Electronic Supporting Information (ESI) for

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

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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 chloroform as 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.

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\text{Br} \quad \text{Si} \quad \text{Br}
\]

Compound 1 was prepared according to modified procedure from the literature.\(^{20}\) 1,4-Dibromobenzene (4.20 g, 17.8 mmol) was dissolved in 15 mL 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): \(\delta\) (ppm) = 7.57-7.52 (m, 8H), 7.48-7.38 (m, 10H). \(^1\)C NMR (CDCl\(_3\), 100 MHz): \(\delta\) (ppm) = 137.93, 136.32, 134.98, 133.36, 131.14, 129.88, 128.02, 124.82.

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

\[
\text{H} \quad \text{I} \quad \text{I}
\]

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 °C 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): \(\delta\) (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). \(^1\)C NMR (CDCl\(_3\), 100 MHz): \(\delta\) (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(triphenylphosphine)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

$\begin{align*}
\text{H NMR (400 MHz, CDCl}_3\text{)) } \delta [\text{ppm}]: & 8.34 (d, J=1.71 \text{ Hz}, 2\text{H}), 8.13 (s, 1\text{H}), 7.66 − 7.73 (m, 6\text{H}), 7.49 − 7.56 (m, 6\text{H}), 1.42 (s, 18\text{H}). \\
\text{C NMR (100 MHz, CDCl}_3\text{)) } \delta [\text{ppm}]: & 149.46, 139.30, 139.16, 132.99, 126.92, 125.72, 125.52, 124.04, 118.71, 110.85, 34.51, 31.44. \text{ HRMS (MALDI-TOF) m/z: [M]+ Calcd for C}_{32}\text{H}_{33}\text{N 431.2613; Found 431.165.}
\end{align*}$

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(triphenylphosphine)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**. ¹H NMR (400 MHz, CDCl₃) 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). ¹³C NMR (100 MHz, CDCl₃) 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]+ Caled for C₂₆H₂₁NO₂ 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**. ¹H NMR (400 MHz, CDCl₃) 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). ¹³C NMR (100 MHz, CDCl₃) 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]+ Caled for C₂₄H₁₅F₂N 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**

**1H NMR (600 MHz, CDCl₃) 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).

**13C NMR (100 MHz, CDCl₃) 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 C₂₆H₂₁NO₂ 379.1572; Found 379.511.**

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

![3,6-diiodo-9-tosyl-9H-carbazole](image)

Compound 8 was prepared according to procedure from the literature. 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**

**1H NMR (400 MHz, CDCl₃) 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).

**13C NMR (100 MHz, CDCl₃) 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 C₁₉H₁₃I₂NO₂S 572.8756; Found 572.885.**

3,6-di-tert-butyl-9H-carbazole, (7), known compound.
In ice bath of 0 °C, carbazole (20 mmol) was suspended in 100 ml chloroform under nitrogen. AlCl₃ (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 Na₂SO₄ and the solvent was removed under reduced pressure to obtain white solid. Yield: 82.6%. Melting point = 230-233 °C. ¹H NMR (400 MHz, CDCl₃) 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). ¹³C NMR (100 MHz, CDCl₃) 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 C₂₀H₂₅N 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. ¹H NMR (400 MHz, CDCl₃) 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). ¹³C NMR (100 MHz, CDCl₃) 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
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.** \(^1\)\(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) [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). \(^1\)\(^3\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) [ppm]: 145.49, 143.02, 139.51, 137.38, 135.02, 134.54, 130.07, 127.09, 127.07, 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\(_3\)O\(_2\)S 875.4484; Found 875.756.

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\(_3\)) \(\delta\) [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\(_3\)) \(\delta\) [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\(_{37}\)H\(_{47}\)N\(_3\)O\(_4\) 921.3567; Found 921.795.

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

![Compound 12](image)

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\(_3\)) \(\delta\) [ppm]: 8.52 (br. s., 1H), 8.18 (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\(_3\)) \(\delta\) [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$_2$CO$_3$ (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 °C. 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$_2$Si 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$_2$CO$_3$ (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 °C. 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,
Bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl), P3. New compound.

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\text{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 } \text{K}_2\text{CO}_3 (0.44 g, 3.2 mmol) \text{ were dissolved in 4 ml anhydrous } \text{o-dichlorobenzene under nitrogen atmosphere. The reaction mixture was refluxed for 72 h at 180 °C. 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.} \]

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\text{1H NMR (600 MHz, CDCl}_3\text{) } \delta \text{ [ppm]: 8.33 – 8.38 (m, 4H), 7.97 (d, } J=8.25 \text{ Hz, 2H), 7.15 – 7.24 (m, 8H).} \]

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\text{13C NMR (100 MHz, CDCl}_3\text{) } \delta \text{ [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]^+ \text{ Caled for } C_{76}H_{58}N_{2}O_{4}Si 1090.4166; \text{ Found 1091.070.} \]

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

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\text{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$_2$CO$_3$ (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 ºC. $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ [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$_3$) $\delta$ [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$_6$O$_8$Si 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$_2$CO$_3$ (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 ºC.**

$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ [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$_3$) $\delta$ [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$_6$Si 1774.9813; Found 1776.242.
III. Copies of 1H and 13C NMR for synthesized compounds

Fig. S1. 1H NMR spectrum (400 MHz) for bis(4-bromophenyl)diphenylsilane (Compound 1) in CDCl₃.

Fig. S2. 13C NMR spectrum (100 MHz) for bis(4-bromophenyl)diphenylsilane (Compound 1) in CDCl₃.
Fig. S3. $^1$H NMR spectrum (400 MHz) for 3,6-diodocarbazole (Compound 2) in CDCl$_3$.

Fig. S4. $^{13}$C NMR spectrum (100 MHz) for 3,6-diodocarbazole (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 CDCl₃.

Figure S37. ¹H NMR spectrum (600 MHz) for bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane/P2 in CDCl₃.

Figure S38. ¹³C NMR spectrum (100 MHz) for bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane/P2 in CDCl₃.
Figure S39. MALDI-TOF MS spectrum for bis(4-(3,6-bis(3-methoxyphenyl)-9H-carbazol-9-yl)phenyl)diphenylsilane/P2 in CDCl₃.

Figure S40. ¹H NMR spectrum (600 MHz) for bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl)/P3 in CDCl₃.

Figure S41. ¹³C NMR spectrum (100 MHz) for bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl)/P3 in CDCl₃.
Figure S42. MALDI-TOF MS spectrum for bis(4-(3,6-bis(4-fluorophenyl)-9H-carbazol-9-yl)phenyl)/P3 in CDCl3.

Figure S43. 1H 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 CDCl3.

Figure S44. 13C 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 CDCl3.
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 CDCl₃.

Figure S46. ¹H 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 CDCl₃.

Figure S47. ¹³C 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 CDCl₃.
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 CDCl₃.

