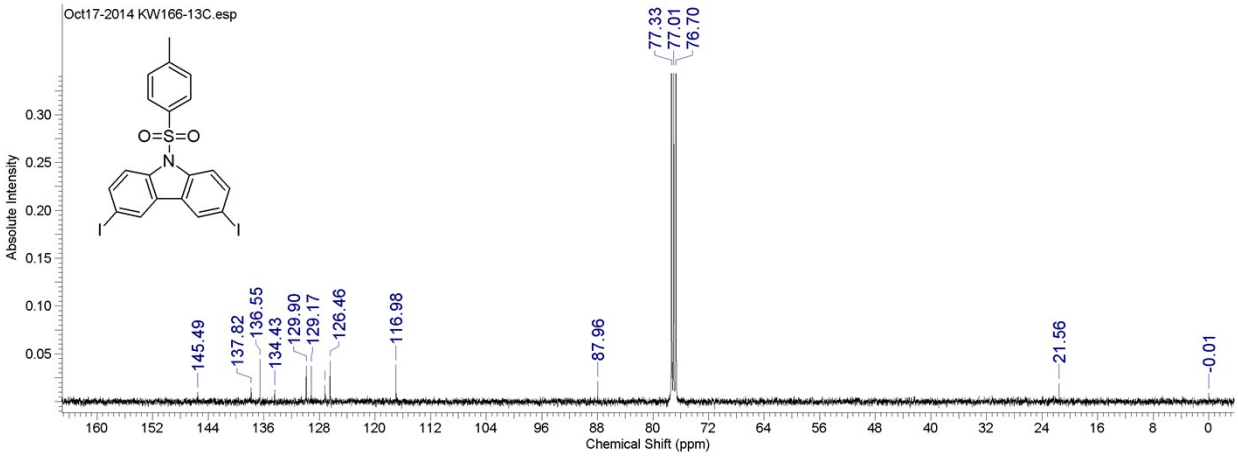


Figure S18. ^{13}C NMR spectrum (100 MHz) for *3,6-diiodo-9-tosyl-9H-carbazole* (Compound **8**) in $CDCl_3$.

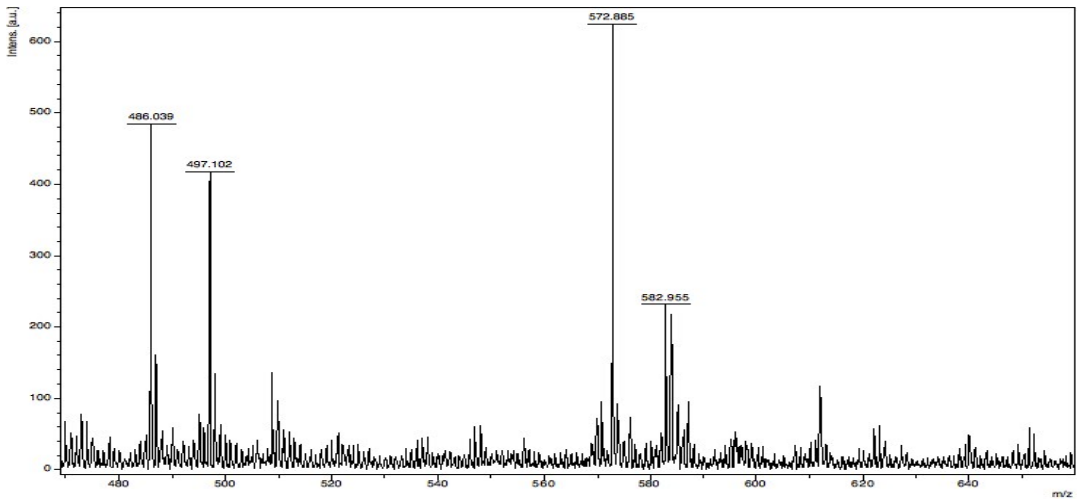


Figure S19. MALDI-TOF MS spectrum for *3,6-diiodo-9-tosyl-9H-carbazole* (Compound **8**) in $CDCl_3$.

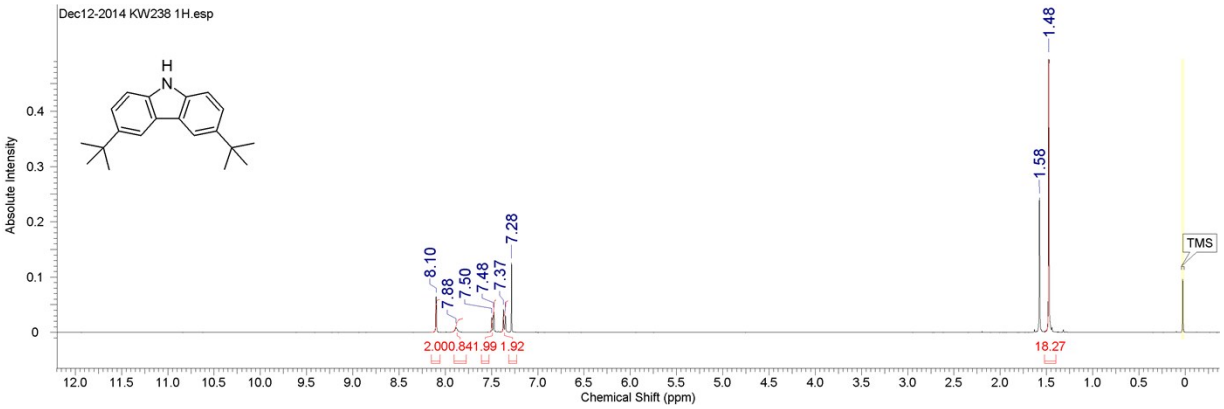


Figure S20. ^{1}H NMR spectrum (400 MHz) for *3,6-di-tert-butyl-9H-carbazole* (Compound **7**) in $CDCl_3$.

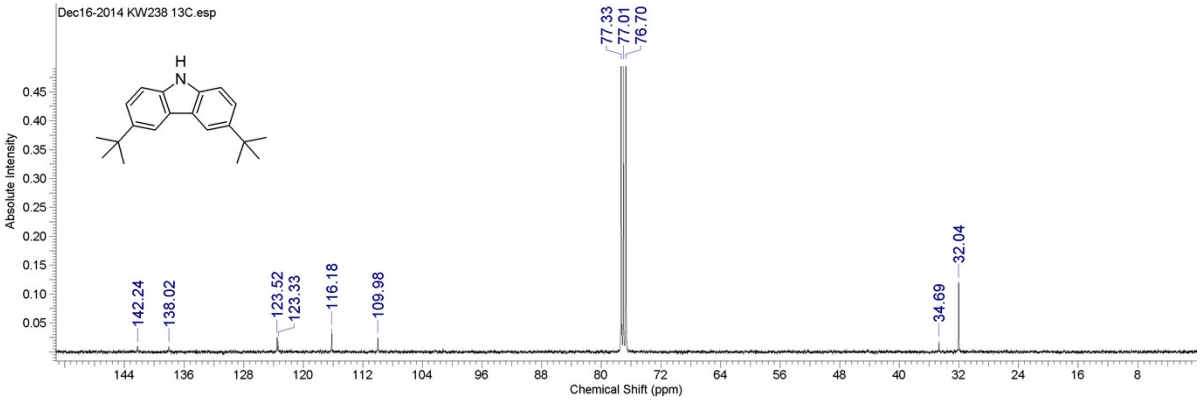


Figure S21. ^{13}C NMR spectrum (100 MHz) for *3,6-di-tert-butyl-9H-carbazole* (Compound **7**) in $CDCl_3$.

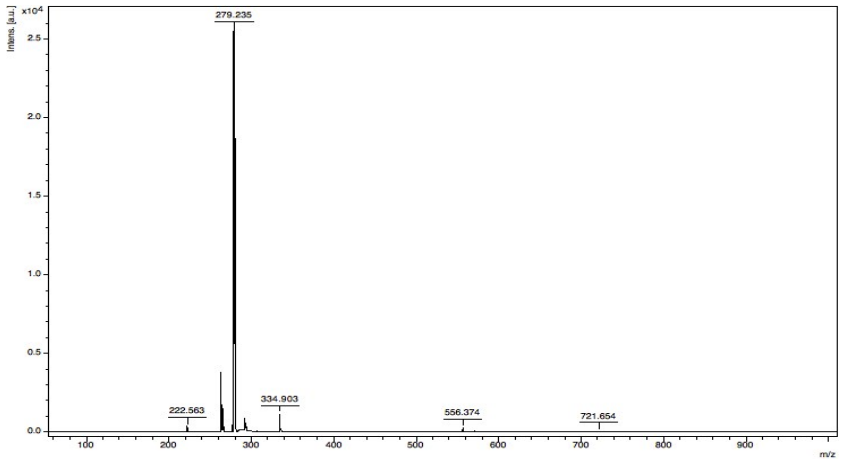


Figure S22. MALDI-TOF MS spectrum for *3,6-di-tert-butyl-9H-carbazole* (Compound **7**) in $CDCl_3$.

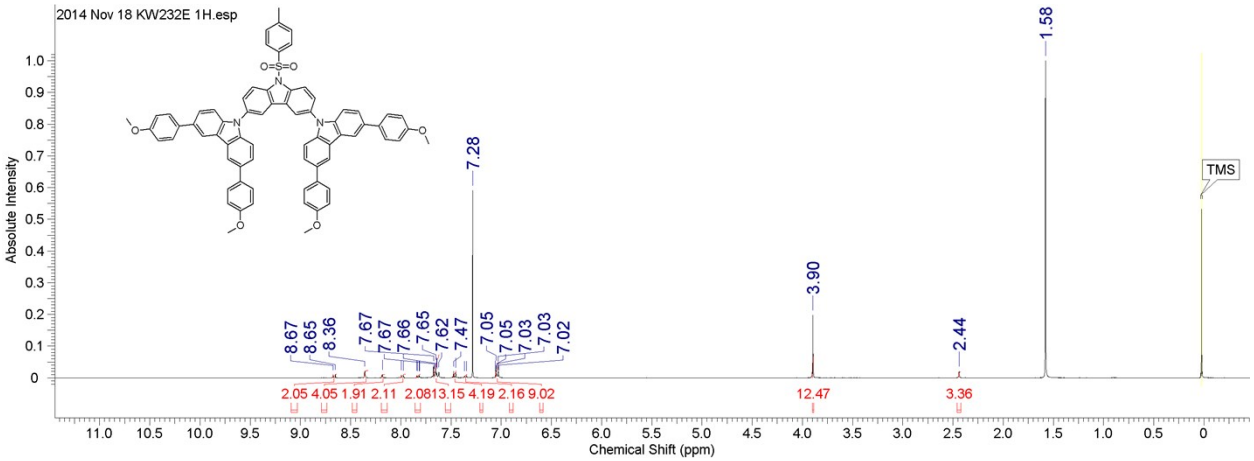


Figure S23. ^{1}H NMR spectrum (400 MHz) for *3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'-tosyl-9'H-9,3':6',9''-tercarbazole* (Compound **9**) in $CDCl_3$.

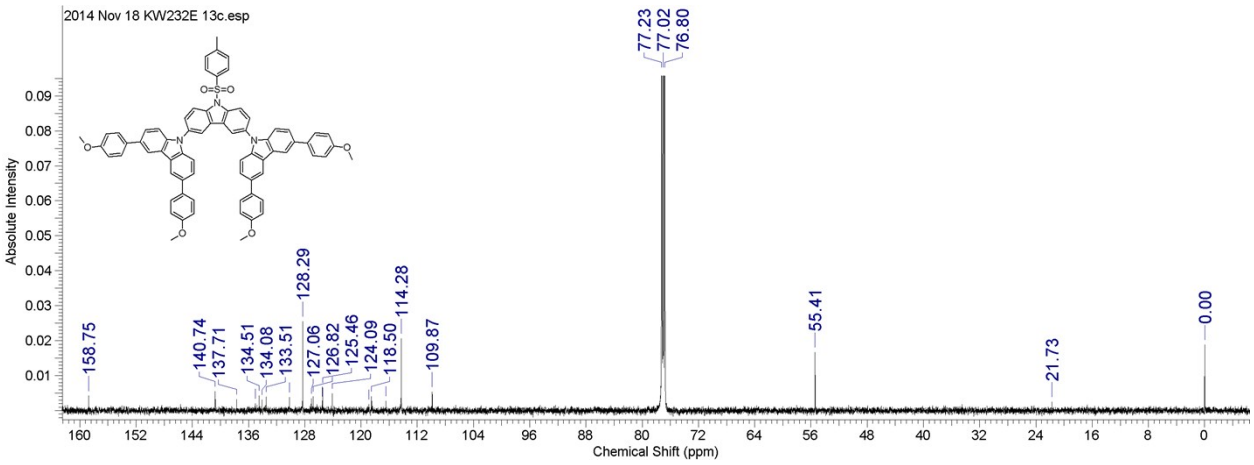


Figure S24. ^{13}C NMR spectrum (100 MHz) for *3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'-tosyl-9'H-9,3':6',9''-tercarbazole* (Compound **9**) in $CDCl_3$.

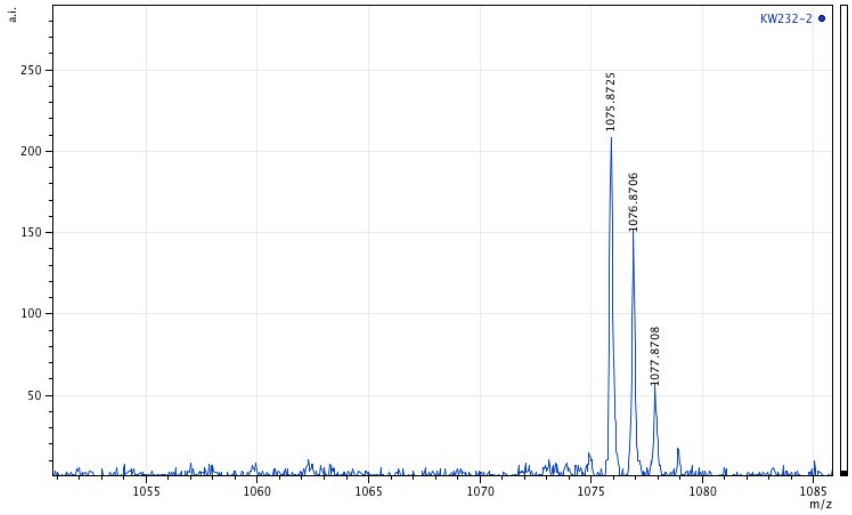


Figure S25. MALDI-TOF MS spectrum for *3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'-tosyl-9'H-9,3':6',9''-tercarbazole* (Compound **9**) in $CDCl_3$.

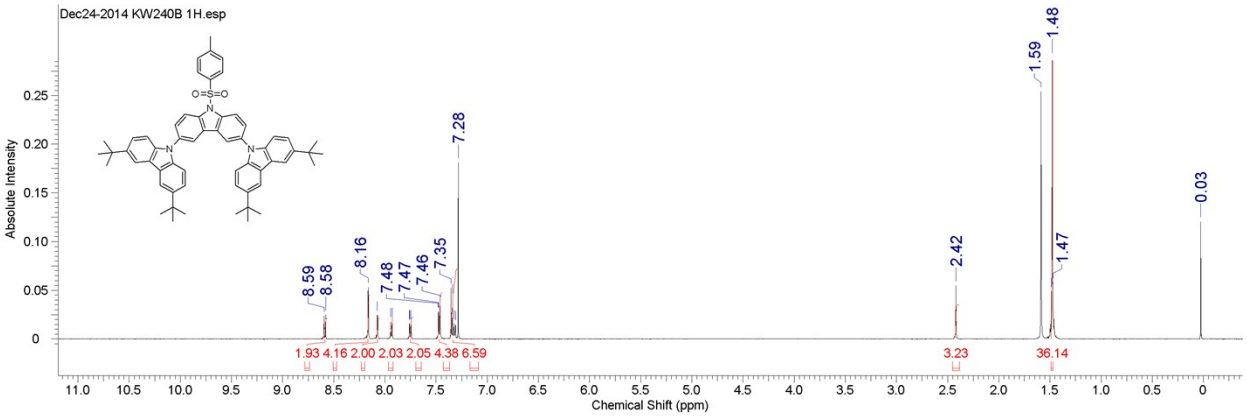


Figure S26. ^{1}H NMR spectrum (600 MHz) for *3,3'',6,6''-tetra-tert-butyl-9'-tosyl-9'H-9,3':6',9''-tercarbazole* (Compound **10**) in $CDCl_3$.

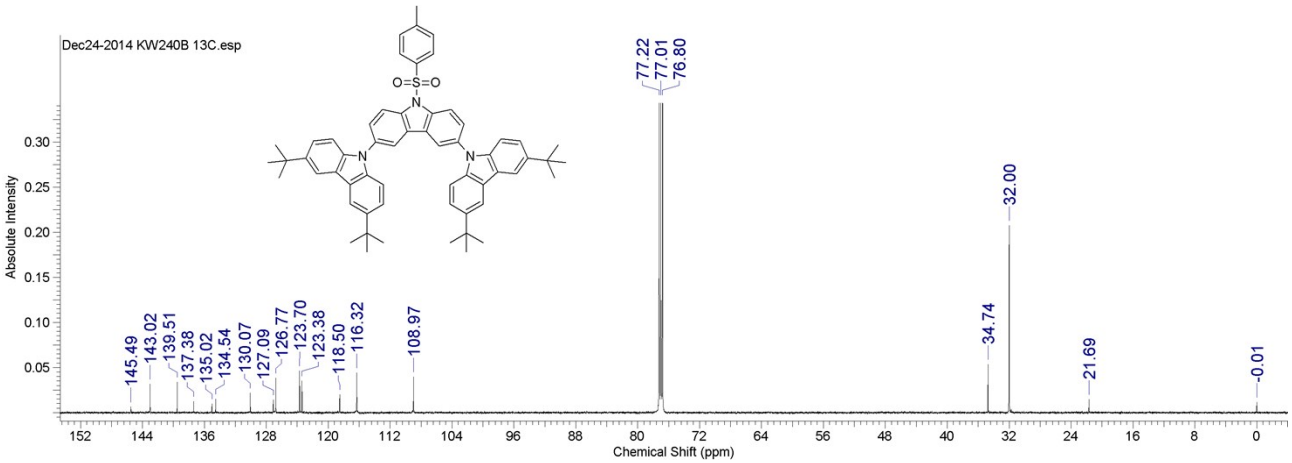


Figure S27. ^{13}C NMR spectrum (100 MHz) for *3,3'',6,6''-tetra-tert-butyl-9'-tosyl-9'H-9,3':6',9''-tercarbazole* (Compound **10**) in $CDCl_3$.

