

Supporting Information

General Strategy for Tuning the Stokes Shifts of Near Infrared Cyanine Dyes

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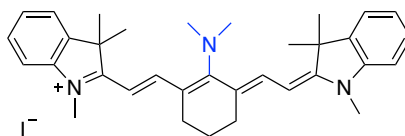
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Materials and General Instrumentations

Solvents and reagents used for reactions were purchased from commercial sources. Acetonitrile (ACN) for reactions was HPLC grade from Sigma-Aldrich. Column chromatography was performed using SiliCycle silica gel (230-400 mesh). Thin layer chromatography (TLC) with fluorescent indicator was purchased from Analtech. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra were obtained on Varian Inova 500 MHz instruments and were reported in parts per million (ppm) relative to the solvent resonances (δ), with coupling constants (J) in Hertz (Hz). HRMS analysis was performed on a Q-TOF Ultima system using electrospray ionization in positive mode. UV-Vis was performed on Agilent Cary 100 series machine and PL was recorded on Fluorolog by ISA instrument. Quantum yield measurement was performed on absolute PL quantum yield spectrometer C11347 by Hamamatsu.

Cyanine Substrates Preparation and Characterization

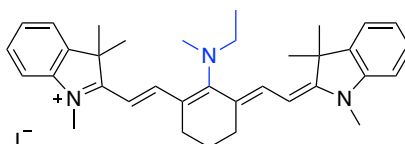
General procedure for cyanine dyes:



2-((*E*)-2-((*E*)-2-(dimethylamino)-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,3,3-trimethyl-3*H*-indol-1-ium iodide (**2**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (40 mg, 0.064 mmol, 64%).

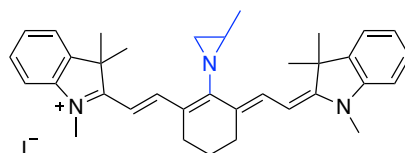
$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 7.40 (d, J = 13.1 Hz, 2H), 7.23 (td, J = 8.1, 7.4, 1.5 Hz, 4H), 7.01 (t, J = 7.4 Hz, 2H), 6.88 (d, J = 7.9 Hz, 2H), 5.56 (d, J = 13.1 Hz, 2H), 3.61 (s, 6H), 3.39 (s, 6H), 2.46 (t, J = 6.6 Hz, 4H), 1.79 (p, J = 6.6 Hz, 2H), 1.59 (s, 12H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform-*d*): δ 175.55, 167.84, 143.54, 140.28, 139.84, 128.22, 122.73, 122.08, 121.97, 108.50, 94.06, 53.53, 47.86, 47.60, 29.48, 25.40, 21.56. ϵ (664 nm) = 40,929 $\text{M}^{-1}\text{cm}^{-1}$. HRMS (ESI+): calcd for $\text{C}_{34}\text{H}_{42}\text{N}_3^+$ [M] $^+$ 492.3379, found 492.3378.



2-((*E*)-2-((*E*)-2-(ethyl(methyl)amino)-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,3,3-trimethyl-3*H*-indol-1-ium iodide (**3**).

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (39 mg, 0.062 mmol, 62%).

$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 7.46 (d, J = 13.4 Hz, 2H), 7.33 – 7.24 (m, 4H), 7.08 (t, J = 7.4 Hz, 2H), 6.97 (d, J = 7.9 Hz, 2H), 5.72 (d, J = 13.4 Hz, 2H), 3.79 (q, J = 7.0 Hz, 2H), 3.48 (s, 6H), 3.41 (s, 3H), 2.47 (t, J = 6.5 Hz, 4H), 1.81 (p, J = 6.6 Hz, 2H), 1.60 (s, 12H), 1.37 (t, J = 7.0 Hz, 3H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform-*d*): δ 175.03, 169.15, 143.30, 141.83, 139.94, 128.44, 124.26, 123.41, 121.97, 109.15, 95.86, 53.52, 47.90, 44.73, 31.24, 29.27, 24.94, 21.83, 14.98. ϵ (684 nm) = 30,548 $\text{M}^{-1}\text{cm}^{-1}$. HRMS(ESI+): calcd for $\text{C}_{35}\text{H}_{44}\text{N}_3^+$ [M] $^+$ 506.3535, found 506.3525.

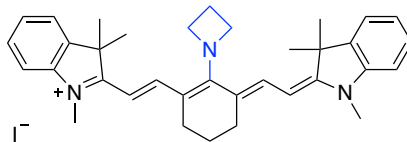


1,3,3-Trimethyl-2-((*E*)-2-((*E*)-2-(2-methylaziridin-1-yl)-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3*H*-indol-1-ium iodide (**4**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (30 mg, 0.047 mmol, 47%).

$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 8.01 (d, J = 13.7 Hz, 2H), 7.38 – 7.26 (m, 4H), 7.14 (t, J = 7.4 Hz, 2H), 7.05 (d, J = 7.9 Hz, 2H), 5.88 (d, J = 13.7 Hz, 2H), 3.57 (s, 6H), 2.57 (t, J = 6.0 Hz, 4H), 1.84 – 1.76 (m,

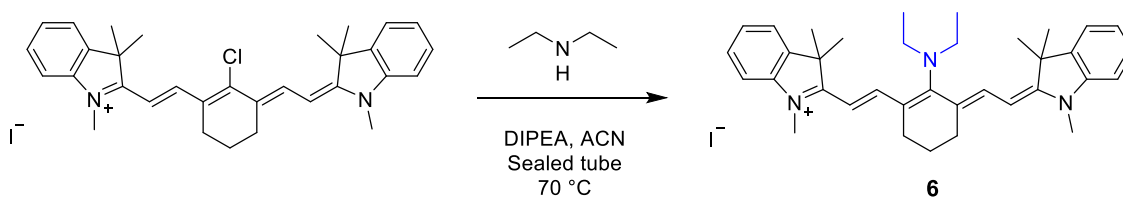
3H), 1.69 – 1.59 (m, 14H), 1.46 (d, $J = 5.4$ Hz, 3H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform- d): δ 170.91, 170.12, 143.07, 140.20, 139.76, 128.61, 124.61, 124.14, 121.99, 109.76, 98.11, 48.27, 39.06, 36.94, 31.66, 28.61, 28.47, 25.95, 20.86, 18.09. ϵ (742 nm) = 63,314 $\text{M}^{-1}\text{cm}^{-1}$. HRMS (ESI+): calcd for $\text{C}_{35}\text{H}_{42}\text{N}_3^+$ $[\text{M}]^+$ 504.3379, found 504.3375.



2-((E)-2-((E)-2-(azetidin-1-yl)-3-(2-((E)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,3,3-trimethyl-3H-indol-1-ium iodide (5)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (49 mg, 0.078 mmol, 78%).

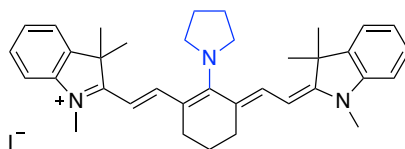
$^1\text{H-NMR}$ (500 MHz, Chloroform- d): δ 7.24 – 7.16 (m, 6H), 6.96 (t, $J = 7.5$ Hz, 2H), 6.77 (d, $J = 7.7$ Hz, 2H), 5.32 (d, $J = 12.8$ Hz, 2H), 4.93 (t, $J = 7.6$ Hz, 4H), 3.25 (s, 6H), 2.71 (p, $J = 7.6$ Hz, 2H), 2.56 – 2.49 (m, 4H), 1.86 – 1.83 (m, 2H), 1.64 (s, 12H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform- d): δ 169.77, 165.86, 143.70, 139.75, 134.78, 127.96, 121.99, 121.95, 107.61, 92.32, 62.46, 47.02, 29.83, 29.27, 27.22, 20.79, 19.31. ϵ (615 nm) = 30,105 $\text{M}^{-1}\text{cm}^{-1}$. HRMS (ESI+): calcd for $\text{C}_{35}\text{H}_{42}\text{N}_3^+$ $[\text{M}]^+$ 504.3379, found 504.3382.



2-((E)-2-((E)-2-(diethylamino)-3-(2-((E)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,3,3-trimethyl-3H-indol-1-ium iodide. (6)

Compound **6** is synthesized according to the previous reported procedures.¹ To a solution of **6** (74 mg, 0.10 mmol), diisopropylethylamine (DIPEA) (35 μL , 2 equiv, 0.20 mmol) in acetonitrile (2 mL) was added freshly distilled diethylamine (206 μL , 20 equiv, 2.0 mmol) under nitrogen. The mixture was stirred at 70 °C and the reaction was monitored by LC-MS. Upon completion, typically in 48 h, the mixture was concentrated under reduced pressure and purified by flash column (100% DCM gradually to 5% MeOH/DCM). The product was isolated as a dark solid (21 mg, 0.032 mmol, 32%).

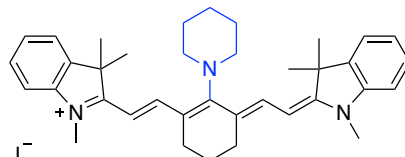
$^1\text{H-NMR}$ (500 MHz, Chloroform- d): δ 7.52 (d, $J = 13.6$ Hz, 2H), 7.34 – 7.26 (m, 4H), 7.11 (m, 2H), 7.02 (d, $J = 7.9$ Hz, 2H), 5.80 (d, $J = 13.6$ Hz, 2H), 3.65 (q, $J = 6.9$ Hz, 4H), 3.52 (s, 6H), 2.49 (t, $J = 6.5$ Hz, 4H), 1.82 (p, $J = 6.5$ Hz, 2H), 1.60 (s, 12H), 1.28 (t, $J = 6.9$ Hz, 6H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform- d): δ 174.15, 169.83, 143.19, 142.52, 140.06, 128.57, 125.76, 123.76, 121.97, 109.50, 96.95, 49.47, 48.03, 31.36, 29.07, 24.88, 21.98, 14.84. ϵ (699 nm) = 65,575 $\text{M}^{-1}\text{cm}^{-1}$. HRMS (ESI+): calcd for $\text{C}_{36}\text{H}_{46}\text{N}_3^+$ $[\text{M}]^+$ 520.3690, found 520.3692.



1,3,3-Trimethyl-2-((E)-2-((E)-2-(pyrrolidin-1-yl)-3-(2-((E)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3H-indol-1-ium iodide (7).

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (15 mg, 0.023 mmol, 23%).

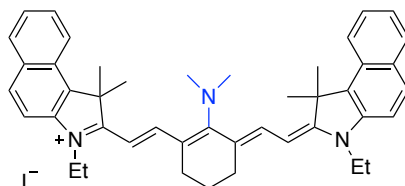
$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 7.42 (d, J = 12.7 Hz, 2H), 7.19 (m, 4H), 6.94 (t, J = 7.4 Hz, 2H), 6.73 (d, J = 8.0 Hz, 2H), 5.27 (d, J = 12.7 Hz, 2H), 4.32 (d, J = 6.5 Hz, 4H), 3.22 (s, 6H), 2.59 (t, J = 6.2 Hz, 4H), 2.10 (m, 4H), 1.79 (t, J = 6.3 Hz, 2H), 1.70 (s, 12H). $^{13}\text{C-NMR}$ (126 MHz, cdCl_3): δ 173.07, 165.22, 143.92, 140.02, 135.14, 127.72, 122.03, 121.53, 121.22, 107.08, 91.76, 55.86, 46.98, 29.58, 29.43, 28.77, 24.16, 20.91. ϵ (604 nm) = 52,973 $\text{M}^{-1}\text{cm}^{-1}$. HRMS (ESI+): calcd for $\text{C}_{36}\text{H}_{44}\text{N}_3^+$ $[\text{M}]^+$ 518.3535, found 518.3536.



1,3,3-Trimethyl-2-((E)-2-((E)-2-(piperidin-1-yl)-3-(2-((E)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3H-indol-1-ium iodide (8)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (72 mg, 0.054 mmol, 54%).

$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 7.50 (d, J = 13.2 Hz, 2H), 7.33 – 7.22 (m, 4H), 7.06 (t, J = 7.4 Hz, 2H), 6.95 (d, J = 7.9 Hz, 2H), 5.68 (d, J = 13.2 Hz, 2H), 3.85 (t, J = 5.0 Hz, 4H), 3.46 (s, 6H), 2.47 (t, J = 6.7 Hz, 4H), 1.96-1.92 (m, 2H), 1.90-1.86 (m, 4H), 1.84-1.82 (m, 2H), 1.62 (s, 12H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform-*d*): δ 175.57, 168.39, 143.43, 140.15, 139.75, 128.36, 123.79, 123.06, 121.89, 108.84, 95.03, 56.80, 47.63, 28.96, 28.15, 24.94, 24.28, 21.63, 18.91. ϵ (668 nm) = 61,734 $\text{M}^{-1}\text{cm}^{-1}$. HRMS (ESI+): calcd for $\text{C}_{37}\text{H}_{46}\text{N}_3^+$ $[\text{M}]^+$ 532.3692, found 532.3690.

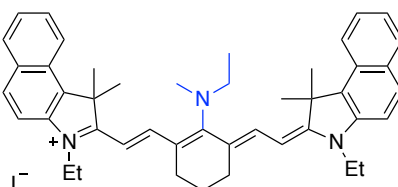


2-((E)-2-((E)-2-(dimethylamino)-3-(2-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3-ethyl-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (9).

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (41 mg, 0.055 mmol, 55%).

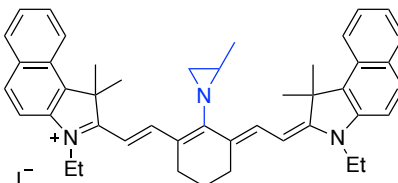
$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 8.07 (d, J = 8.5 Hz, 2H), 7.83 (dd, J = 8.5, 4.4 Hz, 4H), 7.57 (d, J = 13.3 Hz, 2H), 7.51 (ddd, J = 8.3, 6.8, 1.3 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 5.69 (d, J = 13.3 Hz, 2H), 4.04 (q, J = 7.2 Hz, 4H), 3.65 (s, 6H), 2.50 (t, J = 6.6 Hz, 4H), 1.93 (s, 12H), 1.86 – 1.81 (m, 2H), 1.40 (t, J = 7.2 Hz, 6H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform-*d*): δ 174.46, 168.95, 140.52, 139.85,

131.82, 130.89, 130.18, 129.89, 128.49, 127.41, 123.90, 122.00, 121.91, 109.74, 93.65, 49.72, 47.83, 38.59, 28.97, 25.34, 21.74, 12.03. HRMS (ESI+): calcd for C₄₄H₅₀N₃⁺ [M]⁺ 620.4005, found 620.4008.



3-Ethyl-2-((E)-2-((E)-2-(ethyl(methyl)amino)-3-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (10).

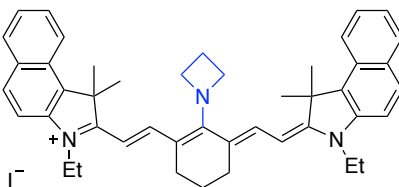
The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (57 mg, 0.075 mmol, 75%). ¹H-NMR (500 MHz, Chloroform-*d*): δ 8.06 (d, *J* = 8.4 Hz, 2H), 7.86 (dd, *J* = 8.7, 2.1 Hz, 4H), 7.63 (d, *J* = 13.6 Hz, 2H), 7.53 (ddd, *J* = 8.4, 6.8, 1.3 Hz, 2H), 7.36 (ddd, *J* = 8.1, 6.9, 1.1 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 5.82 (d, *J* = 13.6 Hz, 2H), 4.11 (q, *J* = 7.2 Hz, 4H), 3.80 (q, *J* = 7.0 Hz, 2H), 3.42 (s, 3H), 2.50 (t, *J* = 6.4 Hz, 4H), 1.92 (s, 12H), 1.85 (p, *J* = 6.5 Hz, 2H), 1.43 – 1.40 (m, 9H). ¹³C-NMR (126 MHz, Chloroform-*d*): δ 173.76, 170.16, 141.76, 139.68, 132.27, 131.18, 130.46, 130.02, 128.35, 127.53, 124.33, 124.23, 121.83, 110.09, 95.39, 53.44, 49.99, 44.59, 39.03, 24.99, 21.96, 15.12, 12.24. HRMS (ESI+): calcd for C₄₅H₅₂N₃⁺ [M]⁺ 634.4161, found 634.4171.



3-Ethyl-2-((E)-2-((E)-3-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)-2-(2-methylaziridin-1-yl)cyclohex-1-en-1-yl)vinyl)-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (11)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (36 mg, 0.047 mmol, 47%).

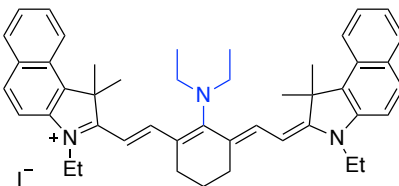
¹H-NMR (500 MHz, Chloroform-*d*): δ 8.14 (d, *J* = 13.7 Hz, 2H), 8.10 – 8.04 (m, 2H), 7.88 (dd, *J* = 8.5, 4.2 Hz, 4H), 7.55 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 2H), 7.39 (ddd, *J* = 8.0, 6.8, 1.0 Hz, 2H), 7.35 (d, *J* = 8.8 Hz, 2H), 5.94 (d, *J* = 13.7 Hz, 2H), 4.18 (q, *J* = 7.3 Hz, 4H), 2.79 – 2.77 (m, 1H), 2.70 (d, *J* = 5.8 Hz, 1H), 2.58 (t, *J* = 6.2 Hz, 4H), 2.43 (d, *J* = 3.5 Hz, 1H), 1.98 (d, *J* = 7.4 Hz, 13H), 1.86 – 1.82 (m, 2H), 1.56 (d, *J* = 5.4 Hz, 3H), 1.44 (t, *J* = 7.2 Hz, 6H). ¹³C-NMR (126 MHz, Chloroform-*d*): δ 170.68, 170.28, 139.50, 139.11, 132.75, 131.45, 130.61, 130.07, 128.30, 127.64, 124.54, 124.01, 121.93, 110.27, 97.17, 50.26, 39.37, 37.12, 28.16, 28.04, 25.94, 20.92, 18.37, 12.33. HRMS (ESI+): calcd for C₄₅H₅₀N₃⁺ [M]⁺ 632.4005, found 632.4009.



2-((E)-2-((E)-2-(azetidin-1-yl)-3-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3-ethyl-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (**12**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (64 mg, 0.084 mmol, 84%).

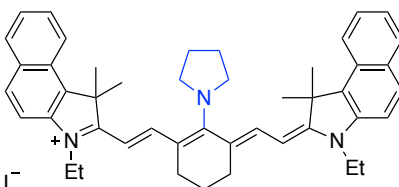
¹H-NMR (500 MHz, Chloroform-*d*): δ 8.07 (d, *J* = 8.6 Hz, 2H), 7.78 (dd, *J* = 13.7, 8.4 Hz, 4H), 7.48 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 2H), 7.38 (d, *J* = 12.8 Hz, 2H), 7.29 (ddd, *J* = 8.0, 6.8, 1.0 Hz, 2H), 7.11 (d, *J* = 8.7 Hz, 2H), 5.43 (d, *J* = 12.7 Hz, 2H), 5.01 (t, *J* = 7.5 Hz, 4H), 3.88 (q, *J* = 7.2 Hz, 4H), 2.75 (p, *J* = 7.5 Hz, 2H), 2.55 (t, *J* = 6.2 Hz, 4H), 1.96 (s, 12H), 1.90 – 1.84 (m, 2H), 1.31 (t, *J* = 7.2 Hz, 6H). ¹³C-NMR (126 MHz, Chloroform-*d*): δ 169.26, 166.64, 140.07, 134.72, 131.06, 130.49, 129.81, 129.72, 128.65, 127.24, 123.39, 122.06, 117.62, 109.25, 91.46, 62.48, 49.04, 37.71, 28.66, 27.22, 20.84, 19.31, 11.59. HRMS (ESI⁺): calcd for C₄₅H₅₀N₃⁺ [M]⁺ 632.4005, found 632.4007.



2-((E)-2-((E)-2-(diethylamino)-3-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3-ethyl-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (**13**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (36 mg, 0.046 mmol, 46%).

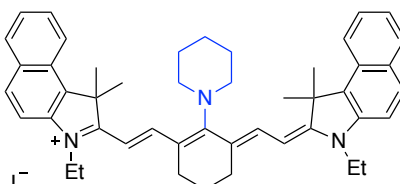
¹H-NMR (500 MHz, Chloroform-*d*): δ 8.07 (d, *J* = 8.5 Hz, 2H), 7.89 (d, *J* = 8.9 Hz, 4H), 7.69 (d, *J* = 13.7 Hz, 2H), 7.58 – 7.51 (m, 2H), 7.42 – 7.37 (m, 2H), 7.34 (d, *J* = 8.8 Hz, 2H), 5.89 (d, *J* = 13.7 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 4H), 3.70 (q, *J* = 6.9 Hz, 4H), 2.53 (t, *J* = 6.4 Hz, 4H), 1.93 (s, 12H), 1.89 – 1.85 (m, 2H), 1.44 (t, *J* = 7.2 Hz, 6H), 1.35 (t, *J* = 6.9 Hz, 6H). ¹³C-NMR (126 MHz, Chloroform-*d*): δ 173.00, 170.56, 142.05, 139.64, 132.46, 131.29, 130.56, 130.10, 128.33, 127.57, 125.62, 124.37, 121.82, 110.20, 96.22, 50.06, 49.39, 39.18, 28.59, 28.44, 25.01, 22.05, 14.96, 12.31. HRMS (ESI⁺): calcd for C₄₆H₅₄N₃⁺ [M]⁺ 648.4319, found 648.4318.



3-Ethyl-2-((E)-2-((E)-3-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)-2-(pyrrolidin-1-yl)cyclohex-1-en-1-yl)vinyl)-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (**14**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (56 mg, 0.072 mmol, 72%).

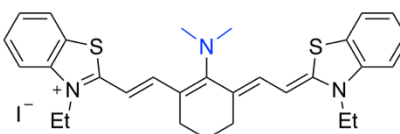
$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 8.08 (d, J = 8.6 Hz, 2H), 7.75 (dd, J = 16.0, 8.4 Hz, 4H), 7.53 (d, J = 12.7 Hz, 2H), 7.44 (dd, J = 8.4, 6.8 Hz, 2H), 7.25 (t, J = 7.5 Hz, 2H), 7.08 (d, J = 8.7 Hz, 2H), 5.38 (d, J = 12.7 Hz, 2H), 4.34 (d, J = 6.4 Hz, 4H), 3.84 (q, J = 7.6, 7.0 Hz, 4H), 2.62 (t, J = 6.1 Hz, 4H), 2.12 (q, J = 4.7, 3.1 Hz, 4H), 1.99 (s, 12H), 1.81 (p, J = 6.4 Hz, 2H), 1.29 (t, J = 7.3 Hz, 6H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform-*d*): δ 172.74, 165.92, 140.25, 135.05, 130.89, 130.28, 129.65, 129.62, 128.76, 127.03, 123.10, 122.11, 120.64, 109.17, 91.03, 55.93, 48.99, 37.51, 28.81, 28.78, 24.30, 20.89, 11.50. HRMS (ESI+): calcd for $\text{C}_{46}\text{H}_{52}\text{N}_3^+$ [M] $^+$ 646.4161, found 646.4163.



3-Ethyl-2-((E)-2-((E)-3-((E)-2-(3-ethyl-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)-2-(piperidin-1-yl)cyclohex-1-en-1-yl)vinyl)-1,1-dimethyl-1H-benzo[e]indol-3-ium iodide (15).

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (66 mg, 0.084 mmol, 84%).

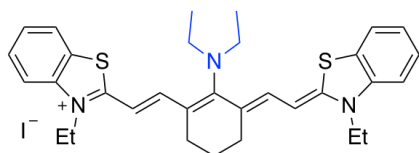
$^1\text{H-NMR}$ (500 MHz, Chloroform-*d*): δ 8.06 (d, J = 8.6 Hz, 2H), 7.84 (d, J = 8.5 Hz, 4H), 7.68 (d, J = 13.3 Hz, 2H), 7.51 (ddd, J = 8.3, 6.8, 1.3 Hz, 2H), 7.34 (ddd, J = 8.0, 6.8, 1.0 Hz, 2H), 7.27 (d, J = 8.7 Hz, 2H), 5.78 (d, J = 13.3 Hz, 2H), 4.07 (q, J = 7.2 Hz, 4H), 3.79 (t, J = 4.8 Hz, 4H), 2.48 (t, J = 6.6 Hz, 4H), 1.95 – 1.80 (m, 20H), 1.40 (t, J = 7.2 Hz, 6H). $^{13}\text{C-NMR}$ (126 MHz, Chloroform-*d*): δ 174.14, 169.56, 140.35, 139.77, 131.99, 131.07, 130.38, 129.99, 128.39, 127.46, 124.08, 124.04, 121.86, 110.03, 94.84, 56.78, 49.78, 38.85, 28.48, 28.23, 25.07, 24.57, 21.83, 12.18. HRMS (ESI+): calcd for $\text{C}_{47}\text{H}_{54}\text{N}_3^+$ [M] $^+$ 660.4318, found 660.4318.



3-Ethyl-2-((E)-2-((E)-3-((Z)-2-(3-ethylbenzo[d]thiazol-2(3H)-ylidene)ethylidene)-2-(pyrrolidin-1-yl)cyclohex-1-en-1-yl)vinyl)benzo[d]thiazol-3-ium iodide (16)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (29 mg, 0.046 mmol, 46%).

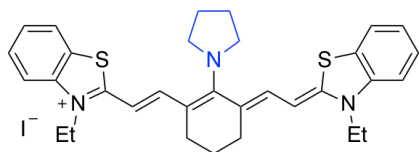
$^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.58 (dd, J = 8.3, 1.2 Hz, 2H), 7.42 (ddd, J = 8.6, 7.6, 1.2 Hz, 2H), 7.36 – 7.31 (m, 2H), 7.27 – 7.20 (m, 4H), 5.87 (d, J = 12.7 Hz, 2H), 4.24 (q, J = 7.3 Hz, 4H), 3.46 (s, 6H), 2.45 (t, J = 6.5 Hz, 4H), 1.84 – 1.80 (m, 2H), 1.47 (t, J = 7.2 Hz, 6H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 141.48, 127.63, 124.71, 124.07, 122.31, 111.13, 92.69, 47.76, 41.33, 29.71, 22.01, 12.31. ϵ (703 nm) = 13,307 $\text{M}^{-1}\text{cm}^{-1}$.



2-((E)-2-((E)-2-(diethylamino)-3-((Z)-2-(3-ethylbenzo[d]thiazol-2(3H)-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3-ethylbenzo[d]thiazol-3-ium iodide (**17**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (38 mg, 0.058 mmol, 58%).

^1H NMR (500 MHz, Chloroform-*d*) δ 7.59 (d, $J = 8.0, 1.2$ Hz, 2H), 7.48 – 7.39 (m, 4H), 7.32 (d, $J = 8.2$ Hz, 2H), 7.26 – 7.20 (m, 2H), 6.02 (d, $J = 13.0$ Hz, 2H), 4.33 (q, $J = 7.3$ Hz, 4H), 3.59 (q, $J = 7.1$ Hz, 4H), 2.51 (t, $J = 6.3$ Hz, 4H), 1.85 (q, $J = 6.4$ Hz, 2H), 1.48 (t, $J = 7.3$ Hz, 6H), 1.31 (t, $J = 7.0$ Hz, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.30, 142.65, 141.53, 127.87, 124.93, 124.41, 122.31, 122.21, 111.69, 111.14, 94.81, 49.60, 41.79, 29.71, 25.77, 21.93, 14.22. ϵ (733 nm) = 16,795 $\text{M}^{-1}\text{cm}^{-1}$.



3-Ethyl-2-((E)-2-((E)-3-((Z)-2-(3-ethylbenzo[d]thiazol-2(3H)-ylidene)ethylidene)-2-(pyrrolidin-1-yl)cyclohex-1-en-1-yl)vinyl)benzo[d]thiazol-3-ium iodide (**18**)

The title compound was prepared according to the general procedure at 0.1 mmol scale. Product was isolated as a dark solid product (54 mg, 0.082 mmol, 82%).

^1H NMR (500 MHz, Chloroform-*d*) δ 7.47 (d, $J = 7.7$ Hz, 2H), 7.31 (t, $J = 7.7$ Hz, 2H), 7.14 – 7.05 (m, 4H), 7.02 (d, $J = 8.2$ Hz, 2H), 5.51 (d, $J = 12.0$ Hz, 2H), 4.17 (s, 4H), 4.04 (q, $J = 7.2$ Hz, 4H), 2.61 – 2.53 (m, 4H), 2.11 (s, 4H), 1.86 – 1.81 (m, 2H), 1.38 (t, $J = 7.2$ Hz, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 156.88, 141.65, 137.22, 126.98, 124.54, 122.91, 122.15, 119.87, 109.86, 88.91, 55.99, 40.37, 28.82, 24.62, 20.94, 11.73. ϵ (636 nm) = 26,513 $\text{M}^{-1}\text{cm}^{-1}$.

Computational Supplementary Figure and Table

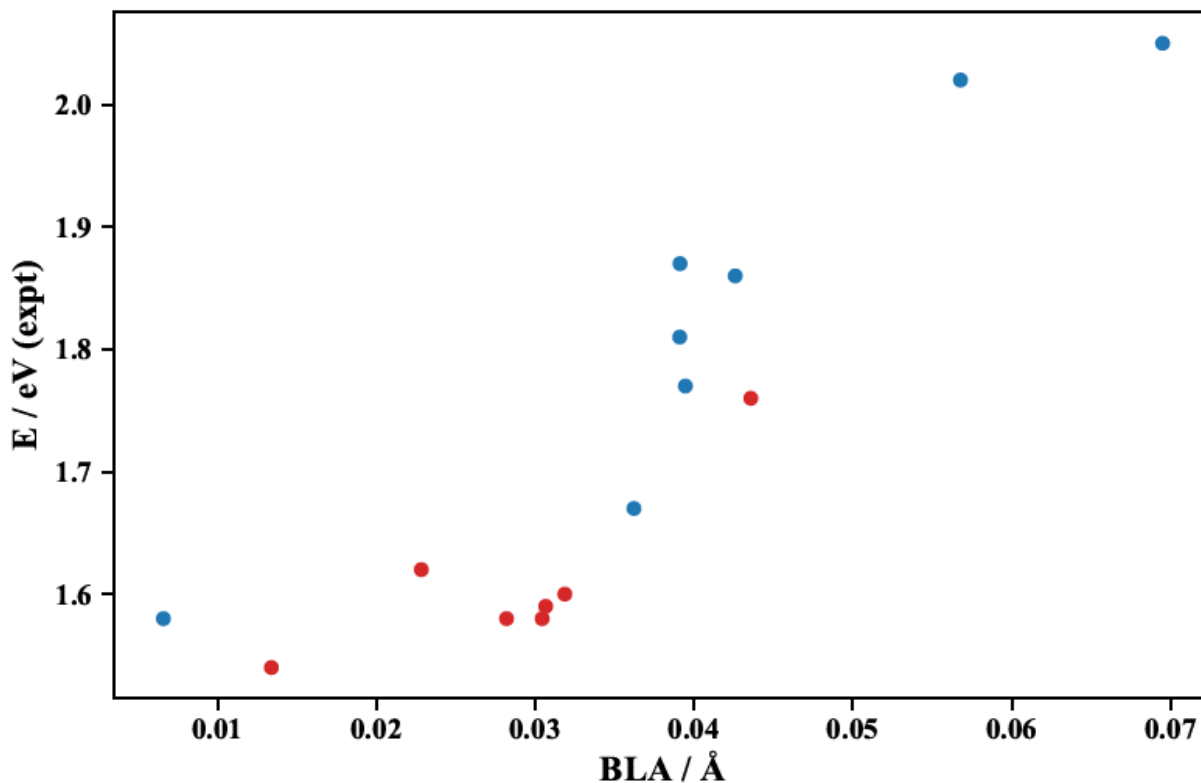


Figure S1. Scatter plot of the experimental spectral energy maxima as a function of the DFT-optimized bond length alternation coordinate (in angstrom). Absorption and emission energies are shown by blue and red dots, respectively.