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.
# Coordinates of Stationary Points in xyz format

| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
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| C    | 3.0557373885 | 1.1057552109  | 0.0001909291 |
| C    | 1.7243864723 | 1.5113887993  | 0.0000102255 |
| C    | 0.725716804  | 0.5330082923  | -0.0000046862|
| C    | 1.0990879868 | -0.8218164867 | 0.0001226625 |
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| C    | -1.0990934929| -0.8218227179 | 0.0001226359 |
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| C    | -3.3967556816| -0.2554006217 | 0.0003350425 |
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| H    | 4.4418811640 | -0.5419697100 | 0.0005091865 |
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| H    | -1.4705665836| 2.5651190309  | -0.0000881201|
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Carb40
48
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| H  | 6.1214336752  | 3.7321085359  | 0.000605317 |
| H  | 7.9547202330  | 2.0751918718  | 0.0014231309 |
| H  | 7.4709156610  | -0.3564959000 | 0.0016734609 |

|    |         |         |         |
|----|---------|---------|---------|
| H  | 7.8193891093  | -4.5884248492 | -0.4309882314 |
| H  | 6.6233881657  | -6.7591967261 | -0.4883518711 |
| H  | 4.1556319159  | -6.8492602257 | -0.4197516565 |
| H  | 2.8201930433  | -4.7678727442 | -0.2909431824 |
| H  | 7.3432972984  | -1.8190630031 | -0.2974831835 |
| H  | 6.1284097343  | 0.7057765580  | -0.1506879213 |
| H  | 1.9496154384  | -2.1296806701 | -0.148045065 |
| H  | 4.2340395631  | 2.7644600117  | -0.005613517 |
| H  | 1.8597787522  | 4.2492625944  | 0.1308045796 |
| H  | -0.1659415769 | -0.3726440377 | -0.0109785425 |
| H  | -0.8466406228 | 4.9806203900  | 0.2427416706 |
| H  | -3.6490813876 | 4.9683709542  | 0.3214626145 |
| H  | -2.8881676281 | -0.0185013942 | 0.0851272571 |
| H  | -6.3288163751 | 4.1401012184  | 0.3730064608 |
| H  | -5.4176300116 | -1.1756114429 | 0.1084409306 |
| H  | -7.8538429984 | -1.6145711030 | 0.1618232804 |
| H  | -9.4667237488 | 0.2522387480  | 0.2913812350 |
| H  | -8.6871617551 | 2.6042459759  | 0.3694556906 |
| C  | 6.7360126608  | -4.6212250497 | -0.4003952056 |
| C  | 6.0569279161  | -5.8368536286 | -0.4322669182 |
| C  | 4.6557399123  | -5.8882738954 | -0.3931194322 |
| C  | 3.9032151909  | -4.7201789005 | -0.3206815969 |
| N  | 6.3862898254  | -2.1286764598 | -0.2830995270 |
| C  | 5.9759192779  | -3.4553711949 | -0.3280252256 |
| C  | 4.5592741066  | -3.4867175527 | -0.2869429228 |
| C  | 5.2316907438  | 0.0967916056  | -0.1502970202 |
| C  | 5.2788856903  | -1.2956041981 | -0.2134984585 |
| C  | 4.1085314817  | -2.1103097343 | -0.2137736836 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 2.8464228679 | -1.5202111095 | -0.1491924971 |
| N    | 3.5910556879    | 1.9910489172    | -0.0170384738 |
| C    | 3.9571600388    | 0.6533761119    | -0.086985675  |
| C    | 2.7662972600    | -0.1323884101    | -0.085698265  |
| C    | 1.4244914253    | 3.2569000580    | 0.1005478763  |
| C    | 2.0563920279    | 2.156868031     | 0.0281490156  |
| C    | 1.6517421012    | 0.7942145862    | -0.0125113413 |
| C    | 0.2701621826    | 0.6197800000    | 0.0197714532  |
| N    | -0.9781487118   | 3.9843117958    | 0.2009021570  |
| C    | 0.0471419216    | 3.0480081655    | 0.1312167536  |
| C    | -0.537687890    | 1.7507941857    | 0.0921024535  |
| C    | -3.4858701499   | 3.8979541013    | 0.2708087469  |
| C    | -2.2102878525   | 3.3435362654    | 0.2093449877  |
| C    | -1.9782165103   | 1.9374542544    | 0.2118345886  |
| C    | -3.0518267503   | 1.0522670001    | 0.1350709998  |
| N    | -5.9059481289   | 3.2293757812    | 0.3120713304  |
| C    | -4.5408152042   | 2.9854891094    | 0.2621990455  |
| C    | -4.343290426    | 1.5748825479    | 0.1952991002  |
| C    | -6.6010935588   | 2.0266221483    | 0.2818767058  |
| C    | -5.6603856693   | 0.9689006061    | 0.2080867357  |
| C    | -6.1192196200   | -0.3504531694   | 0.1648401212  |
| C    | -7.4887111028   | -0.5948605744   | 0.1953055710  |
| C    | -8.4042485136   | 0.4653940448    | 0.2686482915  |
| C    | -7.9741554824   | 1.7892800514    | 0.3129539471  |

**Carb5N**

62

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -8.3718197174 | 3.9704020020 | 0.4615907237 |
| C    | -8.9110395746 | 2.6871112728 | 0.3997394803 |
| C    | -8.0863048392 | 1.5552778031 | 0.3106604696 |
| C    | -6.7010597602 | 1.6862186944 | 0.2814868909 |
| C    | -6.1347221729 | 2.9622444646 | 0.3417766486 |
| C    | -6.9840567779 | 4.0932973247 | 0.4317935329 |
| C    | -4.7720564489 | 3.4577212225 | 0.3335051687 |
| C    | -4.8514930119 | 4.8784720712 | 0.4196712819 |
H  6.2797708850 -6.4357283203  -0.5467296170
H  0.8980077309  -6.0505056760  -0.3784399857
H  0.6978880753 -8.5161080338  -0.5182043663
H  2.7152812114 -9.9361524770  -0.6551817434
H  4.9820747724 -8.9295096215  -0.6566858530