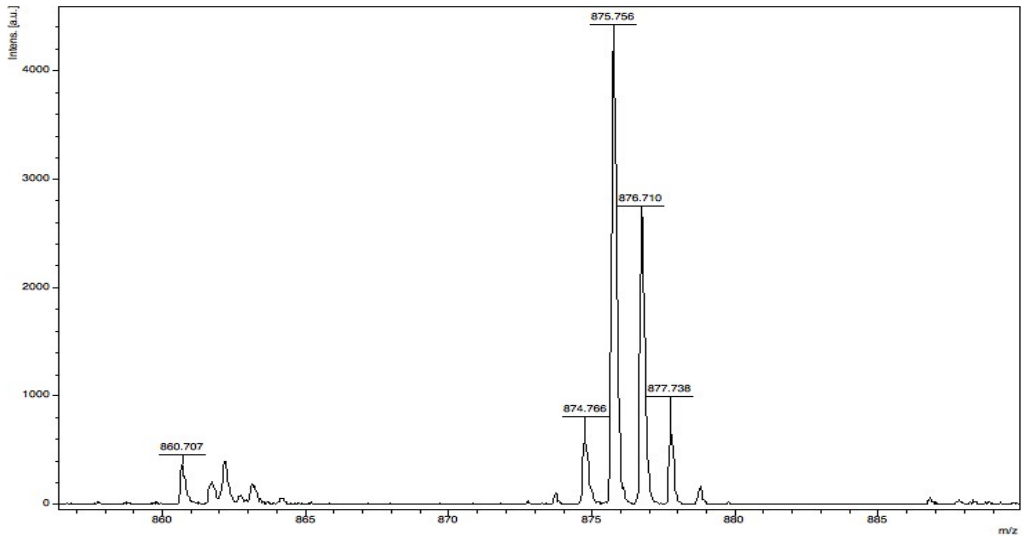


Figure S28. MALDI-TOF MS spectrum for *3,3'',6,6''-tetra-tert-butyl-9'-tosyl-9'H-9,3':6',9''-tercarbazole* (Compound **10**) in $CDCl_3$

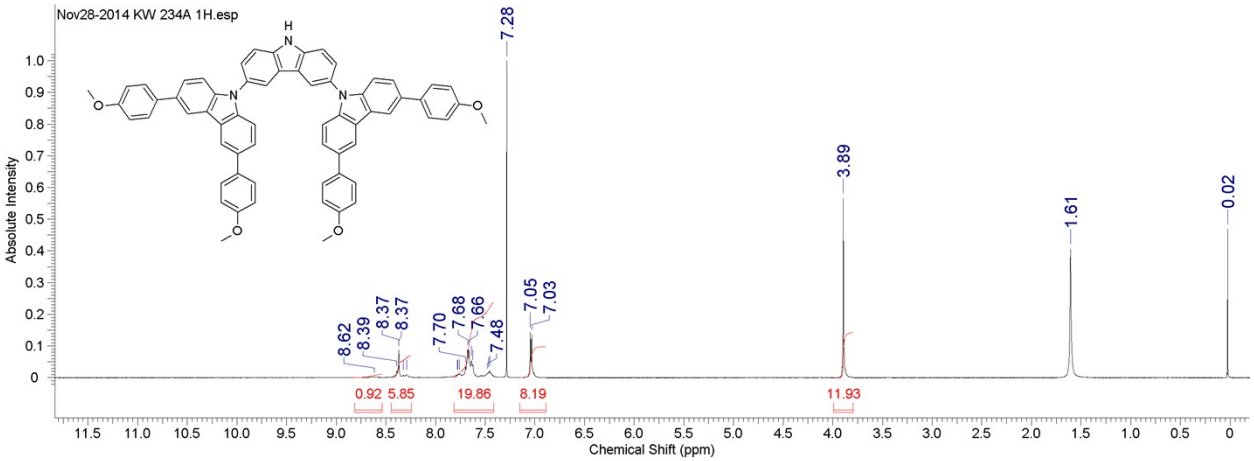


Figure S29. ^{1}H NMR spectrum (600 MHz) for *3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-9,3':6',9''-tercarbazole* (Compound **11**) in $CDCl_3$.

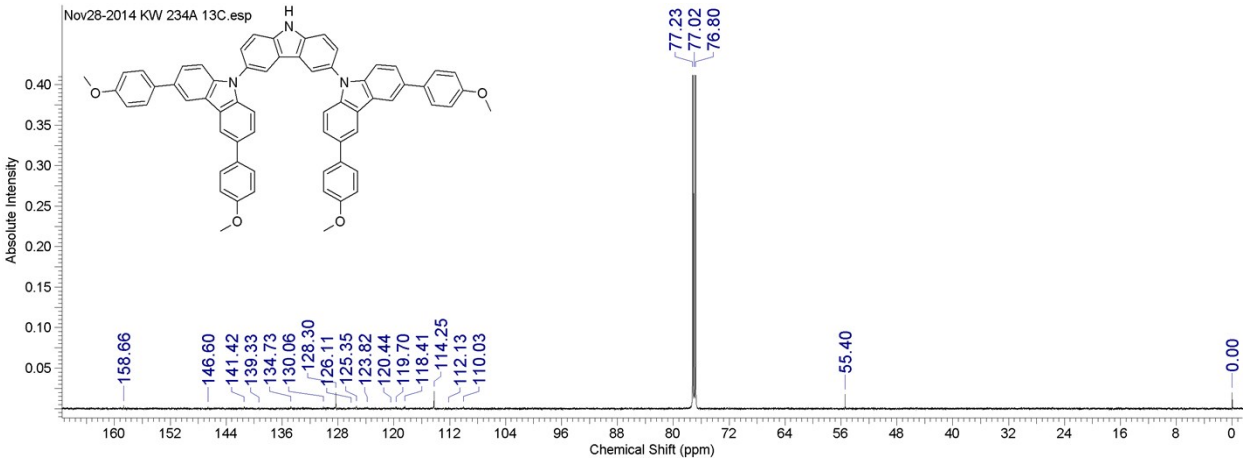


Figure S30. ^{13}C NMR spectrum (100 MHz) for *3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-9,3':6',9''-tercarbazole* (Compound **11**) in $CDCl_3$.

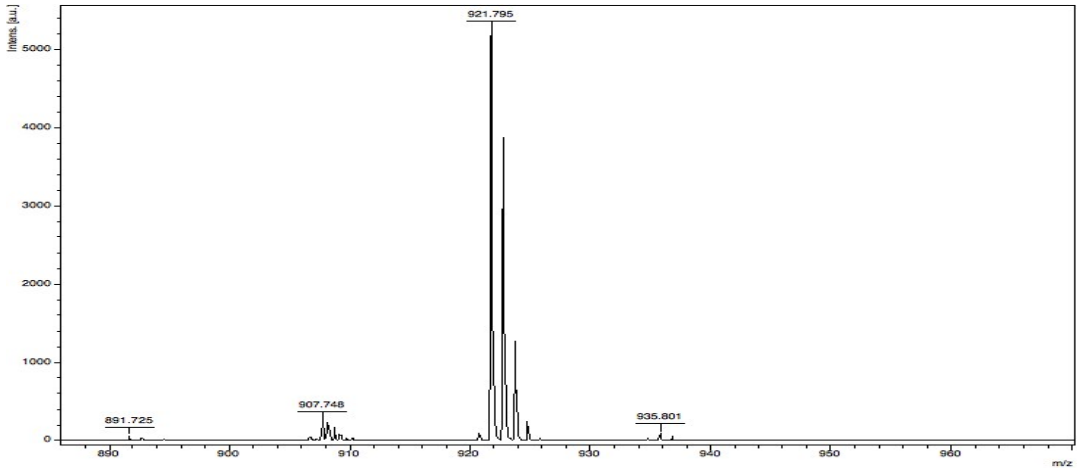


Figure S31. MALDI-TOF MS spectrum for *3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-9,3':6',9''-tercarbazole* (Compound **11**) in $CDCl_3$.

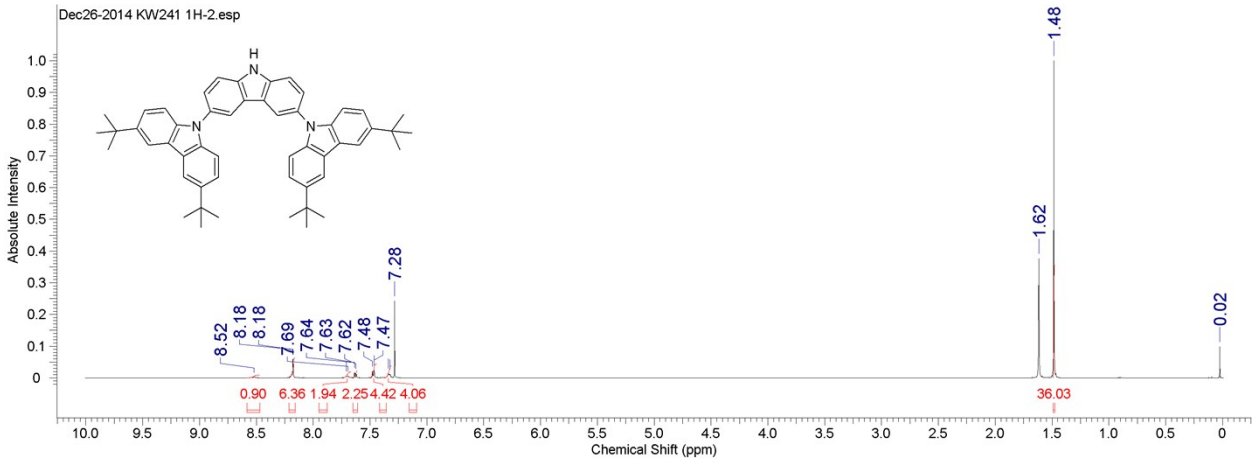


Figure S32. ^{1}H NMR spectrum (600 MHz) for *3,3'',6,6''-tetra-tert-butyl-9'H-9,3':6',9''-tercarbazole* (Compound **12**) in $CDCl_3$.

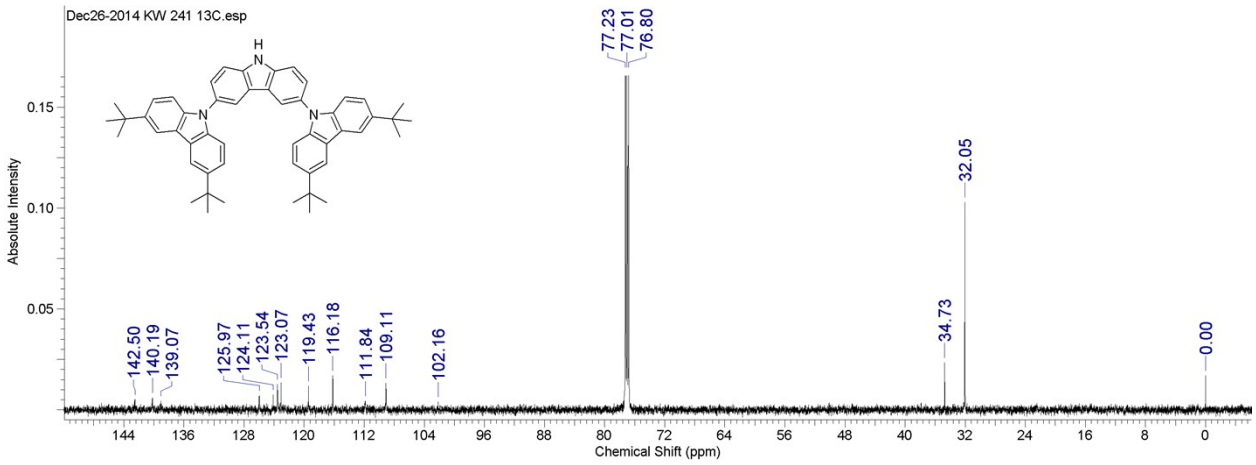


Figure S33. ^{13}C NMR spectrum (100 MHz) for *3,3'',6,6''-tetra-tert-butyl-9'H-9,3':6',9''-tercarbazole* (Compound **12**) in $CDCl_3$.

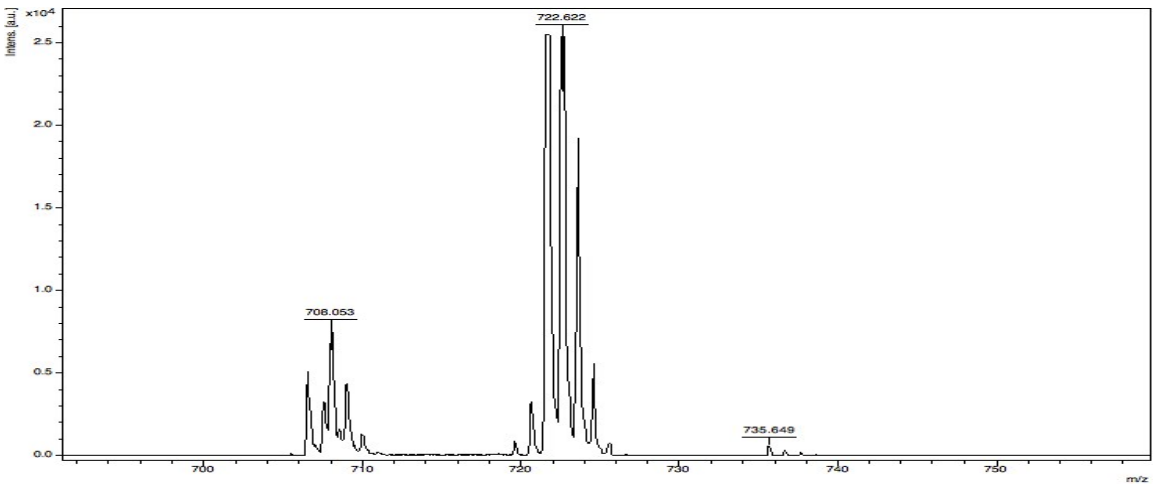


Figure S33. MALDI-TOF MS spectrum for *3,3'',6,6''-tetra-tert-butyl-9'H-9,3':6',9''-tercarbazole* (Compound **12**) in $CDCl_3$.

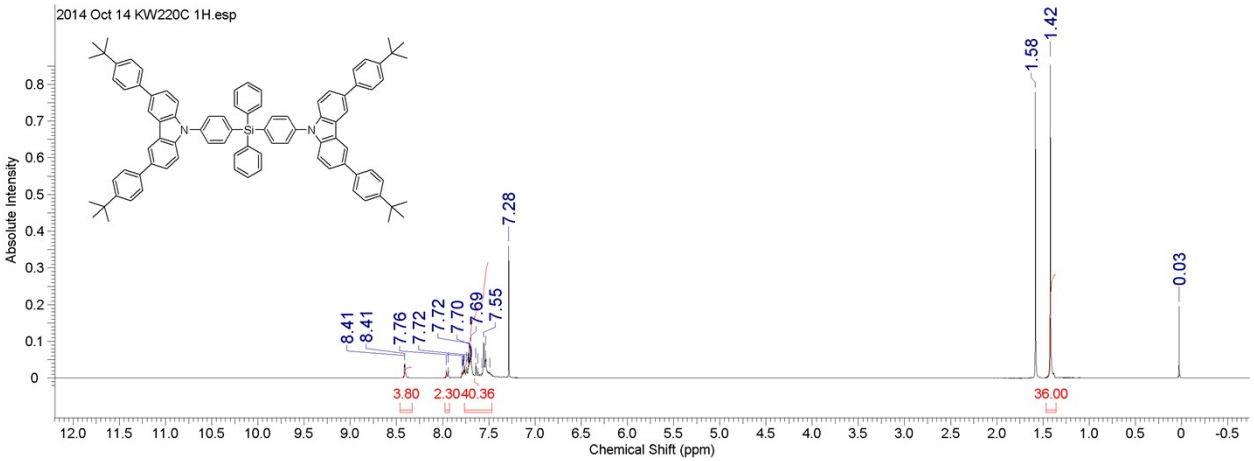


Figure S34. ^{1}H NMR spectrum (400 MHz) for *bis(4-(3,6-bis(4-(tert-butyl)phenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane*/**P1** in $CDCl_3$.

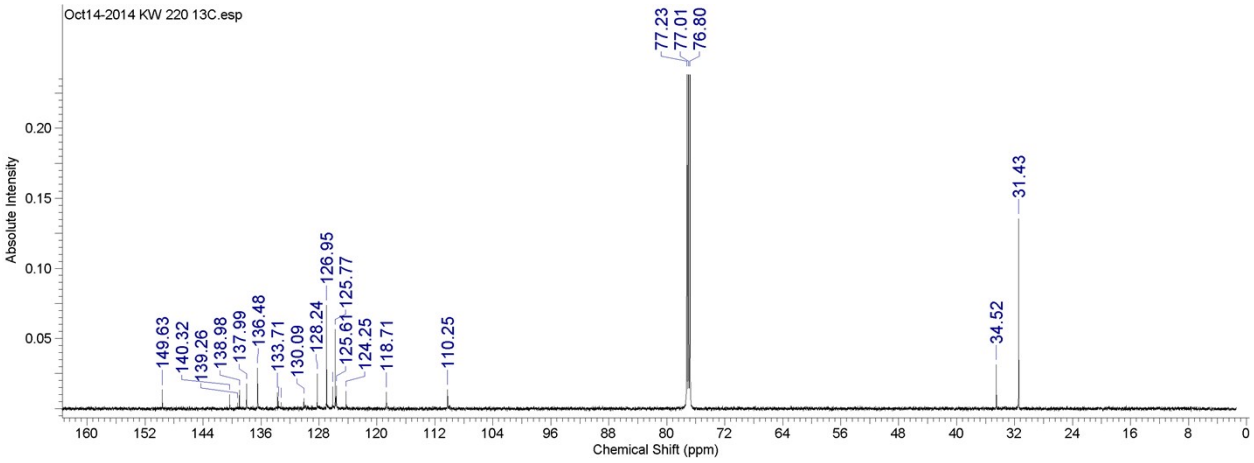


Figure S35. ^{13}C NMR spectrum (100 MHz) for *bis(4-(3,6-bis(4-(tert-butyl)phenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane*/**P1** in $CDCl_3$.