Table S1. Absolute energies of optimized geometries on the DFT level of theory. (CAM-B3LYP/6-31G*)

Molecule	Conformers	Geometries	S ₀ Energy / a.u.	S ₁ Energy / a.u.	S ₁ -S ₀ Gap / a.u.
1	-	Franck-Condon point	-1809.801264	-1809.710549	0.090715
		S ₁ minimum	-1809.800022	-1809.711759	0.088263
2	Bis-dipole	Franck-Condon point	-1484.092954	-1483.994624	0.098330
		S ₁ minimum	-1484.088437	-1483.998166	0.090271
	Cyanine-like	Franck-Condon point	-1484.098962	-1484.002956	0.096006
		S ₁ minimum	-1484.073807	-1484.010546	0.066895
3	Bis-dipole	Franck-Condon point	-1523.376682	-1523.280279	0.096404
		S ₁ minimum	-1523.355859	-1523.287972	0.067887
	Cyanine-like	Franck-Condon point	-1523.388981	-1523.293277	0.095704
		S ₁ minimum	-1523.386699	-1523.295906	0.090793
4	Bis-dipole	Franck-Condon point	-1522.160161	-1522.066705	0.093456
		S ₁ minimum	-1522.158405	-1522.068372	0.090032

	Cyanine-like	Franck-Condon point	-1522.144393	-1522.053229	0.091164
		S ₁ minimum	-1522.143264	-1522.054359	0.088905
5	Bis-dipole	Franck-Condon point	-1522.167762	-1522.069148	0.098614
		S ₁ minimum	-1522.164092	-1522.072413	0.091678
	Cyanine-like	Franck-Condon point	-1522.15922	-1522.06249	0.096730
		S ₁ minimum	-1522.156756	-1522.065402	0.091353
6	Bis-dipole	Franck-Condon point	-1562.663326	-1562.567549	0.095776
		S ₁ minimum	-1562.638213	-1562.577772	0.060441
	Cyanine-like	Franck-Condon point	-1562.679046	-1562.583593	0.095453
		S ₁ minimum	-1562.676662	-1562.586636	0.090026
7	Bis-dipole	Franck-Condon point	-1561.475774	-1561.377488	0.098285
		S ₁ minimum	-1561.467923	-1561.382244	0.085679
	Cyanine-like	Franck-Condon point	-1561.476323	-1561.383757	0.092565
		S ₁ minimum	-1561.474749	-1561.385506	0.089244
8	Bis-dipole	Franck-Condon point	-1600.75445	-1600.657514	0.096936
		S ₁ minimum	-1600.735358	-1600.666551	0.068807
	Cyanine-like	Franck-Condon point	-1600.764007	-1600.667421	0.096586
		S ₁ minimum	-1600.761831	-1600.671054	0.090777

Table S2. Important geometric parameters for CAM-B3LYP/6031G* structures.^a

Dye	State ^b	BLA (Å) ^c	Pyr. Ang. (°) ^d
2	GS	0.03912	0.002
	ES	0.03187	0.001
3	GS	0.03910	0.014
	ES	0.03066	0.177
4	GS	0.03622	43.354
	ES	0.02284	49.371
5	GS	0.05677	7.156
	ES	0.04358	15.927
6	GS	0.03948	0.002
	ES	0.03046	0.162
7	GS	0.06949	2.115
	ES	0.02820	0.1421
8	GS	0.04259	0.011
	ES	0.03044	0.002

[a] Geometric parameters are computed at the TD-CAM-B3LYP/6-31G* level.

[b] Ground and excited state structures are abbreviated GS and ES, respectively.

[c] BLA is defined:

$$\text{BLA} = (r_{2-3} + r_{4-5} + r_{5-6} + r_{7-8}) - (r_{1-2} + r_{3-4} + r_{6-7} + r_{8-9})$$

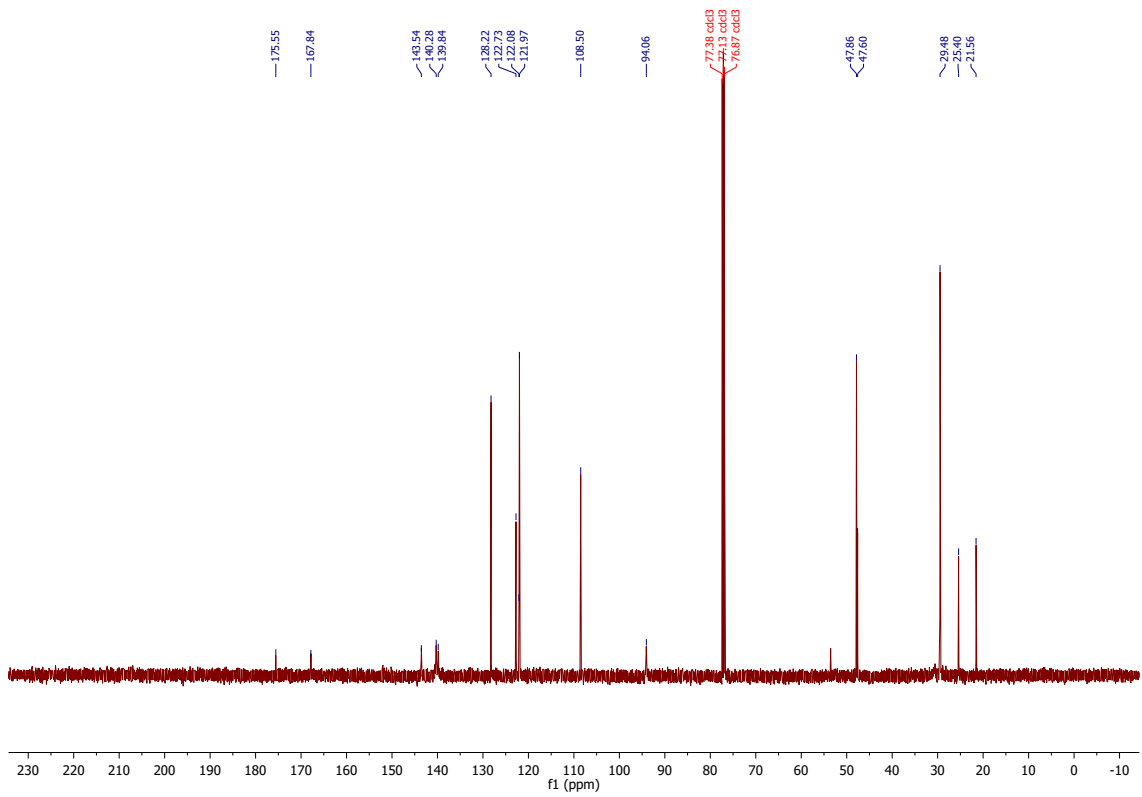
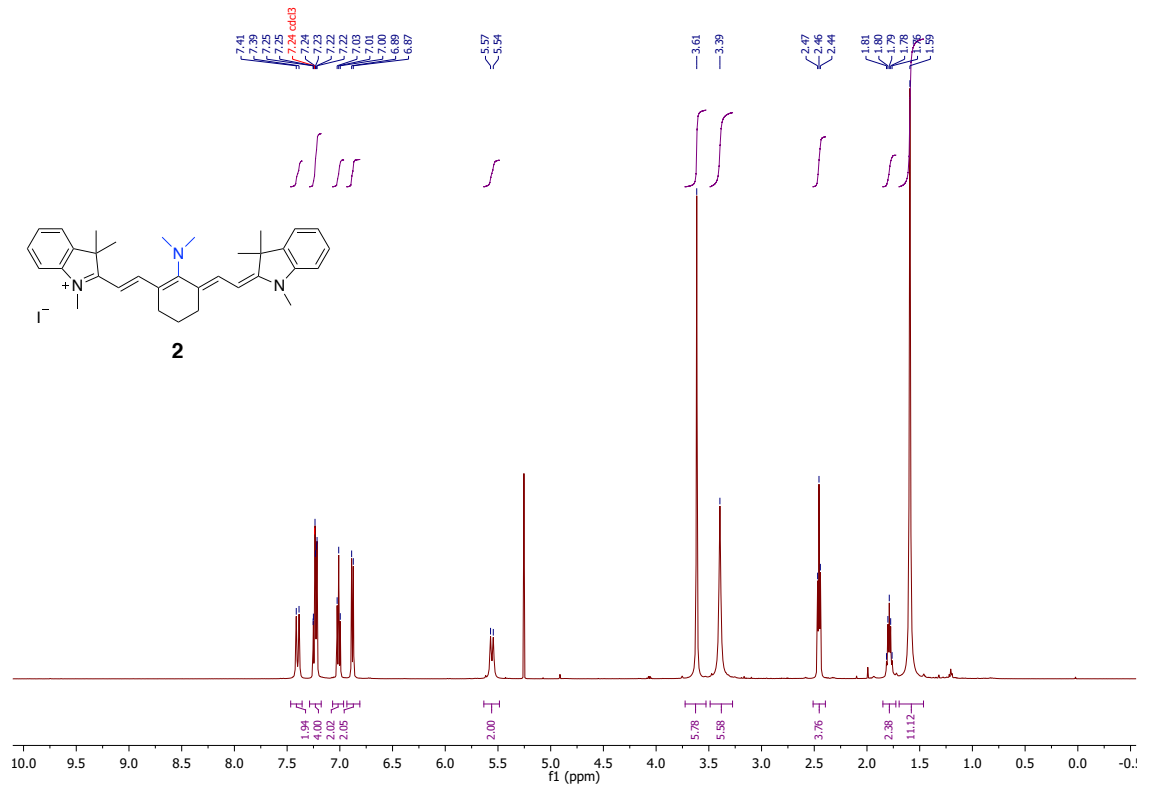
where r_{m-n} is the distance between carbon atoms m and n of the heptamethine chain.

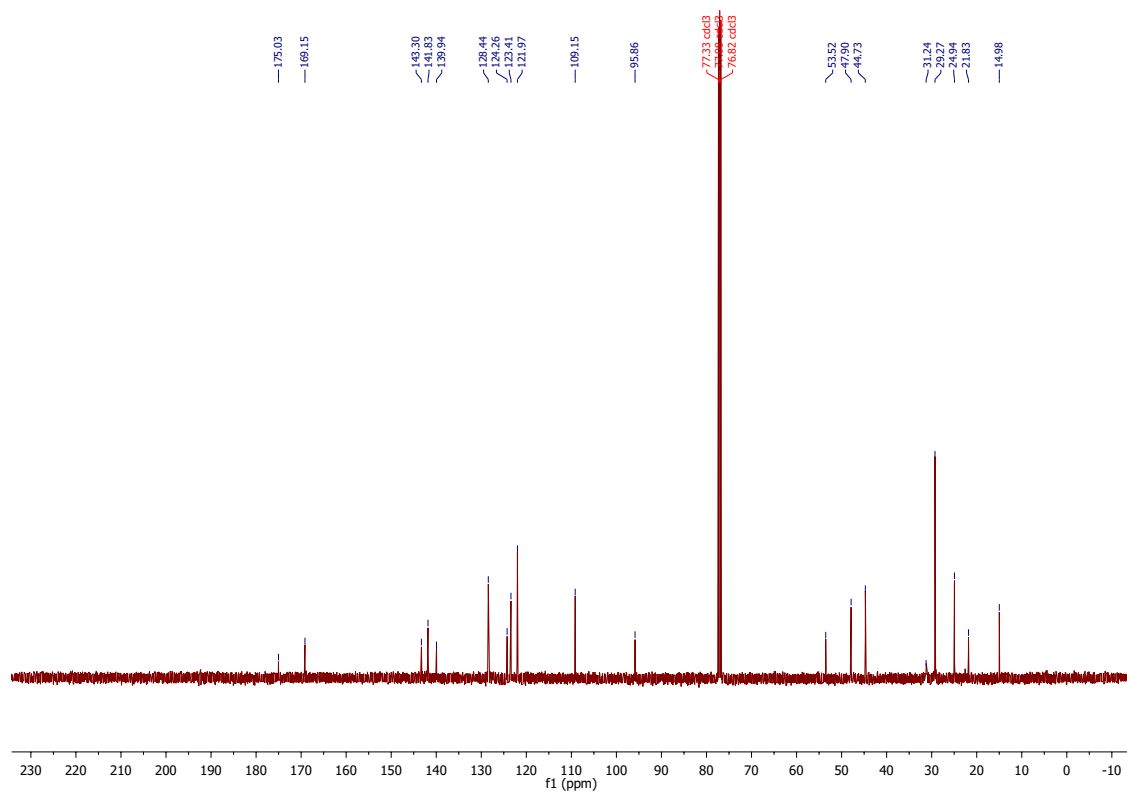
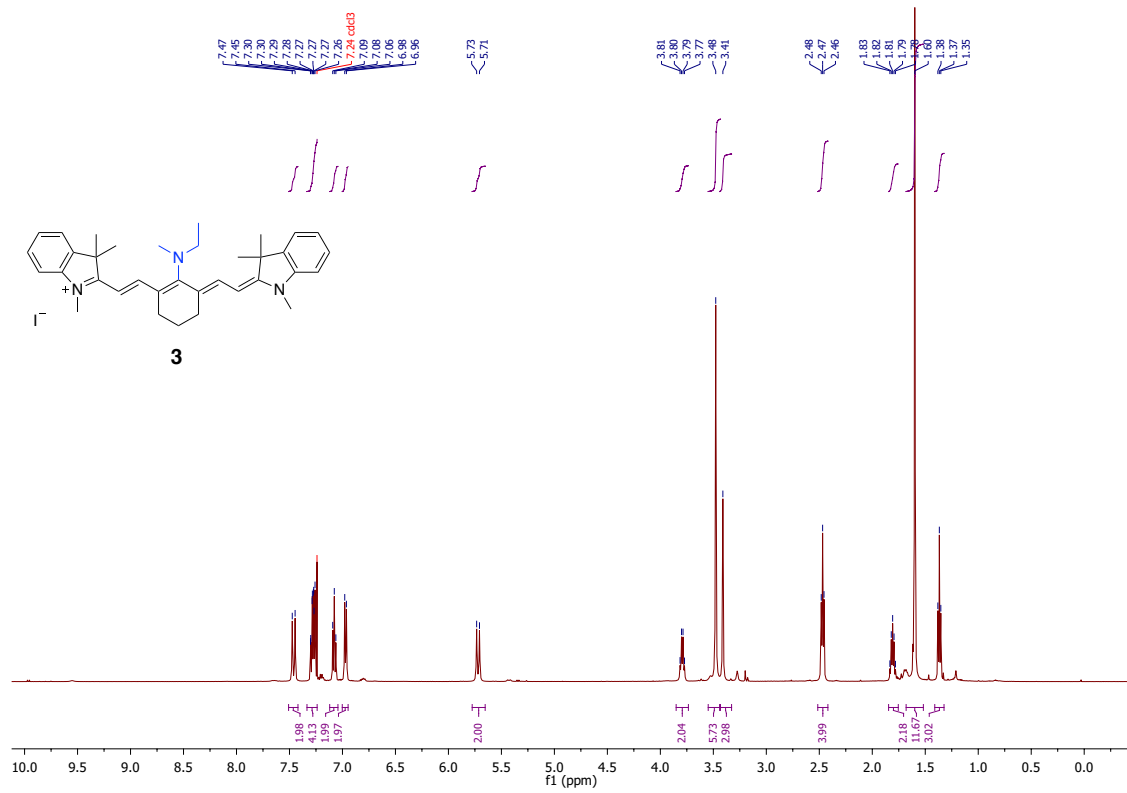
[d] Pyramidalization angle is defined:

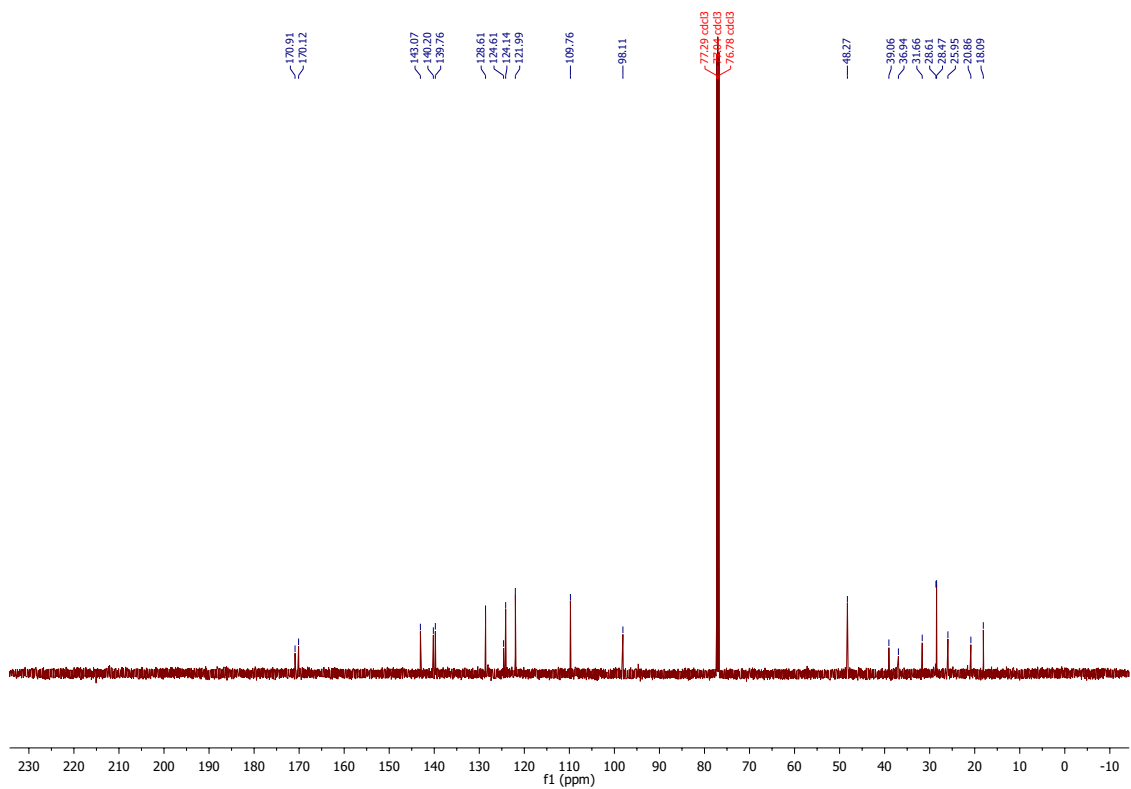
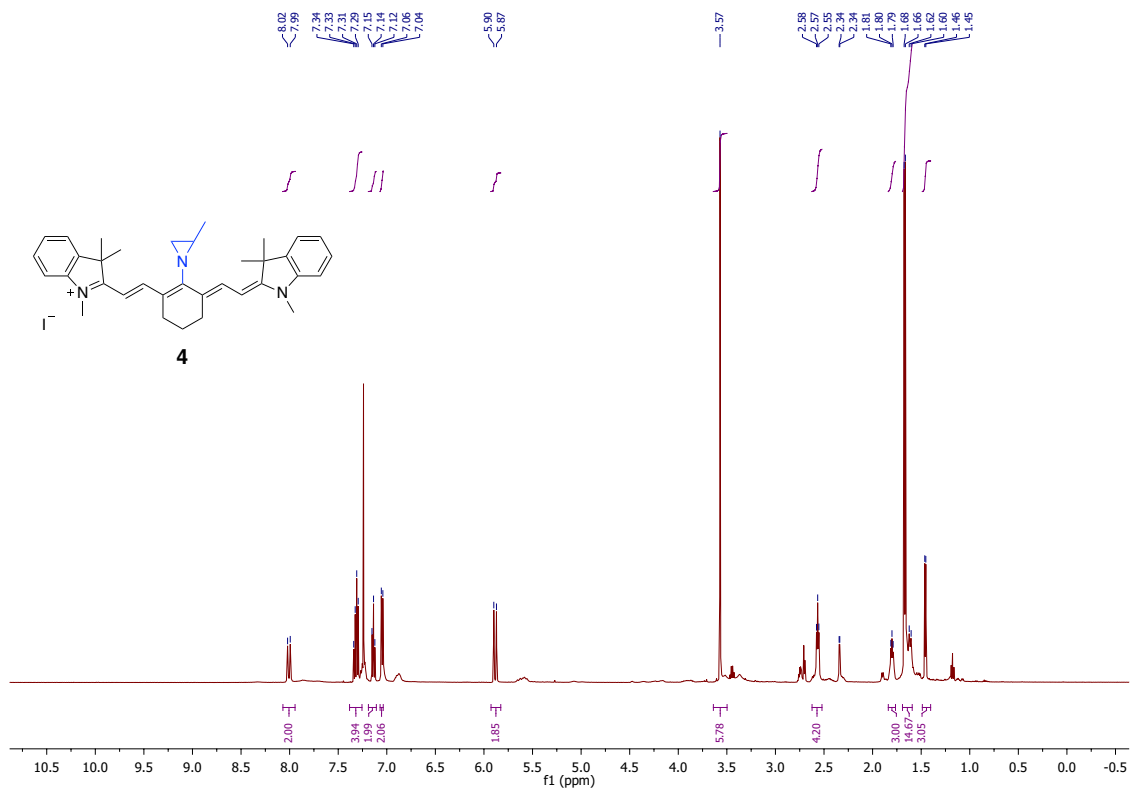
$$\text{Pyr. Ang.} = 360 - (\theta_{C_a-N-C_b} + \theta_{C_a-N-C_c} + \theta_{C_b-N-C_c})$$

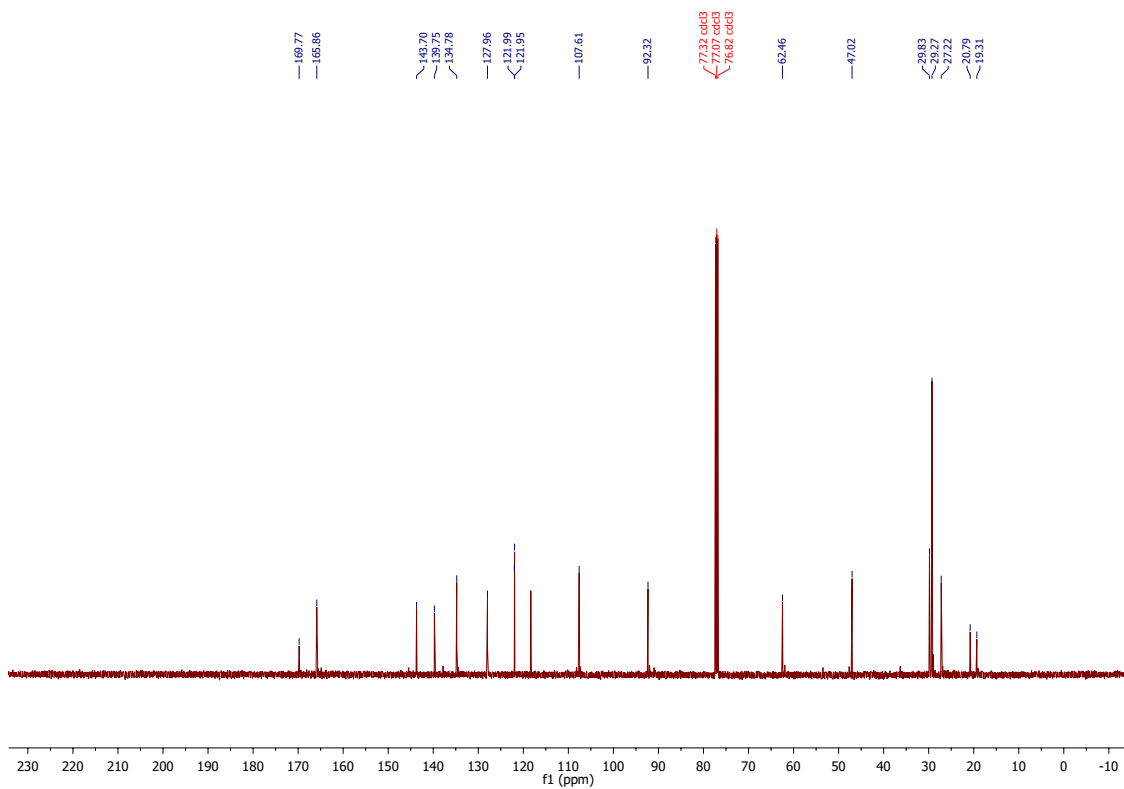
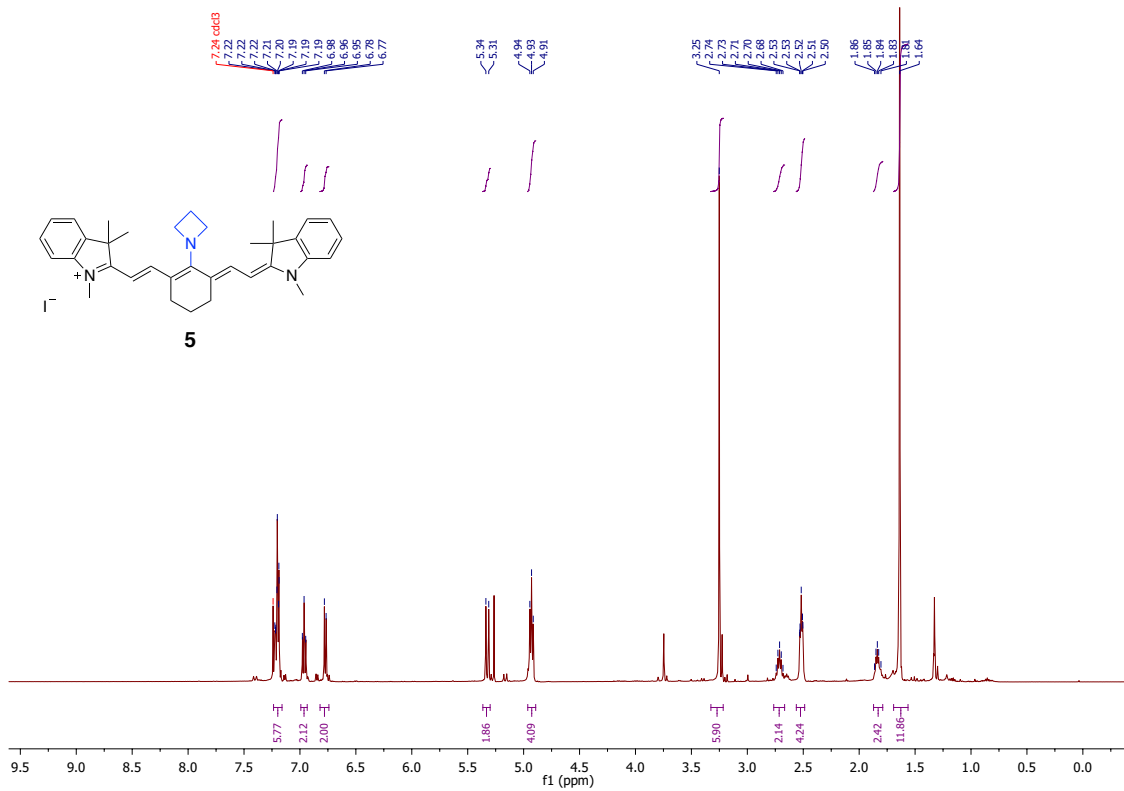
where $\theta_{C_m-N-C_n}$ is the angle formed by carbon atom m , the amine nitrogen atom, and carbon atom n . Carbon atoms a, b, and c are the three atoms bound to the amine nitrogen.