Carb6N

72

C  -7.8123078399  6.0419160133  0.5770391556
C  -8.4495326654  4.8055054657  0.5026971607
C  -7.7158467492  3.6136773226  0.4062962185
C  -6.3247949259  3.6354607787  0.3818517110
C  -5.6600141637  4.8625568549  0.4550724519
C  -6.4189622820  6.0558975357  0.5525506760
C  -4.2628437018  5.2504311786  0.4552896710
C  -4.2313752525  6.6726123889  0.5541310860
N  -5.5402079711  7.1302617975  0.6116203656
C  -3.0710932893  4.5299865238  0.3809929939
C  -1.8698234354  5.2317178334  0.4063441590
C  -1.8732724983  6.6548332889  0.5065649821
C  -3.0441619705  7.4044981225  0.5823405261
C  -0.4804595091  4.8179179112  0.3486457085
C  0.3085264592  6.0017103256  0.4157970920
N  -0.5538764381  7.0892898482  0.5104957723
C  0.1353058850  3.5734331454  0.2472263148
C  1.5263739349  3.5234117247  0.2146743215
C  2.2881957558  4.7249348981  0.2840705919
C  1.7019812553  5.9860143985  0.3851945301
C  2.4720584379  2.4291239865  0.1193054328
C  3.7754663699  3.0038138529  0.1347441359
H  -0.2802910187 -10.8836127395 -0.7537969630
CarbC

23

C  2.5416394921  1.1687312957  -0.0000571221
C  3.4586627194  0.1143097594  -0.0000882137
C  3.0157219259 -1.2110776198  -0.0000463033
C  1.6526516254 -1.5057863854  0.0000165714
C  0.7347973375 -1.5057863854  0.0000298840
C  1.1829879465  0.8808889882  0.000021538
C -0.7347970777 -0.4545837610  0.0000301293
C -1.1829875130  0.8808888170  0.000021822
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
C -2.5416384857  1.1687319449  -0.0000572170
H  2.8929251980  2.1954733475  -0.0000898421
H  4.5220200875  0.3257807102  -0.0001504261
H  3.7398580772 -2.0180827497  -0.0000704466
H  1.3198662049 -2.5379669491  0.0000457598
H -0.0000003654  2.4812134894  0.8785318020
H -0.0000004551  2.4812738689  -0.8784386816
H -1.3198670957 -2.5379669688  0.0000457279
H -3.7398583318 -2.0180827618  -0.0000705342
H -4.5220204107  0.3257812417  -0.0001505124
H -2.8929248242  2.1954736991  -0.0000896984
|   |        |        |        |
|---|--------|--------|--------|
| C | 4.8181221147 | 0.4573363938 | 0.0002611441 |
| C | 5.3490863395 | -0.8355328236 | -0.0001732248 |
| C | 4.5050648808 | -1.9493197584 | -0.0005338106 |
| C | 3.1198292461 | -1.7910983855 | -0.0004271962 |
| C | 2.5879080818 | -0.5012229364 | 0.0000031562 |
| C | 3.4390671635 | 0.6202859011 | 0.0003088191 |
| C | 1.1950208244 | -0.0353439611 | 0.0000056260 |
| C | 1.1945740377 | 1.3761241235 | 0.0001996742 |
| C | 2.6182397990 | 1.8930404556 | 0.0005751461 |
| C | -0.0000012426 | -0.7544350002 | -0.0000208864 |
| C | -1.1950210548 | -0.0353426923 | -0.0000917797 |
| C | -1.1945736719 | 1.3761213199 | -0.0002306125 |
| C | -0.0000000890 | 2.0906472436 | -0.000155523 |
| C | -2.5879072402 | -0.5012213424 | -0.0000189726 |
| C | -3.4390667560 | 0.6202845308 | -0.0003050049 |
| C | -2.6182394680 | 1.8930399163 | -0.0005883770 |
| C | -3.1198294939 | -1.7910968905 | 0.0004234876 |
| C | -4.5050641772 | -1.9493209635 | 0.0005655509 |
| C | -5.3490859638 | -0.8355337215 | 0.0002276767 |
| C | -4.8181218564 | 0.4573363772 | -0.0002215093 |
| H | 5.4797994212 | 1.3179348604 | 0.0005218525 |
| H | 6.4240063595 | -0.9763132825 | -0.0002592767 |
| H | 4.9328078157 | -2.9456507132 | -0.0009243088 |
| H | 2.4714034995 | -2.6604412678 | -0.0007312980 |
| H | 2.8290655761 | 2.5116020230 | 0.8808008595 |
| H | 2.8294044686 | 2.5122338350 | -0.8791180972 |
| H | 0.0000000669 | -1.8389579474 | -0.0000219429 |
| H | -0.0000001587 | 3.1765633532 | -0.0000126753 |
| H | -2.8290785666 | 2.5115971984 | -0.8808146929 |
| H | -2.8293923908 | 2.5122385735 | 0.8791045451 |
| H | -2.4714023248 | -2.6604415564 | 0.0007121388 |
| H | -4.9328076831 | -2.9456521719 | 0.0009679798 |
| H | -6.4240074618 | -0.9763145910 | 0.0003440888 |
| H | -5.4798002265 | 1.3179354666 | -0.0004633785 |

Carb2C
| H     | -0.0000221083 | -3.6576870559 | -0.8777624709 |
|-------|---------------|---------------|---------------|
| H     | 0.0000085646  | -3.6570502848 | 0.8782860488  |
| H     | 1.3081841135  | 1.3689409890  | -0.0020067422 |
| H     | 2.8805946011  | -3.3938534568 | 0.0008947689  |
| H     | 5.3597315059  | -1.8797477775 | -0.8771243949 |
| H     | 5.3587747181  | -1.8792544196 | 0.8796007789  |
| H     | 3.4059205102  | 2.9260108320  | -0.0016006615 |
| H     | 5.6550547032  | 3.9610567408  | -0.0002057786 |
| H     | 7.6864520032  | 2.5533931289  | 0.0017813610  |
| H     | 7.5013905214  | 0.0788375392  | 0.0023091252  |

![Chemical Structure](image)