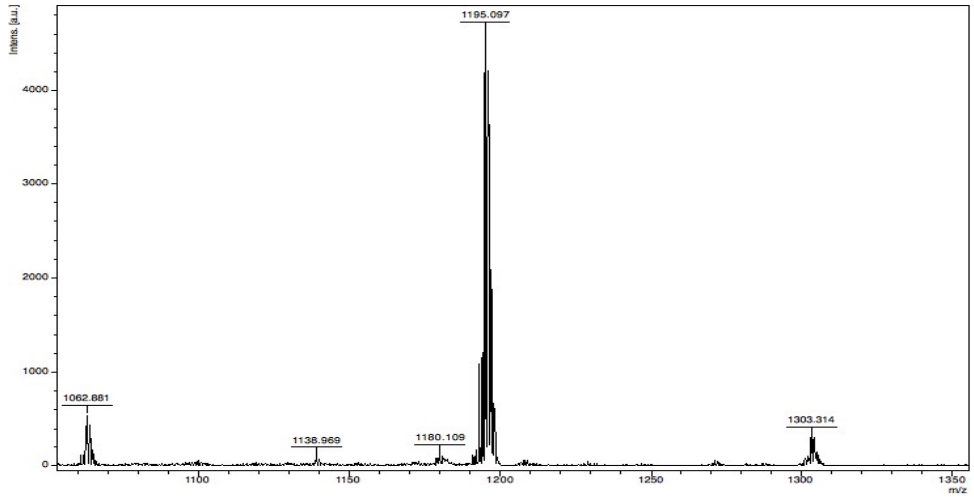


Figure S36. MALDI-TOF MS spectrum for *bis(4-(3,6-bis(4-(tert-butyl)phenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane*/**P1** in $CDCl_3$.

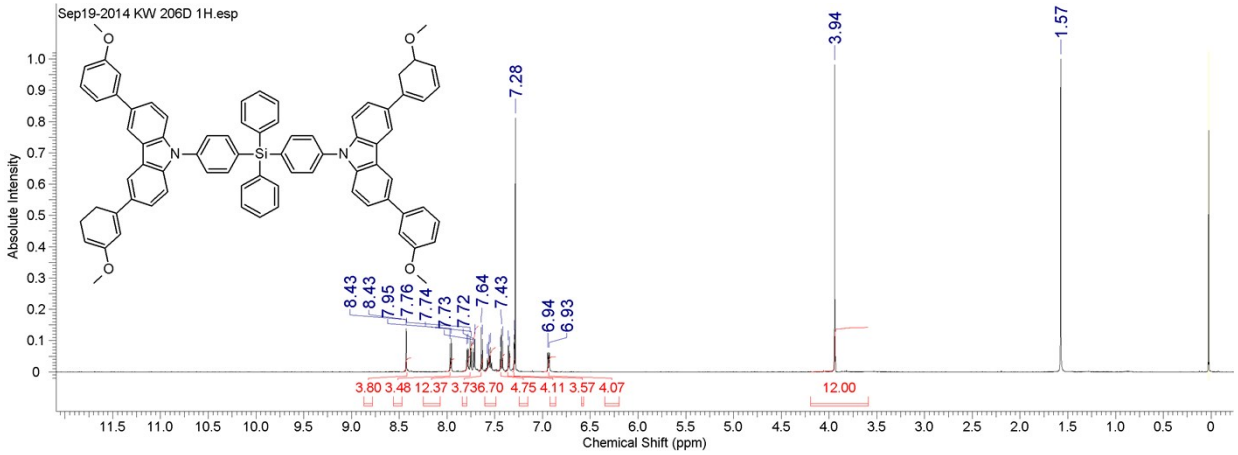


Figure S37. ^{1}H NMR spectrum (600 MHz) for *bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane*/**P2** in $CDCl_3$.

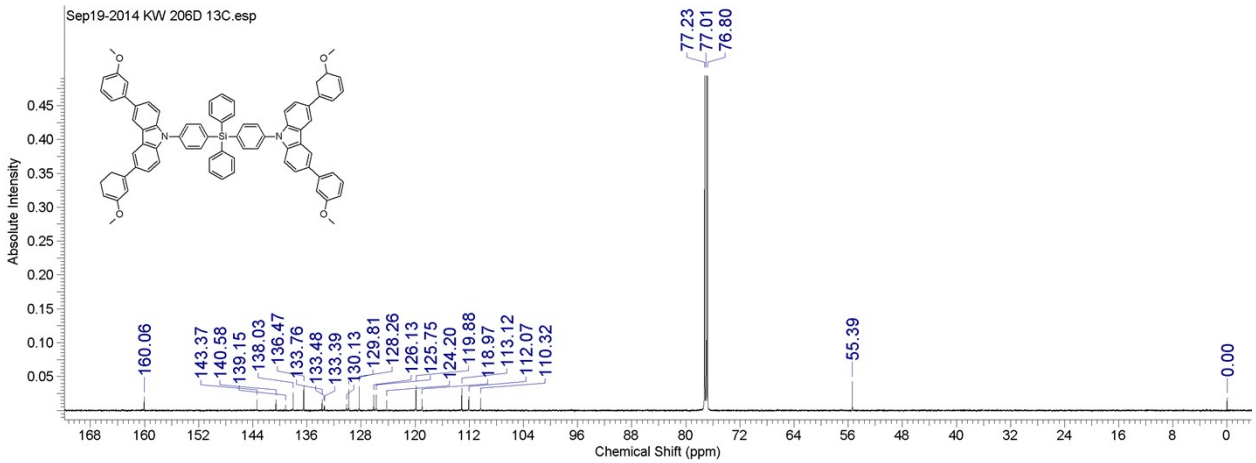


Figure S38. ^{13}C NMR spectrum (100 MHz) for *bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-*

*yl)phenyl)diphenylsilane/***P2** in $CDCl_3$.

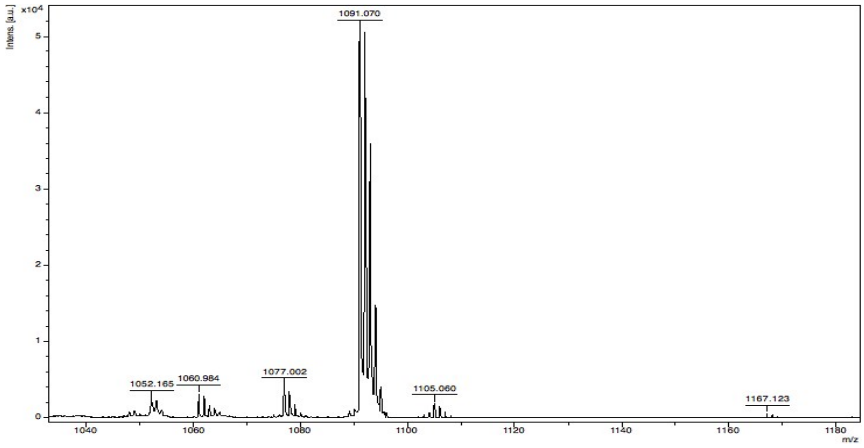


Figure S39. MALDI-TOF MS spectrum for *bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane/***P2** in $CDCl_3$.

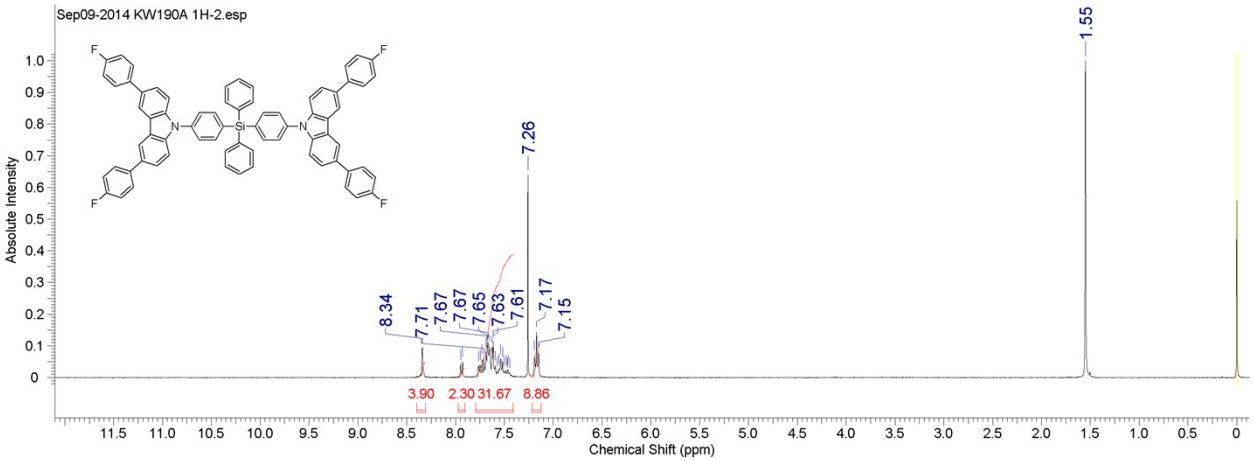


Figure S40. ^{1}H NMR spectrum (600 MHz) for *bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl)*/**P3** in $CDCl_3$.

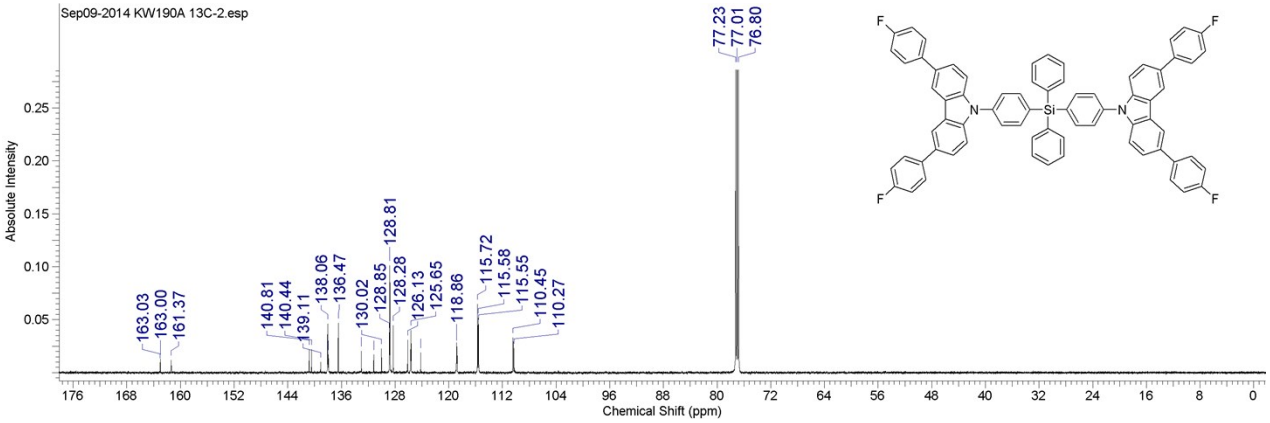


Figure S41. ^{13}C NMR spectrum (100 MHz) for *bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl)*/**P3** in $CDCl_3$.

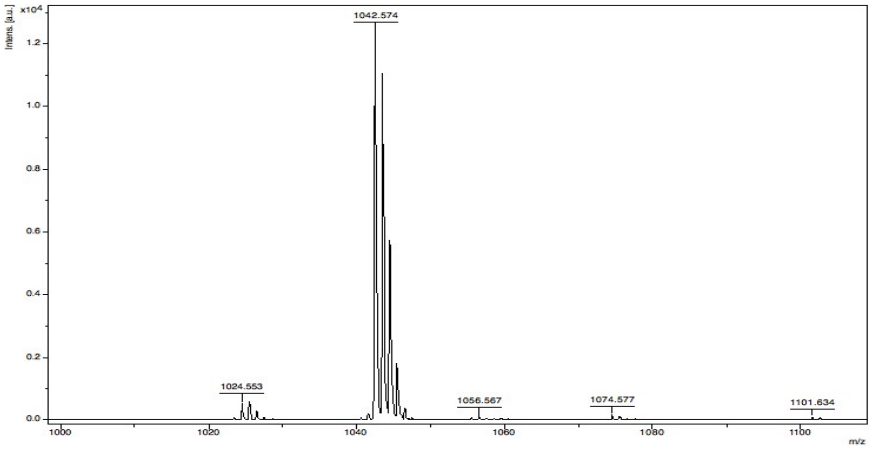


Figure S42. MALDI-TOF MS spectrum for *bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl)*/**P3** in $CDCl_3$.

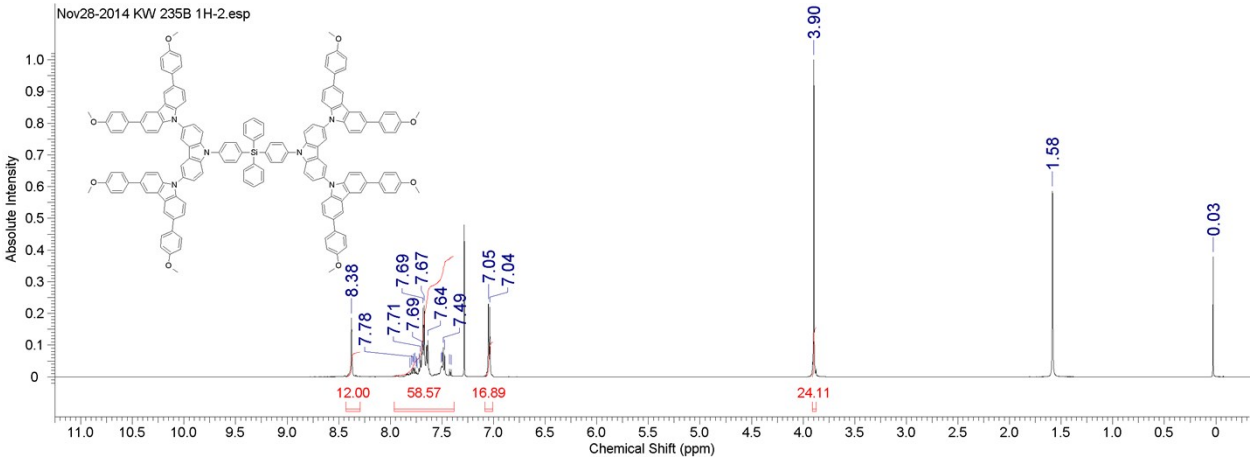


Figure S43. ^{1}H NMR spectrum (600 MHz) for *diphenylbis(4-(3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane*/**P4** in $CDCl_3$.

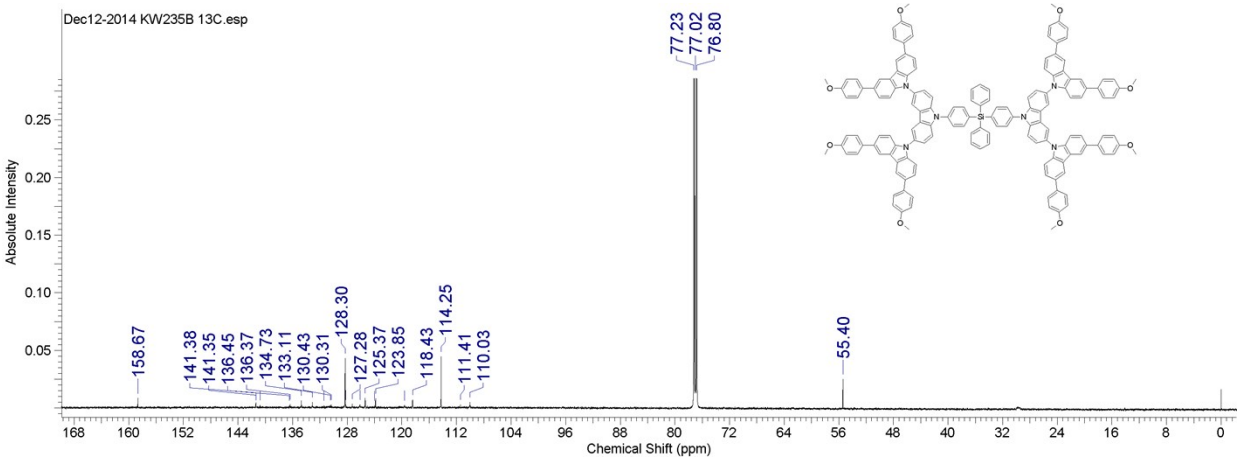


Figure S44. ^{13}C NMR spectrum (100 MHz) for *diphenylbis(4-(3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane*/**P4** in $CDCl_3$.

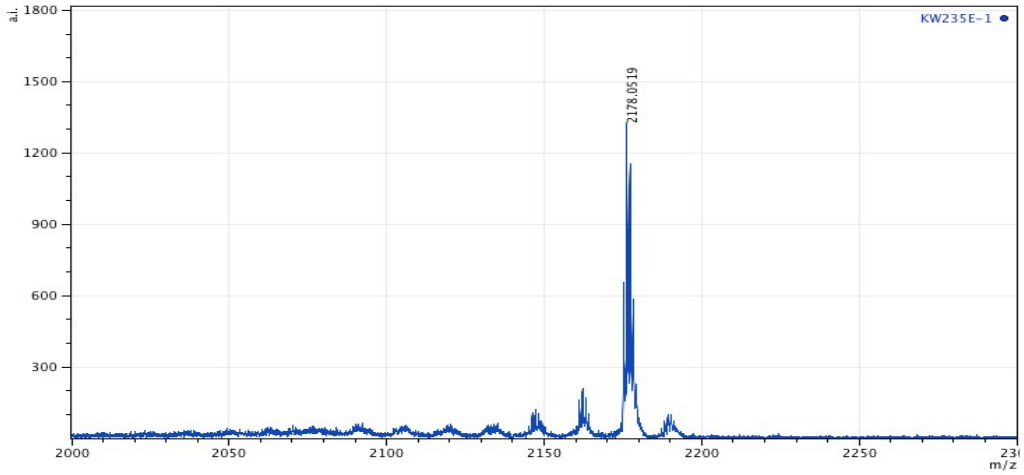


Figure S45. MALDI-TOF MS spectrum for *diphenylbis(4-(3,3'',6,6''-tetrakis(4-methoxyphenyl)-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane*/**P4** in $CDCl_3$.