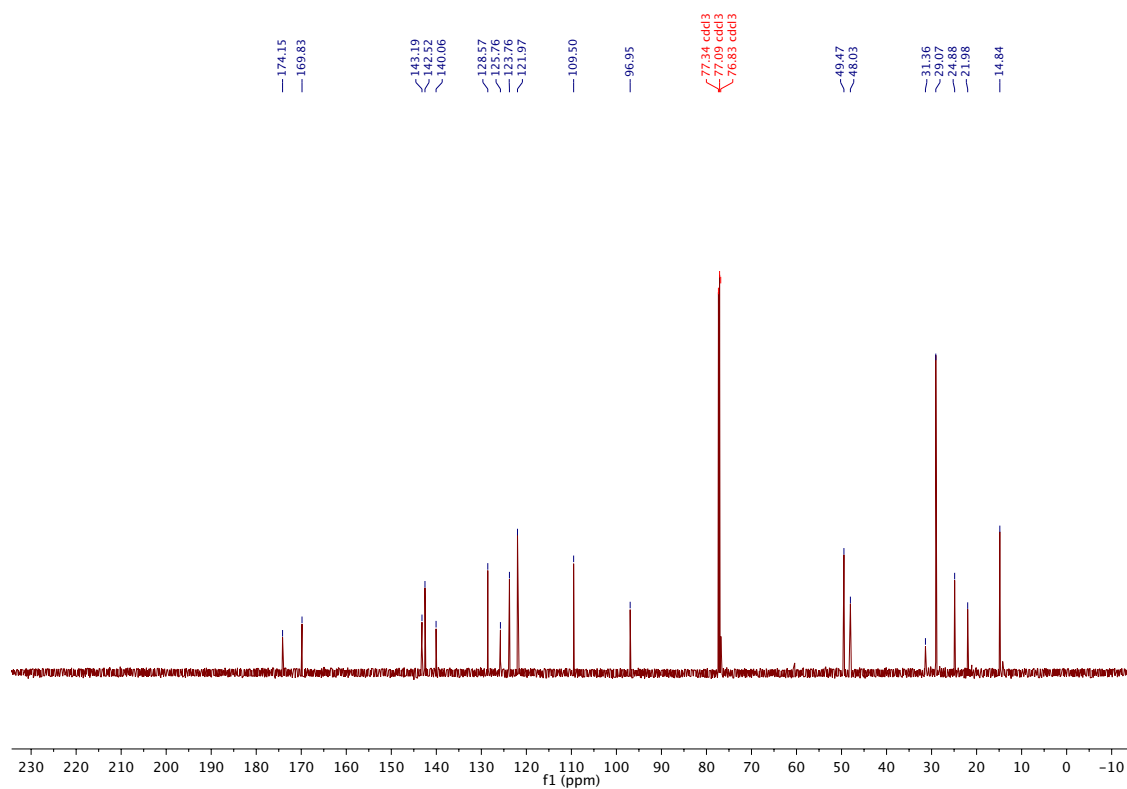
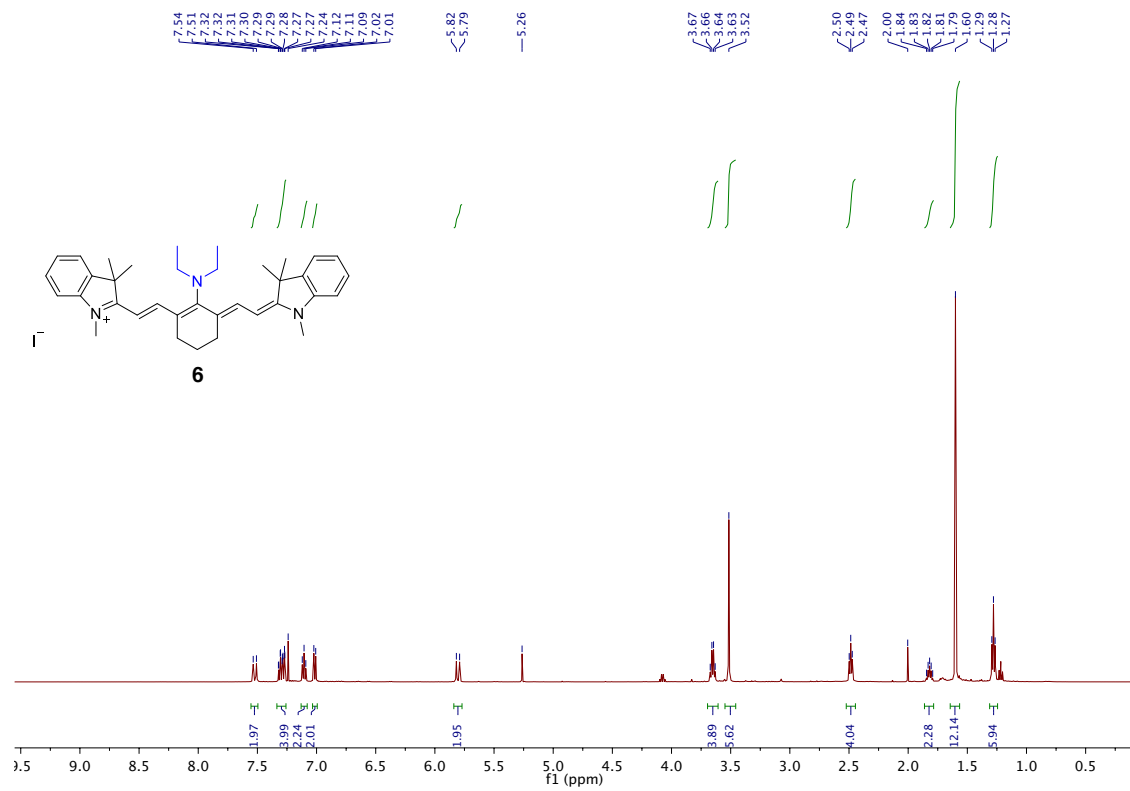
NMR data

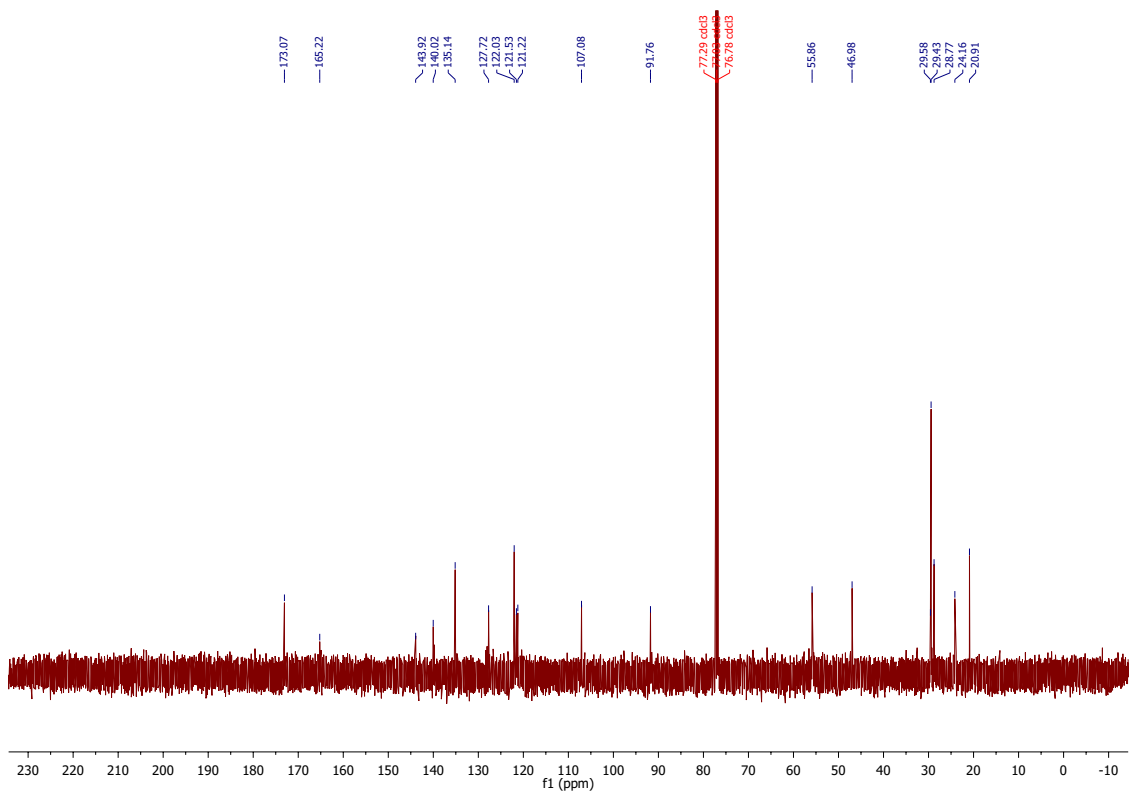
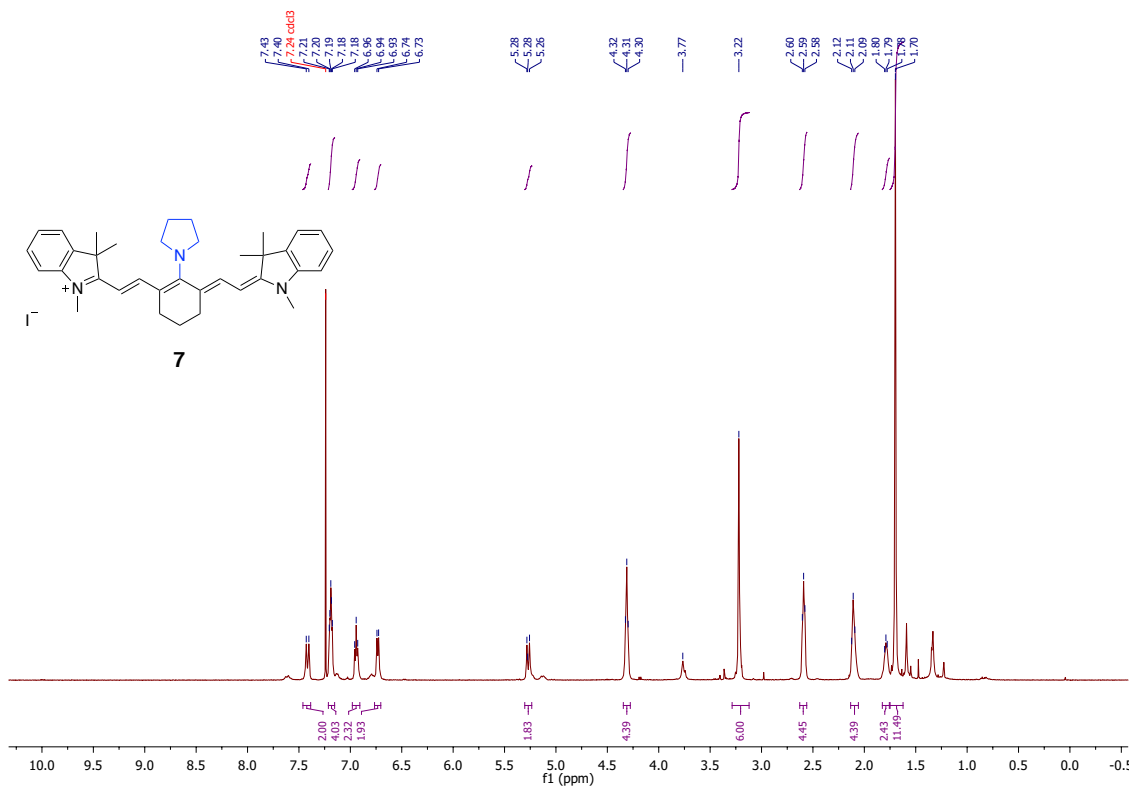


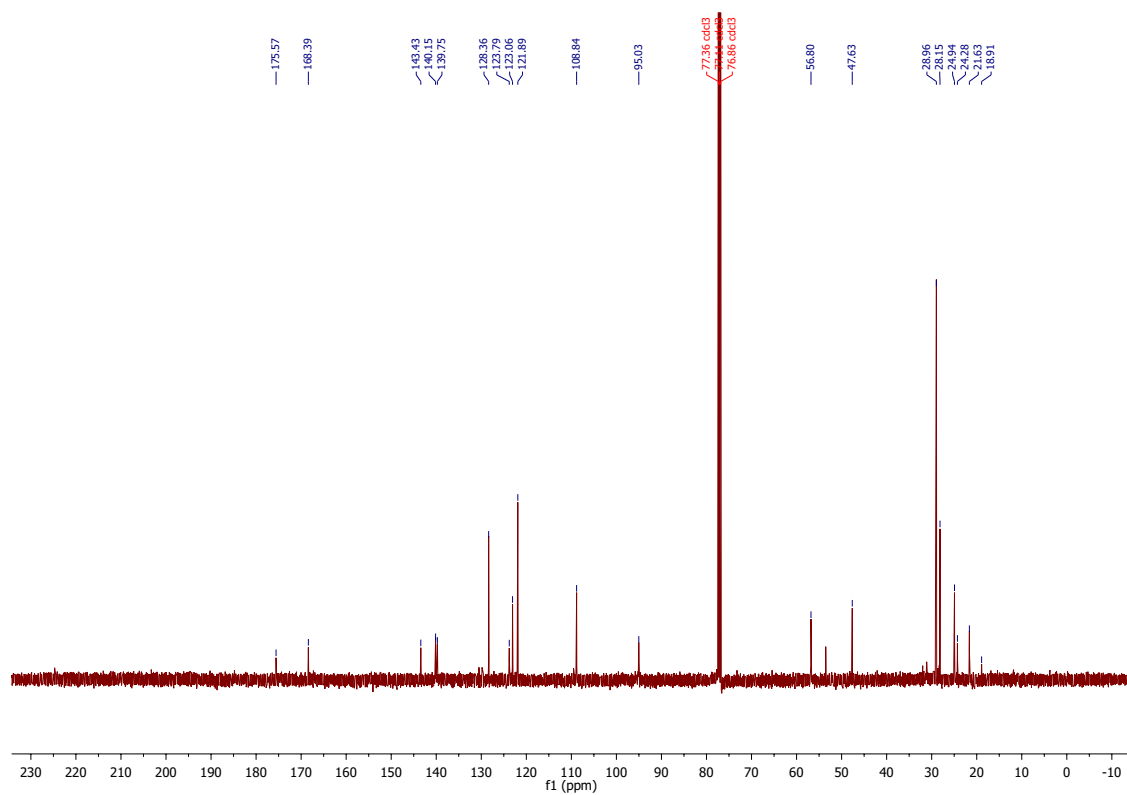
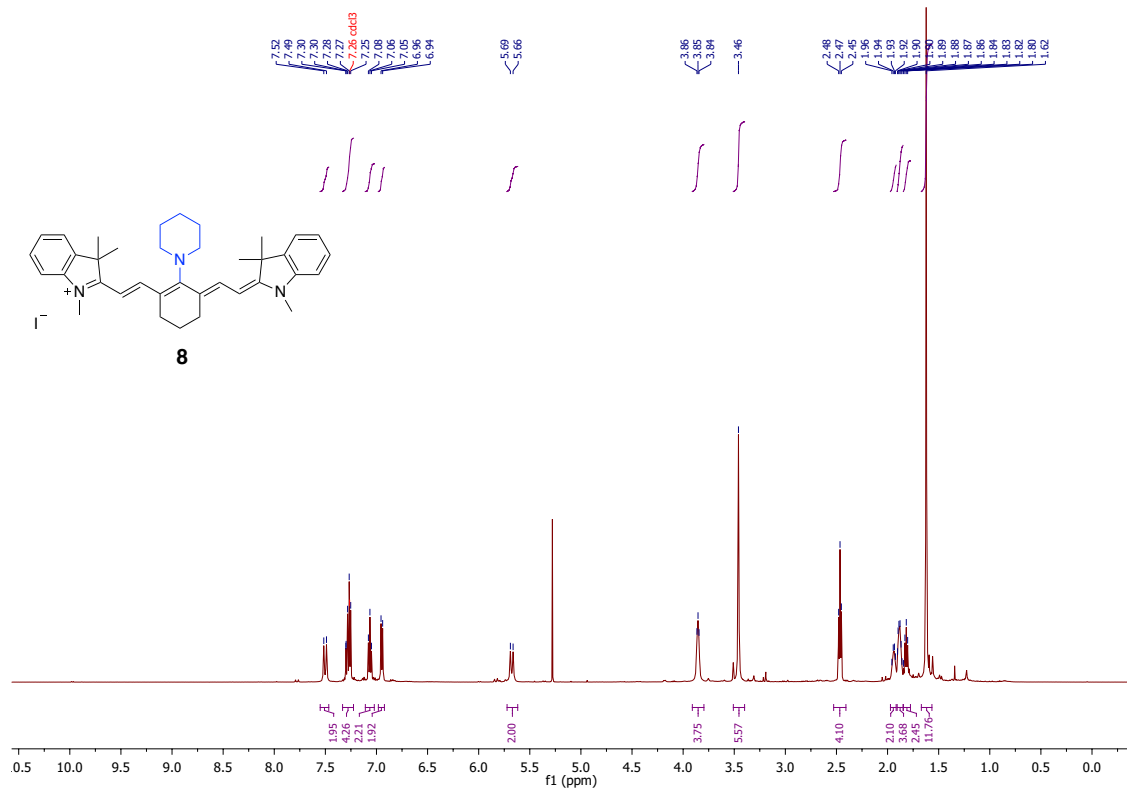


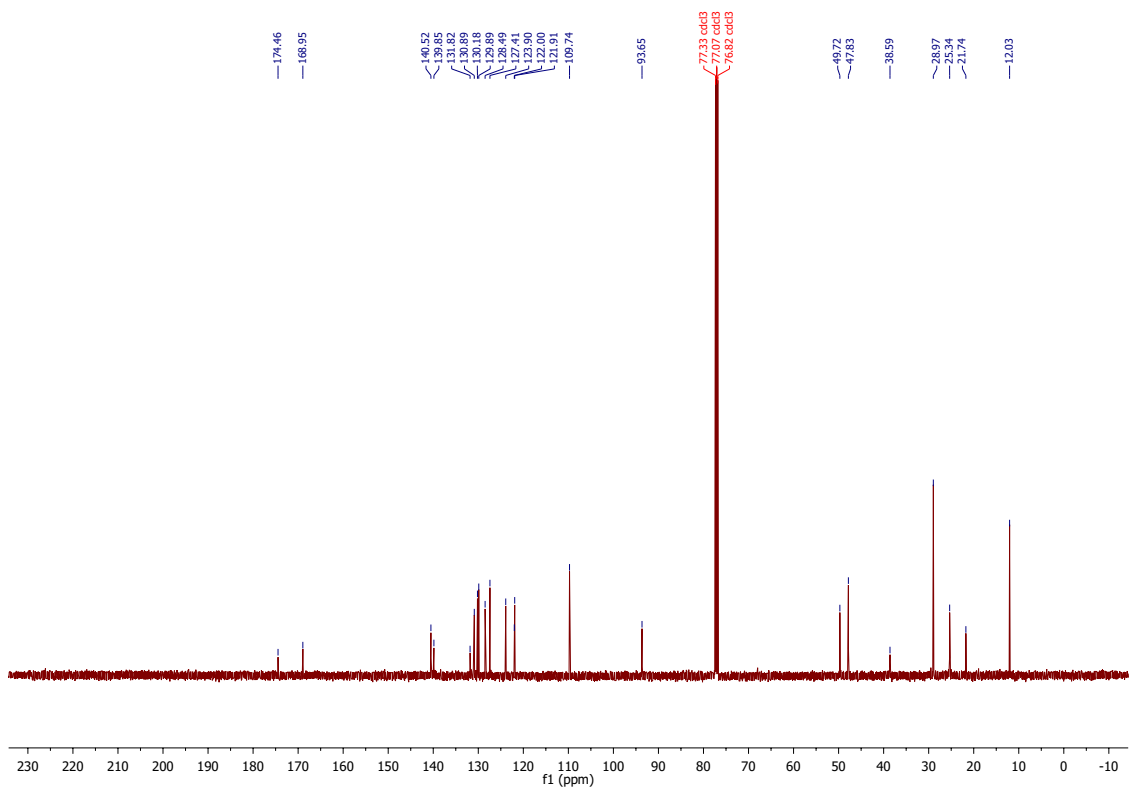
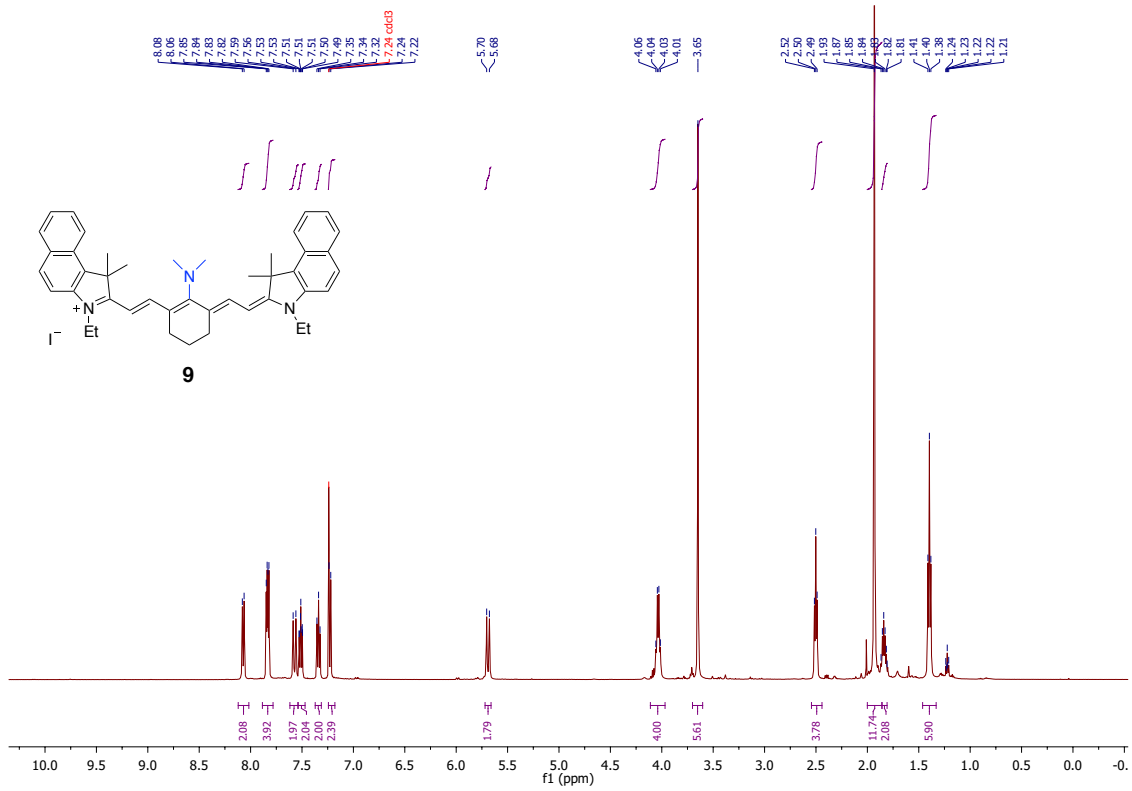


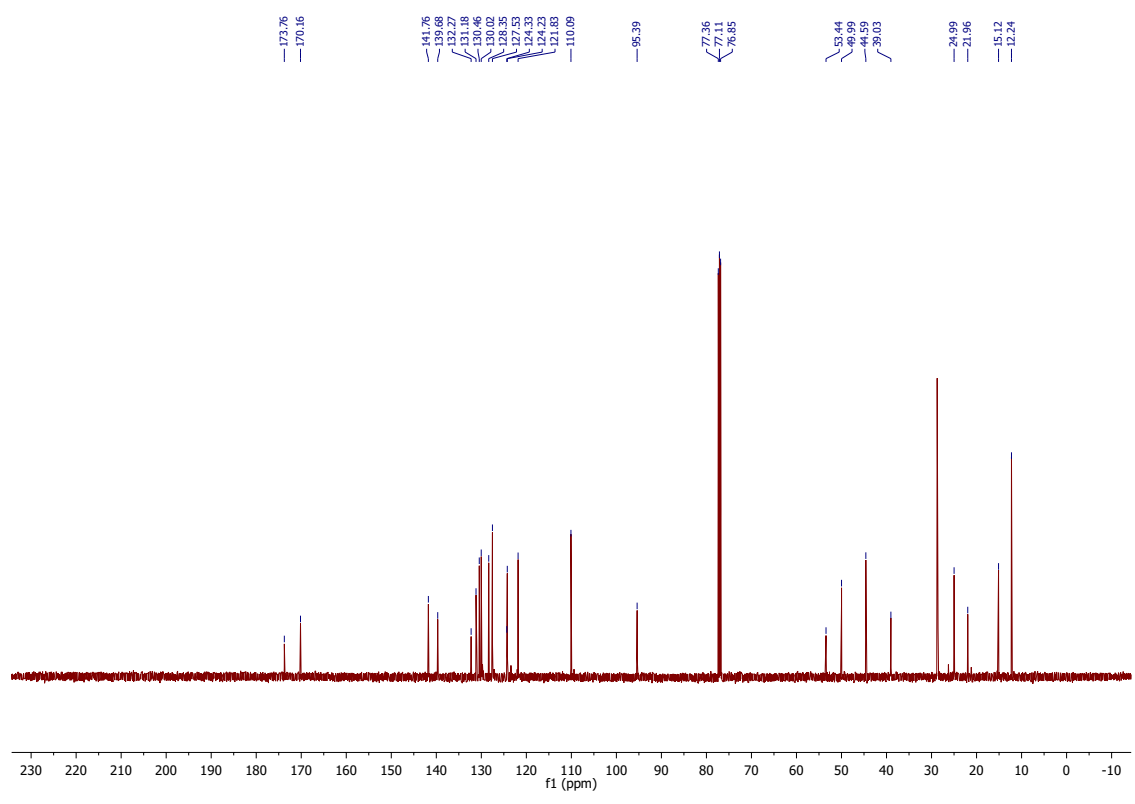
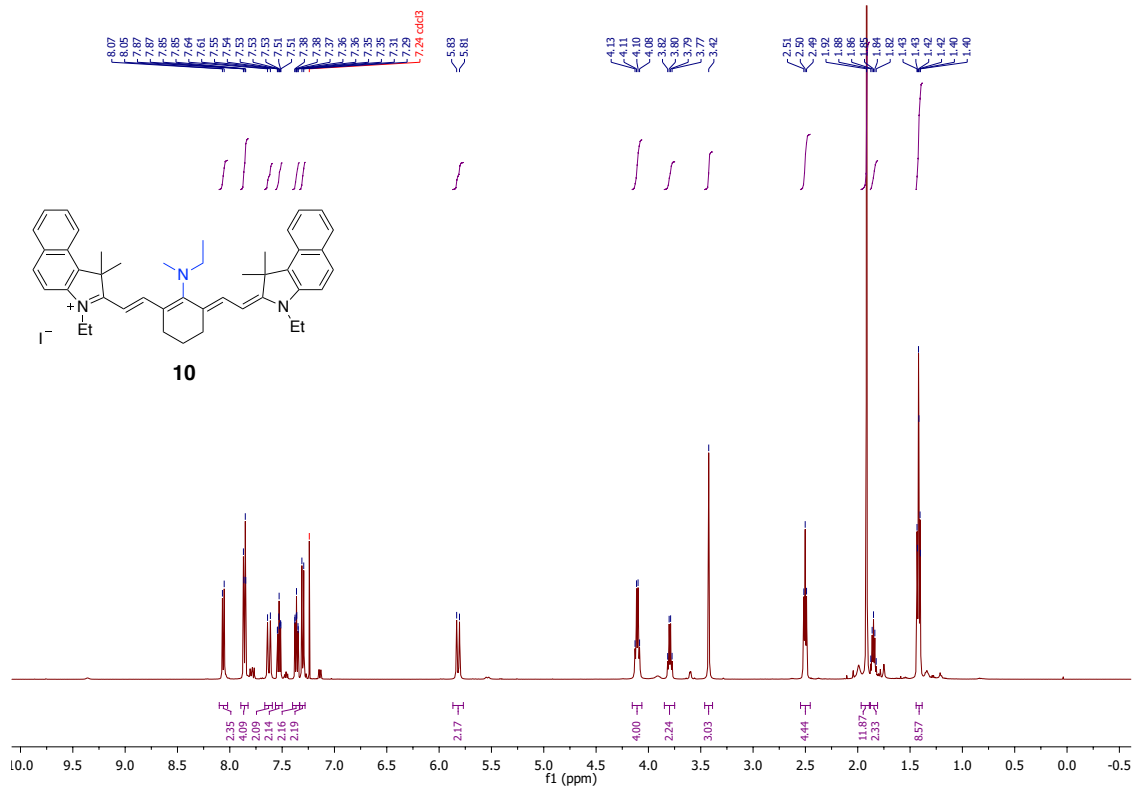


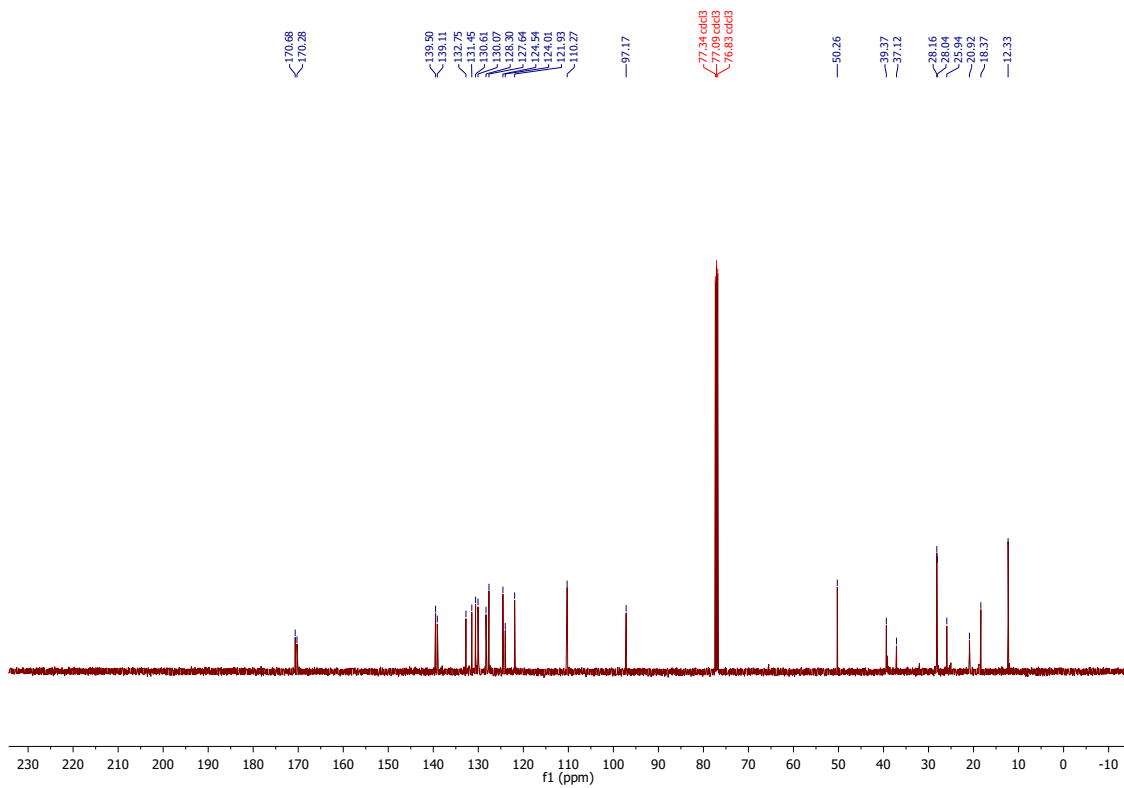
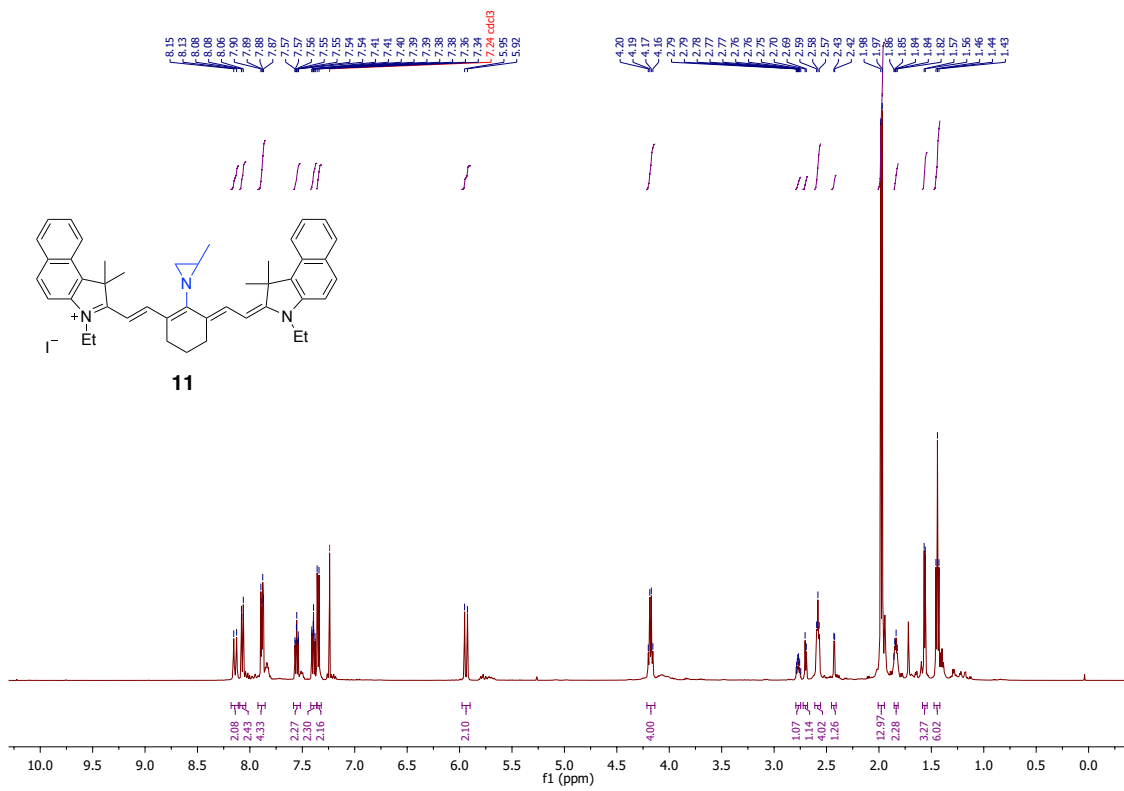