Carb4C

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| C     | -7.9037704885 | 1.1541397568 | 0.2795653877 |
|-------|---------------|---------------|---------------|
| C     | -8.1358871487 | -0.2227124562 | 0.2150159184  |
| C     | -7.0664044805 | -1.1191265101 | 0.1389484750  |
| C     | -5.7508534438 | -0.6571341960 | 0.1265314919  |
| C     | -5.5168816523 | 0.7171256786  | 0.1910914628  |
| C     | -6.5957755950 | 1.6192341847  | 0.2670494896  |
| C     | -4.2624302600 | 1.4819656275  | 0.1957218914  |
| C     | -4.5774341506 | 2.8556768849  | 0.2738939609  |
| C     | -6.0791341649 | 3.0411698394  | 0.325293509   |
| C     | -2.9366343866 | 1.0514830582  | 0.1380543459  |
| C     | -1.9324895068 | 2.0198394961  | 0.1595778858  |
| C     | -2.2506732284 | 3.3927239432  | 0.2383022414  |
| C     | -3.5736639568 | 3.8190625314  | 0.2957202155  |
| C     | -0.4702519637 | 1.8808605312  | 0.1113543198  |
| C     | 0.1051987477  | 3.1687819928  | 0.160995085  |
| C     | -0.9820829585 | 4.2184567217  | 0.2463682444  |
| C     | 0.3298223924  | 0.7406243673  | 0.0307468510 |
| C     | 1.7141366395  | 0.9124085082  | 0.0015237357 |
| C     | 2.2861858552  | 2.2019438556  | 0.0514913366 |
| C     | 1.4858824534  | 3.3372073969  | 0.1311383759 |
| C     | 2.7981770180  | -0.0765634685 | -0.0783476265 |
| C     | 4.0324000260  | 0.6084096756  | -0.0766840241 |
C  3.7959814514  2.1009048932  0.0062914417
C  2.7520622049 -1.4689705902 -0.1494778761
C  3.9613068787 -2.1610282035 -0.2196155198
C  5.1941178426 -1.4733879699 -0.2182460740
C  5.2368645333 -0.0844662974 -0.1463723874
C  4.2329864452 -3.6019873662 -0.3041298156
C  5.6269009434 -3.7967105023 -0.3553368516
C  6.3385313228 -2.4610573472 -0.3065739294
C  3.3669070246 -4.6955204213 -0.3369477306
C  3.9041917282 -5.9794235325 -0.4211955555
C  5.2875513032 -6.1712094915 -0.4718845682
C  6.1569132737 -5.0772352367 -0.4389635785
H -8.7380637940  1.8455681208  0.3385476939
H -9.1528152894 -0.5985344423  0.2238282518
H -7.2625904049 -2.1844345787  0.0891228869
H -4.9266426531 -1.3596116371  0.0670897325
H -6.3969282808  3.5541124858  1.2407455792
H -6.4464661953  3.6446932665 -0.5130514620
H -2.6948056510 -0.0041624199  0.0781691944
H -3.8159164490  4.8759475016  0.3561642068
H -0.8956005546  4.8236332235  1.1566778561
H -0.9447134789  4.9183148474 -0.5968390832
H -0.1128057705 -0.2490359019 -0.0078254874
H  1.9281643367  4.3283278982  0.1692193560
H  4.2619716249  2.5397796092  0.8964842102
H  4.2167381814  2.6292149103 -0.8575373030
H  1.8046370488 -1.9969409314 -0.1503213315
H  6.1853400804  0.4448454106 -0.1459341047
H  7.0131165237 -2.3889892264  0.5546992525
H  6.9535512391 -2.2941734018 -1.1986756853
H  2.2920638710 -4.5557211324 -0.2984167341
H  3.2425831369 -6.8381306840 -0.4477412506
H  5.6891807275 -7.1761449990 -0.5374026293
H  7.2302357241 -5.2326432949 -0.4778935197

Carb5C

67
C  -8.2915675704  2.9613865563  0.3964370922
C  -8.5762317288  1.5951842414  0.3190028673
C  -7.5422062333  0.6590133060  0.2344360972
C  -6.2099246605  1.0698950748  0.2262777049
C  -5.9232927089  2.4334217622  0.3038302767
C  -6.9664922204  3.3756039398  0.3882244285
C  -4.6403660581  3.1489928697  0.3161799967
C  -4.9014964278  4.5331965532  0.4074261302
C  -6.3950595703  4.7755750370  0.4597855194
C  -3.3326706583  2.6679928638  0.2549491247
C  -2.2922651475  3.5965828947  0.2862184578
C  -2.5556249808  4.9799931307  0.3784405075
C  -3.8611888656  5.4571189730  0.4394493527
C  -0.8377640380  3.3991373242  0.2368821175
C  -0.2092059975  4.6610775396  0.2995498132
C  -1.2538290899  5.7531317698  0.3954107371
C  -0.0872909185  2.2269813316  0.1449652224
C  -1.3025976420  2.3403904206  0.1181756386
C  -1.929331451  3.6032609529  0.1821598123
C  -1.1778236607  4.7711950239  0.2726738266
C  -2.3413861211  1.3058697004  0.0289986396
C  -3.6048970927  1.9344718268  0.0405458860
C  -3.4334881647  3.4356603190  0.1381529078
C  -2.2311771948  0.0818133295  -0.0582018009
C  -3.4071311664  -0.8281355269  -0.1338067915
C  -4.6696416532  -0.1977039578  -0.1216738893
C  -4.7765652184  1.1871006493  -0.0341707377
C  -3.6085800236  -2.2795216080  -0.2334280740
C  -4.9949294041  -2.5390893290  -0.2817072983
C  -5.7661505260  -1.2376568180  -0.2174185749
C  -2.6810921743  -3.3203237474  -0.2802689421
C  -3.1661240054  -4.6244704798  -0.3755288397
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
C  -1.6192758312  -8.5569778365  -0.5936415834
C  -2.9870191356  -8.2695724989  -0.6076463662
H  -9.0993217597  3.6831615917  0.4618333233
H  -9.6067380404  1.2587007850  0.3242800637
H  -7.7790844685  -0.3973269341  0.1744033084
H  -5.4135351397  0.3367127336  0.1603490595
H  -6.6922441108  5.2906829992  1.3808641376
H  -6.7372141443  5.3987841953  -0.3747662989
H  -3.1302019646  1.6046413395  0.1858136144
|   | x                  | y                  | z                  |
|---|--------------------|--------------------|--------------------|
| 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      |
| H | 3.9147376089       | 3.8445648093      | 1.0345299845      |
| H | 3.8770635119       | 3.9523671677      | -0.7212784278     |
| H | 1.2605446623       | -0.5657176695     | -0.0668521266     |
| H | 5.7486105782       | 1.6716946982      | -0.0257212686     |
| H | 6.4397538005       | -1.2046103566     | 0.6471148864      |
| H | 6.3889788393       | -1.0908196233     | -1.1078780444     |
| H | 1.6155366271       | -3.1208822438     | -0.2445290993     |
| H | 6.5430951258       | -4.0404811666     | -0.4135617002     |
| H | 5.3917884428       | -6.7480103442     | 0.3154644638      |
| H | 5.3487211437       | -6.6315212393     | -1.4398189895     |
| H | 0.3510263839       | -5.4028384484     | -0.3602573006     |
| H | -0.3784688745      | -7.7659442991     | -0.4946393206     |
| H | 1.2847480471       | -9.5864400079     | -0.6527372500     |
| H | 3.7119041362       | -9.0741935267     | -0.6770666174     |

**Carb6C**

|   | x                  | y                  | z                  |
|---|--------------------|--------------------|--------------------|
| C | -2.8871081912      | 4.0805004916      | 0.3585367755      |
| C | -5.8772006140      | 6.2882042132      | 0.5714988229      |
| C | -4.3920867202      | 5.9964322928      | 0.5234820944      |
| C | -4.1776248858      | 4.6050322800      | 0.4191096129      |
| 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      |