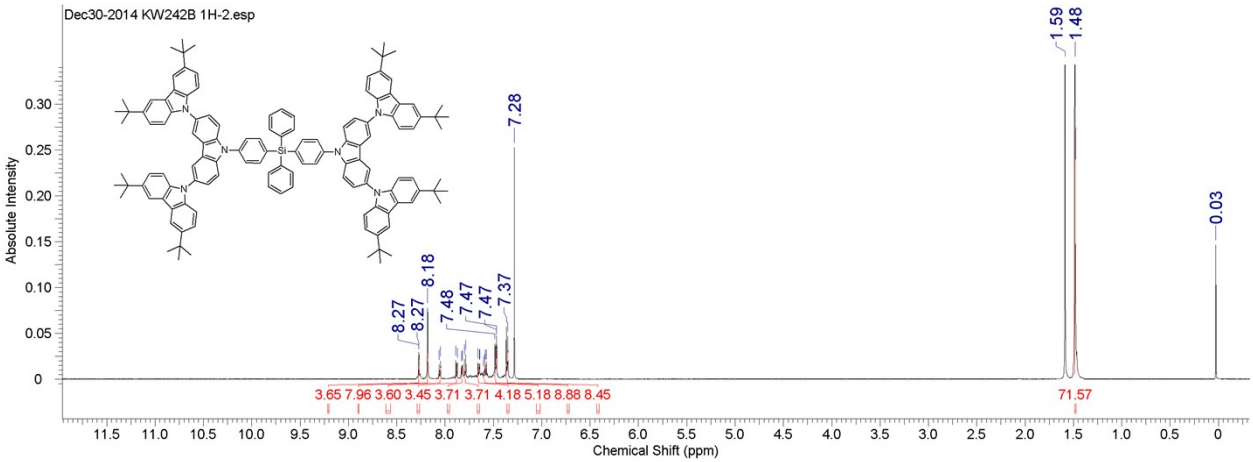


Figure S46. ^{1}H NMR spectrum (600 MHz) for *diphenylbis(4-(3,3'',6,6''-tetra-tert-butyl-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane*/**P5** in $CDCl_3$.

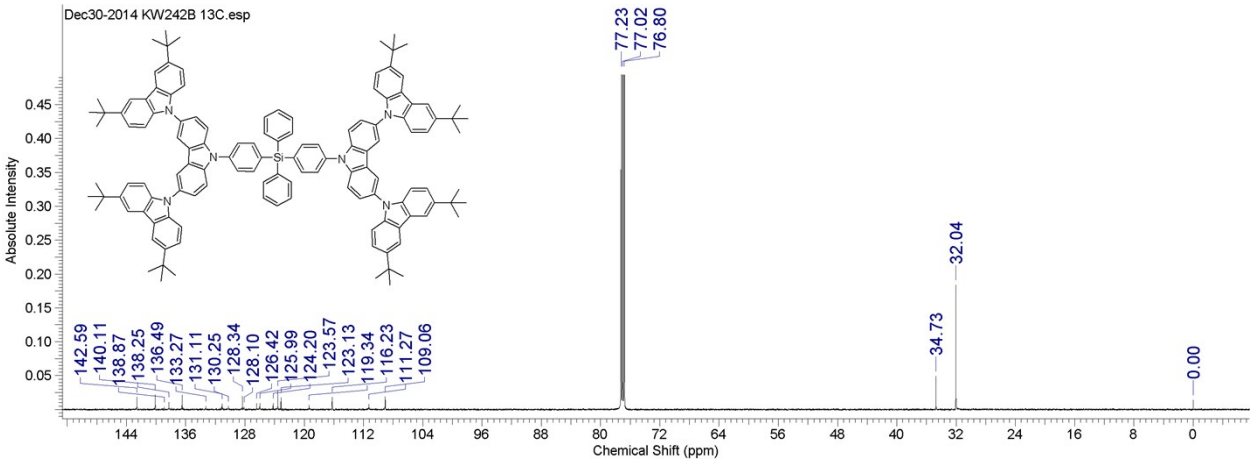


Figure S47. ^{13}C NMR spectrum (100 MHz) for *diphenylbis(4-(3,3'',6,6''-tetra-tert-butyl-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane*/**P5** in $CDCl_3$.

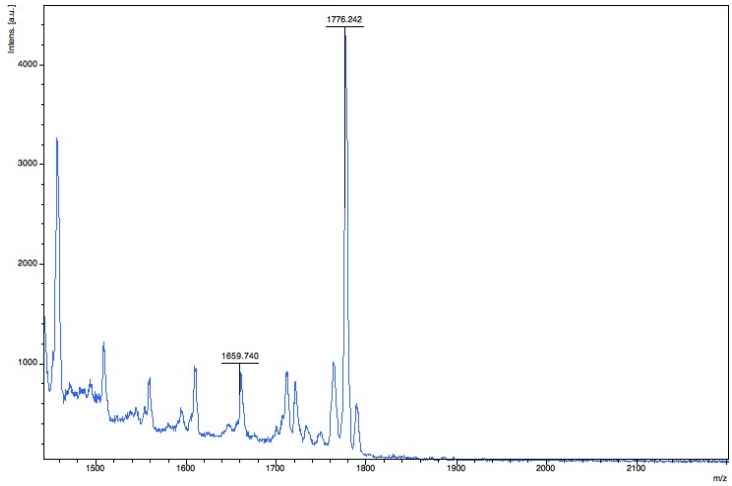


Figure S48. MALDI-TOF MS spectrum for *diphenylbis(4-(3,3'',6,6''-tetra-tert-butyl-9'H-[9,3':6',9''-tercarbazol]-9'-yl)phenyl)silane*/**P5** in $CDCl_3$.

Reference

1. El-Khouly, M. E.; Lee, S.-H.; Kay, K.-Y.; Fukuzumi, S. *New Journal of Chemistry* **2013**, *37*, 3252.

IV . **Torsional angle**

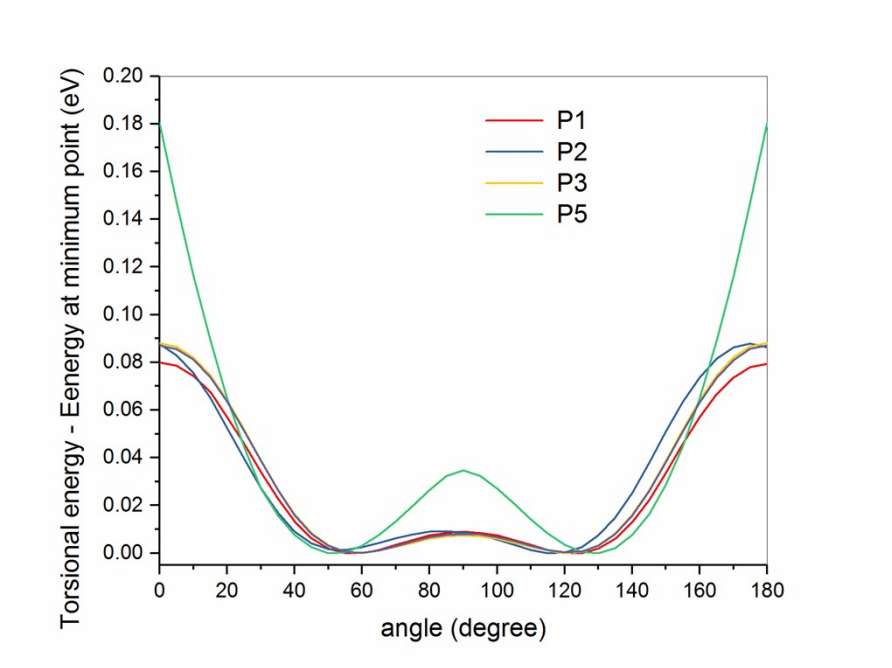
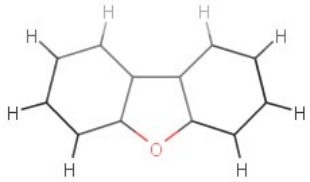


Figure S49 : Torsional angle between the carbazole and moiety at the 3,6 positions of the carbazole. The data is subtracted with its minimum torsional energy for ease of comparison.

I. Coordinates of Stationary Points in xyz format



CarbO
21

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C	1.7243864723	1.5113887993	0.0000102255
C	0.7257168804	0.5330082923	-0.0000046862
C	1.0990879868	-0.8218164867	0.0001226625
C	-0.7257162672	0.5330133265	-0.0000047035
C	-1.0990934929	-0.8218227179	0.0001226359
O	0.0000015300	-1.6498189807	0.0001542002
C	-1.7243921532	1.5113830032	0.0000102925
C	-3.0557313321	1.1057589467	0.0001911045
C	-3.3967556816	-0.2554006217	0.0003350425
C	-2.4173969642	-1.2477633266	0.0002881364
H	2.6661686001	-2.3013337485	0.0004140595
H	4.4418811640	-0.5419697100	0.0005091865
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H	-1.4705665836	2.5651190309	-0.0000881201
H	-3.8429439162	1.8505236491	0.0002454528
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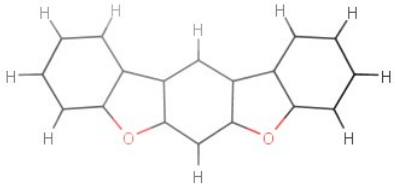

Carb2O
30

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C	-5.3857331947	0.4609247901	-0.0000149854
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C	-3.3331724545	1.7672150125	-0.0004281545
C	-2.6021187067	0.5760765411	-0.0003728671
C	-3.2948636631	-0.6455615821	-0.0001731532
C	-1.1923153522	0.2266735917	-0.0003794225
C	-1.1608095122	-1.1877429267	-0.0002055218
O	-2.4279645941	-1.7170932831	-0.0001139631
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C	1.1607947445	-1.1877838920	-0.0000167369
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C	3.2948643517	-0.6456848506	0.0004043788
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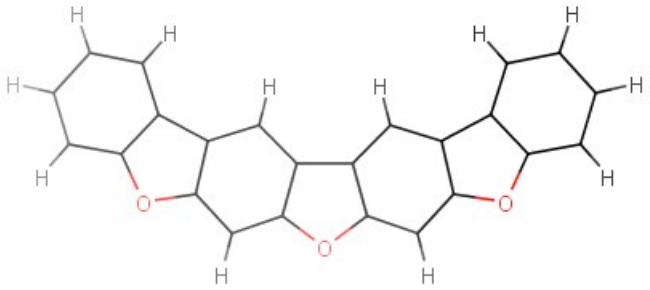
H	6.4690567243	0.4355474232	0.0013420913
H	5.1730517641	-1.7016528178	0.0010910625



Carb3O

39

C	6.6526210459	0.1235437801	0.0008789601
C	7.0476488070	1.4609608474	0.0007948565
C	6.1040571483	2.4984465705	0.0008673656
C	4.7384720526	2.2269367219	0.0009740967
C	4.3200692519	0.8933393373	0.0009031252
C	5.2900223983	-0.1222007027	0.0009021473
C	3.0384920535	0.2099402768	0.0006071543
C	3.3533933659	-1.1686178147	0.0004772924
O	4.7111522247	-1.3731184063	0.0007328020
C	1.7046296070	0.6195745070	0.0002977050
C	0.7264047382	-0.3737218527	-0.0000906942
C	1.1019673426	-1.7363783690	-0.0001954146
C	2.4120116731	-2.1869219405	0.0000518218
C	-0.7264034423	-0.3737243818	-0.0002722157
C	-1.1019657127	-1.7364008025	-0.0004159264
O	0.0000129231	-2.5600103651	-0.0004614907
C	-1.7046371756	0.6195511838	-0.0002016561
C	-3.0384956697	0.2099152645	-0.0001832255
C	-3.3533773142	-1.1686752493	-0.0002599724
C	-2.4119855825	-2.1869308554	-0.0004032405
C	-4.3200847497	0.8932946461	-0.0002414464
C	-5.2900450430	-0.1222653265	-0.0003632872
O	-4.7111390474	-1.3731677772	-0.0002890298
C	-4.7385163112	2.2268850635	-0.0003671922
C	-6.1040936373	2.4983750162	-0.0007629669
C	-7.0476798434	1.4608672715	-0.0009565066
C	-6.6526159681	0.1234707786	-0.0007009361
H	7.3685604652	-0.6884636076	0.0008488110
H	8.1043873758	1.7006591844	0.0006227060
H	6.4451375953	3.5270806909	0.0007887885
H	4.0174907511	3.0364056874	0.0010605925
H	1.4395052954	1.6700520289	0.0003642605
H	2.6780058364	-3.2347889292	-0.0000701102
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H	-2.6779779461	-3.2348221471	-0.0004892377
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H	-6.4451922326	3.5270010001	-0.0009725240
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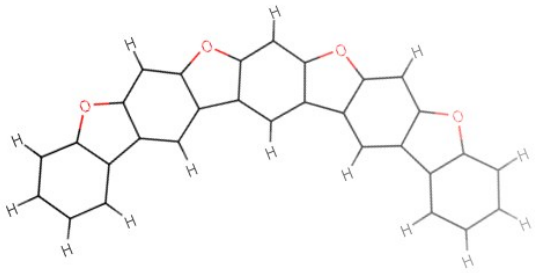

Carb4O

48

C	-7.9050166380	2.4801693309	0.3406720777
C	-8.5268747760	1.2319685579	0.3225569727
C	-7.7785026846	0.0471478570	0.2675133904
C	-6.3871592790	0.0775906645	0.2294921614
C	-5.7431447303	1.3180381244	0.2469588725
C	-6.5212175775	2.4859196493	0.3014384481
C	-4.3628187519	1.7692360832	0.2187495038
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O	-5.7348729856	3.6173271530	0.3087717388
C	-3.1212313732	1.1342520253	0.1642926731
C	-1.9848105904	1.9425330354	0.1474320596
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C	0.2429043653	0.5500125622	0.0365419217
C	1.6259630807	0.7283376602	-0.0131778280
C	2.1678219196	2.0333253771	-0.0035374073
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C	2.9381665233	-1.5482324994	-0.1306947026
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C	5.3349917211	-1.1406020287	-0.2279778126
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O	6.5326189407	-1.8068774535	-0.3045277139
C	4.3553949131	-4.6741127426	-0.2955240426
C	5.2698636684	-5.7212515336	-0.3732568385
C	6.6494155375	-5.4746742015	-0.4298445380
C	7.1528509884	-4.1744366777	-0.4098218976

H	-8.4687961575	3.4033231070	0.3823743277
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H	-8.2934109361	-0.9062905842	0.2538015661
H	-5.8181121955	-0.8439031576	0.1861943628
H	-3.0442656557	0.0538470953	0.1356874219
H	-3.4065189946	5.0984062867	0.2708599330
H	-0.1974328305	-0.4400800612	0.0304269147
H	1.8543968991	4.1832006351	0.0585464425
H	2.0870305672	-2.2185853508	-0.1109767328
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H	3.2912972757	-4.8763367862	-0.2534846199
H	4.9122015987	-6.7440283870	-0.3909212667
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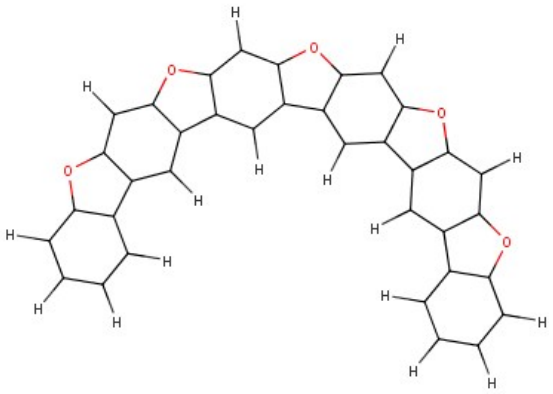

Carb5O

57

C	-8.2096118285	4.9262874484	0.5905832879
C	-8.9722697492	3.7587248848	0.5654702763
C	-8.3681412318	2.4969854751	0.4663048526
C	-6.9839354483	2.3671497336	0.3936385701
C	-6.2000859890	3.5239425021	0.4197965260
C	-6.8358267574	4.7728202433	0.5139392295
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C	-4.6821012207	5.2207350269	0.4290287804
O	-5.9213199395	5.8044667070	0.5195574504
C	-3.6196099569	3.0367744003	0.2838657954
C	-2.3969239777	3.7073322229	0.2577407597
C	-2.3661289147	5.1197905752	0.3112596540
C	-3.4887222860	5.9260113353	0.4003959203
C	-1.0057686056	3.2941079327	0.1794648429
C	-0.2575889669	4.4928671350	0.1836317571
O	-1.0759137708	5.5949204779	0.2659000773

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O	3.0960223935	3.1228781223	-0.0292454828
C	2.0704561686	-0.3354752884	-0.0737539044
C	3.3041342494	-0.9800572188	-0.1654979729
C	4.4948017635	-0.2205706158	-0.2116678088
C	4.5436103169	1.1636801102	-0.1698696693
C	3.7284925459	-2.3677898781	-0.2428923941
C	5.1388737857	-2.3245140867	-0.3308963747
O	5.6026062184	-1.0293545317	-0.3111436889
C	3.0681755104	-3.5961888690	-0.2519664234
C	3.8506992245	-4.7472963792	-0.3510831491
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C	3.5740517797	-6.1720449717	-0.4007341660
C	4.8266412376	-6.7978037095	-0.5103305491
O	5.8507532493	-5.8749405035	-0.5313483444
C	2.4233705944	-6.9645324862	-0.3677461181
C	2.5629922451	-8.3475188381	-0.4452223821
C	3.8285433583	-8.9419660762	-0.5538048816
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H	-8.6617893477	5.9070409169	0.6657628912
H	-10.0520318849	3.8293080942	0.6229813975
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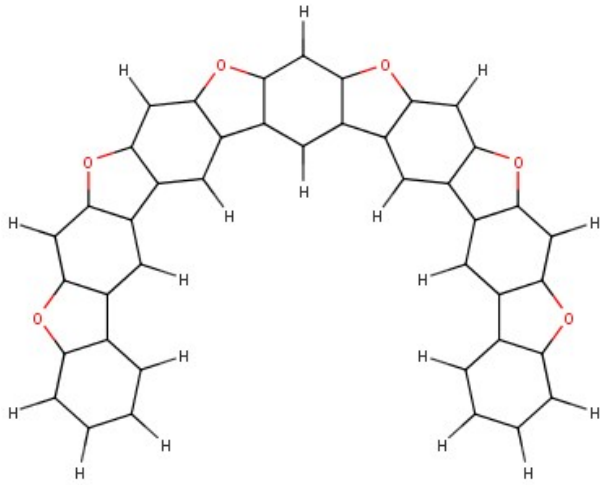