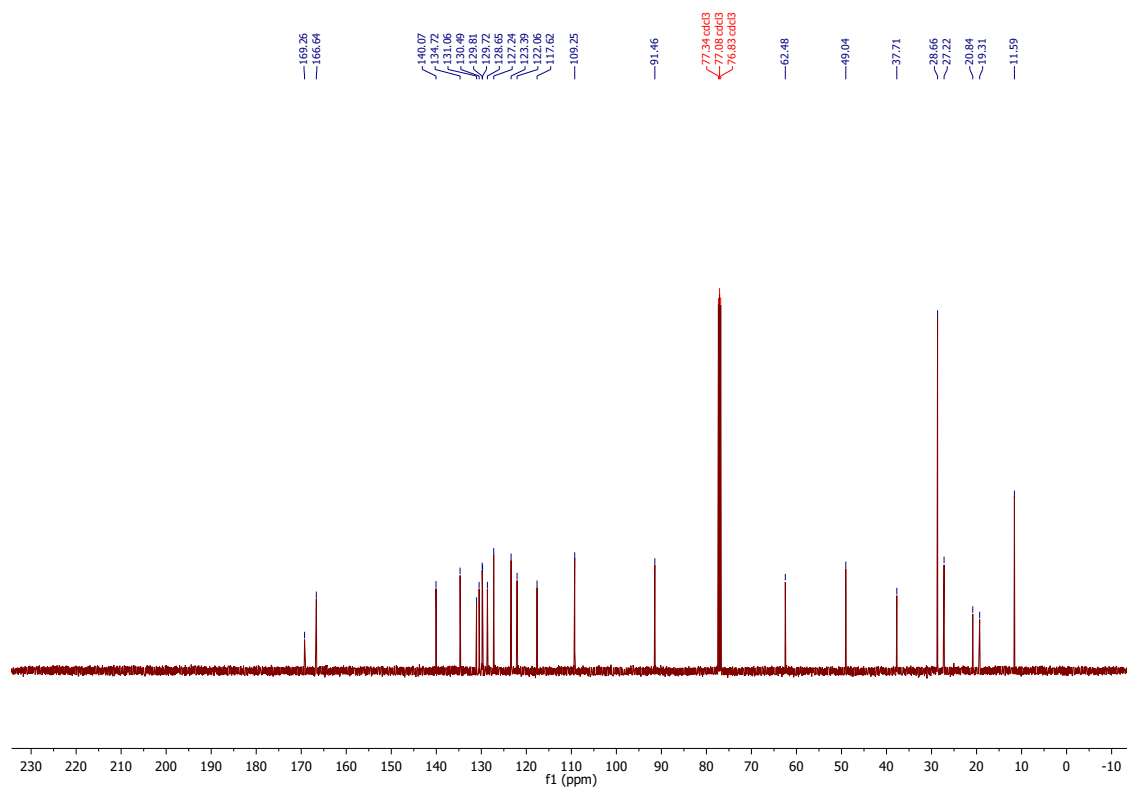
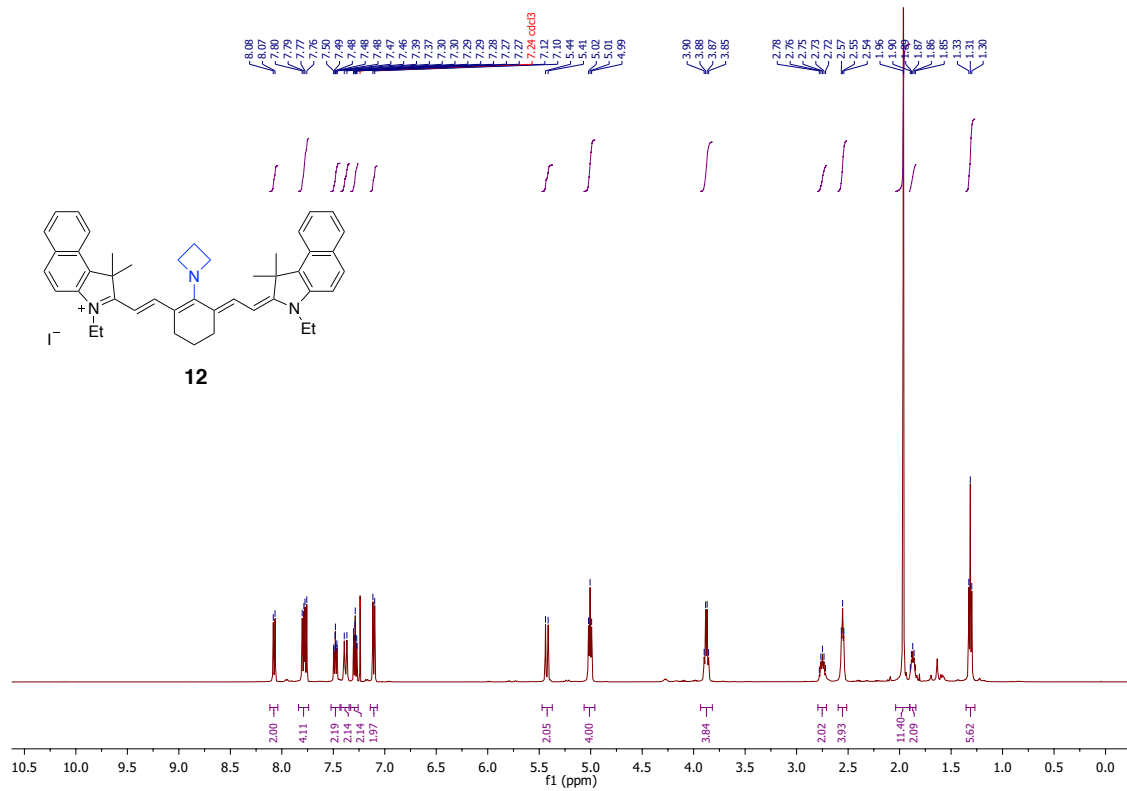


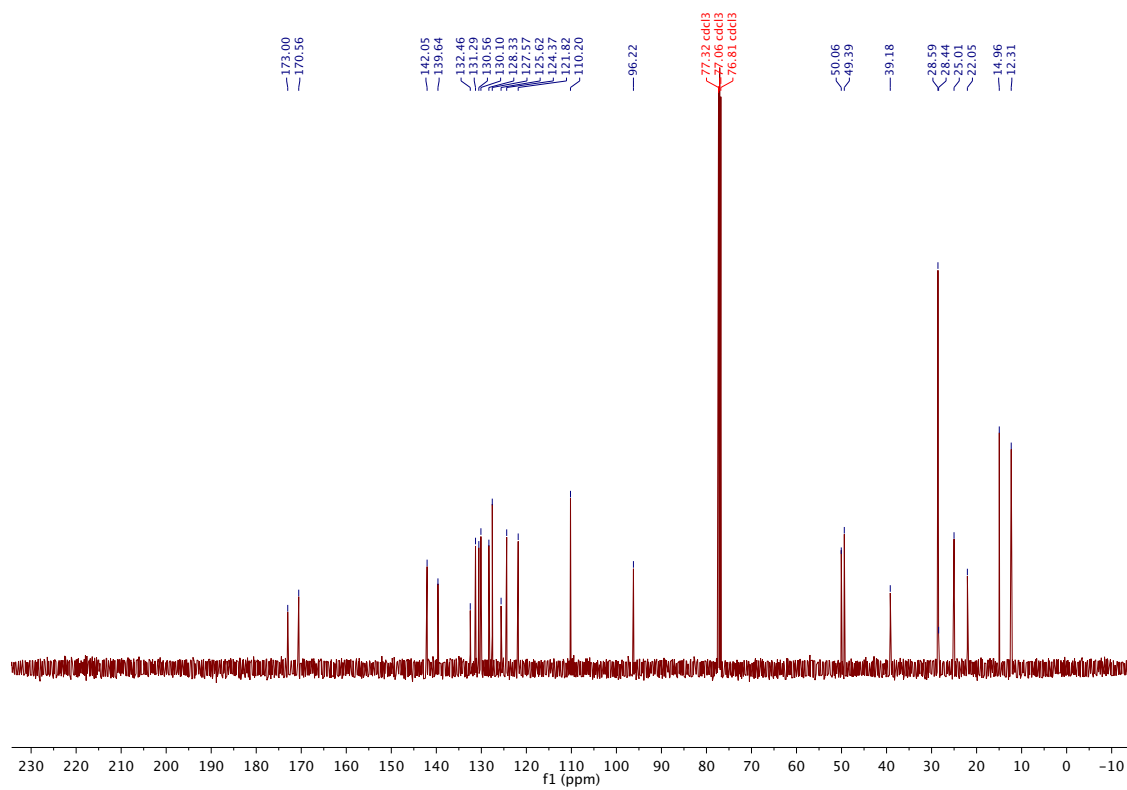
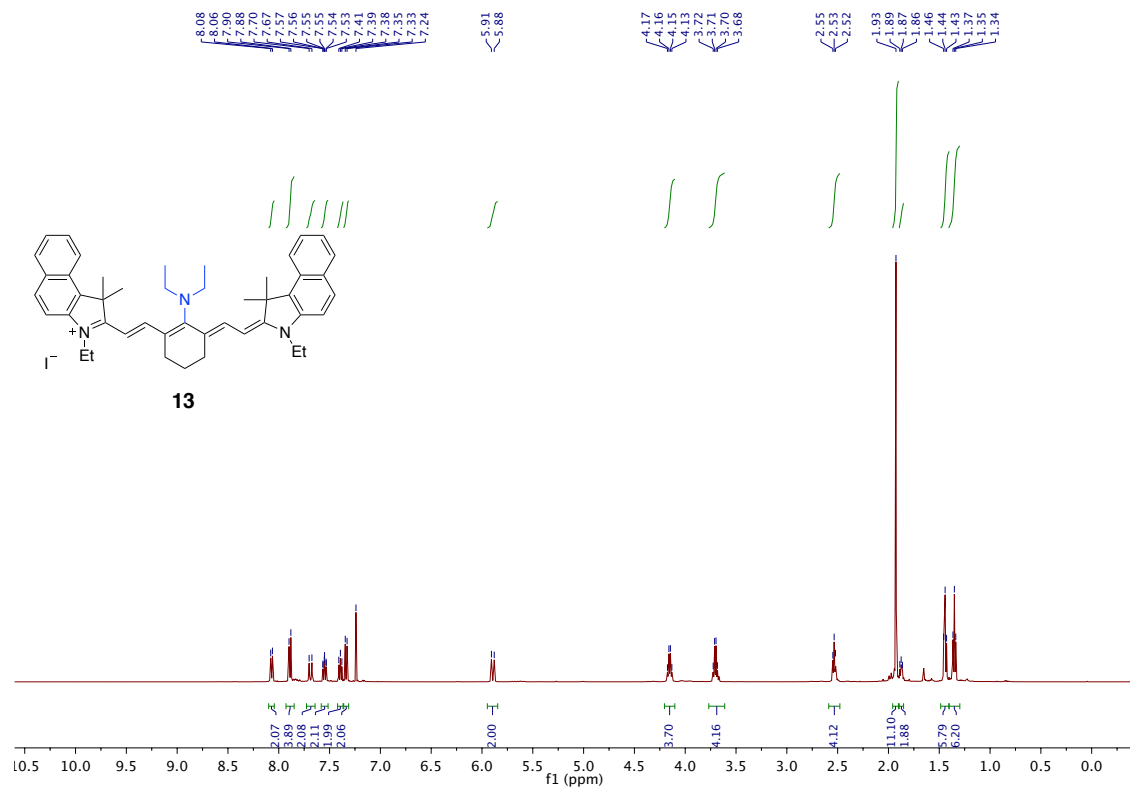


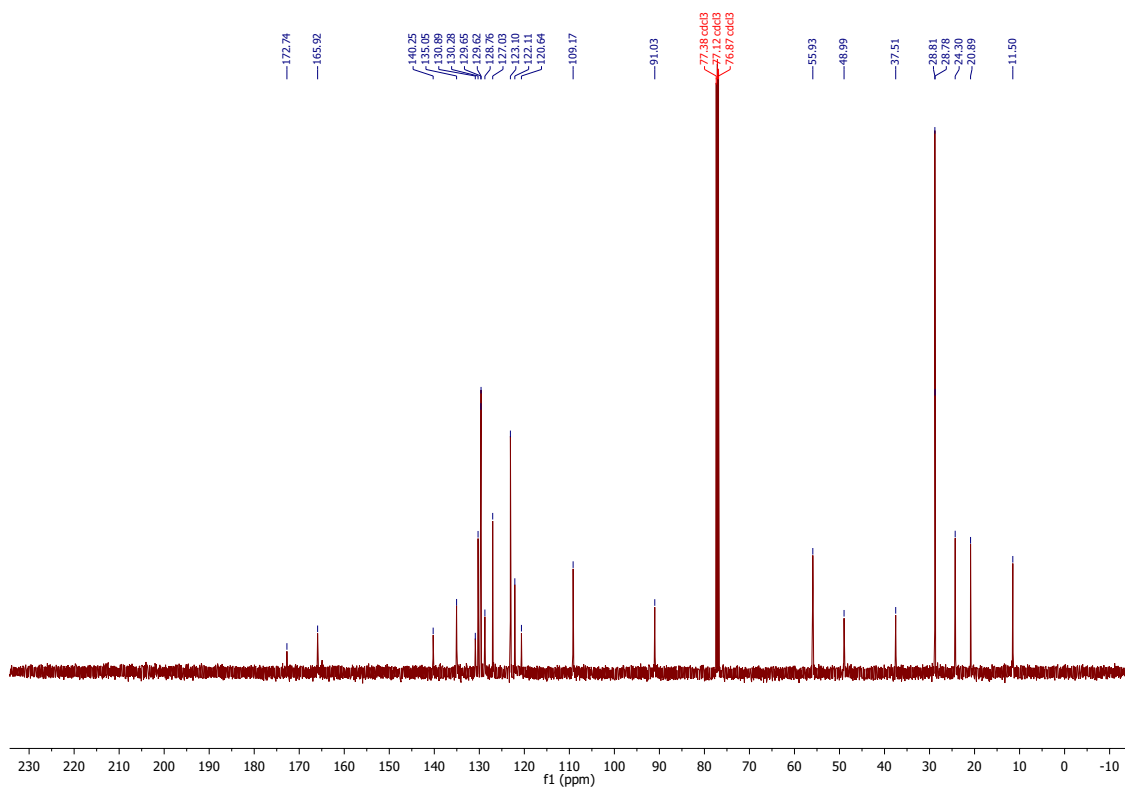
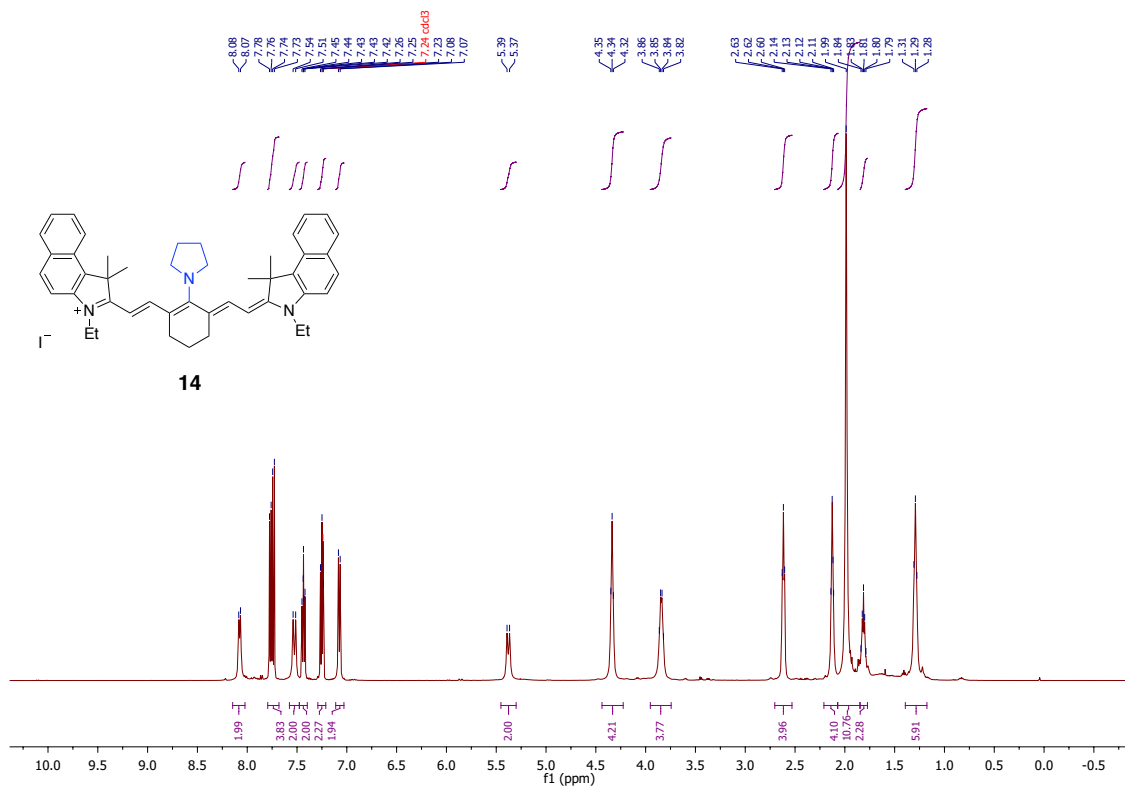


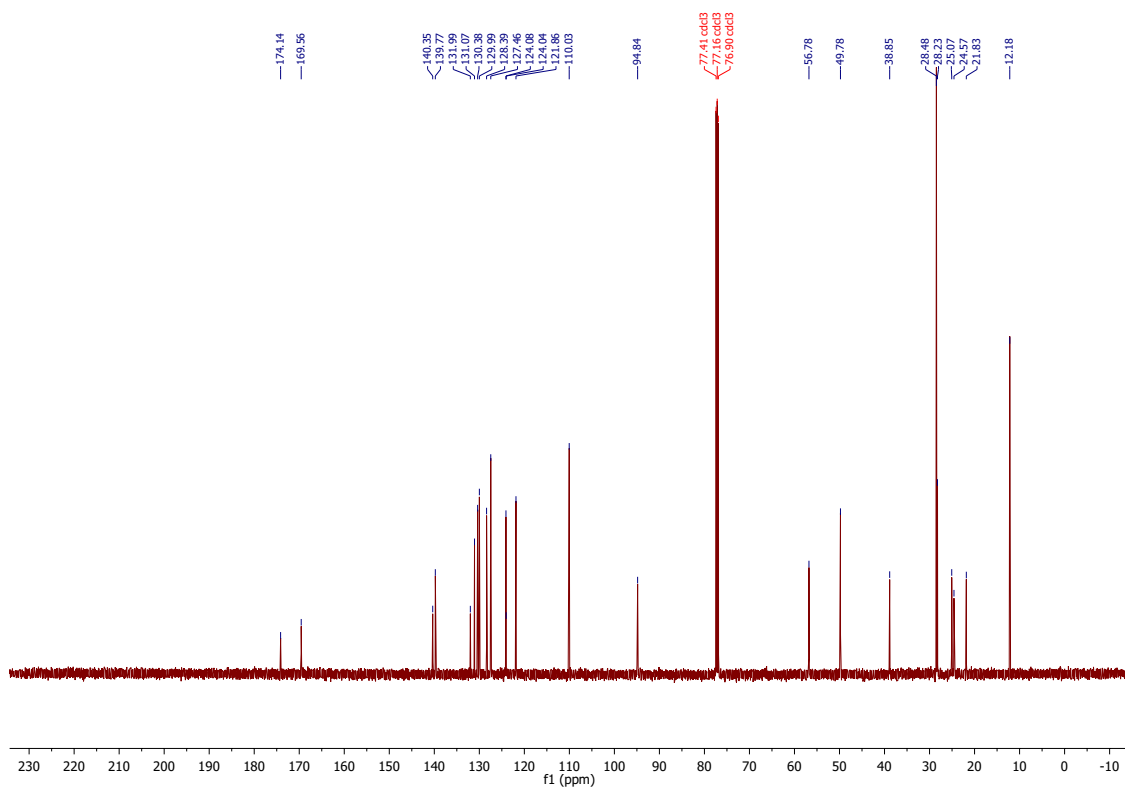
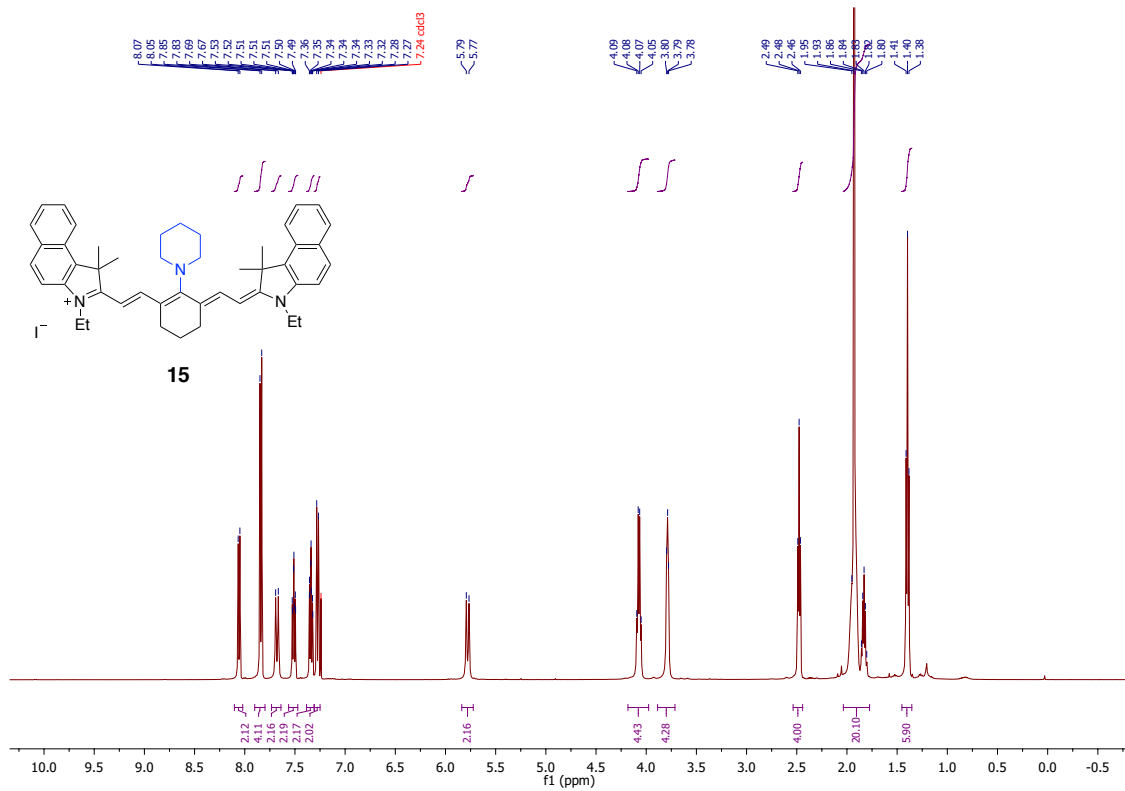


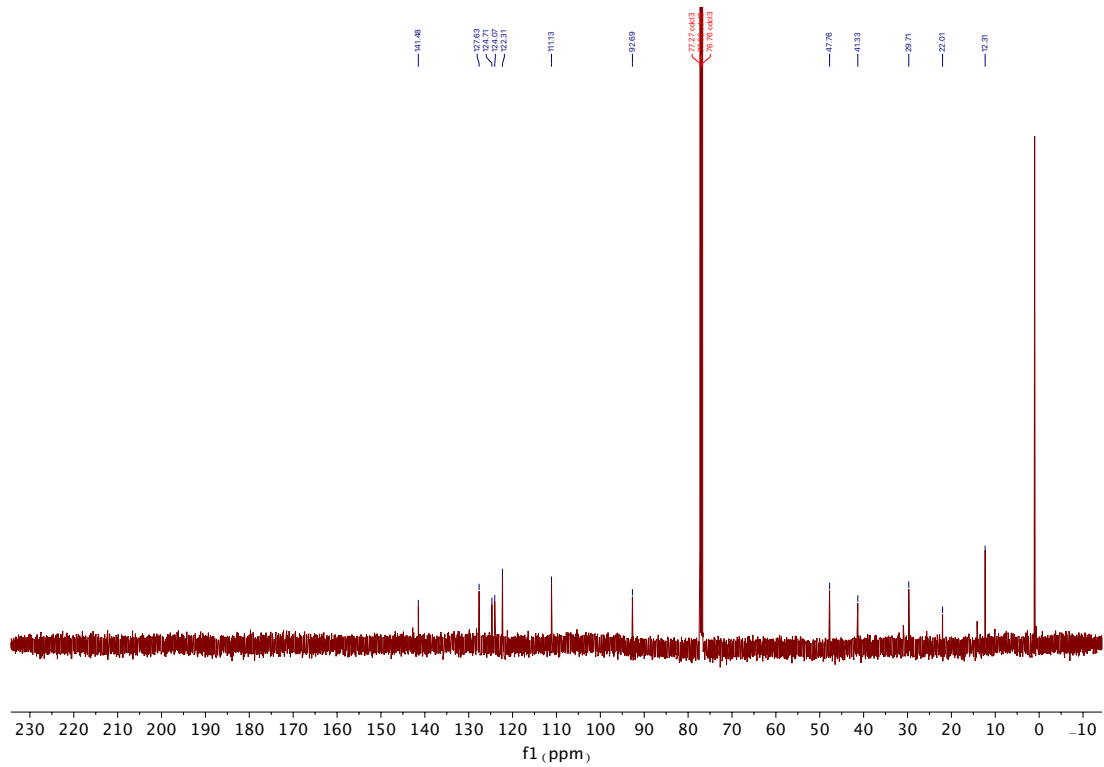
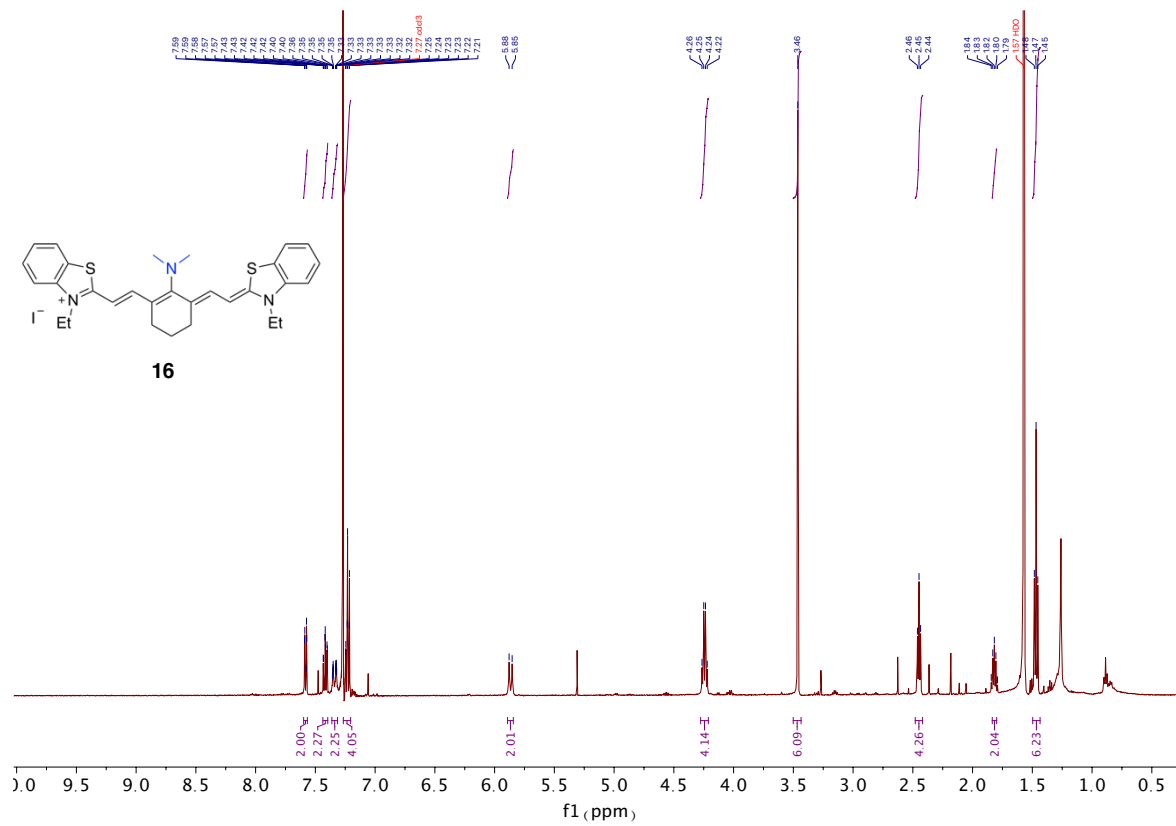


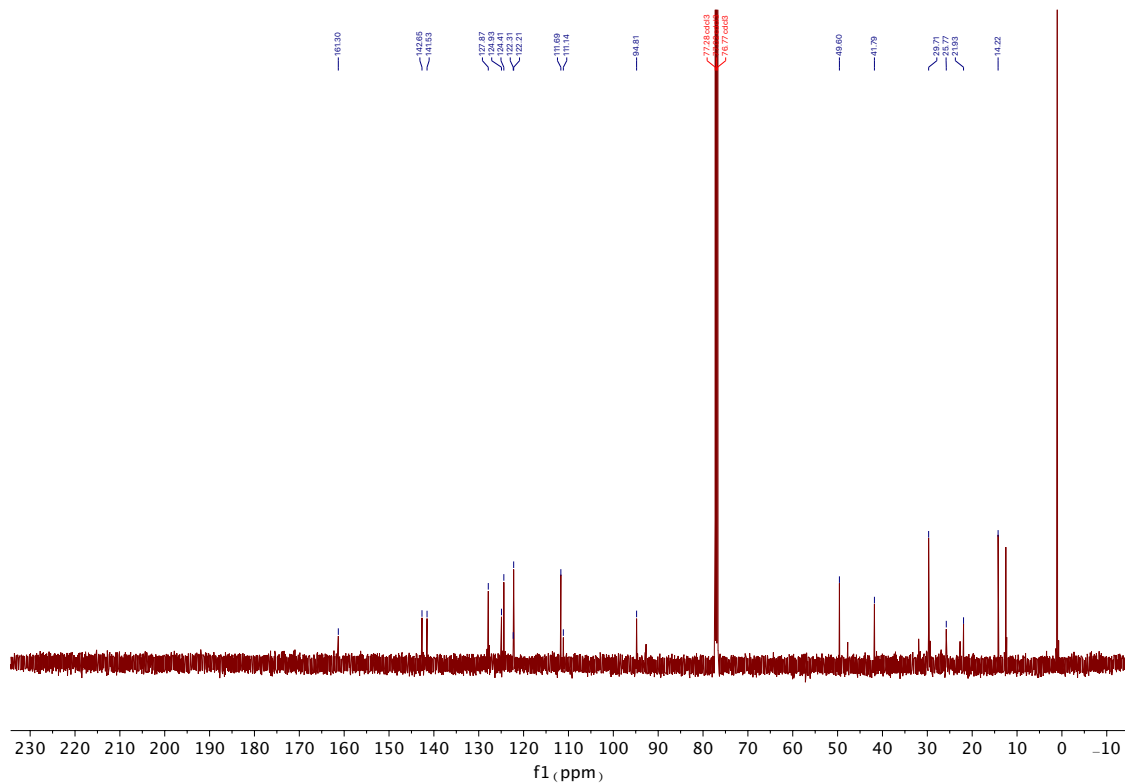
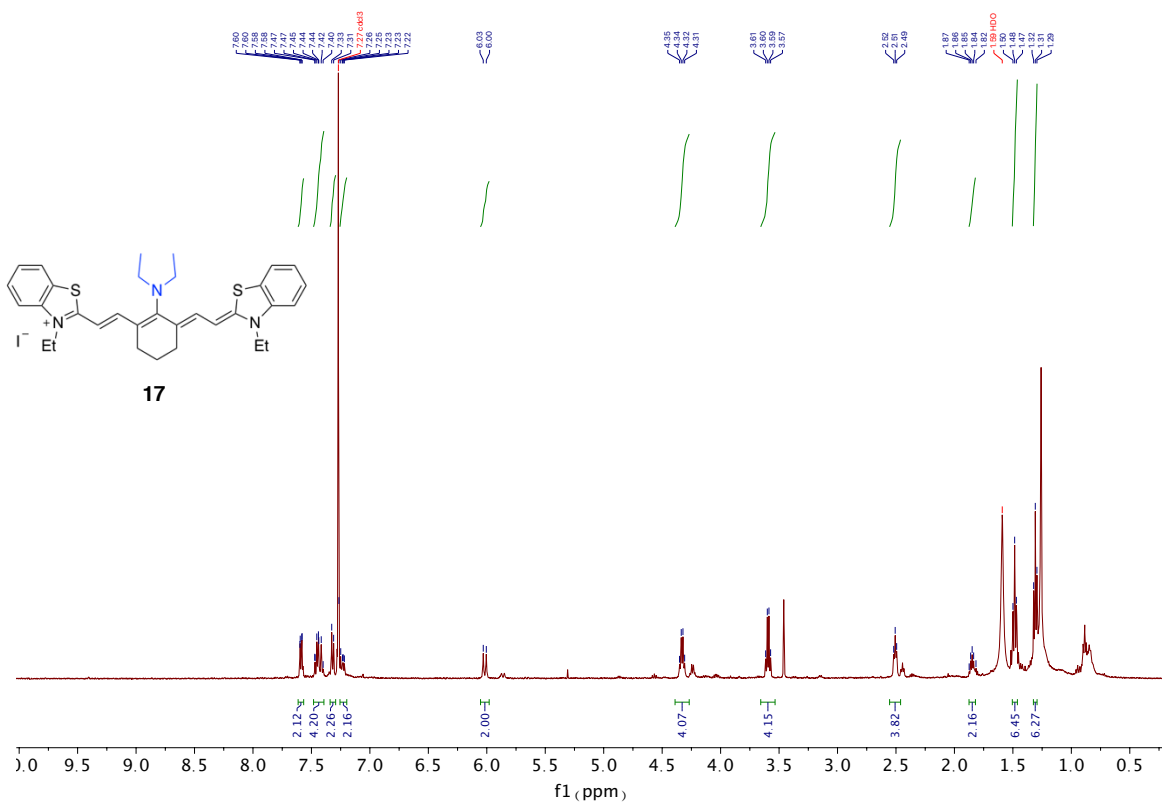