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| 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  |
| C   | 1.7283440806   | 3.5278289341  | 0.2586931334  |
| 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   | 3.900567290    | 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  | -0.205364162  |
| C   | 3.2781455805   | -3.4292553325  | -0.3093054403 |
| C   | 4.6506236283   | -3.7541146598  | -0.3509589589 |
| C   | 5.6232877605   | -2.7598145700  | -0.2893505616 |
| C   | 2.4982654008   | -4.669921591   | -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 |
| C   | -0.7236313321  | -6.7021861247  | -0.5018969655 |
| C   | -0.6727897647  | -8.105009888   | -0.6118213196 |
| C   | 0.7685459538   | -8.5671595171  | -0.6693618829 |
| C   | -1.9515761783  | -6.0430256284  | -0.4316000637 |
| C   | -3.1243918652  | -6.7957856973  | -0.4722189168 |
| C   | -3.0733050333  | -8.1881042518  | -0.5815061497 |
| C   | -1.8441229146  | -8.8502228906  | -0.6519414461 |
| H   | -8.6174993243  | 5.2843884818   | 0.5519922585 |
| H   | -9.2030892019  | 2.8796212099   | 0.3899115593 |
| H   | -7.4297953258  | 1.1656500396   | 0.2295401958 |
| H   | -5.0424630785  | 1.8212171179   | 0.2318319200 |
| H   | -6.1616435632  | 6.8064840126   | 1.4947339987 |
| H   | -6.1948658104  | 6.9314996121   | -0.2574078983 |
| H   | -2.7200676723  | 3.0116446764   | 0.2797767849 |
| H   | -3.4876678690  | 7.9545129668   | 0.6501550320 |
| H   | -0.5753527038  | 7.6677332464   | 1.4638521055 |
| H   | -0.6084467814  | 7.8030103685   | -0.2876262615 |
| H   | -0.1808391126  | 2.5760654730   | 0.1982691109 |
| H   | 2.2111669523   | 6.9751773744   | 0.4799378122 |
|   | x          | y          | z          |
|---|------------|------------|------------|
| H | 4.3935638498 | 4.9842006793 | 1.1824339817 |
| H | 4.3685904607  | 5.1095830678  | -0.5697576401 |
| H | 1.5654683665  | 0.6956315001  | 0.0242417966 |
| H | 6.1439116581  | 2.7408882375  | 0.1137371098 |
| H | 6.7064768487  | -0.1741278159 | 0.7620562082 |
| H | 6.6725538315  | -0.0453483202 | -0.9894580289 |
| H | 1.8017962250  | -1.8546820476 | -0.1740622307 |
| H | 6.6795108057  | -3.0103718219 | -0.3221601389 |
| H | 5.3882598864  | -5.6698016609 | 0.3726077086 |
| H | 5.3653897279  | -5.5329811780 | -1.3788077737 |
| H | 0.4312907307  | -4.0351787327 | -0.3147166456 |
| H | 3.6083874612  | -7.9008920241 | -0.6582929175 |
| H | 1.0135558567  | -9.2463545255 | 0.1555032713 |
| H | 0.9865126800  | -9.1107158530 | -1.5960104817 |
| H | -1.9994650216 | -4.9629085464 | -0.3466824905 |
| H | -4.0856716748 | -6.2969152428 | -0.4189146868 |
| H | -3.9948520127 | -8.7583316544 | -0.6116388269 |
| H | -1.8129360923 | -9.9316301936 | -0.7365503999 |
### Carbs

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| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 3.4695992339 | 0.4545846616 | 0.0952825389 |
| C    | 3.0324049422  | -0.8749388036 | 0.1793295743  |
| C    | 1.6771461825  | -1.1750454851 | 0.1522054825  |
| 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 |
| 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  |
| H    | -4.5760821084 | 0.1533699950  | -0.1846539425 |
| H    | -3.1519872637 | 2.1768983194  | -0.2842741902 |
Carb2S

C  -5.2374633943  -1.0757244862  0.0715475613
C  -4.6810152414   0.2105922184  0.0710974152
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  -0.0861290817  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  0.0300709245
C   4.7721233495   2.4116880111  0.0546898660
C   4.8310971006   1.0223620800  0.0665641574
H  -6.3142984482  -1.1981960602  0.0869365741
H  -5.3319178044   1.0769697579  0.0860807437
H  -2.8825190130   1.3830111683  0.0511222838
H  -4.8516583955  -3.1952415264  0.0521661606
H  -0.4504819925   1.2955928560  0.0176769894
H   1.1953082101  -3.4341750795  0.0427261761
H   1.3997403399   2.8747701396  0.0004012222
H   3.5087250683   4.1570898767  -0.0217011440
H   5.6919030656   2.9849948623  -0.0644016824
H   5.7861982657   0.5106510522  -0.0853644771
| Atom | Coordinates | Atomic Number | Charge |
|------|-------------|---------------|--------|
| C    | -5.929058518 | 3.1470055791  | 0.1055811233 |
| C    | -5.4940191527 | 1.8160153652  | 0.0551080601 |
| C    | -4.1382190380 | 1.5161794641  | 0.0480812049 |
| 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 |
| C    | -0.9298840599 | 1.3319430094  | 0.0505263599 |
| C    | 0.4583833352  | 1.4676164133  | 0.062464853 |
| C    | 1.0247900830  | 2.7665843183  | 0.1191850192 |
| C    | 0.2443739521  | 3.9157770654  | 0.1624360759 |
| S    | 2.7891529007  | 0.9672084005  | 0.0535825964 |
| C    | 2.7911733362  | 2.7323031066  | 0.1273916006 |
| C    | 1.3133377769  | -0.9559497813 | -0.0350319518 |
| C    | 2.4327970460  | -1.7893788460 | -0.0637590516 |
| C    | 3.7276400089  | -1.2120854742 | -0.0327318240 |
| C    | 3.9229807251  | 0.1639140537  | 0.0257694516 |
| C    | 2.4863348989  | -3.2421872367 | -0.1244718646 |
| 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 |
| C    | 4.0913083025  | -5.0921163403 | -0.1950333870 |
| H    | -6.9903815116 | 3.3674147746  | 0.1102194776 |
| H    | -6.2223249951 | 1.0141298932  | 0.0214843761 |
| H    | -3.8132847709 | 0.4824793546  | 0.0087837461 |
| H    | -5.3484420025 | 5.2203012158  | 0.1901593985 |
| H    | -1.3809509798 | 0.3469083135  | 0.0083839470 |
| H    | 0.6934295496  | 4.9004820810  | 0.2045672471 |
| H    | 0.3185763452  | -1.3865956866 | -0.0587021508 |
| H    | 4.9175662818  | 0.5921721685  | 0.0480221115 |
| H    | 0.4048531584  | -3.8195966754 | -0.1562256871 |
Carb4S