Carb6O

66

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C	-5.6479326764	5.7522574819	0.6743729867
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O	-5.0993144580	7.9811084546	0.8318552590
C	-3.1486860686	4.9709300661	0.4401521293
C	-1.8557846623	5.4925737161	0.4073664121
C	-1.6555066981	6.8879665015	0.5147954645
C	-2.6719418703	7.8179453841	0.6571271037
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O	-0.3189751277	7.2086260113	0.4664870232
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C	2.1980761556	4.6184148196	0.1228562475
C	1.7402465803	5.9201513629	0.2482657891
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O	3.5261672758	4.2732294649	0.0310054515
C	2.0999784803	0.9622907733	-0.1145590446
C	3.2505263012	0.1795218793	-0.2153214591
C	4.5221502256	0.7953683421	-0.2438421222
C	4.7322995927	2.1628897572	-0.1691789269
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O	5.5284775784	-0.1360883519	-0.3499985170
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O	5.2119231577	-4.9764763023	-0.6167635976
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H	1.6332752703	-2.3242346910	-0.2522817898
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H	0.7534103759	-5.0770641164	-0.3194169682
H	5.0414569874	-7.7230418295	-0.7739726869
H	-1.3231167217	-7.1182024009	-0.2819944262
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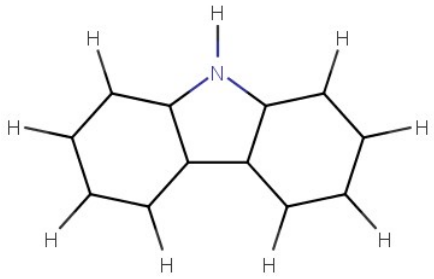

CarbN

22

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N	-0.0000005683	1.6577472650	-0.0000000084
C	-1.6947942659	-1.5065638474	-0.0000000506
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C	-3.4243609070	0.1987313236	0.0000000079
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H	4.4785419382	0.4513536735	0.0000000469
H	3.7994726690	-1.9237671096	-0.0000000028
H	1.4050545239	-2.5515037064	-0.0000000497
H	0.0000004329	2.6635967115	0.0000000178
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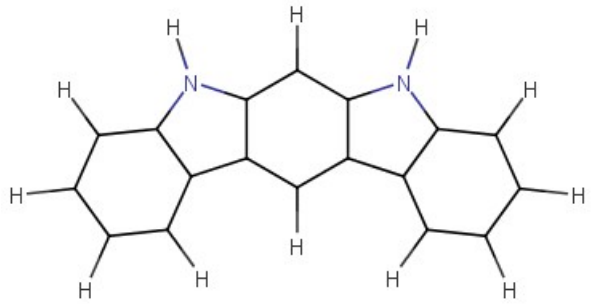

Carb2N

32

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C	-3.3602562836	-0.6466748875	0.0001956378
C	-1.1972165325	0.1470421067	-0.0011079044
C	-1.1784352248	-1.2808063975	-0.0006723980
N	-2.4897906298	-1.7292426874	-0.0001146112
C	0.0000008436	0.8600244156	-0.0014360649
C	1.1972208807	0.1470442533	-0.0011155902
C	1.1784419179	-1.2808041881	-0.0006832781
C	0.0000039116	-2.0239742445	-0.0005633579
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C	3.3602644225	-0.6466683719	0.0001704166
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C	4.6408422248	1.8072241005	0.0007135997
C	5.3825798859	0.6163481414	0.0015671569
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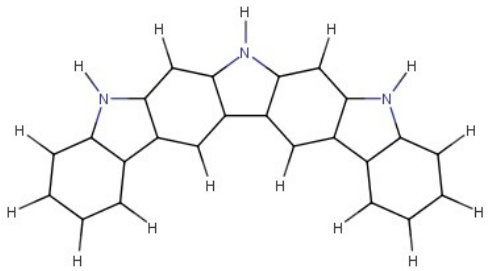

Carb3N

42

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N	-4.7897547668	-1.3168879272	0.0004951136
C	-1.6815198176	0.4880742623	-0.0009813810
C	-0.7267232205	-0.5250651822	-0.0008318827
C	-1.1383547203	-1.8912095288	-0.0003362415
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C	0.7267112960	-0.5250676184	-0.0008292143
C	1.1383386321	-1.8912133615	-0.0003309229
N	-0.0000094694	-2.6859903401	-0.0001937482
C	1.6815110922	0.4880692349	-0.0009776578
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C	3.4051184268	-1.2444179323	-0.0000051995
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C	5.8851265003	2.6744991204	0.0001678493
C	6.9260096471	1.7337480114	0.0009251002
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H	-0.0000110706	-3.6917148054	0.0004671151

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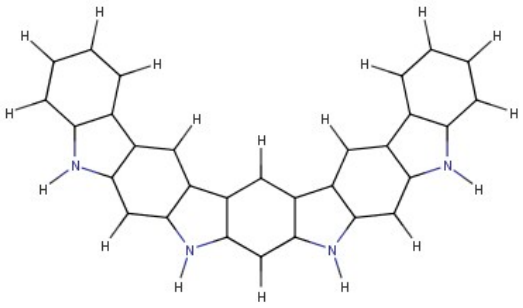

Carb4N

52

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H	6.1284097343	0.7057765580	-0.1506879213
H	1.9496154384	-2.1296806701	-0.1480945065
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H	-5.4176300116	-1.1756114429	0.1084409306
H	-7.8538429984	-1.6145711030	0.1618232804
H	-9.4667237488	0.2522387480	0.2913812350
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C	6.0569279161	-5.8368536286	-0.4322669182
C	4.6557399123	-5.8882738954	-0.3931194322
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C	4.5592741066	-3.4867175527	-0.2869429228
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C	3.9571600388	0.6533761119	-0.0869085675
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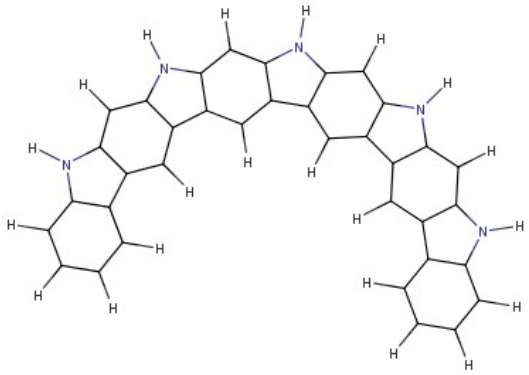

Carb5N

62

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C	-6.1347227129	2.9622244646	0.3417766486
C	-6.9840567779	4.0932973247	0.4317935329
C	-4.7720564489	3.4577212225	0.3335051687
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N	-6.1914622742	5.2331823371	0.4775383513
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C	-0.2741488245	4.5608320310	0.2714702467
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C	1.1364091968	2.1832680126	0.0954172256
C	1.7993224957	3.4430232851	0.1500013387
C	1.1158422363	4.6547002383	0.2387495468
C	2.1686067125	1.1673656769	0.0093358002
C	3.4201322671	1.8477847491	0.0145244408
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C	3.3351344653	-0.9169743114	-0.1432303624
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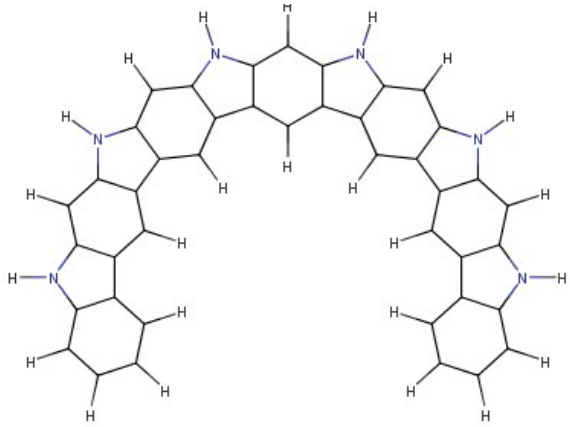

Carb6N

72

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C	2.2881957558	4.7249348981	0.2840705919
C	1.7019812553	5.9860143985	0.3851945301
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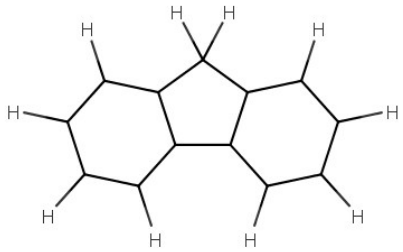

CarbC

23

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C	-0.7347970777	-0.4545837610	0.0000301293
C	-1.1829875130	0.8808888170	0.0000021822
C	-0.0000000883	1.8255363401	0.0000230467
C	-1.6526515020	-1.5057860734	0.0000165568
C	-3.0157221002	-1.2110770733	-0.0000464373
C	-3.4586624176	0.1143109767	-0.0000883738
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H	4.5220200875	0.3257807102	-0.0001504261
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H	-3.7398583318	-2.0180827618	-0.0000705342
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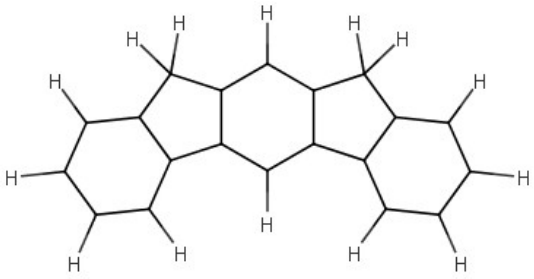

Carb2C

34

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C	1.1945740377	1.3761241235	0.0001996742
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C	-2.5879072402	-0.5012213424	-0.0000189726
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C	-3.1198294939	-1.7910968905	0.0004234876
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H	5.4797994212	1.3173948604	0.0005218525
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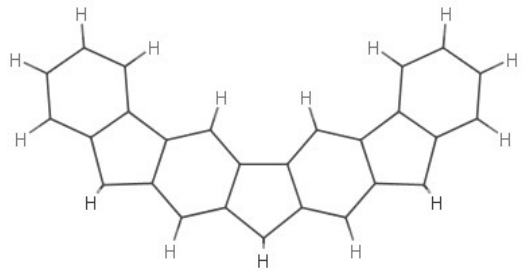

Carb3C

45

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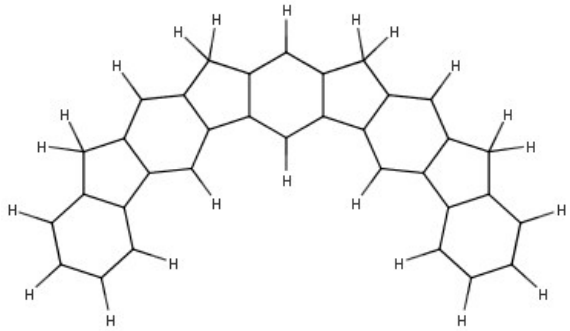

Carb4C

56

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C	-6.0791341649	3.0411698394	0.3252993509
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C	-1.9324895068	2.0198394961	0.1595778858
C	-2.2506732284	3.3927239432	0.2383022414
C	-3.5736639568	3.8190625314	0.2957202155
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C	2.2861858552	2.2019438556	0.0514913366
C	1.4858824534	3.3372073969	0.1311383759
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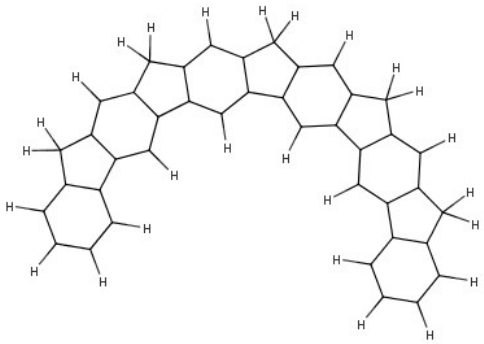

Carb5C

67

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C	-5.9232927089	2.4334217622	0.3038302767
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C	-4.6403660581	3.1489928697	0.3161799967
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C	-0.0872909185	2.2269813316	0.1449652224
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C	5.7661505260	-1.2376568180	-0.2174185749
C	2.6810921743	-3.3203237474	-0.2802689421
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C	4.5531918851	-4.8818553509	-0.4232628806
C	5.4760749456	-3.8411405104	-0.3767914478
C	2.4524632636	-5.9067324312	-0.4424290228
C	3.3986998620	-6.9458497820	-0.5315350385
C	4.7995768427	-6.3721086392	-0.5271000028
C	1.0873788154	-6.1960811143	-0.4287841901
C	0.6790625961	-7.5270023315	-0.5047325512
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H	-6.7372141443	5.3987841953	-0.3747662989
H	-3.1302019646	1.6046413395	0.1858136144

H	-4.0635561167	6.5218926377	0.5097814254
H	-1.1432263947	6.3425036318	1.3134196072
H	-1.1881131842	6.4581934793	-0.4417375617
H	-0.5700003548	1.2569030455	0.0966404291
H	1.6610126114	5.7427640412	0.3213103892
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H	1.2605446623	-0.5657176695	-0.0668521266
H	5.7486105782	1.6716946982	-0.0257212686
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H	1.6155366271	-3.1208822438	-0.2445290993
H	6.5430951258	-4.0404811666	-0.4135617002
H	5.3917884428	-6.7480103442	0.3154644638
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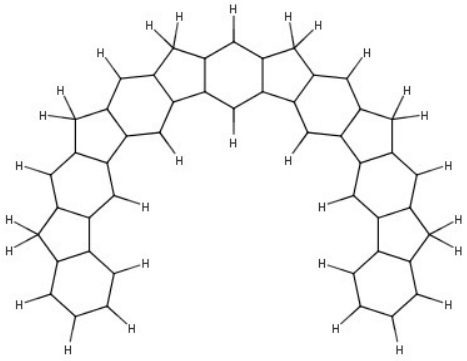

Carb6C

78

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C	-6.4950147888	4.9085224767	0.4838558383
C	-5.4832956071	3.9329539552	0.3941121695
C	-5.8139378234	2.5802353663	0.3019946724
C	-7.1590107734	2.2131487318	0.3011376631
C	-8.1620438888	3.1820533645	0.3909506350
C	-7.8332459054	4.5375472083	0.4828069604
C	-1.8165529679	4.9731134612	0.4040471677

C	-2.0318972779	6.3637989461	0.5096017690
C	-3.3210043985	6.8843164601	0.5698440042
C	-0.3706651844	4.7252998940	0.3592548389
C	0.3030297335	5.9628256477	0.4377243372
C	-0.7031041107	7.0905646038	0.5404219904
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C	1.7283440806	3.5912305574	0.2396757857
C	2.4025801587	4.8280022994	0.3198675620
C	1.6938330723	6.0221984833	0.4187909327
C	2.7247606173	2.5185792068	0.1451070899
C	4.0129635770	3.0942045420	0.1699305402
C	3.9000567290	4.6013077631	0.2813117292
C	2.5551977128	1.1389182096	0.0433977517
C	3.6982117463	0.3449514630	-0.0325403097
C	4.9870510453	0.9188078906	-0.0070830661
C	5.1525607718	2.2976352156	0.0945514712
C	3.8335090935	-1.1116669728	-0.1437801079
C	5.2059848511	-1.4356930649	-0.1856827592
C	6.0359915617	-0.1704116872	-0.1054137964
C	2.8567067906	-2.1045028305	-0.2053664162
C	3.2781455805	-3.4292553325	-0.3093054403
C	4.6506236283	-3.7541146598	-0.3509589589
C	5.6232877605	-2.7598145700	-0.2893505616
C	2.4982654008	-4.6699921591	-0.3933773852
C	3.3920588049	-5.7579656094	-0.4889724142
C	4.8208310561	-5.2546498580	-0.4687412068
C	1.1182791369	-4.8712984161	-0.3890295833
C	0.6491197114	-6.1809694751	-0.4825932460
C	1.5433526012	-7.2686396825	-0.5799927623
C	2.9204675470	-7.0638129144	-0.5836744294
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C	0.7685459538	-8.5671595171	-0.6693618829
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H	-3.4876678690	7.9545129668	0.6501550320
H	-0.5753527038	7.6677332464	1.4638521055
H	-0.6084467814	7.8030103685	-0.2876262615
H	-0.1806311262	2.5760654730	0.1982691109
H	2.2111669523	6.9751773744	0.4799378122

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H	6.1439116581	2.7408882375	0.1137371098
H	6.7064768487	-0.1741278159	0.7620562082
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H	1.8017962250	-1.8546820476	-0.1740622307
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H	1.0135558567	-9.2463545255	0.1555032713
H	0.9865126800	-9.1107158530	-1.5960104817
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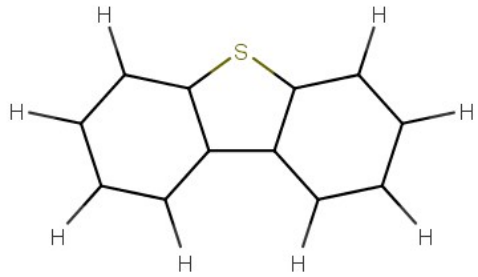

CarbS

21

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C	0.7353079581	-0.1427408277	0.0397607364
C	1.1949023857	1.1887460439	-0.0446186941
C	2.5556745319	1.4959977521	-0.0173244561
C	-0.7153151830	-0.2255504942	-0.0082753132
C	-1.3174215542	1.0451415877	-0.1286811147
S	-0.1283016323	2.3496781628	-0.1846186208
C	-1.5385261112	-1.3587765069	0.0474167773
C	-2.9178991272	-1.2156554516	-0.0167435684
C	-3.4976738385	0.0554725900	-0.1362885841
C	-2.7031250500	1.1948055651	-0.1929635182
H	4.5306186869	0.6751419773	0.1178620833
H	3.7589369933	-1.6745059926	0.2657401559
H	1.3497322646	-2.2065734942	0.2180477099
H	2.8945414108	2.5231590342	-0.0833340097
H	-1.0993569469	-2.3457544406	0.1400332941
H	-3.5527858230	-2.0929642266	0.0260976654
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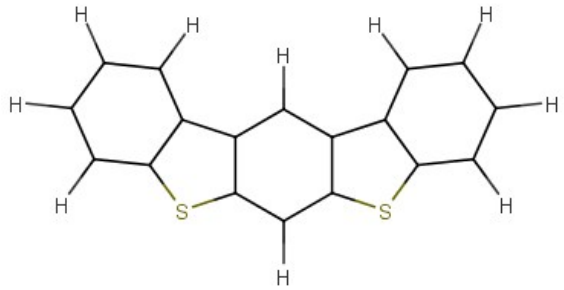
H	-3.1519872637	2.1768983194	-0.2842741902