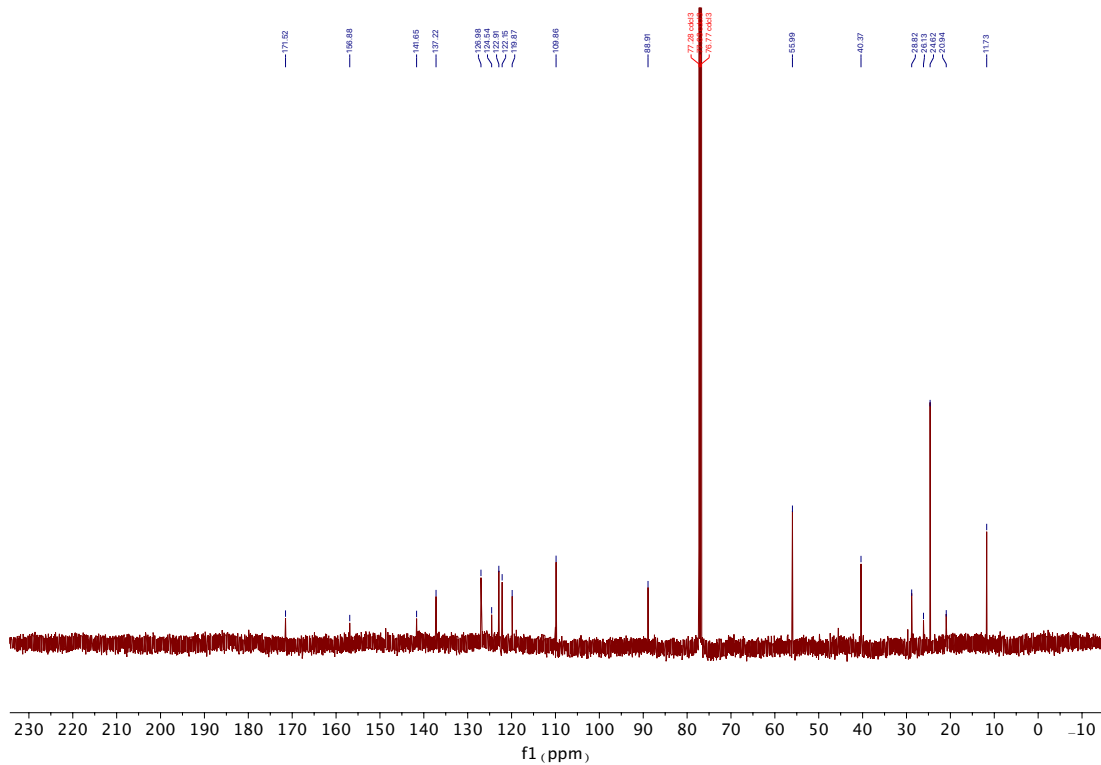
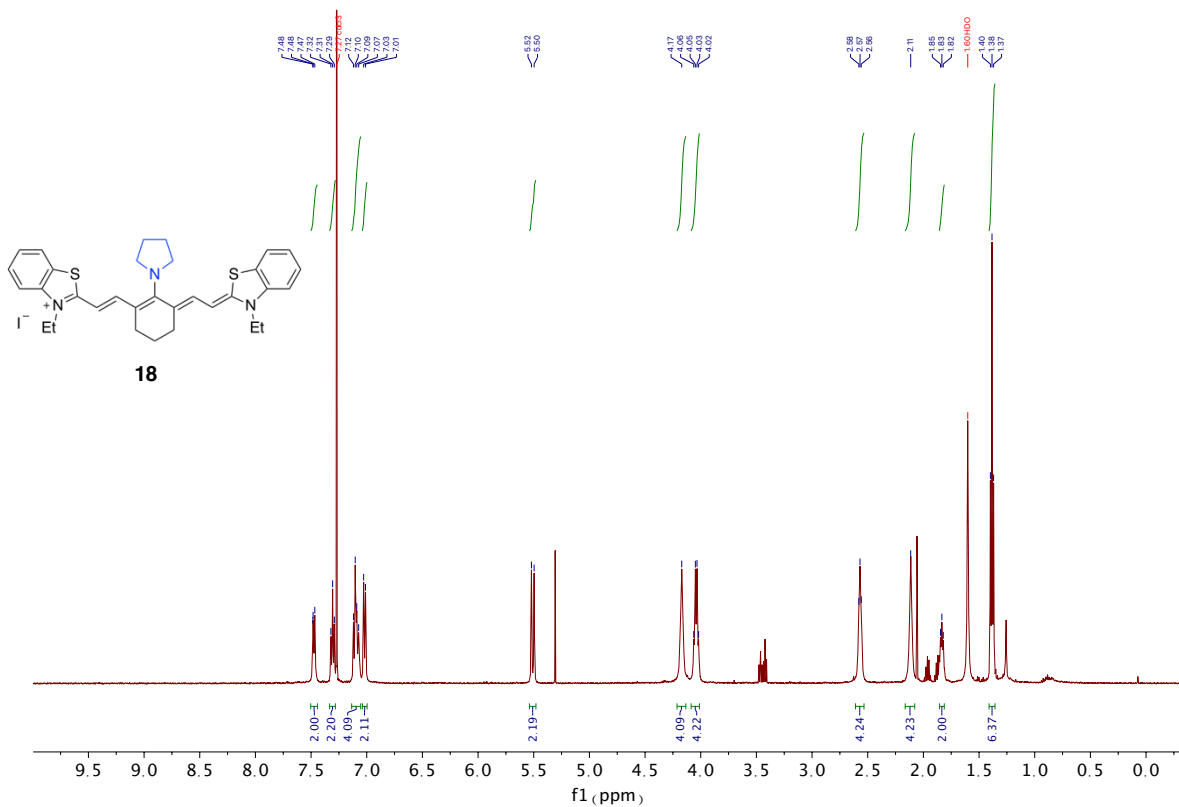












Optimized Geometries (In Angstrom) (CAM-B3LYP/6-31G*)

Dye 1

Franck-Condon point

H	-1.8122047363	7.8617759991	-4.0734638064
C	-1.8885658517	7.7571257269	-2.9973907038
C	-2.0977123043	7.5195855010	-0.1943131131
C	-1.5805410273	6.5780285207	-2.3396678174
C	-2.3097886635	8.8313210674	-2.2157363357
C	-2.4145080632	8.7186427030	-0.8326841532
C	-1.6790260316	6.4475976258	-0.9601939778
H	-2.5590540209	9.7698981915	-2.6989994384
H	-2.7445781100	9.5695668987	-0.2469190732
H	-2.1801280010	7.4365187621	0.8852505761
N	-1.1359439550	5.3464790509	-2.8765985895
C	-0.9387562285	4.4246386930	-1.9133545507
C	-1.2744680110	5.0457991120	-0.5529266509
H	-1.1551375073	6.0086721239	-4.8500764667
C	-0.9174701179	5.1068385910	-4.2909018971
H	0.1276003042	4.8444456937	-4.4778789502
H	-1.5610139722	4.2968443002	-4.6450756158
C	-0.5017049820	3.1374727919	-2.2094924200
H	-0.3360393304	2.9025363361	-3.2531726356
C	-0.2798926230	2.1399929468	-1.2605499057
H	-0.4665483542	2.3886580210	-0.2264750225
C	0.1454077917	0.8390089862	-1.5253280819
C	0.2794583552	-0.1178267988	-0.5026038540
C	0.5903489564	-1.4743302652	-0.7115233929
C	0.6536917349	-2.3836175520	0.3427695877
H	0.5043600367	-1.9852434443	1.3352902400
C	0.4363151090	0.4064599149	-2.9482137777
H	0.8922958286	1.2384331164	-3.4929264928
H	-0.5058554220	0.1762746719	-3.4647046816
C	0.8274638321	-1.9281220617	-2.1372975518
H	1.5401348873	-2.7572357300	-2.1432805184
H	-0.1072651408	-2.3153014421	-2.5655569153
C	1.3637691501	-0.7991433504	-3.0070891423
H	2.3592303343	-0.5105714808	-2.6511314735
H	1.4771424668	-1.1375048655	-4.0408753162
H	1.5758340317	-8.7045217548	1.8190082965
C	1.4527127162	-7.9816488751	2.6171381168
C	1.1494634786	-6.1236986440	4.7177388518
C	1.2446640308	-6.6340116734	2.3756319053
C	1.5055398628	-8.3895241746	3.9487167137
C	1.3557432969	-7.4765064793	4.9881711833
C	1.0967381914	-5.7080187554	3.4004053067
H	1.6677492483	-9.4382214228	4.1735790517
H	1.4014334988	-7.8190314629	6.0161303798
H	1.0344842690	-5.4151223072	5.5325471140
C	0.8863612996	-4.3284344901	2.8109007433
C	0.9583644703	-4.6308128373	1.3099608594
C	0.8727221603	-3.7566275751	0.2315561753
H	0.9806089092	-4.1831337698	-0.7575574117

N	1.1449076117	-5.9547676222	1.1385293714
Cl	0.0120114314	0.4141819222	1.1538988063
C	1.2437514955	-6.6043483577	-0.1550247418
H	2.1508599693	-6.2900184855	-0.6798795186
H	0.3713736927	-6.3607615168	-0.7665754440
H	1.2751958137	-7.6824307864	-0.0149812576
C	-2.4578987655	4.3284773985	0.1237101245
H	-2.2025001414	3.3121237346	0.4306222355
H	-3.3221027256	4.2792217449	-0.5437393294
H	-2.7545389226	4.8839698407	1.0176428033
C	-0.0438630977	5.0971373052	0.3724897326
H	0.7984062891	5.5902284603	-0.1195417588
H	0.2760956659	4.1018117033	0.6876470504
H	-0.2910738697	5.6703325922	1.2702073256
C	-0.4987013169	-3.7899176515	3.2194589581
H	-0.5503939565	-3.7226099313	4.3095047813
H	-1.2953986228	-4.4597538971	2.8857935991
H	-0.6926494535	-2.7950278773	2.8128676601
C	2.0130656832	-3.3790876646	3.2597204089
H	2.9911838790	-3.7504596551	2.9433988209
H	2.0155832364	-3.3124722575	4.3510355982
H	1.8832463071	-2.3702311327	2.8623844067

S₁ minimum

H	-1.7241524533	7.8930069682	-4.1316849236
C	-1.8260832499	7.7949377547	-3.0571133251
C	-2.1029990560	7.5739591453	-0.2543158667
C	-1.5445436713	6.6086944850	-2.3861205184
C	-2.2518489680	8.8749753254	-2.2921565627
C	-2.3906397709	8.7726115231	-0.9079041561
C	-1.6792274520	6.4917050975	-1.0008073740
H	-2.4793540858	9.8142764470	-2.7852696682
H	-2.7244412866	9.6316545439	-0.3358828787
H	-2.2117474073	7.4987183821	0.8234939032
N	-1.1054072088	5.3843068006	-2.8984719857
C	-0.9413415946	4.4562093194	-1.9140516424
C	-1.3024613236	5.0904276637	-0.5715751863
H	-1.0517800776	6.0316862379	-4.8765022882
C	-0.8525848635	5.1297153301	-4.3024375016
H	0.1913878298	4.8401872717	-4.4572698724
H	-1.5030233524	4.3302340316	-4.6704664546
C	-0.5136058327	3.1624174296	-2.1900467168
H	-0.3288967220	2.9201599333	-3.2298873522
C	-0.3197106793	2.1589897674	-1.2319493192
H	-0.5196159596	2.4083152150	-0.2007049485
C	0.0966863475	0.8482053819	-1.4921153764
C	0.2203687965	-0.1151037525	-0.4650101192
C	0.5350985785	-1.4791998609	-0.6712131395
C	0.6035534205	-2.3927176160	0.3852771127
H	0.4503401196	-1.9981098223	1.3786186673
C	0.3973315399	0.4092694466	-2.9081701072
H	0.8494602025	1.2382766894	-3.4599477924
H	-0.5445845793	0.1702478955	-3.4227719088
C	0.7763829264	-1.9256021368	-2.0957294985

H	1.4769579096	-2.7644348934	-2.1066405211
H	-0.1638342362	-2.2956809243	-2.5291760769
C	1.3246374855	-0.7971955320	-2.9593686595
H	2.3183915629	-0.5116069223	-2.5966035916
H	1.4425301115	-1.1358833387	-3.9925776808
H	1.6371710632	-8.7379443644	1.7713074575
C	1.5177820321	-8.0251180489	2.5789972098
C	1.2266384319	-6.1898442552	4.7067251560
C	1.2832808435	-6.6724250524	2.3507318899
C	1.6027491931	-8.4435386555	3.9019884434
C	1.4594250338	-7.5425672459	4.9573821272
C	1.1406978672	-5.7584722433	3.3973434203
H	1.7859037933	-9.4917905491	4.1138613671
H	1.5315707359	-7.8964312555	5.9801586427
H	1.1167938018	-5.4920828683	5.5315395721
C	0.8961334508	-4.3756805601	2.8327114093
C	0.9497463554	-4.6550051288	1.3313256540
C	0.8382922812	-3.7697383551	0.2662583029
H	0.9400264854	-4.1871259063	-0.7284633812
N	1.1537932546	-5.9894019185	1.1384975327
Cl	-0.0684044162	0.4126970597	1.1854427190
C	1.2334987925	-6.6182348829	-0.1643407009
H	2.1215136949	-6.2787607268	-0.7077420939
H	0.3428397738	-6.3811331555	-0.7532101028
H	1.2886490736	-7.6978361355	-0.0433265298
C	-2.5104927074	4.3927952959	0.0873717461
H	-2.2744222423	3.3726702553	0.3970955130
H	-3.3637699928	4.3561344407	-0.5945885533
H	-2.8128869295	4.9521698583	0.9772567524
C	-0.0971289943	5.1341926226	0.3905908313
H	0.7627859309	5.6192217414	-0.0780556902
H	0.2050981685	4.1358413974	0.7133761356
H	-0.3647665304	5.7084017766	1.2820895302
C	-0.4923947328	-3.8660635922	3.2744820293
H	-0.5224269534	-3.8011437447	4.3657582562
H	-1.2826200326	-4.5501261224	2.9549363730
H	-0.7132935131	-2.8743323284	2.8734518010
C	2.0076547691	-3.4067169122	3.2847932551
H	2.9908702025	-3.7542081746	2.9578437105
H	2.0154437800	-3.3479934562	4.3767681087
H	1.8530012353	-2.3980600949	2.8962004464

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Bis-dipole Franck-Condon point

H	6.3215188475	5.2264514052	2.1358302896
C	6.1269240781	4.3127500461	2.6858437135
C	5.6481488793	1.9475159330	4.1400563841
C	4.9542238981	3.5916666244	2.5321672990
C	7.0686429214	3.8231802533	3.5901424000
C	6.8378971539	2.6568304957	4.3115582237
C	4.7084307916	2.4236246717	3.2458439196
H	7.9958032916	4.3683442955	3.7323458773
H	7.5850434739	2.2976902929	5.0106645933

H	5.4697101027	1.0371917864	4.7051846563
N	3.8486140666	3.8574264656	1.7000103461
C	2.8700943747	2.9211343375	1.8484456025
C	3.3501037935	1.8707404110	2.8596199716
H	4.6868880383	5.5382607524	0.8066374368
C	3.7489759976	4.9867668484	0.8024484355
H	3.5533467437	4.6461386758	-0.2190520522
H	2.9439288453	5.6619464684	1.1106797833
C	1.6830060082	2.9938809261	1.1605693252
H	1.5484799781	3.8397382323	0.4986545677
C	0.6130511729	2.0647857587	1.2445386823
H	0.7545608521	1.2119530056	1.8954050845
C	-0.5394581445	2.1320713466	0.5059629066
C	-1.5224544028	1.0588295908	0.5172710949
C	-2.0283064989	0.6538850000	-0.7858666546
C	-2.1337696566	-0.6661759609	-1.1389490185
H	-1.8958576847	-1.4150077323	-0.3949327601
C	-0.7223370154	3.2292361447	-0.5259077088
H	0.0827933283	3.1810717003	-1.2722333782
H	-0.6240377296	4.2021997322	-0.0302970623
C	-2.2196011665	1.7412271147	-1.8261153981
H	-1.4955150932	1.6137252512	-2.6430152198
H	-3.2127908390	1.6290215187	-2.2765976841
C	-2.0674735268	3.1318115977	-1.2291149152
H	-2.1469717956	3.8937491290	-2.0088085038
H	-2.8775068505	3.3216225170	-0.5139709873
H	-3.3141529468	-4.5092885177	-6.3566313334
C	-3.0610030773	-4.9628087878	-5.4051925557
C	-2.4095736757	-6.1770295345	-2.9475415726
C	-2.7961652364	-4.2107803283	-4.2724655018
C	-2.9937929818	-6.3505866767	-5.2855427082
C	-2.6732464333	-6.9557245063	-4.0752128776
C	-2.4733758141	-4.8008281260	-3.0552623514
H	-3.1993080818	-6.9651415074	-6.1556623327
H	-2.6287691375	-8.0372477398	-4.0074773609
H	-2.1598696571	-6.6517475750	-2.0029487630
C	-2.2370934370	-3.7219056130	-2.0162456894
C	-2.4932474604	-2.4493495848	-2.8352614130
C	-2.4497027580	-1.1339522930	-2.4411741920
H	-2.6740125141	-0.3867533100	-3.1916146488
N	-2.7955859667	-2.8106208773	-4.1136429689
N	-1.9274524637	0.4726691006	1.6558644866
C	-1.4848551160	0.9032436024	2.9822399895
C	-2.9665741377	-0.5561501123	1.7041261233
H	-3.6023906478	-0.4935225088	0.8237057186
H	-2.5373485092	-1.5611841516	1.7686316615
H	-1.1425072106	1.9352108877	2.9499542564
H	-0.6806665694	0.2674224255	3.3659974103
C	-3.0797554117	-1.8628860803	-5.1683426102
H	-2.2337505338	-1.1830320633	-5.3107272104
H	-3.9714878804	-1.2734453146	-4.9317505492
H	-3.2542690222	-2.3967960613	-6.1000179403
C	-0.7846582708	-3.7898074986	-1.5109326697

H	-0.0782838078	-3.6795224159	-2.3374733078
H	-0.6052433715	-4.7615694186	-1.0422796804
H	-0.5677217574	-3.0142346887	-0.7720212631
C	-3.2403691337	-3.8751764339	-0.8600061976
H	-3.1004093136	-4.8480321425	-0.3805460626
H	-4.2697913759	-3.8234138254	-1.2234872705
H	-3.1097947914	-3.1032088409	-0.0975863704
C	2.4395273569	1.7946574543	4.0968085643
H	1.4500405630	1.4006210534	3.8537393142
H	2.3125016016	2.7792075235	4.5539871532
H	2.8895242416	1.1324792229	4.8418232955
C	3.5130845349	0.4890972641	2.1999459214
H	4.1687145231	0.5480041277	1.3275681592
H	2.5555626630	0.0719361146	1.8778855322
H	3.9626554266	-0.2071867880	2.9135717077
H	-2.3292483128	0.8298112021	3.6692245379
H	-3.5737903434	-0.3907413097	2.5951343671

Bis-dipole S₁ minimum

H	6.2944724021	5.2700623033	2.1738075222
C	6.1159697783	4.3449909334	2.7097477896
C	5.6809946465	1.9436900340	4.1263940721
C	4.9489631451	3.6067236002	2.5499563118
C	7.0674585898	3.8550344990	3.5990521876
C	6.8595781457	2.6702952739	4.3020482201
C	4.7270369559	2.4185210046	3.2478866723
H	7.9874803581	4.4108962050	3.7457530566
H	7.6175654992	2.3112952746	4.9896047000
H	5.5217270798	1.0203958240	4.6757287419
N	3.8412265205	3.8673581456	1.7375857120
C	2.8792513357	2.9018284268	1.8704704128
C	3.3783455557	1.8484001071	2.8605876884
H	4.6279695639	5.6074657642	0.9117437325
C	3.7181550208	5.0132102830	0.8637192406
H	3.5685964175	4.6910939639	-0.1718063269
H	2.8732985834	5.6419105456	1.1639390162
C	1.6903028115	2.9590635877	1.1736690867
H	1.5450007948	3.8198111841	0.5318619846
C	0.6405629208	2.0074368296	1.2063559355
H	0.7662675307	1.1326004042	1.8318516237
C	-0.5289922578	2.1133096296	0.4748553140
C	-1.5761216493	1.1090073508	0.5213241513
C	-1.9918855208	0.6588668658	-0.7951063673
C	-2.0561722059	-0.6807338324	-1.1343076607
H	-1.7873457226	-1.4048723601	-0.3749789816
C	-0.7026193655	3.2245845651	-0.5422291651
H	0.1144685821	3.1904070001	-1.2761281288
H	-0.6177252757	4.1943457865	-0.0359407534
C	-2.2057661612	1.7323639370	-1.8435466018
H	-1.4993896670	1.5917301524	-2.6735890103
H	-3.2086891674	1.6211510530	-2.2746373751
C	-2.0413558183	3.1297129207	-1.2614419011
H	-2.1040393383	3.8825158953	-2.0518452081
H	-2.8550742037	3.3348783475	-0.5565518198

H	-3.3653181364	-4.4946063491	-6.3577917813
C	-3.0902335136	-4.9576037353	-5.4171315638
C	-2.3837605445	-6.1971547799	-2.9824869073
C	-2.8061775901	-4.2143868300	-4.2772229871
C	-3.0133887492	-6.3431831644	-5.3141212270
C	-2.6653642312	-6.9620075113	-4.1154290450
C	-2.4561961114	-4.8207673062	-3.0698052354
H	-3.2312528780	-6.9496361739	-6.1869791819
H	-2.6137669246	-8.0440505651	-4.0626508143
H	-2.1132967775	-6.6825961504	-2.0492823849
C	-2.2064414034	-3.7557824937	-2.0221464206
C	-2.4805291429	-2.4797493499	-2.8191056731
C	-2.4244964557	-1.1622885345	-2.4149020090
H	-2.6795144812	-0.4164233483	-3.1584308599
N	-2.8107485067	-2.8273393918	-4.1017984256
N	-1.9954739498	0.5157664020	1.6787091377
C	-1.5754592741	0.9782354697	2.9921946294
C	-3.0747941454	-0.4593876945	1.7107105916
H	-3.6406132764	-0.4347191137	0.7815819324
H	-2.7024400092	-1.4791479973	1.8702698711
H	-1.1652607425	1.9845923254	2.9312102890
H	-0.8233624472	0.3166698040	3.4402020808
C	-3.1175832437	-1.8705141571	-5.1422817171
H	-2.2722789839	-1.1930926949	-5.3004550050
H	-4.0002057287	-1.2789212332	-4.8776420124
H	-3.3182761276	-2.3961625479	-6.0731531417
C	-0.7457117444	-3.8271664084	-1.5342246608
H	-0.0479510872	-3.7100155228	-2.3671922176
H	-0.5616602168	-4.8023835893	-1.0740223819
H	-0.5251480280	-3.0569610952	-0.7915062296
C	-3.1885677799	-3.9206828030	-0.8470924270
H	-3.0267146114	-4.8898034801	-0.3666416814
H	-4.2247234481	-3.8841885227	-1.1928878953
H	-3.0522257030	-3.1424178121	-0.0923973930
C	2.4666184450	1.7379409591	4.0965692310
H	1.4803650673	1.3461463793	3.8379838774
H	2.3343126284	2.7107832784	4.5767576597
H	2.9177048182	1.0595719194	4.8263981706
C	3.5619789022	0.4738453358	2.1857634710
H	4.2183518854	0.5501356938	1.3152690746
H	2.6095808086	0.0489161538	1.8600947501
H	4.0193445677	-0.2230073348	2.8942785740
H	-2.4424303045	0.9966556558	3.6576259708
H	-3.7499567241	-0.2164932098	2.5355081436

Cyanine-like Franck-Condon point

H	7.8399089996	1.0278848789	-4.4058463663
C	7.6869688737	1.5416551392	-3.4637916045
C	7.3239505095	2.8913625955	-1.0157629315
C	6.5322419732	1.3904069421	-2.7142348293
C	8.6697853026	2.3929924040	-2.9609109413
C	8.4957938634	3.0617104887	-1.7536791329
C	6.3423353640	2.0508671574	-1.5061946335
H	9.5854390807	2.5328272539	-3.5255669212

H	9.2754177071	3.7184468904	-1.3836024409
H	7.1915032763	3.4138980614	-0.0729351548
N	5.3902017048	0.6049292118	-2.9847304591
C	4.4574066214	0.7232998580	-2.0087365980
C	4.9919631498	1.6739685957	-0.9306460581
H	6.1069609319	-0.1290505191	-4.7954123024
C	5.2252898101	-0.2185257542	-4.1648692185
H	5.0995565331	-1.2691152322	-3.8865708182
H	4.3515789202	0.1035736100	-4.7396118049
C	3.2464804299	0.0600079245	-2.0724514297
H	3.0756938026	-0.5655453879	-2.9395131120
C	2.2120324196	0.1413881802	-1.1212948336
H	2.3960672273	0.7180832264	-0.2241229486
C	0.9487403591	-0.4021460087	-1.2672166687
C	-0.0312733741	-0.1984542065	-0.2438649364
C	-1.4223956996	-0.2281738623	-0.5865117230
C	-2.3835831770	-0.4582513256	0.3776812687
H	-2.0209857252	-0.6394338082	1.3816151612
C	0.5682548176	-1.0594573238	-2.5807017850
H	1.1377399934	-1.9877462045	-2.7165667780
H	0.8821288091	-0.3932059469	-3.3939710765
C	-1.7299241805	-0.2133094288	-2.0642021939
H	-2.7949907743	-0.3556624834	-2.2495472765
H	-1.4581663504	0.7502157005	-2.5144867196
C	-0.9275719338	-1.3362233445	-2.7247905860
H	-1.1936609190	-2.2841362891	-2.2447120829
H	-1.1836413135	-1.4314900622	-3.7842734693
H	-8.8601125116	-1.2298646051	1.2478749849
C	-8.1874562275	-1.4041660965	2.0798153031
C	-6.4689079897	-1.8675700564	4.2653949643
C	-6.8147712799	-1.2549007594	1.9693684536
C	-8.6919375792	-1.7948116864	3.3194661145
C	-7.8486346722	-2.0250609270	4.4013737003
C	-5.9584475874	-1.4813073094	3.0405052059
H	-9.7631091190	-1.9204805225	3.4365383872
H	-8.2656005876	-2.3285841472	5.3553696145
H	-5.8122197509	-2.0482254971	5.1114428211
C	-4.5283696000	-1.2285535756	2.6072794284
C	-4.7194456261	-0.8474745692	1.1335076683
C	-3.7783057430	-0.5193966017	0.1792784700
H	-4.1516356701	-0.2844805431	-0.8090251908
N	-6.0469018271	-0.8751314570	0.8481113998
N	0.3684279600	0.0530629951	1.0458984945
C	1.4689163581	-0.6451679652	1.6929493439
H	1.1008963868	-1.1106851585	2.6157992688
H	2.2812702991	0.0374820038	1.9703441738
C	-0.2558424258	1.0508357797	1.9008757159
H	-0.7126102020	0.6008008875	2.7905771657
H	-1.0140682186	1.6034137501	1.3496287685
H	1.8628751851	-1.4217816528	1.0406041243
H	0.5118777826	1.7543017555	2.2473177485
C	-6.6002442164	-0.5585262264	-0.4519335895
H	-6.2300143875	-1.2556281632	-1.2100101420

H	-6.3326128217	0.4609916853	-0.7450690605
H	-7.6846346704	-0.6334951240	-0.4120742630
C	4.1082913911	2.9237004799	-0.7744188655
H	3.1219281770	2.6799426858	-0.3738683611
H	3.9721058230	3.4315985504	-1.7325794895
H	4.5879942388	3.6259038901	-0.0867804061
C	5.1825520191	0.9482858585	0.4142327046
H	5.8133578050	0.0635704285	0.2966484756
H	4.2302969227	0.6343664433	0.8474003026
H	5.6725627685	1.6197148063	1.1248150227
C	-3.6870855884	-2.5068438106	2.7681215073
H	-4.1096775468	-3.3301024821	2.1866193555
H	-3.6773889548	-2.8079321353	3.8194772764
H	-2.6521943541	-2.3604224133	2.4500717621
C	-3.9378364474	-0.0616786254	3.4196572667
H	-3.9298940590	-0.3228463586	4.4816267316
H	-4.5378733999	0.8439467139	3.2996203077
H	-2.9127690856	0.1656068243	3.1201827405

Cyanine-like S₁ minimum

H	7.8867440429	1.4306295802	-4.3619226738
C	7.7842137971	1.6510528981	-3.3055001663
C	7.5596192683	2.2375803184	-0.5605414500
C	6.5944444373	1.4589443099	-2.6205787053
C	8.8711343874	2.1461934408	-2.5854891377
C	8.7678721672	2.4381738766	-1.2301791680
C	6.4765985169	1.7467190080	-1.2636220944
H	9.8137414783	2.3044653832	-3.0989195307
H	9.6275933827	2.8221861985	-0.6920409672
H	7.4794835080	2.4659385098	0.4985762435
N	5.3630803106	0.9770794774	-3.0949144042
C	4.4221008253	0.9269067718	-2.0970471488
C	5.0660435490	1.4367235595	-0.8001117400
H	6.0125542450	0.6840329215	-5.0470177954
C	5.1079437583	0.5636403580	-4.4544324634
H	4.8075933892	-0.4892091427	-4.4904411184
H	4.3152750893	1.1707736943	-4.9044416800
C	3.1455955579	0.4829365694	-2.3191304838
H	2.9052867494	0.1855711575	-3.3321829493
C	2.1041600460	0.3771441031	-1.3536613714
H	2.3510054259	0.7111317669	-0.3535198458
C	0.8300158198	-0.1028864548	-1.5953561684
C	-0.1772178526	-0.1576014883	-0.5938955130
C	-1.5279914485	-0.5744540399	-0.7452652114
C	-2.4358757314	-0.5803146994	0.2969747836
H	-2.0941144434	-0.3033896581	1.2872325180
C	0.4203591646	-0.5894666796	-2.9684977195
H	1.2750358934	-1.0647820672	-3.4563577662
H	0.1454375530	0.2725676040	-3.5913634236
C	-1.9227925728	-1.0100553349	-2.1390061918
H	-2.7077959723	-1.7673688187	-2.0763475969
H	-2.3500179821	-0.1577354001	-2.6846297046
C	-0.7399918125	-1.5775207293	-2.9166101532
H	-0.4065546052	-2.5057868023	-2.4386666899