48

C  -5.8501031805  4.6644713476  0.1603176390
C  -5.4035924645  3.3810874499  0.0907491640
C  -4.0453829746  3.0501851122  0.0949789412
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
C   0.5448262226  3.0315422317  0.1595473118
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
C   1.5139011243  -6.3129372820  -0.2991138600
S   3.2734949125  -6.1539681912  -0.2706754841
C    -0.5423673996   -5.0416434369   -0.2539524910
C    -1.2545359554   -6.2313959970   -0.3292136093
C    -0.5842934607   -7.4605739507   -0.3900077520
C     0.8048978851   -7.5110109070   -0.3748932746
H    -6.9129372528    4.8762992481    0.1553997031
H    -6.1242227144    2.5308068003    0.0333146397
H    -3.7098614205    2.0206422700    0.0404009137
H    -5.2896841689    6.7403746338    0.2904131821
H    -1.2878884867    1.9030587616    0.0653978884
H     0.7613575662    6.4625986302    0.3663207545
H     0.4120301297    0.1817967978    0.0041137789
H     5.0057756770    2.1669742730    0.1637844106
H     0.5027949239   -2.2344852335   -0.0977738773
H     5.2391391685   -3.8610735765   -0.1365493868
H    -1.0711294794   -4.0962565734   -0.2083790375
H    -2.3379013052   -6.2101588190   -0.3423471213
H    -1.1512427994   -8.3822547282   -0.4502476292
H     1.3235244301   -8.4611885955   -0.4226399178

Carb5S

57

C    -5.1268232331   5.7295992218    0.2079415007
C    -4.6789744396   4.4048581516    0.1160063463
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    0.2074888333
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 -0.0224935180
C -0.4855446731 -6.968227701 -0.4103545123
C  0.2142609099 -6.377833626 -0.3379243635
C  1.6040682039 -6.4409159785 -0.3117003978
C -1.9270013702 -5.3356864937 -0.3387488042
C -2.2834491110 -6.6986227701 -0.4372027886
S -0.8736441336 -7.7648246059 -0.4258353636
C -2.9462764333 -4.3740976773 -0.3167983013
C -4.2757121525 -4.7723904614 -0.3651173082
C -4.6092667145 -6.1317713969 -0.4372027886
C -3.6164020905 -7.1050475599 -0.4606704015
H -6.1896418500  5.9416161774  0.1971159025
H -5.3994556426  3.5993850521  0.0344697078
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  0.5185785389
H  1.1588773280  1.2522166241  0.0696057583
H  5.7380973817  3.2604324656  0.3194218332
H  1.2644692366 -1.1583183088 -0.0477925988
H  6.0064767657 -2.7644074902 -0.0494959114
H -0.2845409332 -3.0032370224 -0.1930516896
H  2.1258391877 -7.3894155256 -0.3444021657
H -2.6986706068 -3.3199262525 -0.2617362957
H -5.0624645798 -4.0272671653 -0.3471840031
H -5.6505398101 -6.4299706754 -0.4757205042
H -3.8748861453 -8.1557442544 -0.5178186895
|   |   |   |   |   |
|---|---|---|---|---|
| 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 |
| C | -5.8461524148 | -1.6357111484 | -0.0341011350 |
| C | -7.0000349249 | -2.4242301138 | -0.1195634278 |
| C | -6.9065193493 | -3.8015670238 | -0.2741378314 |
| H | -5.1939923002 | 6.3947361169 | -0.1219275713 |
| H | -4.4100774589 | 4.0498147104 | -0.2756645591 |
| H | -2.0103682814 | 3.5168558114 | -0.0915864324 |
| H | -3.5758749699 | 8.2372606974 | 0.2195735651 |
| H | 0.4193725715 | 3.3831198972 | 0.1370521132 |
| H | 2.4331022058 | 7.9243916275 | 0.7556612872 |
| H | 2.1307290823 | 1.6593302391 | 0.1580127936 |
| H | 6.6910937443 | 3.6562336793 | 0.6771406046 |
| H | 2.2462133893 | -0.7577213441 | 0.0132626258 |
| H | 6.9943338600 | -2.3413449724 | 0.0058581583 |
| H | 0.7091886375 | -2.6162414491 | -0.1568175287 |
| H | 3.1611121845 | -6.9656572732 | -0.5084758748 |
| H | -1.6867467949 | -2.9581455325 | -0.1934157228 |
| H | -2.8124324424 | -7.8102783321 | -0.6939079566 |
| H | -3.7015878966 | -1.5948125179 | -0.0356492471 |
| H | -5.9369931301 | -0.5617554401 | 0.0871728659 |
| H | -7.9777523916 | -1.9577517738 | -0.0645980388 |
| H | -7.8005640465 | -4.4117005830 | -0.3397278465 |
| Atom | X       | Y       | Z       | Coordinates |
|------|---------|---------|---------|-------------|
| C    | 3.3424565363 | -1.0580626846 | 0.1987914884 |             |
| C    | 3.1710798065 | 0.7846236006 | -0.4231406452 |             |
| C    | 1.8990755193 | 0.2304235897 | -0.3142125983 |             |
| 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 |             |
| P    | -0.6327269919 | -2.0071039733 | 1.039546465  |             |
| 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 |             |
| H    | -4.4511298065 | 1.1274212613 | -0.0341673642 |             |
| H    | -3.5757525607 | -1.0290363273 | 0.8099548106  |             |
Carb2P