Carb2S

30

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C	-3.3031685904	0.3836165311	0.0514998905
C	-2.4586814205	-0.7345782313	0.0320252602
C	-3.0380907517	-2.0205297218	0.0324238047
C	-4.4205874928	-2.2010720097	0.0521249711
C	-1.0048358238	-0.7852090440	0.0097901700
C	-0.5199399524	-2.1179510299	-0.0070685881
S	-1.8253836959	-3.3067068661	0.0049928260
C	-0.0943312340	0.2717939417	0.0039147618
C	1.2755722166	0.0086129081	-0.0191723759
C	1.7235249909	-1.3372002092	-0.0361608479
C	0.8396210338	-2.4112500047	-0.0300825051
C	2.3829908717	0.9519470851	-0.0291515745
C	3.6357479236	0.3045374437	-0.0536269188
S	3.4848154221	-1.4569923108	-0.0651134068
C	2.3500561986	2.3530024703	-0.0178697681
C	3.5370693494	3.0738000559	-0.0305070924
C	4.7721233495	2.4116880111	-0.0546898660
C	4.8310971006	1.0223620880	-0.0665641574
H	-6.3142984482	-1.1981960602	0.0869365741
H	-5.3319178044	1.0769697579	0.0860807437
H	-2.8825190130	1.3830111683	0.0511222283
H	-4.8516583955	-3.1952415264	0.0521661606
H	-0.4504819925	1.2955928560	0.0176769894
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H	1.3997403399	2.8747701396	0.0004012222
H	3.5087250683	4.1570898767	-0.0217011440
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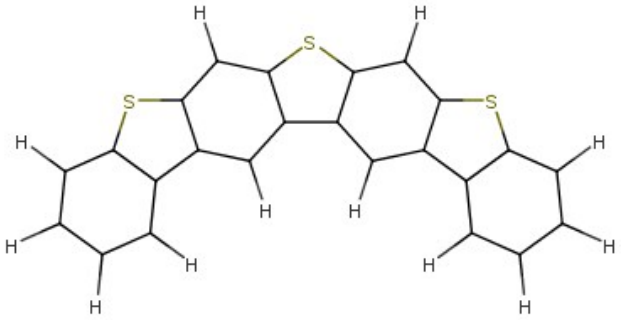

Carb3S

39

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C	-3.1933839992	2.5503338313	0.0918551245
C	-3.6519503489	3.8833316612	0.1434500761
C	-5.0119570282	4.1910018052	0.1502754677
C	-1.7408040399	2.4673320287	0.0938688048
C	-1.1365839526	3.7490345248	0.1488941475
S	-2.3269408816	5.0513276588	0.1971949841
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C	1.0247900830	2.7665843183	0.1191850192
C	0.2443739521	3.9157770654	0.1624360759
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C	2.7891529007	0.9672084005	0.0535825964
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C	2.4327970460	-1.7893788460	-0.0637590516
C	3.7276400089	-1.2120854742	-0.0327318240
C	3.9229807251	0.1639140537	0.0257694516
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C	3.8108344986	-3.7274065114	-0.1389584186
S	5.0064506056	-2.4276532828	-0.0777223222
C	1.4325482497	-4.1651653320	-0.1670770863
C	1.7053111623	-5.5255663085	-0.2228257678
C	3.0282148558	-5.9871462122	-0.2369578415
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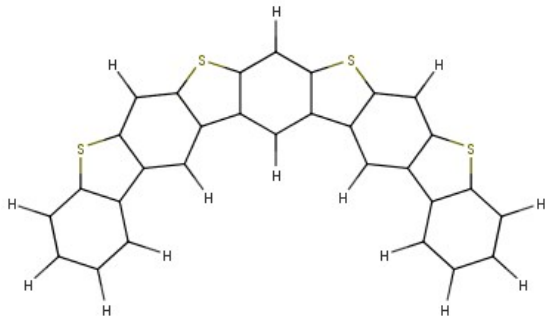

Carb4S

48

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C	-3.1107487810	4.0915181648	0.1695135839
C	-3.5800401023	5.4194327859	0.2406923844
C	-4.9427166901	5.7153529839	0.2359990969
C	-1.6584569904	4.0189604743	0.1866799963
C	-1.0626010907	5.3027659216	0.2723978148
S	-2.2635963815	6.5953978947	0.3331331149
C	-0.8419283885	2.8890685312	0.1308764565
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C	1.1045178527	4.3317874399	0.2436754287
C	0.3176023009	5.4765818099	0.3018052173
C	1.5675147703	1.9966554620	0.1149148157
C	2.8759707380	2.5392933062	0.1612363243
S	2.8711419157	4.3030384777	0.2631764171
C	1.4062630803	0.6127394254	0.0396397162
C	2.5266231529	-0.2183351087	0.0126227808
C	3.8188107359	0.3627193624	0.0565095903
C	4.0118819628	1.7378012785	0.1305096229
C	2.5817144983	-1.6719953060	-0.0562048340
C	3.9153219854	-2.1535833837	-0.0665529307
S	5.1035981375	-0.8485910351	0.0092240609
C	1.5285300572	-2.5855665360	-0.1076239831
C	1.7965662893	-3.9540386667	-0.1718709168
C	3.1440324817	-4.3963784650	-0.1818151146
C	4.2146340064	-3.5096215734	-0.1287605695
C	0.8589849905	-5.0650245411	-0.2387230186
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H	0.4120301297	0.1817967978	0.0041137789
H	5.0057756770	2.1669742730	0.1637844106
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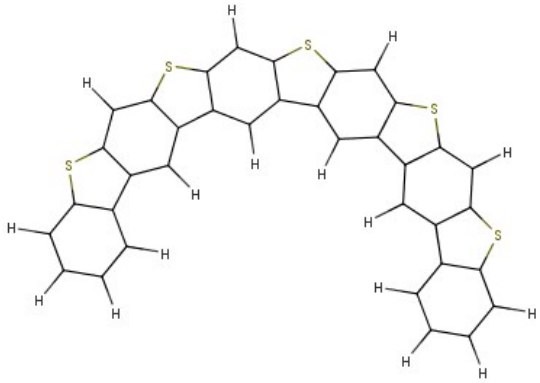
H	1.3235244301	-8.4611885955	-0.4226399178



Carb5S

57

C	-5.1268232331	5.7295992218	0.2079415007
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C	-3.3204973159	4.1167194618	0.1288126772
C	-2.3865036086	5.1563060979	0.2341546153
C	-2.8576221708	6.4827084421	0.3250507361
C	-4.2202272472	6.7786653168	0.3131098213
C	-0.9338867192	5.0845964694	0.2682863264
C	-0.3420890665	6.3681842822	0.3827008809
S	-1.5443557263	7.6585119312	0.4516864238
C	-0.1126995735	3.9575668391	0.2074888833
C	1.2736221960	4.1031691532	0.2599710942
C	1.8279459304	5.4037917532	0.3704566269
C	1.0368498868	6.5448675605	0.4335550727

C	2.3016136160	3.0727284175	0.2182097181
C	3.6069594038	3.6206449286	0.2912668262
S	3.5939459958	5.3824605994	0.4169405776
C	2.1498409090	1.6887646992	0.1239473112
C	3.2756111966	0.8643423677	0.1022383126
C	4.5640269323	1.4510487658	0.1706435035
C	4.7475073683	2.8258698665	0.2661832630
C	3.3399301600	-0.5875316953	0.0177465826
C	4.6753238396	-1.0622585709	0.0177651169
S	5.8562184866	0.2473816110	0.1231135800
C	2.2914732509	-1.5056289397	-0.0519617661
C	2.5659719565	-2.8719143350	-0.1213705718
C	3.9146827576	-3.3078529424	-0.1188993998
C	4.9805572884	-2.4172715297	-0.0511752324
C	1.6309825112	-3.9852072737	-0.1958706659
C	2.2952810415	-5.2369123506	-0.2425288438
S	4.0539623993	-5.0670646294	-0.2032358373
C	0.2368316617	-3.9531359810	-0.2249351806
C	-0.4855446731	-5.1451294714	-0.2967021650
C	0.2142609099	-6.3777833626	-0.3379243635
C	1.6040682039	-6.4409159785	-0.3117003978
C	-1.9270013702	-5.3356864937	-0.3387488042
C	-2.2834491110	-6.6986227701	-0.4103545123
S	-0.8736441336	-7.7648246059	-0.4265835363
C	-2.9462764333	-4.3740976773	-0.3167983013
C	-4.2757121525	-4.7723904614	-0.3651173082
C	-4.6092667145	-6.1317713969	-0.4372027886
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H	-6.1896418500	5.9416161774	0.1971159025
H	-5.3994556426	3.5993850521	0.0344593078
H	-2.9849683619	3.0881770989	0.0563922661
H	-4.5675218837	7.8025473450	0.3851331116
H	-0.5538491655	2.9709887216	0.1207404083
H	1.4762862231	7.5311147051	0.5185875839
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H	5.7380973817	3.2604324656	0.3194218332
H	1.2644692366	-1.1583183088	-0.0477925988
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H	-2.6986706068	-3.3199262525	-0.2617362957
H	-5.0624645798	-4.0272671653	-0.3471840031
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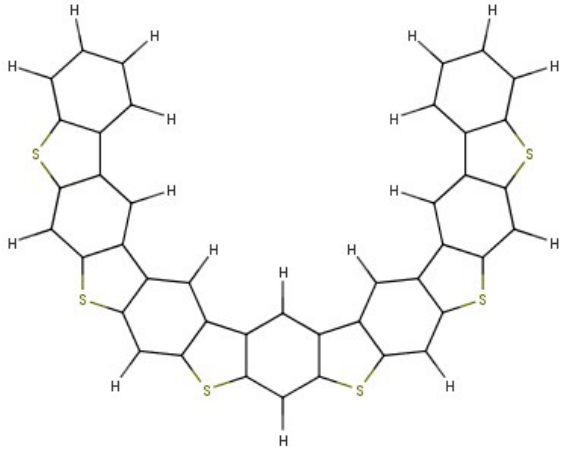

Carb6S

66

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C	-2.3409226670	4.5480184454	-0.0208678066
C	-1.4092294490	5.5762848452	0.1721828301
C	-1.8770524559	6.9037684006	0.2566050025
C	-3.2322337833	7.2109059514	0.1533597486
C	0.0367194173	5.4948385599	0.3029361417
C	0.6246067457	6.7727378972	0.4815208693
S	-0.5708673303	8.0618997071	0.4955080226
C	0.8567495791	4.3666567680	0.2724160710
C	2.2370599670	4.5041984304	0.4144167509
C	2.7869626436	5.7997790632	0.5856817929
C	1.9968380065	6.9409655025	0.6246963371
C	3.2643743669	3.4733479491	0.4050178256
C	4.5640592974	4.0178663730	0.5573929435
S	4.5413150504	5.7693128027	0.7268914181
C	3.1188527026	2.0927101811	0.2710204705
C	4.2438980348	1.2681690427	0.2814428203
C	5.5270791950	1.8531075092	0.4223816362
C	5.7036170523	3.2233919843	0.5668533509
C	4.3157332082	-0.1797811031	0.1568828941
C	5.6524587593	-0.6496051086	0.1866382151
S	6.8163717881	0.6556111975	0.3844891069
C	3.2755599906	-1.1000389349	0.0290238441
C	3.5585134362	-2.4617809443	-0.0758787155
C	4.9093487968	-2.8902691528	-0.0592225385
C	5.9663014086	-1.9987117606	0.0764419766
C	2.6341305429	-3.5775082706	-0.2071068728
C	3.3099425924	-4.8194185266	-0.3021265897
S	5.0587870276	-4.6366754590	-0.2202813646
C	1.2398907174	-3.5590501948	-0.2358545328
C	0.5290586001	-4.7522501856	-0.3606522510

C	1.2417955203	-5.9727264735	-0.4650870993
C	2.6300423374	-6.0237314196	-0.4354603784
C	-0.9108945093	-4.9562742418	-0.3952670530
C	-1.2507490463	-6.3257385399	-0.5332248571
S	0.1708689975	-7.3610663604	-0.6189790734
C	-1.9300657500	-4.0095660417	-0.3036853142
C	-3.2639151326	-4.4149754373	-0.3482826942
C	-3.5638246742	-5.7929525112	-0.4937840332
C	-2.5690295918	-6.7595505627	-0.5875156007
C	-4.4666247433	-3.6035652619	-0.2577194723
C	-5.6405140405	-4.3801624715	-0.3403355927
S	-5.2955456613	-6.0978849215	-0.5305697998
C	-4.5882519159	-2.2167564677	-0.1031649163
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H	0.4193725715	3.3831198972	0.1370521132
H	2.4331022058	7.9243916275	0.7556612872
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H	6.9943338600	-2.3413449724	0.0958581583
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H	3.1611121845	-6.9656572732	-0.5084758748
H	-1.6867467949	-2.9581455325	-0.1934157228
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H	-3.7015878966	-1.5948125179	-0.0356492471
H	-5.9369931301	-0.5617554401	0.0871728659
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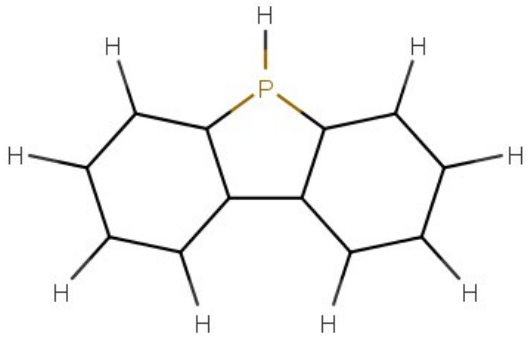

CarbP

22

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C	0.7812036510	0.0439729082	-0.0246694276
C	0.9593878089	-1.2582000841	0.4893429439
C	2.2367743123	-1.8006187815	0.6118314520
C	-0.6274160505	0.4619624237	-0.0754266903
C	-1.5197212402	-0.5230826447	0.3989066671
P	-0.6327269919	-2.0071039733	1.0339546465
C	-1.1325234338	1.6841529837	-0.5318917854
C	-2.5051346978	1.9138690597	-0.5185537758
C	-3.3841178105	0.9365587039	-0.0441215411
C	-2.8912188651	-0.2801285939	0.4261902497
H	4.3378578457	-1.4789827494	0.2825958768
H	4.0358900464	0.8055537967	-0.6250573609
H	1.7805516944	1.7860595163	-0.8212080286
H	2.3755838800	-2.7934969441	1.0260138593
H	-0.8437215448	-2.8599977950	-0.0907531487
H	-0.4619204887	2.4527620722	-0.8994481310
H	-2.8943677207	2.8610606988	-0.8744515124
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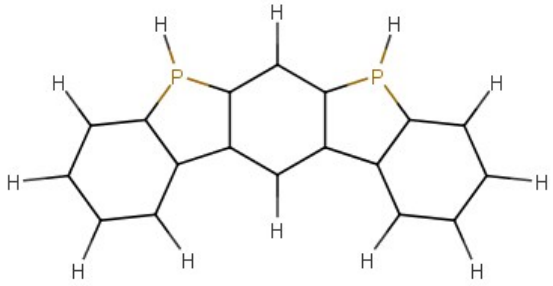
H	-3.5757525607	-1.0290363273	0.8099548106



Carb2P

32

C	-5.1604651876	1.0889571368	-0.8944024875
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C	-2.8223387515	1.6432800746	-0.5914730412
C	-2.5256717043	0.2894692070	-0.4000209753
C	-3.5654212583	-0.6626888986	-0.4582747109
C	-4.8791492171	-0.2615554887	-0.6913844041
C	-1.2060675881	-0.3034714448	-0.1364834279
C	-1.2460160236	-1.7097906280	0.0066787533
P	-2.9645857661	-2.3639251854	-0.0876109076
C	0.0110255060	0.3728227497	-0.0330783336
C	1.1827104823	-0.3444667272	0.2147523321
C	1.1297501686	-1.7495048824	0.3668311905
C	-0.0810169751	-2.4297801875	0.2604188755
C	2.5409963930	0.2016411667	0.3526043811
C	3.5168239431	-0.7839915783	0.6125775439
P	2.8026911463	-2.4816466770	0.6027987350
C	2.9284208060	1.5425922807	0.2547907709
C	4.2657846502	1.8901920418	0.4205407990
C	5.2282734607	0.9095927639	0.6746587290
C	4.8566352683	-0.4315120167	0.7601192720
H	-6.1794355133	1.4057108598	-1.0854057516
H	-4.3610853913	3.0848801567	-0.9930652070
H	-2.0373727099	2.3900534427	-0.5485091120
H	-5.6816612671	-0.9910288576	-0.7160827941
H	-2.9177527258	-2.8522238119	-1.4278953591
H	0.0449457072	1.4505282055	-0.1457375745
H	-0.1164877820	-3.5086146274	0.3731818091
H	2.7363101225	-2.6740104994	2.0154731630
H	2.1945346251	2.3146948857	0.0521665518
H	4.5627594617	2.9301632643	0.3464636182
H	6.2680586948	1.1903094957	0.7973949022
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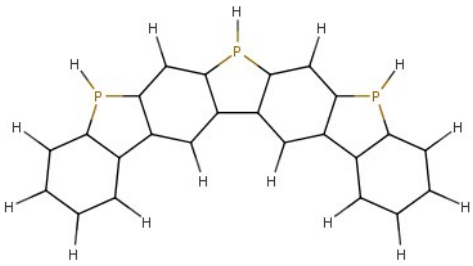