H	-1.0519280112	-1.8368337902	-3.9321963911
H	-8.7545223417	-2.0027405156	1.5591207356
C	-8.0779696344	-1.8071576807	2.3832391700
C	-6.3447813468	-1.3231742308	4.5491473570
C	-6.7470612519	-1.4759187507	2.1839975395
C	-8.5323145679	-1.8911595089	3.6990893107
C	-7.6827136585	-1.6524081694	4.7733660876
C	-5.8834250984	-1.2394066828	3.2499251721
H	-9.5697369533	-2.1511103673	3.8817974079
H	-8.0593660417	-1.7247861624	5.7878047181
H	-5.6805711331	-1.1397797525	5.3890611342
C	-4.5014562286	-0.9072264716	2.7187540764
C	-4.7185590496	-1.0318207434	1.2041868658
C	-3.8162610864	-0.9120867718	0.1818907620
H	-4.1929922524	-1.0841855428	-0.8185317785
N	-6.0405121236	-1.3249034219	0.9800107455
N	0.1983686313	0.2978865212	0.7059609227
C	0.7411606824	-0.6439628153	1.6487584498
H	0.0570719091	-1.4946349300	1.7205405601
H	0.9034053898	-0.1846080340	2.6224399401
C	0.0229827944	1.6886651866	1.0328133130
H	-1.0476771458	1.9159132927	0.9736179500
H	0.5216086427	2.2871523450	0.2646712702
H	1.6844404696	-1.0250934801	1.2399413632
H	0.4107292995	1.9180803166	2.0239089023
C	-6.6111796974	-1.4887548666	-0.3358720135
H	-6.2069011103	-2.3759772581	-0.8361693880
H	-6.3996461889	-0.6101866579	-0.9533445765
H	-7.6911221864	-1.5962882804	-0.2539558364
C	4.3856948172	2.7211745336	-0.2948229966
H	3.3543807511	2.5386249750	0.0189538139
H	4.3733663736	3.4880949272	-1.0731465478
H	4.9352874861	3.1198472298	0.5629428366
C	5.0978136466	0.3561204127	0.2936437482
H	5.5694135702	-0.5587954979	-0.0732574396
H	4.0944398313	0.1032561654	0.6462609357
H	5.6754727068	0.7134365736	1.1511432734
C	-3.4724470739	-1.9241271903	3.2393870539
H	-3.7408901335	-2.9406525344	2.9417566364
H	-3.4368705438	-1.8897318278	4.3322434592
H	-2.4678346809	-1.7148448163	2.8623166950
C	-4.1179888931	0.5269627094	3.1253233881
H	-4.0961797237	0.6085481877	4.2159873999
H	-4.8464782049	1.2493838538	2.7487100789
H	-3.1311796901	0.8093883297	2.7474994184

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Bis-dipole Franck-Condon point

H	0.1920462294	8.4317605281	-1.1078050535
C	0.5720494048	7.9964559653	-0.1905949021
C	1.5747010760	6.8994798327	2.2014151804
C	0.3453891486	6.6725299956	0.1493570626
C	1.3178745463	8.7713856112	0.6971617382

C	1.8155104831	8.2362899704	1.8800250590
C	0.8377316179	6.1226363100	1.3284567389
H	1.5100552564	9.8114154828	0.4549518207
H	2.3925946572	8.8590533091	2.5547393279
H	1.9642897817	6.4818034087	3.1254881811
N	-0.3638830172	5.6827977382	-0.5548601426
C	-0.3600999040	4.4875580421	0.1110024596
C	0.4298103351	4.6641175402	1.4172001170
H	-0.8781768090	6.9179315523	-2.1458285163
C	-1.0132567106	5.8858109670	-1.8291055396
H	-0.5838778020	5.2290312277	-2.5931694872
H	-2.0870622010	5.6847455907	-1.7543157255
C	-0.9848247217	3.3774699128	-0.3892271325
H	-1.4877318775	3.4859248069	-1.3416263665
C	-1.0355557380	2.0949263387	0.2352831481
H	-0.5614260943	2.0199253799	1.2079656105
C	-1.5649690546	0.9500565922	-0.2797057048
C	-1.4222861005	-0.3184782174	0.4491315839
C	-0.8032913401	-1.4128052238	-0.2866409200
C	0.1623061583	-2.1898518900	0.3000501190
H	0.4189523059	-1.9596491487	1.3268253035
C	-2.0684565200	0.8153041246	-1.6989021287
H	-2.0671574713	1.7855773368	-2.1962737617
H	-3.1095631009	0.4650383315	-1.7032350485
C	-1.1670746961	-1.5247492977	-1.7564935110
H	-0.4656043595	-2.1861096166	-2.2665109806
H	-2.1554587831	-1.9962220875	-1.8474842580
C	-1.1980219689	-0.1747848298	-2.4707864257
H	-0.1812521655	0.2255960490	-2.5479315155
H	-1.5772833236	-0.3041587699	-3.4894848526
H	4.5248856260	-6.9748976954	-0.9022278732
C	4.5352421802	-6.4741292991	0.0590587290
C	4.5881680010	-5.1982374667	2.5704980977
C	3.6478316715	-5.4586683970	0.3755761381
C	5.4621720384	-6.8442380850	1.0328018063
C	5.4934321507	-6.2181785362	2.2741011044
C	3.6656331114	-4.8234285938	1.6122904688
H	6.1692136251	-7.6370551183	0.8124188778
H	6.2240208206	-6.5238043793	3.0149930411
H	4.6142772466	-4.7109995028	3.5409866031
C	2.5758929042	-3.7697414351	1.6560954686
C	1.9562358109	-3.9132178004	0.2581626089
C	0.9158075403	-3.2240524850	-0.3160183330
H	0.6452324610	-3.5046056936	-1.3251377958
N	2.6229194471	-4.8958697551	-0.4107741150
N	-1.8475648574	-0.4467786493	1.7064891941
C	-2.6416000711	0.5856624595	2.4172196590
H	-2.3111369530	1.5774463984	2.1390802721
C	-1.8373720156	-1.7175076431	2.4359143398
H	-0.9850060261	-1.7732312925	3.1191486000
H	-1.8021102247	-2.5567937248	1.7450348019
H	-2.4304628951	0.4607675122	3.4818457389
C	2.3133402620	-5.2984355792	-1.7649351601

H	2.4135734389	-4.4512496674	-2.4508480279
H	1.2929550383	-5.6894418080	-1.8309333906
H	3.0034335775	-6.0788990452	-2.0781490010
C	-0.4533071459	4.4424489065	2.6579581046
H	-0.7585849409	3.3981579770	2.7643488327
H	-1.3537394252	5.0606262457	2.6150754495
H	0.1021843479	4.7189687059	3.5586334711
C	1.6801458991	3.7675661471	1.4590519373
H	2.3023028173	3.9210655849	0.5736788076
H	1.4227146705	2.7068226130	1.5146061526
H	2.2794909495	4.0163679457	2.3395217453
C	3.1921805171	-2.3761275035	1.8686470760
H	3.9114511771	-2.1418171324	1.0797715912
H	3.7218404486	-2.3505538542	2.8253803278
H	2.4338242322	-1.5894855693	1.8822323760
C	1.5674642229	-4.1126087557	2.7671598565
H	2.0810155845	-4.1406750740	3.7323000551
H	1.1149956442	-5.0931527017	2.5982431113
H	0.7649556790	-3.3742473126	2.8367870417
H	-2.7507044175	-1.7800264964	3.0287246837
C	-4.1307422769	0.4369705616	2.1288401351
H	-4.3361219559	0.6199469743	1.0709200920
H	-4.6913115553	1.1689925384	2.7161723427
H	-4.5065656223	-0.5567573812	2.3873734796

Bis-dipole S₁ minimum

H	-0.4532525559	8.5786797297	-1.0704564991
C	0.1180083780	8.1684684061	-0.2463105941
C	1.6424716894	7.1234910824	1.8904819167
C	0.0668152499	6.8272897032	0.1050174762
C	0.9540494412	8.9882635779	0.5050680393
C	1.7059506410	8.4770200108	1.5611087817
C	0.8165667852	6.2983085393	1.1499973505
H	1.0204303587	10.0423342155	0.2593245141
H	2.3485120888	9.1393467373	2.1307498809
H	2.2333970918	6.7335229580	2.7133880049
N	-0.6929361082	5.7885422128	-0.4724475533
C	-0.4527172852	4.6042674828	0.1276482441
C	0.5500170447	4.8133705716	1.2634035274
H	-1.7703470656	7.0511795549	-1.7279398917
C	-1.6116404624	5.9856554875	-1.5809381117
H	-1.2069375659	5.5539547096	-2.5003093511
H	-2.5747185682	5.5248989088	-1.3536450397
C	-1.0635256978	3.4281088617	-0.3019269808
H	-1.7410642502	3.5060109116	-1.1433015491
C	-0.8717340758	2.1529661314	0.2575939215
H	-0.2083210704	2.0576705694	1.1085215263
C	-1.4990762239	0.9939571199	-0.1566213093
C	-1.2210034282	-0.3011688339	0.5095357307
C	-0.3666715342	-1.1664521797	-0.2166985757
C	0.4107270457	-2.1279807851	0.4062686962
H	0.4682457011	-2.0617397140	1.4873770941
C	-2.1753479186	0.8173246897	-1.4721063686
H	-2.5275336826	1.7404204024	-1.9417964615

H	-3.0241955577	0.1327989040	-1.3772334788
C	-0.4612436932	-1.1103422935	-1.7400184374
H	0.5238784542	-1.2728971369	-2.1892936565
H	-1.0775037898	-1.9638107782	-2.0563404667
C	-1.0627163765	0.1695143975	-2.3439881812
H	-0.2745249467	0.9177676140	-2.4799728684
H	-1.4696156421	-0.0463369645	-3.3368654584
H	4.5206067783	-7.1251273994	-0.8832533029
C	4.4879734046	-6.6992332237	0.1132092196
C	4.4508219831	-5.5971330974	2.7039363311
C	3.6158175238	-5.6746018218	0.4503108907
C	5.3475780046	-7.1695128177	1.1056059002
C	5.3355572456	-6.6299029874	2.3867671902
C	3.5944403075	-5.1232064061	1.7298439727
H	6.0418998756	-7.9683015674	0.8660605529
H	6.0177748155	-7.0070074676	3.1407203254
H	4.4434862345	-5.1741756045	3.7044999223
C	2.5503961411	-4.0247643797	1.7909539448
C	2.0300683031	-4.0172854837	0.3479986770
C	1.1264722528	-3.1713931290	-0.2400618506
H	0.9536010289	-3.3030973819	-1.3031846450
N	2.6613052045	-5.0254084999	-0.3442886575
N	-1.8489380832	-0.6413597270	1.6975658000
C	-2.4543068791	0.3626628885	2.5598116825
H	-1.7933054939	1.2324541548	2.6066552567
C	-2.3293460069	-1.9963348600	1.9382871043
H	-2.0111943273	-2.3480127021	2.9258606402
H	-1.9311411289	-2.6748211506	1.1873285739
H	-2.4841645401	-0.0585613726	3.5707978246
C	2.3968602266	-5.3366039608	-1.7273455211
H	2.7800269086	-4.5572123249	-2.3971531045
H	1.3196949195	-5.4401416258	-1.8909869741
H	2.8725194173	-6.2818530779	-1.9845585781
C	-0.0727283832	4.4878544772	2.6355820375
H	-0.2875026236	3.4230716980	2.7439679572
H	-1.0002228132	5.0448476928	2.7906432370
H	0.6271127262	4.7729807525	3.4253543849
C	1.8530936020	4.0233207546	1.0356750717
H	2.2892079335	4.2538306188	0.0604349234
H	1.6963818126	2.9447401322	1.0954218061
H	2.5805588329	4.3016885068	1.8027959794
C	3.2075462256	-2.6871013993	2.1726877206
H	4.0167449179	-2.4411113960	1.4802499531
H	3.6327205253	-2.7568656156	3.1785767615
H	2.4892326358	-1.8646799306	2.1622691737
C	1.4469322250	-4.4093089401	2.7940676086
H	1.8813543015	-4.5362296972	3.7900350270
H	0.9763851692	-5.3545836482	2.5112563111
H	0.6679365984	-3.6458512713	2.8593249000
H	-3.4251631690	-2.0376251868	1.9008934514
C	-3.8610105062	0.7985463781	2.1515380613
H	-3.8543824717	1.2837245372	1.1708956817
H	-4.2665043269	1.5078836608	2.8794107771

H	-4.5451399896	-0.0528919475	2.1034539423
Cyanine-like Franck-Condon point			
H	-2.1005241148	-4.7622497151	-7.3991372083
C	-1.8907795622	-3.7019818633	-7.4808085848
C	-1.3488160721	-0.9468748815	-7.7319381318
C	-1.5880776930	-2.9169382047	-6.3807155187
C	-1.9176060082	-3.0757053449	-8.7261106551
C	-1.6508486131	-1.7167005830	-8.8556635321
C	-1.3183978156	-1.5582053445	-6.4926317738
H	-2.1512618813	-3.6641150189	-9.6070480070
H	-1.6775437117	-1.2528607769	-9.8355983383
H	-1.1415411654	0.1140687677	-7.8365363781
N	-1.4927143871	-3.2864422202	-5.0209809218
C	-1.1663449335	-2.2310423835	-4.2361346069
C	-1.0313359815	-0.9845679304	-5.1196438513
H	-1.9760894589	-5.2837226062	-5.3471667033
C	-1.7015509728	-4.6302398972	-4.5222140191
H	-0.7879868553	-5.0162567535	-4.0595579426
H	-2.5079084206	-4.6431797820	-3.7833049730
C	-0.9885172228	-2.3634980052	-2.8716853373
H	-1.1087442046	-3.3557035574	-2.4549430569
C	-0.6529071314	-1.3278351999	-1.9800078063
H	-0.5981058570	-0.3205734530	-2.3724701834
C	-0.3270607356	-1.4974951296	-0.6463692796
C	0.0187370023	-0.3587836033	0.1474907682
C	0.8471979016	-0.5360398889	1.3037718195
C	0.8274151905	0.3875079052	2.3291079663
H	0.1480349166	1.2217337008	2.2055727973
C	-0.1903543239	-2.9019266367	-0.0877179213
H	0.4174582235	-3.4858099465	-0.7901701731
H	-1.1713923640	-3.3935081163	-0.0606714930
C	1.5315775139	-1.8760658079	1.4167527753
H	2.2814444865	-2.0036333788	0.6255470444
H	2.0570542121	-1.9747032808	2.3670642510
C	0.4619648561	-2.9635415378	1.2936192334
H	0.8935728812	-3.9565318392	1.4514179590
H	-0.2840314147	-2.8101531348	2.0808401879
H	3.2219132597	1.6027463397	8.3341318739
C	2.4337720742	2.2332131627	7.9388140414
C	0.3775487044	3.8861507157	6.9467272032
C	1.8927896380	2.0430568889	6.6779328395
C	1.9216646577	3.2795832700	8.7046593880
C	0.9073119997	4.0986629843	8.2201144143
C	0.8772408410	2.8509586445	6.1796518474
H	2.3248642773	3.4528156785	9.6968330645
H	0.5252517638	4.9056511779	8.8356787001
H	-0.4158572676	4.5264208367	6.5720674984
C	0.5056946470	2.3932461411	4.7829562335
C	1.4505889743	1.1995672511	4.5934654760
C	1.5695284827	0.3327845348	3.5270960440
H	2.2980480167	-0.4614916209	3.6260540390
N	2.2200635114	1.0744053940	5.7058401301
N	-0.4357245103	0.8884999883	-0.2107539562

C	0.3989497102	2.0918338845	-0.1582115458
H	-0.0551046996	2.8270635131	0.5199076602
C	-1.8078395211	1.1170270608	-0.6478456973
H	-2.2357284377	1.9317129005	-0.0503550591
H	-2.4005859698	0.2177948590	-0.4896161633
H	1.3671591172	1.8151492223	0.2560976690
H	-1.8850085714	1.4042077206	-1.7006666506
C	3.2365967768	0.0576351879	5.8751823804
H	3.9670742169	0.1086199845	5.0626365994
H	2.7897176437	-0.9415729631	5.8902115007
H	3.7573232526	0.2207202211	6.8162004744
C	-2.0859470243	0.0809929000	-4.7692871967
H	-1.9115796245	0.5214155691	-3.7851677950
H	-3.0937187106	-0.3419723010	-4.7824424673
H	-2.0484857507	0.8858377074	-5.5085644724
C	0.3918581898	-0.4022046741	-5.0686434205
H	1.1364053041	-1.1597246487	-5.3264488151
H	0.6350879035	-0.0073330767	-4.0795379694
H	0.4797924548	0.4150587646	-5.7901357418
C	0.8007629770	3.5153538382	3.7707151242
H	1.8513944759	3.8141360559	3.8106060746
H	0.1916321156	4.3919266691	4.0087637388
H	0.5701771173	3.2130126951	2.7468030600
C	-0.9723039258	1.9688819478	4.7337436276
H	-1.6055997601	2.8182999203	5.0048418029
H	-1.1724178117	1.1597880819	5.4407100813
H	-1.2686019070	1.6326064673	3.7372698977
C	0.5979544677	2.7262383099	-1.5326762986
H	1.2747421460	3.5807697203	-1.4445949285
H	-0.3375751835	3.0929698044	-1.9627704872
H	1.0451576755	2.0110627188	-2.2299502246

Cyanine-like S₁ minimum

H	-2.0970446081	-4.6902095948	-7.4782609148
C	-1.9021996453	-3.6260813122	-7.5451102684
C	-1.3854720052	-0.8588300070	-7.7581772764
C	-1.5956659749	-2.8533611329	-6.4298393378
C	-1.9468348277	-2.9817905848	-8.7770282746
C	-1.6932037751	-1.6156647824	-8.8895928124
C	-1.3367970025	-1.4848865904	-6.5278708430
H	-2.1825661647	-3.5581028278	-9.6654884833
H	-1.7349384697	-1.1382159683	-9.8625478033
H	-1.1875515728	0.2048936526	-7.8502189386
N	-1.4872054978	-3.2373196669	-5.0900133043
C	-1.1493215210	-2.1834508791	-4.2888999153
C	-1.0419746810	-0.9267371683	-5.1516846738
H	-2.0700901405	-5.2065655661	-5.4212701803
C	-1.6914873016	-4.5879389045	-4.6104672367
H	-0.7531453661	-5.0195167960	-4.2458605031
H	-2.4243132813	-4.5939809003	-3.7984661582
C	-0.9311178750	-2.3395435227	-2.9278107831
H	-1.0067926177	-3.3484292438	-2.5383924732
C	-0.6105318512	-1.3246390990	-2.0097442447
H	-0.5847418988	-0.3012846746	-2.3594772977

C	-0.2679060446	-1.5383001260	-0.6705250671
C	0.0068957715	-0.4364066360	0.1874452654
C	0.7173421418	-0.6352124580	1.4221007934
C	0.7061610458	0.3368879953	2.4140193668
H	0.0641848206	1.1903600922	2.2341339558
C	-0.1154677799	-2.9585779392	-0.1670631066
H	0.6343178343	-3.4628485860	-0.7918299216
H	-1.0508939863	-3.5115408531	-0.3188751446
C	1.3561731918	-1.9855660070	1.6106145897
H	2.2195702968	-2.1066173754	0.9424059749
H	1.7216487627	-2.1138315440	2.6305504833
C	0.3113796434	-3.0570290884	1.2945119008
H	0.7072536526	-4.0564652097	1.4980595685
H	-0.5505368086	-2.9115793574	1.9548381476
H	3.2191652402	1.6463332489	8.3681307749
C	2.4530719108	2.2960416596	7.9612410777
C	0.4495655636	4.0011292695	6.9364482210
C	1.8840835775	2.0827433485	6.7089344646
C	1.9980514273	3.3867322351	8.6934920089
C	1.0089007887	4.2333414302	8.1938936532
C	0.8915436710	2.9223335748	6.1963365643
H	2.4227553339	3.5789992387	9.6731129031
H	0.6720687963	5.0766563540	8.7869201306
H	-0.3226201108	4.6614518440	6.5526676619
C	0.4786076907	2.4366175388	4.8226235748
C	1.3693645444	1.2056824785	4.6597798875
C	1.4395991407	0.2965465000	3.6208297427
H	2.1373413430	-0.5226931435	3.7452241340
N	2.1523469083	1.0798884015	5.7771819520
N	-0.4138307717	0.8451831142	-0.1570546973
C	0.5102319947	1.9736960081	-0.2104355894
H	0.0476477606	2.8362976153	0.2892233062
C	-1.7733732207	1.1183231943	-0.5881005168
H	-2.1918711274	1.9329434053	0.0178917163
H	-2.3904697771	0.2312568883	-0.4468425432
H	1.4050127869	1.7146895604	0.3575460660
H	-1.8464600159	1.4225336965	-1.6394494152
C	3.1263227587	0.0264250502	5.9656844603
H	3.8498110905	0.0253302116	5.1446984555
H	2.6364397436	-0.9522878013	6.0082307258
H	3.6616911574	0.1897905190	6.8983055673
C	-2.1045889667	0.1251303952	-4.7736480906
H	-1.9363710906	0.5322028158	-3.7742653267
H	-3.1101520559	-0.3017076038	-4.8059613981
H	-2.0658403312	0.9538259288	-5.4864862180
C	0.3733692790	-0.3198049775	-5.1049298558
H	1.1279974939	-1.0608875930	-5.3801300437
H	0.6152036552	0.0630123933	-4.1111612297
H	0.4410341779	0.5110386917	-5.8132312727
C	0.7870635377	3.5160863397	3.7651769199
H	1.8480259103	3.7783313334	3.7680968181
H	0.2142298338	4.4206335000	3.9889261626
H	0.5170013384	3.1872723276	2.7591877842

C	-1.0175227639	2.0666745421	4.8072486737
H	-1.6163980320	2.9518708180	5.0404420947
H	-1.2404706793	1.3009361502	5.5544094162
H	-1.3313507283	1.6935775965	3.8296443867
C	0.9113533541	2.3611882493	-1.6331406495
H	1.5981337313	3.2128570774	-1.6123407007
H	0.0470026708	2.6504826645	-2.2379443620
H	1.4201589976	1.5296805650	-2.1305704993

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Bis-dipole Franck-Condon point

H	-5.9127742892	-5.5544325253	-3.7623788414
C	-5.3216751816	-5.8525759240	-2.9040518722
C	-3.7981683100	-6.6634609513	-0.6749012102
C	-4.4814805952	-4.9749303783	-2.2391883162
C	-5.3877310236	-7.1608561557	-2.4270548777
C	-4.6385868000	-7.5660617912	-1.3272878752
C	-3.7243998087	-5.3641534627	-1.1403665206
H	-6.0374240386	-7.8720101129	-2.9260896434
H	-4.7086424163	-8.5892724504	-0.9748399247
H	-3.2149063761	-6.9833548169	0.1837474667
N	-4.2266031565	-3.6120317634	-2.5043682255
C	-3.3313803084	-3.0897192842	-1.6298359844
C	-2.9129466155	-4.1852487597	-0.6413875253
H	-5.4144087179	-2.0134122955	-3.1677006144
C	-4.8484603839	-2.8577819231	-3.5729873656
H	-4.0939393900	-2.4798225436	-4.2694395094
H	-5.5327410809	-3.5022112725	-4.1203484788
C	-2.9276423416	-1.7702968940	-1.6998983997
H	-3.3519820658	-1.1712343329	-2.4956820730
C	-2.0087285105	-1.1477251054	-0.8346736365
H	-1.5766405365	-1.7500997762	-0.0466273599
C	-1.5596276116	0.1552200347	-0.9430649063
C	-0.5594951395	0.6431071972	-0.0450186756
C	0.2089884200	1.8061173050	-0.3622671183
C	1.4046895046	2.0690708025	0.2826867827
H	1.7232529198	1.3740629888	1.0469957324
C	-2.0312972889	1.0400630257	-2.0749764256
H	-3.1098413095	0.9093309728	-2.2118349865
H	-1.5625887489	0.7283781504	-3.0192488028
C	-0.2500755328	2.6904155159	-1.5023076818
H	-0.0624859533	3.7373599268	-1.2438208229
H	0.3447187266	2.4846492828	-2.4036407209
C	-1.7279423490	2.5076809199	-1.8146015366
H	-2.3276447732	2.8615761918	-0.9671143437
H	-2.0089646731	3.1133735690	-2.6806694405
H	6.3713988573	6.3771234060	0.3446190681
C	6.3837929446	5.5442554071	1.0381633456
C	6.4442529977	3.3923458411	2.8588207985
C	5.3825578764	4.5876342441	1.0676521066
C	7.4297591100	5.4039317673	1.9489762096
C	7.4647724522	4.3438139795	2.8488316291
C	5.4012588499	3.5229785128	1.9611417553

H	8.2279648390	6.1385540190	1.9528320318
H	8.2894876516	4.2574716683	3.5476205962
H	6.4739586183	2.5670968492	3.5643164838
C	4.1691858826	2.6659687540	1.7516934233
C	3.4655037564	3.4177272757	0.6152945292
C	2.2694948320	3.1383184505	-0.0182895439
H	1.9723317730	3.8116901087	-0.8115010550
N	4.2190418870	4.4919270283	0.2738966074
N	-0.2790543391	-0.0923161706	1.0826490789
C	-0.0080782464	0.4022149355	2.4123710734
H	0.8693332215	-0.0086676145	2.9064810809
C	-1.1990167745	-0.4532513386	2.1570410006
H	-1.1275643701	-1.5003291939	2.4479559668
H	-0.1884454670	1.4599785263	2.5969187637
C	-2.5811753943	0.1415805080	2.2317068883
H	-2.5735930547	1.1957074929	1.9414995352
H	-2.9526780599	0.0697127157	3.2580402075
H	-3.2833605386	-0.3828365285	1.5783670803
C	3.8591394802	5.4351881388	-0.7645687959
H	2.9031140405	5.9154762267	-0.5343843414
H	3.7809661378	4.9308393666	-1.7322463090
H	4.6252011481	6.2039033248	-0.8356558788
C	3.3200289952	2.6444575060	3.0352656900
H	3.0233737202	3.6548112985	3.3284690017
H	3.9049060902	2.2144061895	3.8531430596
H	2.4172114376	2.0426988205	2.9147331624
C	4.5723330101	1.2434648750	1.3221826690
H	5.1751423409	0.7811234545	2.1089167541
H	5.1706967606	1.2646731649	0.4077681824
H	3.7017665157	0.6074515520	1.1456069685
C	-3.3270790223	-3.8369596036	0.8000112463
H	-4.3940857593	-3.6062857253	0.8575041455
H	-2.7697064867	-2.9825103890	1.1909731479
H	-3.1321406752	-4.6928739357	1.4520677234
C	-1.4088105469	-4.4996092767	-0.7332864025
H	-0.7912852399	-3.6619177656	-0.4016340132
H	-1.1231591944	-4.7498711442	-1.7581369521
H	-1.1791653124	-5.3608090683	-0.0995829748

Bis-dipole S₁ minimum

H	-5.9181845748	-5.5528385541	-3.7800354623
C	-5.3268808417	-5.8591882178	-2.9250003642
C	-3.7987232503	-6.6933966382	-0.7027083487
C	-4.4732708841	-4.9860690489	-2.2578474185
C	-5.4025259500	-7.1653815112	-2.4538572374
C	-4.6512760559	-7.5840637253	-1.3565509958
C	-3.7130143517	-5.3923742094	-1.1587665705
H	-6.0601329642	-7.8690475486	-2.9534502172
H	-4.7308173677	-8.6084597164	-1.0092287096
H	-3.2145532199	-7.0244365932	0.1508899382
N	-4.2121316466	-3.6381132196	-2.5125689198
C	-3.3037459743	-3.1234863012	-1.6284498516
C	-2.8888172512	-4.2261956574	-0.6549628000
H	-5.3588585413	-2.0066176140	-3.1618059171

C	-4.8285312267	-2.8710479869	-3.5736901258
H	-4.0742007263	-2.5181849601	-4.2845154704
H	-5.5443475686	-3.4939148340	-4.1053382042
C	-2.8938001660	-1.8031272995	-1.6915001610
H	-3.3260697432	-1.1992548407	-2.4808362924
C	-1.9700203685	-1.1756477489	-0.8309980957
H	-1.5157509773	-1.7694359716	-0.0490430468
C	-1.5532935886	0.1482250623	-0.9288948664
C	-0.5946077513	0.6700589736	-0.0019201607
C	0.1907818724	1.8186848181	-0.3283037812
C	1.4051921556	2.0653965685	0.3090518068
H	1.7310838254	1.3455924262	1.0466754289
C	-2.0305113510	1.0356082198	-2.0534235735
H	-3.1041073377	0.8860056391	-2.2102110519
H	-1.5410260565	0.7413240178	-2.9935116699
C	-0.2798759031	2.7104820454	-1.4551488142
H	-0.1063228748	3.7582872409	-1.1888249635
H	0.3208539944	2.5204366504	-2.3565936237
C	-1.7543444499	2.5061751543	-1.7742092461
H	-2.3619651497	2.8381879294	-0.9240788893
H	-2.0445163593	3.1177930255	-2.6333034634
H	6.3871432187	6.3798043692	0.3056955509
C	6.4039967853	5.5493225572	1.0018945988
C	6.4746261267	3.4023614711	2.8337090242
C	5.3924984399	4.5951456940	1.0464888393
C	7.4573584342	5.4076521221	1.8984916928
C	7.4988441763	4.3501024556	2.8060416141
C	5.4203719231	3.5309084962	1.9505489839
H	8.2601052948	6.1374852473	1.8884706654
H	8.3316405961	4.2648718437	3.4954767937
H	6.5105087861	2.5796966275	3.5417063647
C	4.1885102722	2.6722830460	1.7577795823
C	3.4712207976	3.4232821955	0.6364912958
C	2.2582763978	3.1514771865	0.0268010660
H	1.9385294687	3.8452697779	-0.7413326239
N	4.2317298328	4.5010812552	0.2754237320
N	-0.3102601559	-0.0763480000	1.1342772925
C	-0.1006135875	0.4805847623	2.4558188741
H	0.7566509660	0.0952899834	3.0028326837
C	-1.2772283778	-0.3869828782	2.1895732283
H	-1.2185666951	-1.4214055822	2.5255412397
H	-0.2913222806	1.5445661567	2.5866241345
C	-2.6633905926	0.2040172989	2.1914165125
H	-2.6520418220	1.2439869300	1.8537813358
H	-3.0692742369	0.1776721632	3.2070032816
H	-3.3397552772	-0.3556535567	1.5397468392
C	3.8674500870	5.4336342204	-0.7695224813
H	2.9436720521	5.9631896677	-0.5134829362
H	3.7231795843	4.9068127694	-1.7177852135
H	4.6630513811	6.1640966237	-0.8975252288
C	3.3525606008	2.6375582111	3.0518623136
H	3.0570947339	3.6448684199	3.3559059381
H	3.9449890366	2.1991506259	3.8600663139