|   |   |   |   |
|---|---|---|---|
| C | -5.1604651876 | 1.0889571368 | -0.8944024875 |
| C | -4.1338417246 | 2.0356091035 | -0.8422268796 |
| 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 |
| C | -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 | 4.2657848502 | 1.8901920418 | 0.4205407990 |
| C | 5.2282734607 | 0.9095927639 | 0.6746587290 |
| C | 4.8566352683 | -0.4315120167 | 0.7601192720 |
| H | -0.1794355133 | 1.4057108598 | -1.0854057516 |
| H | -4.3610853913 | 3.0848801567 | -0.9930652070 |
| H | -2.0373727099 | 2.3900534427 | -0.5483091120 |
| H | -5.6816612671 | -0.9910288576 | -0.7160827941 |
| H | -2.9177527258 | 2.8522381199 | 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 | 1.190304957 | 0.7973949022 |
| H | 5.6096394630 | -1.1913656273 | 0.9399195798 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -6.042357 | 2.711351  | 0.153448  |
| C    | -5.489231 | 1.428394  | 0.122656  |
| C    | -4.110024 | 1.254898  | 0.057910  |
| C    | -3.268309 | 2.372445  | 0.034759  |
| C    | -3.832080 | 3.665607  | 0.064860  |
| C    | -5.214476 | 3.832553  | 0.111772  |
| C    | -1.798695 | 2.378498  | -0.015274 |
| C    | -1.247123 | 3.680589  | -0.030528 |
| P    | -2.550106 | 4.980586  | -0.078503 |
| C    | -0.957064 | 1.265680  | -0.050829 |
| C    | 0.426916  | 1.445031  | -0.087503 |
| C    | 0.967877  | 2.751392  | -0.102654 |
| C    | 0.131662  | 3.865288  | -0.100994 |
| C    | 1.452306  | 0.392158  | -0.123793 |
| P    | 2.771563  | 0.899329  | -0.164559 |
| C    | 2.802702  | 2.737979  | -0.256171 |
| P    | 1.236460  | -0.987116 | -0.132213 |
| C    | 2.326603  | -1.858066 | -0.165155 |
| C    | 3.641897  | -1.340253 | -0.204494 |
| C    | 3.861784  | 0.034947  | -0.230902 |
| C    | 2.282751  | -3.327788 | -0.171791 |
| C    | 3.560246  | -3.925745 | -0.211953 |
| P    | 4.904018  | -2.672809 | -0.347659 |
| C    | 1.144115  | -4.140291 | -0.140467 |
| C    | 1.281563  | -5.525020 | -0.139276 |
| C    | 2.549051  | -6.112149 | -0.180161 |
| C    | 3.690502  | -5.312753 | -0.228718 |
| H    | -7.118143 | 2.835789  | 0.201693  |
| H    | -6.139300 | 0.560917  | 0.144482  |
| H    | -3.695781 | 0.253241  | 0.028348  |
| H    | -5.649626 | 4.826177  | 0.117494  |
| H    | -2.502536 | 5.360004  | 1.296912  |
| H    | -1.379873 | 0.267318  | -0.045657 |
| H    | 0.549811  | 4.865390  | -0.153754 |
| H    | 3.118005  | 2.999553  | 1.111452  |
| H    | 0.227376  | -1.383150 | -0.110737 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 4.87056 | 0.42865 | -0.30335 |
| H    | 5.32840 | -2.69226 | 1.01495 |
| H    | 0.15407 | -3.69886 | -0.11451 |
| H    | 0.39783 | -6.15252 | -0.11120 |
| H    | 2.64533 | -7.19189 | -0.18135 |
| H    | 4.67143 | -5.77331 | -0.27706 |

**Carb4P**

| C    | -6.02093 | 4.02829 | 0.21828 |
| C    | -5.42111 | 2.76897 | 0.13346 |
| C    | -4.03579 | 2.64835 | 0.07965 |
| C    | -3.23512 | 3.79471 | 0.12069 |
| C    | -3.84577 | 5.06399 | 0.20629 |
| C    | -5.23388 | 5.17894 | 0.24277 |
| C    | -1.76626 | 3.85377 | 0.09055 |
| C    | -1.26186 | 5.17365 | 0.14783 |
| P    | -2.60957 | 6.42797 | 0.13899 |
| C    | -0.88428 | 2.77445 | 0.01460 |
| C    | 0.49277 | 3.00467 | 0.01415 |
| C    | 0.98624 | 4.32847 | 0.07189 |
| C    | 0.11020 | 5.41065 | 0.11143 |
| C    | 1.55658 | 1.99162 | -0.04510 |
| C    | 2.85724 | 2.54663 | -0.03267 |
| P    | 2.82213 | 4.38748 | -0.04856 |
| C    | 1.39234 | 0.60721 | -0.11391 |
| C    | 2.51430 | -0.22234 | -0.15185 |
| C    | 3.81036 | 0.34328 | -0.14052 |
| C    | 3.97979 | 1.72534 | -0.10651 |
| C    | 2.52248 | 1.69151 | -0.21202 |
| C    | 3.82494 | -2.24011 | -0.25172 |
| P    | 5.12328 | -0.93595 | -0.31180 |
| C    | 1.41023 | -2.35320 | -0.23541 |
| C    | 1.59136 | -3.91849 | -0.28265 |
| C    | 2.89888 | -4.45631 | -0.32330 |
| C    | 4.01102 | -3.61792 | -0.33422 |
| C    | 0.54174 | -4.94819 | -0.29856 |
| At. | X        | Y        | Z        |
|-----|----------|----------|----------|
| 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  |
| H   | -7.1011284500  | 4.1115679736   | 0.2558567980   |
| H   | -6.0394928330  | 1.8790379364   | 0.103535086    |
| H   | -3.5845860092  | 1.6651138243   | 0.0083454498   |
| H   | -5.7049180842  | 6.1548977702   | 0.2901637917   |
| H   | -2.5914275009  | 6.7508666962   | 1.5290166419   |
| H   | -1.2686504219  | 1.7619330790   | -0.0383937533  |
| H   | 0.4928460285   | 6.4262319752   | 0.1154734425   |
| H   | 3.1079565710   | 4.6048033917   | 1.3331110325   |
| 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  | -0.403806608   |
| H   | 3.1835154600   | -6.6133836030  | 0.8712691587   |
| H   | -1.2541253427  | -3.7444759772  | -0.2340635167  |
| H   | -2.7737731789  | -5.6831059488  | -0.2526320185  |
| H   | -1.8718540944  | -7.9882961078  | -0.3399169290  |
| H   | 0.5722323401   | -8.3664445563  | -0.4307140547  |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| C | -5.4154903363 | 4.6406924691 | 0.2015499184 |
| C | -4.7383961287 | 3.4202701040 | 0.1315434327 |
| C | -3.3476642950 | 3.8470056900 | 0.1161879585 |
| C | -2.6201223454 | 4.5780835646 | 0.1822199673 |
| C | -3.0797174360 | 5.8075223781 | 0.2581181813 |
| C | -4.7013008180 | 5.8373998111 | 0.2533626561 |
| C | -1.1581712039 | 4.7259823076 | 0.1857270369 |
| C | -0.7314177867 | 6.0719447648 | 0.2664250214 |
| P | -2.1526026830 | 7.2436582229 | 0.2407473049 |
| C | -0.2148367973 | 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 | 3.8736464345 | 0.1262295354 |
| P | 3.3994203667 | 5.5120306020 | 0.1318344795 |
| C | 2.1603404042 | 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 | -3.9697428634 | -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 |