Carb3P

42

C	-6.0423579501	2.7113517969	0.1534481602
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C	-4.1100248631	1.2548984585	0.0579106177
C	-3.2683097621	2.3724455073	0.0347588903
C	-3.8320801892	3.6656073858	0.0648607110
C	-5.2144762091	3.8325537920	0.1117720283
C	-1.7986959176	2.3784985293	-0.0152739867
C	-1.2471235992	3.6805895078	-0.0305276235
P	-2.5501063485	4.9805866623	-0.0781886905
C	-0.9570641420	1.2656807515	-0.0508290109
C	0.4269163740	1.4450306369	-0.0875026928
C	0.9678768754	2.7513916455	-0.1026543072
C	0.1316623114	3.8652879748	-0.1009937446
C	1.4523062720	0.3921583258	-0.1237937192
C	2.7715633906	0.8993292462	-0.1645590573
P	2.8027023917	2.7379794369	-0.2561719834
C	1.2364601244	-0.9871165054	-0.1322135997
C	2.3266035717	-1.8580664808	-0.1651559581
C	3.6418974553	-1.3402539895	-0.2044940754
C	3.8617846454	0.0349473584	-0.2309027156
C	2.2827513469	-3.3277873241	-0.1717913378
C	3.5602460151	-3.9257445950	-0.2119530497
P	4.9040183519	-2.6728095041	-0.3476590622
C	1.1441154830	-4.1402913755	-0.1404672470
C	1.2815633733	-5.5250200433	-0.1392760249
C	2.5490511562	-6.1121492932	-0.1801613868
C	3.6905023219	-5.3127531369	-0.2287182568
H	-7.1181433529	2.8357891679	0.2016938308
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H	-3.6957812898	0.2532413317	0.0283482088
H	-5.6496269904	4.8261774499	0.1174948122
H	-2.5025360218	5.3600454204	1.2969126941
H	-1.3798739076	0.2673182309	-0.0456579018
H	0.5498118583	4.8653905390	-0.1537544983
H	3.1180057900	2.9995538316	1.1114525675
H	0.2273766690	-1.3831508827	-0.1107366851

H	4.8705600014	0.4286593107	-0.3033510544
H	5.3284001000	-2.6922693189	1.0149517930
H	0.1540682002	-3.6988867251	-0.1145114632
H	0.3978261955	-6.1525180820	-0.1112010249
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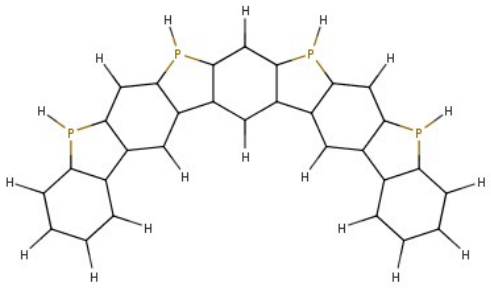
H	4.6714297041	-5.7733104403	-0.2770059011



Carb4P

52

C	-6.0209338836	4.0282930438	0.2182805343
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C	-4.0359729217	2.6483465826	0.0796513362
C	-3.2351248796	3.7947077727	0.1206928179
C	-3.8457669463	5.0639955148	0.2062974253
C	-5.2338763687	5.1789389634	0.2427761617
C	-1.7662593476	3.8537676223	0.0905547216
C	-1.2618630928	5.1736508618	0.1478296776
P	-2.6095766902	6.4279735376	0.1389918343
C	-0.8842797493	2.7744486912	0.0146055593
C	0.4927677464	3.0046655025	0.0141557172
C	0.9862473984	4.3284717234	0.0718887015
C	0.1102024069	5.4106426711	0.1114326172
C	1.5565783599	1.9916216731	-0.0451079253
C	2.8572386798	2.5466394457	-0.0326726204
P	2.8221276279	4.3874811621	-0.0485607323
C	1.3923444827	0.6072194230	-0.1139192606
C	2.5143008214	-0.2223496761	-0.1518551266
C	3.8103645428	0.3432860188	-0.1405251769
C	3.9797917133	1.7253439781	-0.1065142250
C	2.5224795093	-1.6915112975	-0.2120225546
C	3.8249464472	-2.2401193387	-0.2517205341
P	5.1232852656	-0.9359573927	-0.3118084944
C	1.4102337570	-2.5352034895	-0.2354188463
C	1.5913582583	-3.9184974321	-0.2826506200
C	2.8988821734	-4.4563173774	-0.3233070818
C	4.0110222258	-3.6179229450	-0.3342224058
C	0.5417391742	-4.9481945964	-0.2985654671

C	1.0491795481	-6.2640474828	-0.3473954365
P	2.8854230312	-6.2900758342	-0.4865156587
C	-0.8425227464	-4.7471877579	-0.2675625026
C	-1.7016512378	-5.8418924698	-0.2776919531
C	-1.1937065486	-7.1425933146	-0.3280340818
C	0.1833953198	-7.3553537142	-0.3745272775
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H	-3.5845860092	1.6651138243	0.0083454498
H	-5.7049180842	6.1548977020	0.2901637917
H	-2.5914275009	6.7508666962	1.5290166419
H	-1.2686504219	1.7619330790	-0.0383937533
H	0.4928460285	6.4262319752	0.1154734425
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H	0.3979409305	0.1756114199	-0.1349037121
H	4.9749352315	2.1573938590	-0.1369031233
H	5.5273739726	-0.9936927443	1.0560655448
H	0.4105109535	-2.1160852628	-0.2111427478
H	5.0112364423	-4.0332319108	-0.4038806608
H	3.1835154600	-6.6133836030	0.8712691587
H	-1.2541253427	-3.7444759772	-0.2340635167
H	-2.7737731789	-5.6831059488	-0.2526320185
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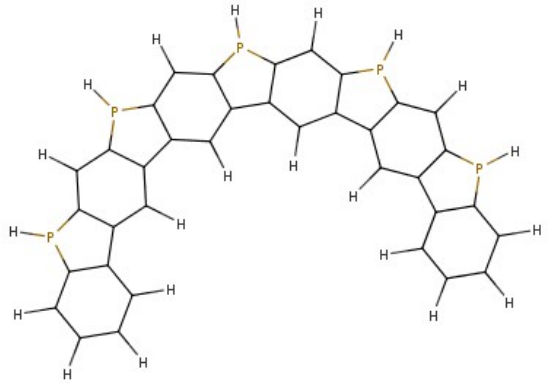

Carb5P

62

C	-5.4154903363	4.6406924691	0.2015499184
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C	-3.3476864295	3.3847005690	0.1161879585
C	-2.6201223454	4.5780835646	0.1822199673
C	-3.3079717436	5.8075223781	0.2581181813
C	-4.7013008180	5.8373399811	0.2533626561
C	-1.1581712039	4.7259823076	0.1857270369
C	-0.7314177867	6.0719447648	0.2664250214
P	-2.1526026830	7.2436582229	0.2407473049
C	-0.2148346797	3.7014572283	0.1135048631
C	1.1454801356	4.0114040083	0.1397520081
C	1.5648662002	5.3585391073	0.2224410413
C	0.6261467806	6.3881411226	0.2591541834
C	2.2598217865	3.0574363752	0.0848700218
C	3.5314387393	3.6736464345	0.1262295354
P	3.3994203667	5.5120306020	0.1318344795
C	2.1603440402	1.6696292337	-0.0029189206
C	3.3190100402	0.8945855870	-0.0290870224
C	4.5878588983	1.5159608202	0.0138990265
C	4.6927228128	2.9049023669	0.0652141218
C	3.3872427775	-0.5695583142	-0.1025321303
C	4.7089165156	-1.0697833323	-0.1135063896
P	5.9546023778	0.2885076385	-0.1379599542
C	2.3067689145	-1.4490182473	-0.1638066921
C	2.5378406123	-2.8228784782	-0.2193028331
C	3.8619729296	-3.3177347746	-0.2260755762
C	4.9452768409	-2.4408306824	-0.1993184536
C	1.5189179966	-3.8777665507	-0.2828236791
C	2.0635406038	-5.1808858289	-0.3347497548
P	3.9057336854	-5.1514144711	-0.4064469943
C	0.1357320516	-3.6967428634	-0.3067455243
C	-0.7057180970	-4.8070729076	-0.3686905979
C	-0.1540315624	-6.1080349043	-0.4221061187
C	1.2276126039	-6.2922324508	-0.4290677158
C	-2.1748771834	-4.7948975385	-0.4008456963

C	-2.7437998024	-6.0831756321	-0.4827761749
P	-1.4565347289	-7.3964436564	-0.6153311929
C	-3.0105640109	-3.6733745953	-0.3620665386
C	-4.3915043648	-3.8378279780	-0.4020946331
C	-4.9508781308	-5.1153442478	-0.4908741701
C	-4.1274276996	-6.2397230389	-0.5419909836
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H	-5.3001208968	2.4942326577	0.0827623043
H	-2.8362137809	2.4304604520	0.0561103251
H	-5.2336418736	6.7816947440	0.2900434417
H	-2.1862026785	7.5423465822	1.6359394903
H	-0.5359227887	2.6688134287	0.0387612711
H	0.9486231682	7.4240548867	0.2842015400
H	3.6547639783	5.7239638294	1.5200995132
H	1.1867048859	1.1951104410	-0.0440387988
H	5.6674925267	3.3817781421	0.0601470051
H	6.3303101418	0.2385538500	1.2379111433
H	1.2924641096	-1.0663103466	-0.1645090222
H	5.9608816625	-2.8208041685	-0.2434372530
H	4.1661708804	-5.4766704377	0.9588346182
H	-0.2862688398	-2.6985287086	-0.2782301760
H	1.6479626055	-7.2897366546	-0.5070763881
H	-1.4915554974	-7.8456884352	0.7387878949
H	-2.5901604312	-2.6758062321	-0.2992838700
H	-5.0376055722	-2.9677024941	-0.3708767818
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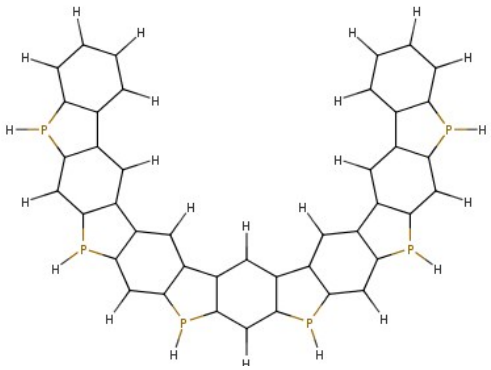

Carb6P

72

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C	-1.8423291098	4.8905366849	0.3083534013
C	-2.5496060937	6.1114248873	0.3227154385

C	-3.9420290726	6.1217802744	0.3643062691
C	-0.3830728400	5.0620020263	0.2615505937
C	0.0171381344	6.4186555256	0.2603145861
P	-1.4234892421	7.5619593275	0.1836584742
C	0.5803881296	4.0527734582	0.2208694081
C	1.9352716385	4.3894167900	0.2090721616
C	2.3245474651	5.7488083889	0.2292178607
C	1.3670230704	6.7602178827	0.2236123880
C	3.0747991364	3.4606677924	0.1759425810
C	4.3279617495	4.1156630516	0.2001987756
P	4.1524246005	5.9470599426	0.1374366528
C	3.0193448345	2.0670884898	0.1105957708
C	4.2025060799	1.3263685803	0.0937555962
C	5.4498857042	1.9916996073	0.1371781088
C	5.5115661482	3.3827159099	0.1623485881
C	4.3278233829	-0.1373642644	0.0237370105
C	5.6705606734	-0.5812481212	0.0348802209
P	6.8643001635	0.8196565980	0.0180171653
C	3.2893667585	-1.0668074915	-0.0633333126
C	3.5830874044	-2.4309360366	-0.1167404568
C	4.9293460962	-2.8633504431	-0.0899509708
C	5.9700206874	-1.9391691882	-0.0422228363
C	2.6206952656	-3.5397390350	-0.2059877408
C	3.2380024026	-4.8121034717	-0.2267468161
P	5.0743274989	-4.6904480129	-0.2573233822
C	1.2297309566	-3.4414905281	-0.2772963200
C	0.4550093206	-4.6012846431	-0.3401631284
C	1.0832675486	-5.8684360344	-0.3432579281
C	2.4716264719	-5.9714089201	-0.3162515767
C	-1.0121256322	-4.6815030531	-0.4072385995
C	-1.4954090615	-6.0101563440	-0.4357893725
P	-0.1305173988	-7.2425013320	-0.5086300476
C	-1.9109164854	-3.6136599660	-0.4529702734
C	-3.2833271634	-3.8654681187	-0.5006619300
C	-3.7555789498	-5.1985081683	-0.5083764671
C	-2.8625237203	-6.2670367022	-0.5054971527
C	-4.3643046054	-2.8697820718	-0.5522887812
C	-5.6533576547	-3.4435290972	-0.5763607214
P	-5.5888279628	-5.2827796439	-0.6533410588
C	-4.2328028877	-1.4774776501	-0.5872217989
C	-5.3691056750	-0.6756261199	-0.6346181468
C	-6.6431352353	-1.2488912201	-0.6519374037
C	-6.7865276723	-2.6353731791	-0.6349856822
H	-5.7202313434	4.9174190122	0.4729667528
H	-4.4883774262	2.7688173686	0.4734725887
H	-2.0259008300	2.7378076846	0.3513811544
H	-4.4866328645	7.0597518189	0.3524723201
H	-1.4415827118	7.9551051246	1.5552330651
H	0.2799397734	3.0112354696	0.2060318366

H	1.6695009937	7.8019879668	0.1903256405
H	4.3889159520	6.2205787354	1.5184378808
H	2.0603418478	1.5627074196	0.0744291652
H	6.4707516464	3.8901396840	0.1466249413
H	7.2195700367	0.7982226669	1.4003613918
H	2.2583092924	-0.7322529892	-0.0870687045
H	7.0022401392	-2.2732954202	-0.0701394130
H	5.3182116246	-4.9958134224	1.1155922133
H	0.7517872934	-2.4682941277	-0.2783386673
H	2.9509216667	-6.9438205608	-0.3663210091
H	-0.1519751725	-7.6499003144	0.8591546925
H	-1.5449991276	-2.5929348116	-0.4486193340
H	-3.2274026421	-7.2877240727	-0.5609666528
H	-5.8801027348	-5.5494869930	0.7182158586
H	-3.2510332497	-1.0171189319	-0.5824966661
H	-5.2642392597	0.4027565703	-0.6698089960
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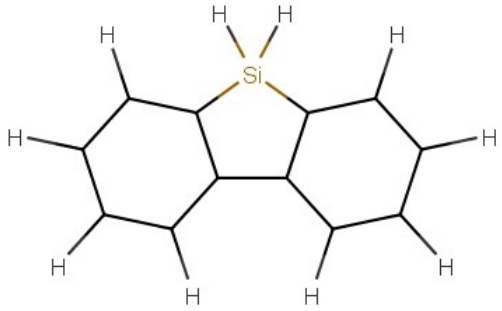

CarbSi

23

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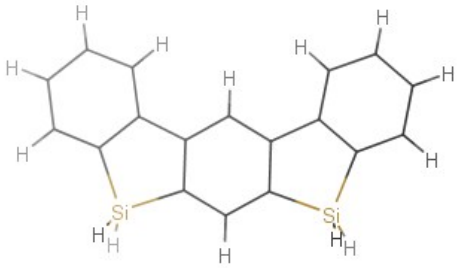
C	0.7824449497	0.2357179607	0.1176860623
C	1.1869619805	-1.1214683648	0.0989982643
C	2.5347253470	-1.4425769003	0.2576835745
C	-0.6758446198	0.4703055702	-0.0626889973
C	-1.4625427386	-0.6961281675	-0.2257242320
Si	-0.3325673919	-2.1952955999	-0.1567074989
C	-1.2919926570	1.7253311816	-0.0818394809
C	-2.6703947056	1.8232184284	-0.2594249418
C	-3.4477699747	0.6763389960	-0.4198086781
C	-2.8409062515	-0.5805602741	-0.4026188106
H	4.5315411332	-0.6893457422	0.5568344823
H	3.8196772744	1.6843776984	0.5904979693
H	1.4508410854	2.2822837274	0.3145806802
H	2.8568941611	-2.4790280400	0.2453875963
H	-0.6192192876	-3.1225663754	0.9694104301
H	-0.3085020274	-2.9984563095	-1.4073617160
H	-0.7078368683	2.6302392238	0.0404559136
H	-3.1400776550	2.8006070519	-0.2725476253
H	-4.5197729466	0.7616206685	-0.5574675971
H	-3.4539598348	-1.4671591381	-0.5299221919



Carb2Si

34

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C	-2.6923742561	1.8015425777	-0.6479124541
C	-2.5083128150	0.4286092013	-0.4582428142
C	-3.6210755794	-0.4434392019	-0.5433835179
C	-4.8864145742	0.0769644359	-0.8142371622
C	-1.2044763450	-0.2270650798	-0.1674191820
C	-1.2536882769	-1.6349582505	-0.0188843423
Si	-3.0298025115	-2.2033566785	-0.2491323985
C	0.0128485719	0.4466441617	-0.0406781366
C	1.1851224799	-0.2627245791	0.2299152219
C	1.1418546506	-1.6711501794	0.3797636400
C	-0.0782868264	-2.3369913589	0.2531049087
C	2.5322339336	0.3519968630	0.3800293448
C	3.5854021967	-0.5551515503	0.6517991452
Si	2.8779632564	-2.2944118807	0.7317612730
C	2.8111800945	1.7181628085	0.2720113829
C	4.1159476413	2.1792003758	0.4316295507
C	5.1545577145	1.2881364157	0.7001533500
C	4.8857437691	-0.0768484471	0.8095137040
H	-6.0461249275	1.8488104631	-1.2123157883
H	-4.0962898609	3.3709733305	-1.0643484017
H	-1.8532408628	2.4849441103	-0.5876976302
H	-5.7462855262	-0.5817219070	-0.8820543830
H	-3.6252351362	-2.8498518170	0.9505267132
H	-3.2360358833	-3.1129336436	-1.4074655803
H	0.0471318930	1.5234942210	-0.1530793312
H	-0.1140486151	-3.4167409272	0.3673279637
H	3.4192395058	-3.2166646346	-0.3016081261
H	3.0358481102	-2.9503647962	2.0571235315
H	2.0195212471	2.4289009380	0.0646080946
H	4.3231627533	3.2401147481	0.3458722167
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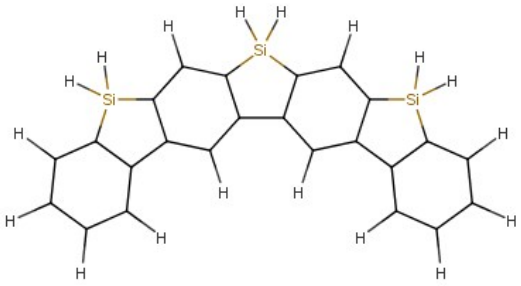
H	5.7000293292	-0.7631026563	1.0189276201