H	2.4496567149	2.0361212199	2.9301199049
C	4.5926696277	1.2478259420	1.3255328646
H	5.2026675494	0.7880864812	2.1085560513
H	5.1829751509	1.2697342677	0.4060629054
H	3.7211464884	0.6109971865	1.1582050601
C	-3.2817488233	-3.8864879493	0.7965452957
H	-4.3465368331	-3.6511827810	0.8701221357
H	-2.7137873668	-3.0361177799	1.1807821190
H	-3.0792986266	-4.7467771680	1.4409232142
C	-1.3848449884	-4.5508513040	-0.7550858929
H	-0.7645625945	-3.7138982882	-0.4272239101
H	-1.1059140739	-4.8035000120	-1.7810233968
H	-1.1556645883	-5.4117065341	-0.1203755000

Cyanine-like Franck-Condon Point

H	-6.3804304284	-5.3975243414	-3.6313602336
C	-5.8736311388	-5.6590494492	-2.7096826333
C	-4.5662620208	-6.3755234511	-0.3153489978
C	-4.9330553148	-4.8334362072	-2.1169016052
C	-6.1535786137	-6.8669714637	-2.0728981621
C	-5.5104141896	-7.2252474613	-0.8921056245
C	-4.2819854114	-5.1747526613	-0.9381063878
H	-6.8862527472	-7.5365266783	-2.5104512502
H	-5.7440510441	-8.1719029775	-0.4174306991
H	-4.0665173561	-6.6595523553	0.6060894203
N	-4.4632233302	-3.5678295596	-2.5399823092
C	-3.5317027098	-3.0741891028	-1.6985235327
C	-3.3188092241	-4.0707198549	-0.5537243162
H	-5.2886910550	-1.8802115991	-3.4693026427
C	-4.9332985601	-2.8810339973	-3.7280090635
H	-4.1336635899	-2.7977911376	-4.4697626499
H	-5.7592375972	-3.4386503155	-4.1637122093
C	-2.9057481131	-1.8540203354	-1.9273713703
H	-3.1605707168	-1.3349274101	-2.8430687034
C	-1.9807154078	-1.2686763113	-1.0626481871
H	-1.7143570081	-1.7910920536	-0.1561076218
C	-1.3397004531	-0.0401809545	-1.2413779583
C	-0.3673607146	0.3801937469	-0.3015608820
C	0.3322965485	1.6150610405	-0.4736088918
C	1.4594182111	1.9679164402	0.2574055694
H	1.7923483947	1.3214241750	1.0505006144
C	-1.6724060689	0.8332675294	-2.4264952025
H	-2.6956038149	0.6396409523	-2.7589872094
H	-1.0179475260	0.5924723019	-3.2759900362
C	-0.1150947773	2.5698548042	-1.5671842868
H	-0.0560075071	3.5960820985	-1.1907418280
H	0.5856153462	2.5125483320	-2.4125883450
C	-1.5248441677	2.3027561407	-2.0662715116
H	-2.2506127133	2.5578307162	-1.2854552216
H	-1.7428720819	2.9385461171	-2.9291960905
H	6.1410100400	6.5763982278	0.5231315403
C	6.0978711949	5.8225686212	1.3007471974
C	6.0078675542	3.8819987666	3.3435982141
C	5.1433928742	4.8189380230	1.3096551997

C	7.0200585501	5.8377987626	2.3460337043
C	6.9798596463	4.8829533565	3.3568559470
C	5.0886868782	3.8576168552	2.3116951310
H	7.7798046275	6.6117422123	2.3677564119
H	7.7072972973	4.9176188119	4.1604015928
H	5.9778070562	3.1389778027	4.1350594899
C	3.9356893930	2.9116583674	2.0425663689
C	3.3588808584	3.4966390780	0.7470030200
C	2.2565167598	3.1015143197	0.0101177437
H	1.9992858105	3.7202130314	-0.8384917437
N	4.1038005419	4.5705138754	0.3876678385
N	-0.1772398302	-0.5461844318	0.7608273237
C	0.2644739794	-0.2576259934	2.1161842511
H	0.5735533827	0.7472268858	2.3804682178
C	1.1010619457	-1.0925956449	1.2149835311
H	1.9904928688	-0.6239339841	0.7986523582
H	-0.3283007726	-0.7491760144	2.8847592588
C	1.1976006141	-2.5875959400	1.3636488571
H	0.2860061190	-2.9913945037	1.8123158778
H	2.0432807282	-2.8543764677	2.0052664538
H	1.3481264998	-3.0667251716	0.3912088799
C	3.8583571556	5.3673861086	-0.7971393038
H	2.8990772451	5.8892172625	-0.7240741292
H	3.8518806494	4.7315435290	-1.6868077937
H	4.6497685531	6.1054323428	-0.9068524437
C	2.9137716363	2.9815661855	3.1908412760
H	2.5468368783	4.0013918572	3.3302528871
H	3.3867543258	2.6619269952	4.1235545220
H	2.0548666264	2.3320167465	3.0078935457
C	4.4606576641	1.4773004579	1.8509298631
H	5.0015486123	1.1663093419	2.7488724380
H	5.1494731458	1.4173544255	1.0045721070
H	3.6508982968	0.7627353053	1.6892181638
C	-3.7122816064	-3.4772047460	0.8126547148
H	-4.7288759474	-3.0759480021	0.7906135204
H	-3.0346781170	-2.6801814070	1.1244437708
H	-3.6790066281	-4.2649682160	1.5704871219
C	-1.8755549256	-4.6069509645	-0.5389923015
H	-1.1546375649	-3.8269214768	-0.2866175188
H	-1.6023781436	-5.0270068900	-1.5106371301
H	-1.7910455766	-5.4023424142	0.2066640906

Cyanine-like S₁ minimum

H	-6.3939553743	-5.4193757773	-3.6474783909
C	-5.8883785675	-5.6764070661	-2.7239847187
C	-4.5796812497	-6.3825681182	-0.3231329633
C	-4.9472285384	-4.8397116569	-2.1318531594
C	-6.1649072499	-6.8798378422	-2.0846058552
C	-5.5227757830	-7.2347603468	-0.8988660770
C	-4.2950339781	-5.1831706689	-0.9459374282
H	-6.8948490682	-7.5535307203	-2.5211115146
H	-5.7574212194	-8.1800363442	-0.4217249239
H	-4.0807355741	-6.6633216402	0.5997025333
N	-4.4875966281	-3.5882758380	-2.5513659558

C	-3.5477860591	-3.0849328685	-1.6994762720
C	-3.3328775176	-4.0806104105	-0.5599214059
H	-5.3109706822	-1.9061185626	-3.4930054530
C	-4.9505489451	-2.9080997167	-3.7432043287
H	-4.1449491725	-2.8227071146	-4.4797149649
H	-5.7712157410	-3.4694177906	-4.1846687971
C	-2.9331610668	-1.8586937168	-1.9197876535
H	-3.2121129808	-1.3256793832	-2.8218263912
C	-1.9867710338	-1.2761999881	-1.0657131272
H	-1.7023971008	-1.8062922989	-0.1694074396
C	-1.3465253596	-0.0436771058	-1.2442239167
C	-0.3650407355	0.3848742756	-0.3017917639
C	0.3420057883	1.6152116013	-0.4807767210
C	1.4737173601	1.9744310101	0.2598168596
H	1.8010122581	1.3272270660	1.0540470146
C	-1.6724560160	0.8326905554	-2.4251389337
H	-2.6891811465	0.6366656034	-2.7746600801
H	-1.0039803787	0.5980664844	-3.2665306353
C	-0.1131534507	2.5683545433	-1.5696160936
H	-0.0455489381	3.5964333144	-1.2003484901
H	0.5804726533	2.5016466265	-2.4211273938
C	-1.5272408235	2.3016082299	-2.0588705577
H	-2.2473977993	2.5523943150	-1.2717212115
H	-1.7520299853	2.9396129066	-2.9185533553
H	6.1592293109	6.5976031597	0.5264136847
C	6.1156939310	5.8410936571	1.3014114477
C	6.0216225112	3.8908391777	3.3416691838
C	5.1535234240	4.8358646055	1.3064978413
C	7.0359324011	5.8501331655	2.3436563097
C	6.9954529861	4.8902643104	3.3544677665
C	5.1003407295	3.8691745898	2.3127021581
H	7.7979405237	6.6220208556	2.3678373918
H	7.7249973174	4.9220283201	4.1563051351
H	5.9914349836	3.1456540018	4.1309830529
C	3.9492663520	2.9235311158	2.0452943652
C	3.3735463992	3.5088467128	0.7551766354
C	2.2701626836	3.1105658579	0.0149912684
H	2.0157105112	3.7270763031	-0.8378184464
N	4.1233021412	4.5932805478	0.3953102473
N	-0.1764659344	-0.5365047503	0.7638555796
C	0.2530989957	-0.2510596302	2.1215747366
H	0.5681664991	0.7522812074	2.3880035459
C	1.0950566653	-1.0876290159	1.2234171939
H	1.9907793623	-0.6192039254	0.8186079998
H	-0.3449436949	-0.7392321608	2.8885423685
C	1.1886431410	-2.5838842060	1.3649809825
H	0.2699017514	-2.9887057943	1.7983597503
H	2.0257786238	-2.8579975878	2.0148857760
H	1.3498451092	-3.0564260272	0.3906832879
C	3.8772495828	5.3923673265	-0.7870897944
H	2.9142141361	5.9082613567	-0.7141726685
H	3.8744040537	4.7592275651	-1.6793265379
H	4.6647699639	6.1352221068	-0.8926025893

C	2.9285034610	2.9860082071	3.1990419258
H	2.5636263915	4.0054499603	3.3471836856
H	3.4033687850	2.6564538734	4.1276687659
H	2.0687896726	2.3390064283	3.0111008844
C	4.4782096351	1.4867720551	1.8578922349
H	5.0208236256	1.1803497755	2.7567230403
H	5.1655924011	1.4248895255	1.0104386863
H	3.6687115812	0.7710151627	1.7003803930
C	-3.7218697820	-3.4889232294	0.8110601509
H	-4.7410016045	-3.0940388760	0.7940849332
H	-3.0467907860	-2.6861294444	1.1136304913
H	-3.6766495492	-4.2747105858	1.5707672344
C	-1.8881605899	-4.6214489146	-0.5358672295
H	-1.1682015834	-3.8416971249	-0.2794294356
H	-1.6095005883	-5.0428932688	-1.5053427465
H	-1.8100554337	-5.4153779402	0.2126588858

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Bis-dipole Franck-Condon point

H	6.1765096223	5.6417629972	2.4354406411
C	6.0223527085	4.7077934497	2.9633603422
C	5.6580359158	2.2808998680	4.3473406960
C	4.9054658295	3.9150804237	2.7564344567
C	6.9651979145	4.2603496671	3.8877396320
C	6.7907022399	3.0638012347	4.5746034646
C	4.7175136570	2.7147616238	3.4326326520
H	7.8497715456	4.8612931486	4.0701807773
H	7.5384514712	2.7367016034	5.2885616548
H	5.5246155711	1.3459254103	4.8836596749
N	3.8108442449	4.1271773749	1.8943287667
C	2.9107451659	3.1085086002	1.9634042008
C	3.4129662636	2.0822927763	2.9882982618
H	4.4752629050	5.9741309190	1.2047140530
C	3.6604400525	5.2754862600	1.0277374133
H	3.6796305701	4.9742829249	-0.0247769991
H	2.7157703967	5.7886014159	1.2320510943
C	1.7703269003	3.0933428444	1.1942102165
H	1.6252766252	3.9247953096	0.5164774572
C	0.7827995734	2.0777424265	1.1888858528
H	0.9377403308	1.2385742938	1.8534934149
C	-0.2988557390	2.0374726975	0.3431085840
C	-1.1711108945	0.8854354614	0.3003748476
C	-1.7931371441	0.5264419762	-0.9550047468
C	-2.0288374380	-0.7880114435	-1.2758863388
H	-1.7620252321	-1.5418280269	-0.5470947604
C	-0.5052256403	3.1222707847	-0.6941442645
H	0.2921535199	3.0802045885	-1.4495573826
H	-0.4162762495	4.1008669507	-0.2096835517
C	-2.0196044046	1.6198371402	-1.9787077314
H	-1.3217102200	1.4992100135	-2.8194748003
H	-3.0256450928	1.5115621590	-2.3993036099
C	-1.8591712644	3.0087984384	-1.3788788447
H	-1.9565315989	3.7716986569	-2.1560870317

H	-2.6581649985	3.1915251651	-0.6495906231
H	-3.9426685462	-4.5786549132	-6.3117737457
C	-3.5822534200	-5.0424342804	-5.4008302113
C	-2.6457601567	-6.2847161641	-3.0516324929
C	-3.1679179665	-4.3033494082	-4.3048900381
C	-3.5202020018	-6.4317144099	-5.2993068281
C	-3.0594196635	-7.0506221550	-4.1423555783
C	-2.7025408963	-4.9070742956	-3.1421600582
H	-3.8385304173	-7.0362370930	-6.1421108777
H	-3.0207137899	-8.1329361993	-4.0874038773
H	-2.2861777181	-6.7698871166	-2.1488162565
C	-2.3314132951	-3.8397973901	-2.1313251375
C	-2.6538782953	-2.5572751987	-2.9100272419
C	-2.5129347777	-1.2435813290	-2.5271783021
H	-2.7828021983	-0.4889335033	-3.2551142709
N	-3.1302831111	-2.9041378109	-4.1369953372
N	-1.3857055309	0.1494961309	1.3981180839
C	-1.1862991786	0.4841954189	2.8213891733
C	-2.4671659454	-0.8076591376	1.7024729009
C	-2.4329654193	-0.3504492343	3.1738386649
H	-2.2839966519	-1.1383443293	3.9117338504
H	-3.2928002885	0.2568585105	3.4580391615
H	-3.3781710233	-0.6143039125	1.1300916527
H	-2.1667415361	-1.8494392877	1.5585144081
H	-1.2234436522	1.5599936857	3.0135486626
H	-0.2552092497	0.0781808650	3.2270815301
C	-3.5428948065	-1.9465954704	-5.1396283091
H	-2.7004816071	-1.3193512124	-5.4486639117
H	-4.3393422838	-1.3036691517	-4.7521504561
H	-3.9199810810	-2.4747587259	-6.0128371201
C	-0.8358327175	-3.9337676521	-1.7819555448
H	-0.2172680160	-3.8154338786	-2.6751990136
H	-0.6202157743	-4.9154008352	-1.3506821631
H	-0.5346647454	-3.1731183067	-1.0575697403
C	-3.2131930678	-3.9819746731	-0.8780373320
H	-3.0398136732	-4.9581747682	-0.4164010346
H	-4.2733774640	-3.9141729280	-1.1350296187
H	-2.9938048159	-3.2133189831	-0.1333928049
C	2.4542728507	1.9587828867	4.1858137900
H	1.4936708217	1.5254889901	3.8971373160
H	2.2646446643	2.9345675972	4.6402991062
H	2.9002609272	1.3135544592	4.9479699119
C	3.6829841680	0.7119012966	2.3418837282
H	4.3586604454	0.8083959862	1.4884449750
H	2.7643976529	0.2319194491	1.9960149569
H	4.1556941476	0.0491573204	3.0722220151
Bis-dipole S₁ minimum			
H	6.1661378899	5.6801872758	2.4689353625
C	6.0265241248	4.7375994479	2.9853103022
C	5.6953565425	2.2869692527	4.3448295152
C	4.9170520322	3.9276310040	2.7660526103
C	6.9713343844	4.2955889680	3.9055661113
C	6.8146887421	3.0864814808	4.5809632811

C	4.7480071495	2.7135954688	3.4350170590
H	7.8457165571	4.9080325007	4.0992428270
H	7.5661355545	2.7659623995	5.2942629103
H	5.5760526342	1.3451688953	4.8723879533
N	3.8287693194	4.1289284328	1.9136885959
C	2.9354659833	3.0923540491	1.9811622333
C	3.4524111338	2.0677085088	2.9909282314
H	4.4962359337	5.9657531653	1.1970397146
C	3.6604119082	5.2835270647	1.0585883631
H	3.6253524052	4.9823206192	0.0063654375
H	2.7348829655	5.8140344215	1.3050666327
C	1.7865232002	3.0687159742	1.2150703815
H	1.6220985340	3.9183236616	0.5627569969
C	0.8197618810	2.0361069019	1.1773101276
H	0.9747897828	1.1744153856	1.8121639420
C	-0.2796581530	2.0149791110	0.3314056833
C	-1.1892094381	0.8995676081	0.3096400692
C	-1.7630127705	0.5166550235	-0.9558489393
C	-1.9744028350	-0.8163129582	-1.2752354379
H	-1.6693106723	-1.5558535713	-0.5467484403
C	-0.4847512644	3.1057642358	-0.6973126018
H	0.3137627022	3.0647770213	-1.4521651721
H	-0.3932584619	4.0836425649	-0.2109114810
C	-2.0050807066	1.6050613179	-1.9782455380
H	-1.3146995530	1.4823395402	-2.8252070682
H	-3.0145493982	1.4951913670	-2.3916437903
C	-1.8398413048	2.9957379665	-1.3818262510
H	-1.9352113939	3.7566713988	-2.1615006112
H	-2.6361778984	3.1808272749	-0.6513205468
H	-3.9743489690	-4.5607247313	-6.3275605270
C	-3.6082432210	-5.0358954412	-5.4248688504
C	-2.6563646594	-6.3058999770	-3.0913048037
C	-3.1792151172	-4.3052614272	-4.3216588481
C	-3.5538754293	-6.4229911451	-5.3357314474
C	-3.0847732681	-7.0572787129	-4.1866314674
C	-2.7067231582	-4.9277137828	-3.1644251555
H	-3.8849883894	-7.0192768397	-6.1795426331
H	-3.0535481621	-8.1405507984	-4.1435363403
H	-2.2912529703	-6.8030334481	-2.1973701151
C	-2.3236517255	-3.8756150018	-2.1449677462
C	-2.6429819269	-2.5885823776	-2.9055909799
C	-2.4949295985	-1.2737475808	-2.5091435028
H	-2.7925769478	-0.5164355484	-3.2251446431
N	-3.1329110271	-2.9207804715	-4.1410061960
N	-1.3770093378	0.1227897525	1.4176353597
C	-1.2761552793	0.5754027474	2.8212682070
C	-2.5731708833	-0.6999952872	1.6987573220
C	-2.4880997688	-0.3031987071	3.1849621711
H	-2.2657769150	-1.1269263412	3.8636872360
H	-3.3521872828	0.2459467225	3.5594736275
H	-3.4610976007	-0.3499902687	1.1628522105
H	-2.4342882304	-1.7651849678	1.4962810495
H	-1.4207953547	1.6551816589	2.9278616688

H	-0.3393139195	0.2930040488	3.3090183792
C	-3.5489054434	-1.9508236513	-5.1303878950
H	-2.7083969754	-1.3129962429	-5.4232867861
H	-4.3514974237	-1.3192752743	-4.7359189722
H	-3.9182766898	-2.4665443793	-6.0140116396
C	-0.8272560498	-3.9882179830	-1.7937160110
H	-0.2043233071	-3.8743144005	-2.6844427395
H	-0.6260652266	-4.9735734483	-1.3634369828
H	-0.5223657975	-3.2339157707	-1.0651174442
C	-3.1983462167	-4.0181808284	-0.8840676007
H	-3.0202188785	-4.9925250489	-0.4200742756
H	-4.2602517096	-3.9507225664	-1.1335174212
H	-2.9706768969	-3.2447734446	-0.1472996110
C	2.4951629151	1.9216732192	4.1896889241
H	1.5334478327	1.5007714271	3.8884209977
H	2.3109107398	2.8884292802	4.6650340980
H	2.9386579577	1.2564348091	4.9360800328
C	3.7335760439	0.6994404562	2.3389016856
H	4.4095258688	0.8025120599	1.4864073318
H	2.8171707803	0.2170757923	1.9922538815
H	4.2080981061	0.0378291190	3.0693820416

Cyanine-like Franck-Condon point

H	4.2935582544	6.8462183223	4.0198453120
C	4.7274082498	5.8569649855	4.1097249385
C	5.8885686757	3.3007466074	4.3570307407
C	4.1416275334	4.7350710410	3.5471646590
C	5.9199619098	5.6749317492	4.8087478338
C	6.4968492700	4.4156145784	4.9348226996
C	4.7066676414	3.4703968331	3.6609017860
H	6.4033220913	6.5351639595	5.2596626417
H	7.4246008202	4.2994089105	5.4842196933
H	6.3418477436	2.3187721962	4.4564733173
N	2.9496206384	4.6325314995	2.7984212555
C	2.7107232265	3.3552574853	2.4063396007
C	3.8366056160	2.4597459995	2.9402756408
H	2.4766942464	6.6538668667	2.9385793361
C	2.0921183690	5.7515068874	2.4684415262
H	2.0583324786	5.9074164899	1.3854549673
H	1.0765252948	5.5756449571	2.8345187677
C	1.6175381353	3.0221743470	1.6329317229
H	0.9631991602	3.8313105196	1.3330617897
C	1.2788926750	1.7261051563	1.1908552469
H	1.8725147882	0.8977527513	1.5557487191
C	0.2915877030	1.4292687669	0.2746943956
C	0.0492434394	0.0622335386	-0.0901029237
C	-0.4395947408	-0.2317277972	-1.4061837453
C	-1.1457152043	-1.3875519173	-1.6593815781
H	-1.3289528157	-2.0324481578	-0.8106598605
C	-0.4088932688	2.5504460116	-0.4710052674
H	0.3469381196	3.3004556813	-0.7311441365
H	-1.1237812971	3.0592195159	0.1883289163
C	-0.3652385430	0.9171118499	-2.3820462920
H	0.6750005697	1.1990595529	-2.5868525307

H	-0.8155917712	0.6548783396	-3.3399207561
C	-1.1121707335	2.0986048360	-1.7559864683
H	-1.1723885846	2.9391008406	-2.4539727620
H	-2.1395483712	1.7841881428	-1.5444865010
H	-4.5486311052	-4.4909732514	-6.3610992038
C	-4.6256175589	-4.8336030141	-5.3356616805
C	-4.8506501255	-5.7519943521	-2.6805849256
C	-3.9260746107	-4.2378758243	-4.2991067180
C	-5.4519200860	-5.9101294640	-5.0161213904
C	-5.5676461965	-6.3670544272	-3.7075472382
C	-4.0294310905	-4.6833672957	-2.9863929060
H	-6.0123889568	-6.3968803213	-5.8072127987
H	-6.2188374531	-7.2049440365	-3.4841415526
H	-4.9427250810	-6.1104478332	-1.6594379158
C	-3.1427572090	-3.8381004875	-2.0937974008
C	-2.5531648340	-2.8443003795	-3.1037199250
C	-1.6994017466	-1.7818075617	-2.8972954166
H	-1.4423131126	-1.1901502979	-3.7663342610
N	-3.0341381390	-3.1459976698	-4.3385454397
N	0.3097371830	-0.9227460345	0.8021386041
C	0.1791893763	-1.0014655507	2.2709121661
C	0.7896849533	-2.3128692354	0.6753698622
C	0.7350703217	-2.4407291696	2.2128284934
H	1.7084904857	-2.5638952497	2.6877601872
H	0.0573830275	-3.2094158073	2.5839515220
H	0.1340965167	-2.9990044194	0.1396544816
H	1.7861737625	-2.3635316101	0.2252087644
H	-0.8665009997	-0.9197755692	2.5855197082
H	0.7700482756	-0.2897886792	2.8462300741
C	-2.6900742759	-2.4138263335	-5.5387804222
H	-1.6111446414	-2.4519108823	-5.7167251479
H	-2.9997444627	-1.3673576048	-5.4557201917
H	-3.1980388584	-2.8573429967	-6.3922520956
C	-2.0513697691	-4.7199894767	-1.4604519603
H	-1.4449535989	-5.2085716265	-2.2272884956
H	-2.5170830483	-5.4991004088	-0.8503104308
H	-1.3867991897	-4.1418933762	-0.8150631179
C	-3.9826243984	-3.1287098855	-1.0178652751
H	-4.4875982634	-3.8736876014	-0.3965042446
H	-4.7482439063	-2.4947143358	-1.4723220931
H	-3.3668200137	-2.5049639984	-0.3656467676
C	3.3183556615	1.4098922926	3.9397984112
H	2.7183435247	0.6393109909	3.4498135586
H	2.7134428284	1.8735468786	4.7232157305
H	4.1667944928	0.9135820095	4.4189048637
C	4.6217910713	1.7965035874	1.7948554972
H	4.9851224093	2.5423276106	1.0835117473
H	4.0097764286	1.0746887499	1.2488569788
H	5.4881610935	1.2683326012	2.2029156808
Cyanine-like S₁ minimum			
H	4.3429114639	6.8394811607	4.0577100929
C	4.7621348699	5.8449623382	4.1569352952
C	5.8898318570	3.2705183953	4.4207065624

C	4.1739526687	4.7276662303	3.5728768178
C	5.9317580934	5.6465176901	4.8828310935
C	6.4936826824	4.3779169799	5.0180851947
C	4.7274122894	3.4516840583	3.6967249780
H	6.4142299755	6.4989300627	5.3495627647
H	7.4061025723	4.2512840820	5.5906346464
H	6.3329793764	2.2846954056	4.5262706530
N	3.0107632986	4.6413732546	2.8041096743
C	2.7707740383	3.3596750257	2.3926606426
C	3.8668425640	2.4525767230	2.9518749103
H	2.5100516580	6.6505206291	3.0092681003
C	2.1709232028	5.7709042087	2.4664367652
H	2.2136533095	5.9816376799	1.3924532475
H	1.1333964862	5.5687056676	2.7475152219
C	1.7010097469	3.0474429809	1.5691352482
H	1.0881874584	3.8775870143	1.2366861787
C	1.3357325654	1.7673657729	1.1119138349
H	1.8799121222	0.9097515777	1.4851607501
C	0.3513929862	1.5164435517	0.1558531272
C	0.0118947858	0.1750296261	-0.1926424590
C	-0.6171584447	-0.1111656686	-1.4515903022
C	-1.2715414786	-1.3165630001	-1.6616270841
H	-1.3607368558	-1.9614768966	-0.7971718911
C	-0.2867840428	2.6755825994	-0.5806873215
H	0.5176611208	3.3018054033	-0.9883139250
H	-0.8340646308	3.3151763306	0.1240154789
C	-0.6460712821	1.0243173667	-2.4402181460
H	0.3617286171	1.2469554006	-2.8152035015
H	-1.2643800680	0.7846451010	-3.3066787258
C	-1.2111666151	2.2532848541	-1.7221023414
H	-1.3363665057	3.0863073201	-2.4203857363
H	-2.2065901884	2.0052802318	-1.3377831765
H	-4.5977281326	-4.6594736653	-6.2721762877
C	-4.6366045746	-4.9928749147	-5.2415781397
C	-4.7746025209	-5.8759994228	-2.5630879763
C	-3.9445114991	-4.3441130080	-4.2230053163
C	-5.4018083046	-6.0996067525	-4.8910143536
C	-5.4743734263	-6.5417401560	-3.5706009573
C	-4.0109257100	-4.7743694414	-2.8952819897
H	-5.9537441358	-6.6252986302	-5.6631305179
H	-6.0800347373	-7.4072838886	-3.3251496894
H	-4.8355595894	-6.2226702750	-1.5357352914
C	-3.1596918747	-3.8714893581	-2.0280974422
C	-2.6371795478	-2.8705230680	-3.0589289240
C	-1.8480828550	-1.7503425817	-2.8772271521
H	-1.6545538126	-1.1480174795	-3.7570126089
N	-3.1130902963	-3.2262916469	-4.2939665955
N	0.3013294619	-0.8532044855	0.6736717343
C	0.1383431060	-1.0073013814	2.1243519975
C	0.9600358436	-2.1532077254	0.4945038295
C	0.7741274966	-2.4122487501	2.0073879997
H	1.7005161278	-2.5476440619	2.5661121116
H	0.0954222684	-3.2322166431	2.2442651977

H	0.4569926735	-2.8564432277	-0.1753398304
H	2.0024631221	-2.0587963593	0.1664156208
H	-0.9118382660	-0.9897546161	2.4383985365
H	0.6904243127	-0.2956364765	2.7450840564
C	-2.8062951756	-2.5154760757	-5.5165671294
H	-1.7242328904	-2.3957456021	-5.6208850150
H	-3.2758644543	-1.5255730009	-5.5257760074
H	-3.1720943152	-3.0852314414	-6.3682707289
C	-2.0201774072	-4.6841493125	-1.3811802105
H	-1.3909611349	-5.1555401418	-2.1403893598
H	-2.4445510853	-5.4736713098	-0.7541458259
H	-1.3872806177	-4.0591909623	-0.7475515903
C	-4.0213605393	-3.1849911445	-0.9501626177
H	-4.4545494334	-3.9418094481	-0.2897265863
H	-4.8406358956	-2.6208963400	-1.4028725826
H	-3.4292423492	-2.4997145605	-0.3398583418
C	3.3145858844	1.3978524678	3.9317233332
H	2.7086802020	0.6458186079	3.4209138761
H	2.7054210217	1.8617733575	4.7116590017
H	4.1481696146	0.8811861981	4.4160372924
C	4.6740832097	1.7800073308	1.8238572122
H	5.0757165123	2.5241122067	1.1315132825
H	4.0596221077	1.0787583009	1.2548013499
H	5.5146219425	1.2269197538	2.2530259592

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Bis-dipole Franck-Condon point

H	0.6349376915	8.2892412142	-1.0881209221
C	0.8789553559	7.8614932833	-0.1224432698
C	1.5287573768	6.7839474921	2.3979682200
C	0.5510003985	6.5586853649	0.2154564513
C	1.5465749165	8.6254137538	0.8342830234
C	1.8704565662	8.0993219342	2.0799823804
C	0.8669294961	6.0181532314	1.4572328156
H	1.8159019870	9.6491800057	0.5965310134
H	2.3901457468	8.7133067675	2.8073439819
H	1.7825135858	6.3747950606	3.3717179713
N	-0.1134695840	5.5817836974	-0.5510622012
C	-0.2493271751	4.4097348641	0.1341235636
C	0.3758491373	4.5846308689	1.5263748223
H	-0.3589664778	6.7942519011	-2.2213757415
C	-0.5907099929	5.7807799542	-1.9010985550
H	-0.1079329920	5.0799359098	-2.5899626290
H	-1.6749017797	5.6388577967	-1.9531656509
C	-0.8577940448	3.3117128975	-0.4193658530
H	-1.2275147063	3.4137224977	-1.4312158533
C	-1.0524915729	2.0590881191	0.2265268587
H	-0.7272413969	1.9993495665	1.2591693647
C	-1.5524330606	0.9128520615	-0.3286030884
C	-1.5813106525	-0.3218787389	0.4504898406
C	-1.0075833460	-1.4986310846	-0.2256223632
C	0.0428195271	-2.1711159728	0.3163040976
H	0.4073976422	-1.8265213465	1.2773865471