Carb5P

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| X  | Y  | Z  |
|----|----|----|
| -2.7437998024 | -6.0831756321 | -0.4827761749 |
| -1.4565347289 | -7.3964436564 | -0.615311929 |
| -3.0105640109 | -3.6733745953 | -0.362065386 |
| -4.3915043648 | -3.8378279780 | -0.4020946331 |
| -4.9508781308 | -5.1153442478 | -0.4908741701 |
| -4.1274276996 | -6.2397230389 | -0.5419690836 |
| -6.4993339894 | 4.6577528894 | 0.2072793067 |
| -5.3001208968 | 2.4942326577 | 0.0827623043 |
| -2.8362137809 | 2.4304604520 | 0.0561103251 |
| -5.2336418736 | 6.7816947440 | 0.2900434417 |
| -2.1862026785 | 7.5423465822 | 1.6359394903 |
| -0.5359227887 | 2.6688134287 | 0.0387612711 |
| 0.9486231682 | 7.4240548867 | 0.2842015400 |
| 3.6547639783 | 5.7239638294 | 1.520095132 |
| 1.1867048859 | 1.1951104410 | -0.0440387988 |
| 5.6674925267 | 3.3817781421 | 0.0601470051 |
| 6.3303101418 | 0.2385538500 | 1.2379111433 |
| 1.2924641096 | -1.0663103466 | -0.1645090222 |
| 5.9608816625 | -2.8208041465 | -0.2434372530 |
| 4.1661708804 | -5.4766704377 | 0.9588346182 |
| -0.2862688398 | -2.6985287086 | -0.2782301760 |
| 1.6479626055 | -7.2897366546 | -0.5070763881 |
| -1.4915554974 | -7.8456884352 | 0.7387787949 |
| -2.5901604312 | -2.6758062321 | -0.2992838700 |
| -5.0376055722 | -2.9677024941 | -0.3708767818 |
| -6.0279349646 | -5.2323019415 | -0.5280494284 |
| -4.5681961175 | -7.2271072458 | -0.6272194071 |

**Carb6P**

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| X  | Y  | Z  |
|----|----|----|
| -4.6373377684 | 4.9150174439 | 0.4258782436 |
| -3.9415328483 | 3.7033920181 | 0.4225473423 |
| -2.5519273045 | 3.6858568136 | 0.3557352336 |
| -1.8423291098 | 4.8905366849 | 0.3083534013 |
| -2.5496060937 | 6.1114248873 | 0.3227154385 |
| Element | X             | Y             | Z             |
|---------|---------------|---------------|---------------|
| 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  | 3.894167900   | 0.2090721616  |
| C       | 2.3245474651  | 5.7488083889  | 0.229178607   |
| 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  | 2.0670884989  | 0.110597708   |
| 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       | 5.6705607634  | -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       | -6.6433152353 | -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  |
|   | 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 | 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 | -0.560966528 |
| H | -5.8801027348 | -5.5494869930 | 0.7182158586 |
| H | -3.2510332497 | -1.0171189319 | -0.5824966661 |
| H | -5.2642392597 | 0.4027565703 | -0.6698089960 |
| H | -7.5217075001 | -0.6152227582 | -0.6915931284 |
| H | -7.7763620343 | -3.0774364694 | -0.6721470522 |
CarbSi

23

C  3.4847108947 -0.4353009525  0.4342545251
C  3.0832663445  0.9002781184  0.4531350260
C  1.7406237034  1.2379773596  0.2964772196
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  0.5558344823
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

C   -5.0605929255   1.4488229033  -1.0017286795
C   -3.9628720752   2.3048751107  -0.9179672554
C   -2.6923742561   1.8015425777  -0.6479124541
C   -2.5083128150   0.4286092013  -0.4582428142
C   -3.6210755794  -0.4434392019  -0.5433835179
C   -4.8664145742   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   0.0646809496
H    4.3231627533   3.2401147481  0.3458722167
H    6.1671598914   1.6553846603  0.8238775643
Carb3Si

Diagram of Carb3Si with atomic coordinates.
H  -1.3401087812  0.2005589638  -0.0364121109  
H   0.3949886245  4.8485921135  0.2796779192  
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  
H   1.9375399680 -7.2717016198  -0.3671434530  
H   4.1200266217 -6.1207688028  -0.2387727334  

Carb4Si  

56  
C  -6.1072867757  3.2049548823  0.0126313213  
C  -5.3116228572  2.0600262672  -0.0289312096  
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   1.4295603884  0.6114191640  0.0862561371  
C   2.5442986770  -0.2303765833  0.0811765887  

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|   |       |       |       |       |
|---|-------|-------|-------|-------|
| C | 3.8468 | 0.3205 | 0.1655 |
| C | 4.0026 | 1.7046 | 0.2488 |
| C | 2.4878 | -1.7154 | -0.0081 |
| C | 3.7438 | -2.3705 | 0.0078 |
| Si | 5.0996 | -1.0788 | 0.1350 |
| C | 1.3122 | -2.4641 | -0.1023 |
| C | 1.3689 | -3.8575 | -0.1800 |
| C | 2.6228 | -4.5172 | -0.1570 |
| C | 3.7929 | -3.7630 | -0.0649 |
| C | 0.1834 | -4.7507 | -0.2903 |
| Si | 2.3340 | -6.3699 | -0.2634 |
| C | -1.4641 | -4.3220 | -0.3426 |
| C | -2.1769 | -5.2537 | -0.4484 |
| C | -1.8950 | -6.6189 | -0.5017 |
| C | -0.5706 | -7.0556 | -0.4506 |
| H | -7.1873 | 3.1173 | -0.9277 |
| H | -5.7757 | 1.0821 | -0.0956 |
| H | -3.3243 | 1.2579 | -0.0189 |
| H | -6.1344 | 5.3488 | 0.1270 |
| H | -3.1780 | 6.8990 | 1.4706 |
| H | -3.1119 | 7.0021 | -0.9277 |
| H | -1.1785 | 1.6140 | 0.0739 |
| H | 0.2023 | 6.3809 | 0.3496 |
| H | 3.2870 | 5.0206 | 1.5886 |
| H | 3.3713 | 5.1315 | -0.8087 |
| H | 0.4343 | 0.1882 | 0.0219 |
| H | 5.0010 | 2.1282 | 0.3097 |
| H | 5.9293 | 1.1822 | 1.3639 |
| H | 6.0202 | 1.0467 | -1.0317 |
| H | 0.3514 | -1.9637 | -0.1151 |
| H | 4.7557 | -4.2657 | -0.0499 |
| H | 2.7974 | -7.1288 | 0.9279 |
| H | 2.9195 | -7.0146 | -1.4680 |
| H | -1.3872 | -3.2659 | -0.3032 |
| H | -3.2055 | -4.9133 | -0.4904 |
| H | -2.7027 | -7.3375 | -0.5833 |
| H | -0.3589 | -8.1192 | -0.4926 |
Carb5Si

|   |   |   |   |
|---|---|---|---|
| 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 | -3.556681369 | 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 | 6.2018816540 | 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   -6.5766601488  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  1.632946158
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  -6.093327243  -0.6273100914

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Carb6Si

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  0.0848158999
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
| Element | X-Crystallographic Position | Y-Crystallographic Position | Z-Crystallographic Position |
|---------|-----------------------------|-----------------------------|------------------------------|
| 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       | -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              | 7.778437123                 | 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              | -0.4971441486               | -1.1038952982               |
| H       | -4.1749487248              | 1.3177933994                | -1.6584385498               |
| H       | -6.5950052234              | 0.8618644043                | -1.9126188280               |
| H       | -7.4604919792              | 1.4348991402                | -1.6108979585               |
| 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              |