Carb3Si

45

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C	-4.0367497330	0.9510437135	-0.0292422175
C	-3.3352262603	2.1586284770	0.0411694316
C	-4.0514139631	3.3795014673	0.0903560981
C	-5.4455158743	3.3638312185	0.0685038298
C	-1.8529160211	2.2865038326	0.0773805755
C	-1.3618167850	3.6128913005	0.1636234385
Si	-2.8207547127	4.7955195984	0.1867863447
C	-0.9606245532	1.2129343486	0.0352576570
C	0.4167187704	1.4405579625	0.0844222041
C	0.9129086348	2.7643457952	0.1760354123
C	0.0155980926	3.8326513566	0.2123354716
C	1.4536231601	0.3733369297	0.0499228738
C	2.7933162693	0.8288222633	0.1167420532
Si	2.7888030190	2.7033519945	0.2301632199
C	1.1845396443	-0.9945656981	-0.0408681190
C	2.2324522001	-1.9175064831	-0.0625621986
C	3.5743361832	-1.4670665932	0.0045168211
C	3.8356207195	-0.0989205698	0.0926718478
C	2.0607340684	-3.3932435488	-0.1521174287
C	3.2615177998	-4.1442892592	-0.1569259263
Si	4.7141444660	-2.9581492174	-0.0479432992
C	0.8325616285	-4.0577755354	-0.2266165011
C	0.7948829177	-5.4481292479	-0.3038559630
C	1.9757798066	-6.1898266156	-0.3076710096
C	3.2061045389	-5.5353334577	-0.2345600222
H	-7.2210317036	2.1463108353	-0.0161952671
H	-5.9656187401	0.0118157507	-0.1030418823
H	-3.5075240790	0.0057857934	-0.0660842158
H	-6.0043673926	4.2934463405	0.1068976747
H	-2.9293947652	5.6121262268	1.4247302042
H	-2.8702346088	5.7219054185	-0.9756675652

H	-1.3401087812	0.2005589638	-0.0364121109
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H	3.3795462053	3.2395269026	1.4852283283
H	3.4535080560	3.3835254312	-0.9131874789
H	0.1598223305	-1.3421543822	-0.0962139405
H	4.8636357418	0.2491586180	0.1440242406
H	5.5498011855	-3.1318850987	1.1697988390
H	5.6172292424	-2.9947435125	-1.2289971267
H	-0.0980425950	-3.5018229533	-0.2246114449
H	-0.1617881908	-5.9555902512	-0.3605789884
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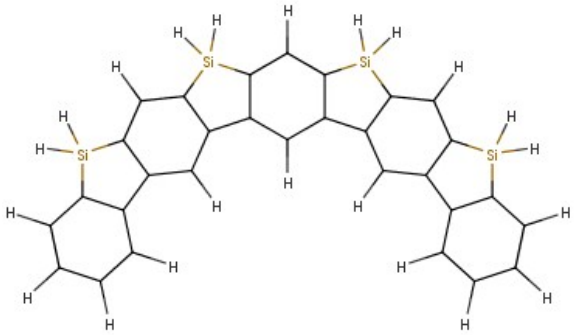
H	4.1200266217	-6.1207688028	-0.2387727334



Carb4Si

56

C	-6.1072867757	3.2049548823	0.0126313213
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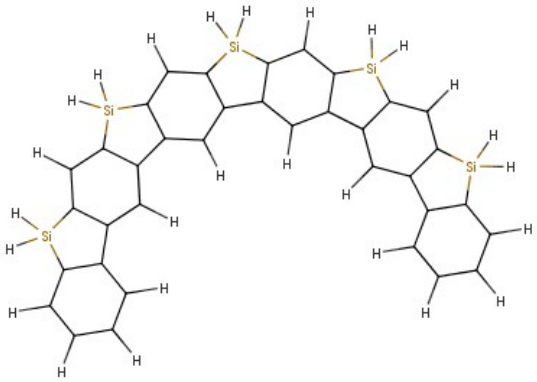
C	-3.9228279647	2.1613048309	0.0148347247
C	-3.3144918445	3.4175138008	0.1004099603
C	-4.1199295325	4.5815606411	0.1395635502
C	-5.5083209393	4.4627979281	0.0962102308
C	-1.8469114640	3.6572043519	0.1546510588
C	-1.4568882766	5.0171615740	0.2324052632
Si	-2.9999489470	6.0868304015	0.2384220459
C	-0.8772256858	2.6527740865	0.1335204211
C	0.4788646729	2.9827058338	0.1889585824
C	0.8741281732	4.3405913739	0.2685400619
C	-0.1003005516	5.3394201506	0.2883747457
C	1.5929996635	1.9959569621	0.1732377045
C	2.8938313737	2.5515947619	0.2524229026
Si	2.7487122270	4.4217269412	0.3393518387
C	1.4295660384	0.6114191640	0.0862561371
C	2.5442986770	-0.2303765833	0.0811765887

C	3.8468957914	0.3205723228	0.1655232796
C	4.0026912248	1.7046589114	0.2488528575
C	2.4878299953	-1.7154038409	-0.0081270374
C	3.7438629109	-2.3705055524	0.0077870653
Si	5.0996035998	-1.0788120847	0.1350488236
C	1.3122088896	-2.4640625074	-0.1022694570
C	1.3689418014	-3.8574939344	-0.1800200906
C	2.6227798757	-4.5171782544	-0.1570495803
C	3.7929743305	-3.7630315477	-0.0649505392
C	0.1834584439	-4.7507400467	-0.2902557839
C	0.4721678647	-6.1362181203	-0.3472405642
Si	2.3340235225	-6.3699186838	-0.2634056026
C	-1.1464164107	-4.3220108643	-0.3426447296
C	-2.1769298383	-5.2537843467	-0.4484788913
C	-1.8950783738	-6.6189618129	-0.5016945935
C	-0.5706717734	-7.0556514843	-0.4506295091
H	-7.1873501748	3.1172990438	-0.0204459660
H	-5.7757379768	1.0821970616	-0.0956480835
H	-3.3243772468	1.2579602766	-0.0188674661
H	-6.1343919386	5.3487569187	0.1270104538
H	-3.1780874843	6.8990586056	1.4706271772
H	-3.1119032682	7.0021296188	-0.9277280059
H	-1.1785103052	1.6140847227	0.0739117726
H	0.2023532351	6.3809477058	0.3496885553
H	3.2870742431	5.0206497923	1.5886340100
H	3.3713896797	5.1315961592	-0.8087523826
H	0.4343317996	0.1882545335	0.0218937745
H	5.0010549306	2.1282747451	0.3097093264
H	5.9293073885	-1.1822216039	1.3639595347
H	6.0202469841	-1.0467446996	-1.0317093071
H	0.3514767884	-1.9637768594	-0.1151293990
H	4.7557602335	-4.2657526933	-0.0499745075
H	2.7974332055	-7.1288201050	0.9279059888
H	2.9195687714	-7.0146259439	-1.4680362531
H	-1.3872657996	-3.2659188325	-0.3032620229
H	-3.2055944605	-4.9132565063	-0.4904982178
H	-2.7027598376	-7.3375660269	-0.5832875737
H	-0.3589952182	-8.1192704053	-0.4926929364

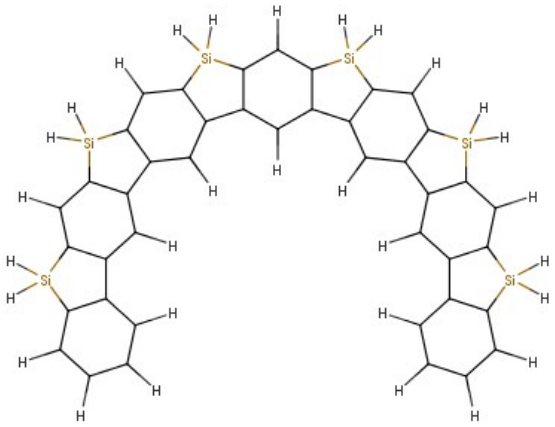


Carb5Si

67

C	-5.5079412970	3.5977129423	0.0287659441
C	-4.6237754429	2.5191858288	0.0218582800
C	-3.2483795330	2.7315323020	0.0811371227
C	-2.7423795121	4.0329518706	0.1488073606
C	-3.6375413659	5.1302110941	0.1594771232
C	-5.0115681369	4.9002588345	0.0984391569
C	-1.2984646730	4.3868950251	0.2084024724
C	-1.0162262369	5.7737987040	0.2712814869
Si	-2.6392600512	6.7207380621	0.2598997308
C	-0.2526296497	3.4617016195	0.2018685672
C	1.0729817851	3.8976399422	0.2547090631
C	1.3619563219	5.2831236354	0.3187321435
C	0.3110640608	6.2018816541	0.3265756188
C	2.2592516461	3.0000014231	0.2524913866
C	3.5139744897	3.6537548947	0.3234453265
Si	3.2256431461	5.5097236022	0.3881031313
C	2.2008825203	1.6064605293	0.1876487349
C	3.3755858822	0.8516277536	0.1971833373
C	4.6331148793	1.4988573298	0.2760167931
C	4.6838429035	2.8924654323	0.3358052494
C	3.4262392535	-0.6333516141	0.1306641043
C	4.7250738679	-1.1974008775	0.1681051315
Si	5.9841994568	0.1930467371	0.2890054853
C	2.3069692237	-1.4625391766	0.0343694466
C	2.4612962566	-2.8487358319	-0.0254191261
C	3.7571299710	-3.4197302833	0.0170810901
C	4.8713836195	-2.5844588473	0.1124785915
C	1.3400119219	-3.8200181987	-0.1346388200
C	1.7218327279	-5.1833861117	-0.1719932456
Si	3.5959202899	-5.2892382064	-0.0781783339
C	-0.0104934681	-3.4693429789	-0.2021240448
C	-0.9898271818	-4.4593448792	-0.3025638156
C	-0.6147418147	-5.8253289923	-0.3299684933
C	0.7367183532	-6.1678688850	-0.2660033147

C	-2.4523564989	-4.1987448271	-0.3891037981
C	-3.2693890793	-5.3525007894	-0.4721390557
Si	-2.1669940784	-6.8754187950	-0.4476058298
C	-3.0453915733	-2.9325039037	-0.4003084347
C	-4.4300682022	-2.8110898430	-0.4919076868
C	-5.2373089184	-3.9454497314	-0.5719392873
C	-4.6538392037	-5.2132543091	-0.5618887622
H	-6.5766660148	3.4238800552	-0.0191064443
H	-5.0083294890	1.5070797353	-0.0304894991
H	-2.5796655315	1.8787576073	0.0737480509
H	-5.7064053810	5.7337238431	0.1038466239
H	-2.8894653407	7.5137525816	1.4925300682
H	-2.8096476304	7.6235042165	-0.9090812316
H	-0.4709247471	2.4016493323	0.1564381649
H	0.5285118412	7.2649597356	0.3766234172
H	3.7149542552	6.1593429341	1.6329446158
H	3.7926143235	6.2524432636	-0.7688132999
H	1.2401615020	1.1093531724	0.1325236048
H	5.6471130877	3.3912590123	0.3929112455
H	6.7956783938	0.1736374861	1.5347654440
H	6.9187885141	0.2676799897	-0.8650969317
H	1.3152156822	-1.0279271789	0.0047085536
H	5.8662195130	-3.0197500003	0.1426072085
H	4.1085113997	-6.0062171309	1.1194784407
H	4.2310444272	-5.8932318860	-1.2794842485
H	-0.2989065931	-2.4255732490	-0.1772530191
H	1.0258172990	-7.2147471238	-0.2900177674
H	-2.3860916876	-7.7658901497	0.7228844840
H	-2.2516371799	-7.7064694819	-1.6776055713
H	-2.4376881206	-2.0369638260	-0.3417585367
H	-4.8824074339	-1.8260293373	-0.5028819502
H	-6.3138098287	-3.8420136423	-0.6433711368
H	-5.2894694022	-6.0903327243	-0.6273100914



Carb6Si

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C	-4.7923744750	3.5890535622	1.3270377464
C	-3.8558770112	2.5569590072	1.2771069602
C	-2.5171010088	2.8301481226	1.0045615123
C	-2.1002523064	4.1462200877	0.7824477032
C	-3.0494756310	5.1962022334	0.8364766851
C	-4.3862238331	4.9059848067	1.1061868902
C	-0.6997832848	4.5661960658	0.5044444339
C	-0.5072864146	5.9619007779	0.3557696347
Si	-2.1662611059	6.8249782815	0.5297555484
C	0.3888772270	3.6960421212	0.4039130474
C	1.6729956918	4.1989645132	0.1799956425
C	1.8731178082	5.5961335918	0.0555629278
C	0.7781597568	6.4572498191	0.1352858887
C	2.9069124155	3.3701337562	0.0894857255
C	4.1132663187	4.1011566313	-0.0423649557
Si	3.7079216615	5.9316940487	-0.1485450489
C	2.9382639530	1.9732716355	0.1380766784
C	4.1594426377	1.2947983896	0.0911528356
C	5.3702068754	2.0269176330	0.0088793444
C	5.3293989135	3.4187344902	-0.0720091753
C	4.3178732941	-0.1859820060	0.1480090374
C	5.6581505994	-0.6426642884	0.2028686150
Si	6.8134593208	0.8310752359	0.0844815899
C	3.2667756062	-1.1083507826	0.1426866371
C	3.5325452768	-2.4792895294	0.2180650130
C	4.8707986576	-2.9333324233	0.3259338290
C	5.9151055292	-2.0094845283	0.3044848521
C	2.5011297914	-3.5556286347	0.1965766113
C	3.0032234174	-4.8709226264	0.3604494673
Si	4.8723764906	-4.8016237084	0.4979494892
C	1.1304521769	-3.3525921361	0.0094444085
C	0.2520509418	-4.4407866351	-0.0050566048
C	0.7500559691	-5.7529877528	0.1907165083
C	2.1194712302	-5.9494893545	0.3652353419

C	-1.2194845551	-4.3514771194	-0.2239789503
C	-1.9135925922	-5.5854954173	-0.1620262188
Si	-0.6826907211	-6.9650572897	0.1513797821
C	-1.9191803687	-3.1725048080	-0.4951923507
C	-3.3012197868	-3.2056377814	-0.7031183795
C	-4.0001125123	-4.4351834127	-0.6198743437
C	-3.2950020438	-5.6084819699	-0.3537112758
C	-4.1431153073	-2.0217719783	-1.0289253894
C	-5.5272698166	-2.2849841256	-1.1793474585
Si	-5.8264731765	-4.1200893578	-0.9199665414
C	-3.6680907839	-0.7189026727	-1.2057698729
C	-4.5514382296	0.3105342770	-1.5249107008
C	-5.9149619164	0.0542077819	-1.6669552063
C	-6.3986531360	-1.2433217724	-1.4943178324
H	-5.8321199451	3.3672749749	1.5389540685
H	-4.1708858950	1.5338591661	1.4458380878
H	-1.8063211400	2.0122264784	0.9746256596
H	-5.1214667994	5.7029749155	1.1504584382
H	-2.2429216676	7.7784837123	1.6682857194
H	-2.6106290812	7.5385643014	-0.6969589415
H	0.2380295399	2.6287803443	0.5149555514
H	0.9304631357	7.5280431767	0.0343753272
H	4.2948329746	6.7559566983	0.9414344343
H	4.0792684159	6.5562043943	-1.4462090406
H	2.0133473793	1.4149746737	0.2226538942
H	6.2565805011	3.9788552745	-0.1534065232
H	7.6916589207	1.0251434482	1.2689076245
H	7.6751928579	0.8214694804	-1.1275989215
H	2.2428742622	-0.7593842444	0.0752098549
H	6.9416482182	-2.3594512899	0.3666351876
H	5.4133906561	-5.2858472317	1.7957570296
H	5.5827013879	-5.5207830512	-0.5928107553
H	0.7490031308	-2.3484281608	-0.1348342340
H	2.5031660748	-6.9567863741	0.4997744468
H	-0.8921298661	-7.6970075554	1.4289299578
H	-0.6066527523	-7.9668904286	-0.9451027735
H	-1.3886822793	-2.2295904314	-0.5553643471
H	-3.8273292239	-6.5537757752	-0.3006847847
H	-6.6947690423	-4.4394857672	0.2443703762
H	-6.3820451029	-4.8157357005	-2.1110245841
H	-2.6118838808	-0.4971414486	-1.1038952982
H	-4.1749487248	1.3177933994	-1.6584385498
H	-6.5950052234	0.8618644043	-1.9126188280
H	-7.4604919792	-1.4348991402	-1.6108979585

Table 1: Computed total energies of optimized structures and their triplet energies

Compound Name	Computed total energies (a.u)	Triplet energies (eV)
CarbO	-5.340439625E+02	3.17639
Carb2O	-7.474.403055E+02	3.08410
Carb3O	-1.140647019E+03	3.06642
Carb4O	-1.443948614E+03	3.05102
Carb5O	-1.747250263E+03	3.04162
Carb6O	-2.050550395E+03	3.03615
CarbN	-5.142178524E+02	3.18084
Carb2N	-7.976928543E+02	3.06827
Carb3N	-1.081167543E+03	3.02863
Carb4N	-1.364642139E+03	3.00474
Carb5N	-1.648116724E+03	2.99370
Carb6N	-1.93780699E+03	2.98780
CarbC	-4.982140790E+02	3.04181
Carb2C	-7.656860958E+02	2.88738
Carb3C	-1.033158737E+03	2.82263
Carb4C	-1.300630562E+03	2.78669
Carb5C	-1.568102331E+03	2.76774
Carb6C	-1.835575000E+03	2.75656
CarbS	-8.566842188E+02	3.09336
Carb2S	-1.482623240E+03	2.92602
Carb3S	-2.108563970E+03	2.85475
Carb4S	-2.309169697E+03	2.82124
Carb5S	-3.360442932E+03	2.80011
Carb6S	-3.986382598E+03	2.78914
CarbP	-8.004745641E+02	2.99534
Carb2P	-1.370205077E+03	2.81544
Carb3P	-1.939936133E+03	2.74207
Carb4P	-2.509667123E+03	2.70558
Carb5P	-3.079397885E+03	2.68481
Carb6P	-3.649127595E+03	2.67782
CarbSi	-7.492687461E+02	2.92038
Carb2Si	-1.267794224E+03	2.71056
Carb3Si	-1.786320061E+03	2.61982
Carb4Si	-2.304845021E+03	2.57345
Carb5Si	-2.823370740E+03	2.54554
Carb6Si	-3.341896263E+03	2.53003