C	-1.9136045988	0.7828042446	-1.7960302057
H	-1.6324393393	1.6899779819	-2.3325559456
H	-3.0047391962	0.6949306987	-1.8936432327
C	-1.5047847372	-1.6923997234	-1.6418172306
H	-1.0080099747	-2.5450278868	-2.1057175498
H	-2.5793872102	-1.9217701077	-1.6404119448
C	-1.2576492517	-0.4266189370	-2.4628908774
H	-0.1782408261	-0.2594780252	-2.5457883288
H	-1.6494567350	-0.5469899241	-3.4779953228
H	4.3637997674	-7.0105924973	-0.8615873391
C	4.4813908585	-6.3953269660	0.0231765766
C	4.8176755520	-4.8160890768	2.3302406177
C	3.6096313845	-5.3618799535	0.3261112871
C	5.5368639699	-6.6279369225	0.9044543132
C	5.7089585867	-5.8519609056	2.0451407832
C	3.7682611366	-4.5769091934	1.4638697668
H	6.2338685867	-7.4314827464	0.6904945142
H	6.5376853664	-6.0520919327	2.7154283270
H	4.9530429819	-4.2104719489	3.2219621449
C	2.6623178888	-3.5396674291	1.5226246765
C	1.8721441327	-3.8622718383	0.2443783523
C	0.7566210504	-3.2619515734	-0.2700917476
H	0.3771803165	-3.6554006835	-1.2042869445
N	2.4780475459	-4.9193808694	-0.3811327649
N	-2.0952169848	-0.3982947956	1.6735809294
C	-2.8084900916	0.7196706213	2.3327525195
H	-2.8195494937	1.5623986803	1.6506131097
C	-2.1393344665	-1.6654905315	2.4479377984
H	-2.3772991084	-1.3836711219	3.4741903318
H	-1.1511303669	-2.1121117927	2.4764844009
H	-2.2304577123	1.0111454721	3.2165813052
C	2.0016619642	-5.4959332094	-1.6164207180
H	2.0109557871	-4.7539314971	-2.4219767373
H	0.9814159943	-5.8763329612	-1.4992568773
H	2.6467100991	-6.3238115798	-1.9034381402
C	-0.6708366488	4.4477764220	2.6469811604
H	-1.0486424453	3.4258873166	2.7358920968
H	-1.5201652220	5.1133297511	2.4731994580
H	-0.2194483600	4.7206804032	3.6050147149
C	1.5601774608	3.6277657025	1.7458009362
H	2.2945001886	3.7240077593	0.9421003291
H	1.2407305972	2.5836100529	1.7914934076
H	2.0588278146	3.8696594277	2.6887935419
C	3.2589573346	-2.1224740615	1.4811710971
H	3.8619627343	-1.9786991268	0.5810735332
H	3.9065942175	-1.9692815911	2.3494455307
H	2.4840178965	-1.3517894393	1.4978332879
C	1.8197430354	-3.7515538759	2.7928258045
H	2.4592144324	-3.6652400839	3.6760329226
H	1.3660311510	-4.7458798063	2.8025889318
H	1.0224021191	-3.0095322751	2.8891041333
C	-3.1577234746	-2.6685450197	1.9201573993
C	-4.2458754689	0.3878184301	2.7192365455

H	-3.1551040483	-3.5522008888	2.5644877394
H	-2.9051128571	-2.9900564365	0.9082426044
H	-4.8357703452	0.1128254601	1.8409454159
H	-4.6950115522	1.2838702079	3.1558907584
H	-4.3262756153	-0.4101168853	3.4599670533
H	-4.1680984670	-2.2558836118	1.9146169260

Bis-dipole S₁ minimum

H	0.2860838718	8.4573592234	-1.3483677394
C	0.3785756838	8.1904280933	-0.3017331995
C	0.6236791619	7.5335170424	2.4248502099
C	0.2025782892	6.8901608443	0.1469112506
C	0.6821992334	9.1663018634	0.6468943473
C	0.8045424105	8.8497434605	1.9950838515
C	0.3218118203	6.5578742818	1.4947111357
H	0.8263454524	10.1910805163	0.3209411342
H	1.0408143417	9.6264998334	2.7139556758
H	0.7217996318	7.2861742446	3.4780178697
N	-0.1038267286	5.7335369017	-0.5840764312
C	-0.1997610055	4.6308700213	0.2323539366
C	0.0783306803	5.0709913381	1.6747492280
H	-0.1147072094	6.6741347171	-2.4366250402
C	-0.2834728156	5.6855187205	-2.0140004614
H	0.4288197219	4.9890157734	-2.4702985543
H	-1.2992864971	5.3653181776	-2.2715399760
C	-0.4861875731	3.3812438366	-0.2554598732
H	-0.6439480729	3.3040024249	-1.3258409024
C	-0.5851264947	2.1822974927	0.4933801176
H	-0.4817188418	2.2357755348	1.5709452146
C	-0.7832076128	0.9129024200	-0.0320141178
C	-1.0765740890	-0.1949114568	0.7894255738
C	-0.8072800179	-1.5227141501	0.1821379081
C	0.2942489546	-2.2721587570	0.5485682227
H	0.9210006823	-1.8559677336	1.3275372196
C	-0.8600462785	0.7094379199	-1.5445043186
H	-0.0327850502	1.2248185814	-2.0435552959
H	-1.7717730152	1.2177794234	-1.8878320238
C	-1.5903842024	-1.7374456270	-1.0651824660
H	-1.5570492662	-2.7509289779	-1.4746902665
H	-2.6380650131	-1.4597544478	-0.9160923489
C	-0.9033895355	-0.7454841950	-2.0479720826
H	0.1155927349	-1.1084248466	-2.2195743712
H	-1.4171902299	-0.7872758483	-3.0132311173
H	3.4524088129	-7.8244417990	-0.9805234658
C	3.8853060320	-7.1559397293	-0.2455368583
C	5.0533562070	-5.4133635058	1.6471117825
C	3.2597964911	-5.9873591852	0.1625602966
C	5.1234028189	-7.4415142207	0.3212816804
C	5.7016301135	-6.5848362373	1.2563983436
C	3.8243656489	-5.1163119763	1.0879933963
H	5.6457763505	-8.3443353158	0.0249552925
H	6.6684774985	-6.8303287340	1.6812116687
H	5.5143132198	-4.7497358266	2.3716432812
C	2.9079404107	-3.9285653971	1.2902491150

C	1.7684552247	-4.2683607800	0.3292017881
C	0.6341004096	-3.5231506204	0.0097555980
H	-0.0296406869	-3.9390422756	-0.7381678966
N	2.0178766160	-5.4593710558	-0.2502350815
N	-1.8035776423	-0.1096753613	1.9709082746
C	-2.9657702903	0.7813086248	2.0763208708
H	-2.6626826914	1.8195592869	1.9212321622
C	-1.6409441472	-1.0905791028	3.0352995503
H	-1.7335979790	-0.5648650214	3.9931751250
H	-0.6149162792	-1.4648278603	2.9945802167
H	-3.3209839846	0.7118080464	3.1077515769
C	1.1400623534	-6.1261535344	-1.1980250776
H	1.1823324434	-5.6393140316	-2.1764242627
H	0.1136481741	-6.1138667502	-0.8276811826
H	1.4522487860	-7.1627342527	-1.3026095550
C	-1.1334018173	4.8380916828	2.5944989824
H	-1.3373107481	3.7741324434	2.7355970561
H	-2.0315505769	5.3077952192	2.1853684922
H	-0.9410431221	5.2769902778	3.5780516075
C	1.3378640970	4.3909583631	2.2411517935
H	2.2016430810	4.5705982532	1.5957386420
H	1.2046242082	3.3110762263	2.3382240547
H	1.5662712709	4.7973672042	3.2311002564
C	3.6326592910	-2.6263714953	0.8957105604
H	3.9754583378	-2.6614538258	-0.1414804837
H	4.5085548070	-2.4965416201	1.5365064666
H	2.9954539343	-1.7484350374	1.0168024821
C	2.4132347255	-3.8719081228	2.7498028862
H	3.2709384332	-3.7518671522	3.4165888426
H	1.8949449626	-4.7927770119	3.0291275271
H	1.7373446011	-3.0306832493	2.9177151749
C	-2.6237230660	-2.2591586516	3.0070685887
C	-4.1027745546	0.4505229346	1.1140153637
H	-2.4163776007	-2.9520509843	3.8288545088
H	-2.5502922542	-2.8125155791	2.0658574350
H	-3.7817544963	0.5746238869	0.0757171106
H	-4.9449238421	1.1285482814	1.2829836538
H	-4.4600762977	-0.5748984183	1.2452414575
H	-3.6556909293	-1.9140436613	3.1161878478
Cyanine-like Franck-Condon point			
H	-2.3741513178	7.3412183402	-4.8119609291
C	-2.0416422170	7.4397967681	-3.7850189082
C	-1.1749442069	7.7337156438	-1.1195130824
C	-1.6814306125	6.3473044259	-3.0133771531
C	-1.9596258981	8.6988231457	-3.1917891425
C	-1.5320663865	8.8499068945	-1.8769555090
C	-1.2519730311	6.4810373400	-1.6980951713
H	-2.2340124652	9.5736181093	-3.7717918512
H	-1.4757008727	9.8401092576	-1.4383036374
H	-0.8414520605	7.8544445378	-0.0929641817
N	-1.6690611268	4.9793715762	-3.3574802034
C	-1.2335445707	4.2061530755	-2.3287026367
C	-0.9406663539	5.1123214899	-1.1255789334

H	-1.1953316249	3.9992034986	-5.1565298976
C	-2.0514758884	4.4596861901	-4.6533843754
H	-2.8449811725	3.7142648795	-4.5471768745
H	-2.4237540414	5.2723382949	-5.2733483898
C	-1.0938743823	2.8398682499	-2.4529885010
H	-1.3332456404	2.4113859622	-3.4178229712
C	-0.6600457063	1.9598003393	-1.4390921958
H	-0.5015132923	2.3802322423	-0.4536506316
C	-0.3770913799	0.6166135509	-1.5755576017
C	0.0753892204	-0.1462578026	-0.4485732035
C	0.8125997341	-1.3516255105	-0.6719051374
C	0.8268844843	-2.3386164366	0.2979845137
H	0.2399148118	-2.1568000239	1.1893707343
C	-0.2902779267	-0.0735097298	-2.9141727975
H	-0.5514716112	0.6030629322	-3.7286262146
H	-0.9879065579	-0.9190821837	-2.9678114487
C	1.4536846660	-1.6285477314	-2.0200581248
H	2.5400062202	-1.7370389245	-1.9064724151
H	1.0898086420	-2.6026344607	-2.3704961828
C	1.1438517411	-0.5782454849	-3.0858181090
H	1.8259907561	0.2741243977	-2.9969733179
H	1.2956638311	-1.0076172985	-4.0806821032
H	3.0845058427	-8.4281320943	1.3319510706
C	2.3990888396	-7.9896803260	2.0480891289
C	0.6204121573	-6.8782889783	3.9318550727
C	1.8844844472	-6.7127415001	1.8977703260
C	2.0021307136	-8.7113355241	3.1727626694
C	1.1240690992	-8.1679700780	4.1049002583
C	1.0073290794	-6.1541445680	2.8199848081
H	2.3878805701	-9.7147312276	3.3184980069
H	0.8299604131	-8.7500898007	4.9713478132
H	-0.0648914831	-6.4572951118	4.6617705237
C	0.6358991343	-4.7524707727	2.3788748982
C	1.4292129195	-4.6249084337	1.0732594884
C	1.4975934691	-3.5699543543	0.1828022024
H	2.1250634774	-3.7090486227	-0.6882119366
N	2.1134268733	-5.7764467592	0.8661335883
N	-0.2113399781	0.2668292723	0.8328254653
C	0.7922926290	0.2317575172	1.9047404390
H	1.7178597836	-0.1484334402	1.4741769918
H	0.4935288408	-0.4677011859	2.6933311880
C	-1.5451908507	0.7562299079	1.2067892088
H	-2.1710105679	0.7128664723	0.3164594336
H	-1.5017004093	1.8059414649	1.5179077940
C	1.0428084997	1.6076682352	2.5156873536
H	1.3285100847	2.3329244994	1.7475662607
H	1.8617511101	1.5403739204	3.2375236241
H	0.1703085085	1.9939743470	3.0494245636
C	-2.1829049817	-0.0738438017	2.3179539513
H	-1.6510962974	0.0197219872	3.2685950591
H	-2.2209954404	-1.1327634611	2.0441206309
H	-3.2082239789	0.2689347590	2.4833265570
C	2.9727943826	-6.0118809786	-0.2761575147

H	3.8018357153	-5.2980687745	-0.2876459092
H	2.4069462126	-5.9160573850	-1.2075484152
H	3.3802667518	-7.0187797127	-0.2209019785
C	-0.8799787884	-4.6497806488	2.1344742848
H	-1.4160568992	-4.8678738836	3.0624935416
H	-1.2065527532	-5.3698443386	1.3798913762
H	-1.1717354387	-3.6506107359	1.8019804868
C	1.1035262085	-3.7299207154	3.4301701312
H	2.1825653360	-3.7959448649	3.5914921148
H	0.6071733074	-3.9337381833	4.3830809285
H	0.8630507264	-2.7055361834	3.1374183992
C	0.5335280672	5.0350683387	-0.6932832991
H	1.2000300784	5.2451951742	-1.5335255780
H	0.7903540597	4.0514497818	-0.2929289442
H	0.7273667448	5.7781207969	0.0854527736
C	-1.8881923943	4.8159457458	0.0512003204
H	-1.7020146242	3.8333306910	0.4907319565
H	-2.9332663476	4.8563012280	-0.2664935789
H	-1.7449526131	5.5669517510	0.8331980492

Cyanine-like S₁ minimum

H	-2.4484752646	7.4003298605	-4.7331659734
C	-2.1293321189	7.4961712208	-3.7018912937
C	-1.2889619137	7.7796976982	-1.0213244276
C	-1.7365951501	6.3995248964	-2.9406497613
C	-2.0931003598	8.7447460964	-3.0914193347
C	-1.6788564273	8.8924441142	-1.7682624496
C	-1.3176902700	6.5325973161	-1.6143366888
H	-2.3913689260	9.6191350056	-3.6601248982
H	-1.6583428622	9.8789565693	-1.3180795934
H	-0.9666183841	7.8999447906	0.0087199016
N	-1.6769962572	5.0527846975	-3.2999487650
C	-1.2102346672	4.2763061515	-2.2730033953
C	-0.9604231850	5.1700835217	-1.0585373223
H	-1.1617916145	4.1647500364	-5.1365313202
C	-2.0421787265	4.5387237832	-4.6025042114
H	-2.7670222745	3.7257802009	-4.4996404304
H	-2.4975058770	5.3322732324	-5.1911827931
C	-1.0072535055	2.9170841909	-2.4224931242
H	-1.2146702351	2.5026209697	-3.4019451466
C	-0.5608567067	2.0228464188	-1.4243343511
H	-0.4407918250	2.4018758845	-0.4165256751
C	-0.2380655341	0.6849310697	-1.6106512190
C	0.1128071452	-0.1479206706	-0.4922488272
C	0.7553686906	-1.4009098379	-0.7036162291
C	0.7728384623	-2.3704701673	0.3051775545
H	0.2192902862	-2.1435900079	1.2074716713
C	-0.1221792797	0.0577318874	-2.9744774493
H	-0.2332120029	0.8014480177	-3.7652195462
H	-0.9101935693	-0.6924126571	-3.1268347566
C	1.3685393215	-1.7301035787	-2.0487015363
H	2.4232735757	-2.0052867225	-1.9220713816
H	0.8711853677	-2.6288581683	-2.4381423128
C	1.2483509656	-0.6115978766	-3.0795657388

H	2.0222239776	0.1463006173	-2.9143688961
H	1.4066576990	-1.0166422025	-4.0835206393
H	3.0422589304	-8.4580622038	1.3978786751
C	2.3847971866	-8.0006919811	2.1282345327
C	0.6663059958	-6.8412394864	4.0450103576
C	1.8731554685	-6.7174043250	1.9681379512
C	2.0175603427	-8.6967136243	3.2748334657
C	1.1698473687	-8.1302931860	4.2256014074
C	1.0207763306	-6.1376847259	2.9101664447
H	2.3997295185	-9.7004593130	3.4278036308
H	0.9004388445	-8.6964532392	5.1106583880
H	0.0054636003	-6.4049596802	4.7882625473
C	0.6389789552	-4.7448187506	2.4546515481
C	1.3878369432	-4.6472829259	1.1274210419
C	1.4174136680	-3.6147161844	0.2017141768
H	1.9977505854	-3.7931504137	-0.6957367416
N	2.0783294885	-5.8085906971	0.9263165300
N	-0.1955658834	0.2791492509	0.7980014734
C	0.8084714758	0.3236229487	1.8587661223
H	1.6597558336	-0.2902798822	1.5604349751
H	0.3995473684	-0.1269679576	2.7722595759
C	-1.5691280815	0.6063890934	1.1767470621
H	-2.1076920855	0.9398696465	0.2876898841
H	-1.5546360587	1.4533805147	1.8727452134
C	1.2885030360	1.7436959042	2.1528290255
H	1.7655385972	2.1769823221	1.2684787681
H	2.0208439361	1.7385667377	2.9662791489
H	0.4646135602	2.3982683032	2.4538663051
C	-2.3119537915	-0.5700126205	1.8072440529
H	-1.8073119895	-0.9308646908	2.7094694601
H	-2.3888712306	-1.4011989086	1.0994991676
H	-3.3261017296	-0.2730235837	2.0923465066
C	2.9166347541	-6.0631966800	-0.2263761090
H	3.6844026197	-5.2890203866	-0.3163043020
H	2.3202913282	-6.0810429472	-1.1444053478
H	3.4084238497	-7.0264626275	-0.1115814835
C	-0.8861176191	-4.6376401720	2.2590998652
H	-1.3920444686	-4.8339230323	3.2089001644
H	-1.2414566471	-5.3692187698	1.5289975457
H	-1.1793133895	-3.6421960035	1.9182207758
C	1.1369138831	-3.6976839414	3.4711022634
H	2.2175111234	-3.7729857680	3.6165959511
H	0.6526324390	-3.8678549595	4.4369966711
H	0.9037894241	-2.6799792343	3.1499670180
C	0.5139475252	5.1372325827	-0.6126105718
H	1.1799928148	5.3923565307	-1.4405808353
H	0.7994330770	4.1532794092	-0.2344249376
H	0.6724896533	5.8664111777	0.1871260485
C	-1.8991515368	4.8194804617	0.1143015804
H	-1.6855533728	3.8302998566	0.5261890056
H	-2.9457034647	4.8422132106	-0.2000229282
H	-1.7715927379	5.5535736252	0.9151483346

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Bis-dipole Franck-Condon point

H	-0.0788502215	8.6143485034	-1.0769606899
C	0.2641587630	8.1868941755	-0.1417019097
C	1.1685372162	7.1107609009	2.2991468835
C	0.1069894603	6.8438753881	0.1602564042
C	0.8893403968	8.9920092272	0.8099558164
C	1.3380726772	8.4671001532	2.0168638923
C	0.5510807867	6.3040131680	1.3626629008
H	1.0256538771	10.0475232758	0.5989792850
H	1.8217472689	9.1135705973	2.7409036312
H	1.5198840178	6.7014463230	3.2420653256
N	-0.4809563032	5.8219020719	-0.6085960561
C	-0.4390952078	4.6175537813	0.0349517111
C	0.2347372230	4.8212467379	1.4002714828
H	-0.9766252048	7.0555999917	-2.2071297147
C	-1.0513425080	6.0079101161	-1.9234548329
H	-0.5173762765	5.4075348515	-2.6675647527
H	-2.1079644053	5.7217327238	-1.9305069806
C	-0.9307764317	3.4730203131	-0.5376141713
H	-1.3542978980	3.5687082617	-1.5285252467
C	-0.9382237968	2.1782516964	0.0566426106
H	-0.5826885111	2.1248177836	1.0768748289
C	-1.2848470556	1.0001348440	-0.5450775956
C	-1.1767954100	-0.2791695116	0.1558689888
C	-0.5752033325	-1.3922813490	-0.5641059433
C	0.2781078020	-2.2430255499	0.0927334597
H	0.4600725466	-2.0375307980	1.1406440131
C	-1.6239987459	0.9007375204	-2.0178237262
H	-1.5413898044	1.8785842222	-2.4923980300
H	-2.6684455087	0.5836719593	-2.1424203137
C	-0.8000040966	-1.4634182552	-2.0603682554
H	-0.0706691776	-2.1340310946	-2.5168973263
H	-1.7889449691	-1.8975328330	-2.2633651418
C	-0.7103314979	-0.0940909985	-2.7268649122
H	0.3226488323	0.2688879153	-2.6845584377
H	-0.9845642650	-0.1744060641	-3.7834520382
H	4.3944203142	-7.3039890220	-0.8184518946
C	4.3764661314	-6.7980145992	0.1400092908
C	4.3562531388	-5.5076892436	2.6445464235
C	3.5327604301	-5.7304099647	0.3990643861
C	5.2214122340	-7.2136135309	1.1685188392
C	5.2161857428	-6.5807555422	2.4067523350
C	3.5151019808	-5.0874580308	1.6318894318
H	5.8933372678	-8.0472676841	0.9935938065
H	5.8832020683	-6.9221958909	3.1907352721
H	4.3538455724	-5.0145955742	3.6124249217
C	2.4910784698	-3.9695945662	1.6052801717
C	1.9518152369	-4.0834593804	0.1718733662
C	0.9982981390	-3.3298726023	-0.4695217076
H	0.7760891165	-3.5971074081	-1.4941609526
N	2.5920273290	-5.1136678781	-0.4495969767
N	-1.6269233341	-0.4341780493	1.4062545248

C	-2.2937722337	0.6274899252	2.1963852653
H	-2.8948579530	1.2399472146	1.5204223390
C	-1.8879861814	-1.7396450634	2.0507193367
H	-1.1117109271	-1.9548326109	2.7937865041
H	-1.8786356045	-2.5299820944	1.3032723670
H	-1.5535222849	1.2769899907	2.6666121771
C	2.3374542048	-5.5095833754	-1.8170481004
H	2.5411533978	-4.6811011251	-2.5029864603
H	1.2970474310	-5.8259977684	-1.9420657712
H	2.9860084737	-6.3424162606	-2.0801424426
C	-0.7282770000	4.5254290430	2.5635101758
H	-0.9856172891	3.4652128528	2.6226965642
H	-1.6546855988	5.0963284804	2.4616661389
H	-0.2595549361	4.8094243883	3.5100360540
C	1.5313927381	4.0031970224	1.5260159605
H	2.2123477456	4.2207153662	0.6993318450
H	1.3388308357	2.9274739899	1.5333420433
H	2.0408062084	4.2614482074	2.4589431917
C	3.1758660773	-2.6145679329	1.8540319320
H	3.9556709316	-2.4277237108	1.1113631399
H	3.6455482111	-2.6161357192	2.8419388042
H	2.4667087180	-1.7839274134	1.8194074118
C	1.3929831319	-4.2415131016	2.6492507171
H	1.8382077645	-4.2901043571	3.6469851339
H	0.8941311116	-5.1946064428	2.4559591379
H	0.6365032288	-3.4538379430	2.6570687723
C	-3.2366787213	-1.5340600593	2.7252180591
C	-3.1299137247	-0.1059334919	3.2543745843
H	-3.4218177379	-2.2712320841	3.5089430979
H	-4.0372237626	-1.6171846242	1.9835435677
H	-4.1002693498	0.3717983362	3.4006447143
H	-2.6105869825	-0.0979207203	4.2171673422

Bis-dipole S₁ minimum

H	-0.1939757702	8.6536866392	-1.0157902563
C	0.1956146783	8.2244210241	-0.1000405494
C	1.2241767923	7.1390600281	2.2938122459
C	0.0905421767	6.8693244724	0.1906468647
C	0.8286928206	9.0327883490	0.8389577016
C	1.3367917276	8.5034676215	2.0237745945
C	0.5993607007	6.3245622540	1.3694881030
H	0.9263736911	10.0948775614	0.6408070219
H	1.8233294661	9.1566105098	2.7399137389
H	1.6236251210	6.7300859781	3.2171488560
N	-0.4963077111	5.8451856252	-0.5625224169
C	-0.3969001073	4.6354994200	0.0655133125
C	0.3468709294	4.8315645666	1.3882931411
H	-1.0605533546	7.0853807001	-2.1357309784
C	-1.1218891407	6.0367289977	-1.8541948962
H	-0.6134146245	5.4403375198	-2.6180109768
H	-2.1763525477	5.7457835341	-1.8185577385
C	-0.8984081644	3.4817389761	-0.5008756986
H	-1.3988015985	3.5884497015	-1.4556114125
C	-0.8206182701	2.1716675077	0.0422626149

H	-0.3545602069	2.0580496152	1.0139343169
C	-1.3048120479	1.0255370580	-0.5433766101
C	-1.2113102803	-0.2787364121	0.1401266357
C	-0.4448678082	-1.2770408709	-0.5457182243
C	0.3811590008	-2.1586286354	0.1370155352
H	0.5225522541	-1.9633933124	1.1932596433
C	-1.7463507156	0.9252511066	-1.9744260769
H	-1.8210807046	1.9015876937	-2.4575319817
H	-2.7348785127	0.4519057445	-2.0326132856
C	-0.5737746348	-1.3223411481	-2.0597610682
H	0.2920812654	-1.8259824813	-2.4966107806
H	-1.4524283401	-1.9299318766	-2.3200066892
C	-0.7193368013	0.0529825595	-2.7141865130
H	0.2473562604	0.5689897485	-2.7028938534
H	-1.0123148848	-0.0624980703	-3.7626103553
H	4.3205625126	-7.3647480864	-0.8171040539
C	4.3225506870	-6.8636253193	0.1441242981
C	4.3597486959	-5.5798421751	2.6538010942
C	3.5034721986	-5.7750332726	0.4148335203
C	5.1673513855	-7.3017374345	1.1610260328
C	5.1914655947	-6.6725773326	2.4026201954
C	3.5170532342	-5.1348560966	1.6538525416
H	5.8178430488	-8.1505177308	0.9766740756
H	5.8603481818	-7.0318243862	3.1771633161
H	4.3812533442	-5.0899955875	3.6231396916
C	2.5233378649	-3.9907069450	1.6427668526
C	1.9718081833	-4.0808445312	0.2172521785
C	1.0528959757	-3.2749389484	-0.4192809235
H	0.8260638391	-3.5207810880	-1.4500208350
N	2.5731369276	-5.1377650515	-0.4154634841
N	-1.7281023511	-0.4474426614	1.3942099958
C	-2.5802570982	0.5712328772	2.0314409837
H	-3.3190389839	0.9422377542	1.3106951780
C	-2.0106699461	-1.7777959792	1.9615718983
H	-1.2236156929	-2.0742088565	2.6651562497
H	-2.0433462330	-2.5232375503	1.1650672073
H	-1.9953043156	1.4283633147	2.3720322339
C	2.2837054687	-5.5299199059	-1.7758825852
H	2.5346630687	-4.7245264589	-2.4745672656
H	1.2226469126	-5.7759653584	-1.8875938067
H	2.8721802489	-6.4077515790	-2.0343667596
C	-0.5139665965	4.4492992369	2.6059983471
H	-0.7101579731	3.3755202339	2.6433901676
H	-1.4717629511	4.9756439243	2.5940337931
H	0.0115521813	4.7242623203	3.5248583439
C	1.6890094638	4.0719055563	1.3996914549
H	2.3007191035	4.3449535800	0.5362205514
H	1.5441189069	2.9892846742	1.3896040832
H	2.2464066004	4.3313322086	2.3041247117
C	3.2449379965	-2.6541175680	1.8959460022
H	4.0283604391	-2.4858776141	1.1525746812
H	3.7147875519	-2.6713208671	2.8838127114
H	2.5551625758	-1.8077133151	1.8629953933

C	1.4249659711	-4.2321763810	2.6958696264
H	1.8731291218	-4.2750963054	3.6928397228
H	0.9103967882	-5.1792891517	2.5151472360
H	0.6825739369	-3.4311834570	2.6931283111
C	-3.3389622378	-1.6004239274	2.6911573500
C	-3.2534009115	-0.1610017896	3.1919956094
H	-3.4734756126	-2.3310567709	3.4918045862
H	-4.1721381841	-1.7108588380	1.9892514547
H	-4.2240731213	0.2737157445	3.4392222825
H	-2.6269665268	-0.1083348086	4.0883417298
Cyanine-like Franck-Condon point			
H	8.8108258670	-0.5040163616	2.8121686602
C	8.5154400847	-0.2616323177	1.7978357994
C	7.7838552654	0.3709967033	-0.8503648442
C	7.1896795799	-0.1199099218	1.4232201651
C	9.4823782828	-0.0785518090	0.8104247837
C	9.1268062121	0.2337646443	-0.4976134201
C	6.8170221233	0.1925706939	0.1211518169
H	10.5298889565	-0.1825548077	1.0725995495
H	9.8979865086	0.3717614945	-1.2474952914
H	7.5100674908	0.6146971238	-1.8727347522
N	6.0228379914	-0.2477667979	2.2088207806
C	4.9021163174	-0.0270127765	1.4813177913
C	5.3063476698	0.2717613986	0.0325712315
H	5.5683148485	0.2523554090	4.1976722265
C	6.0194916388	-0.5623244830	3.6232682754
H	5.4589511936	-1.4829649252	3.8093345489
H	7.0422978232	-0.7034666513	3.9652014282
C	3.6412771374	-0.0731129033	2.0488206860
H	3.5887148347	-0.2853629416	3.1095693865
C	2.4285596037	0.1487833109	1.3751302798
H	2.4566870345	0.3043735058	0.3035444166
C	1.1846357399	0.2434960376	1.9757198198
C	0.0432642575	0.5096590008	1.1630708804
C	-1.1154297610	1.1108434449	1.7399578716
C	-2.3280501886	1.0301815823	1.0824390679
H	-2.3236265731	0.4530183502	0.1655006409
C	1.0737383681	0.2248477069	3.4871058342
H	1.7868935278	0.9555339140	3.8902269865
H	1.3927957315	-0.7507777514	3.8756079890
C	-0.9653849778	1.6466827759	3.1420191840
H	-0.3353688219	2.5457609077	3.1541923329
H	-1.9313455025	1.9340054168	3.5606381552
C	-0.3244182447	0.5582544411	4.0065667918
H	-0.2623936972	0.8760678802	5.0516933642
H	-0.9646199935	-0.3303448906	3.9804998455
H	-8.6791181929	2.6819038475	1.4860400590
C	-8.3516146477	2.0123563839	0.6990459466
C	-7.5367873295	0.2624108402	-1.3549531629
C	-7.0282668488	1.6311450463	0.5508370833
C	-9.2725745901	1.4965964074	-0.2117319120
C	-8.8759065369	0.6329033716	-1.2273382102
C	-6.6156648301	0.7672852547	-0.4567717608

H	-10.3167860995	1.7764336579	-0.1212653766
H	-9.6115597428	0.2446399383	-1.9231746339
H	-7.2303221951	-0.4125583758	-2.1487369243
C	-5.1193350114	0.5481882443	-0.3547361344
C	-4.7707065815	1.4032886879	0.8704091823
C	-3.5519531126	1.5896893321	1.4933416771
H	-3.5432856008	2.2252537711	2.3699528999
N	-5.9036871536	1.9985581255	1.3203807460
N	0.0734315032	0.2179585186	-0.1870422720
C	-0.1972780781	1.2004597392	-1.2525756911
H	-1.0996154180	1.7835980372	-1.0689923211
C	0.4521745979	-1.0907467634	-0.7500848092
H	-0.3832855562	-1.7942224016	-0.6269585790
H	1.3180713452	-1.5278919779	-0.2526669309
H	0.6404869898	1.9098627279	-1.3150958870
C	-5.9512051919	2.8889115178	2.4615865944
H	-6.9582978877	3.2856876671	2.5692147027
H	-5.2625751340	3.7268500038	2.3207021501
H	-5.6837992298	2.3579484089	3.3805848413
C	4.7810055134	-0.8040611060	-0.9356986563
H	3.6907951226	-0.7962851743	-1.0023795917
H	5.0979740747	-1.8026857547	-0.6243844834
H	5.1818117597	-0.6204239198	-1.9365759266
C	4.8677248937	1.6811374431	-0.4022018059
H	5.2336723460	2.4392074536	0.2949096506
H	3.7807023279	1.7694154059	-0.4625299011
H	5.2806367664	1.9051292798	-1.3899095767
C	-4.4287121946	1.0688555713	-1.6289742019
H	-4.6366138701	2.1307065257	-1.7839553378
H	-4.8076762158	0.5225024221	-2.4972939102
H	-3.3455035700	0.9327235399	-1.5932540558
C	-4.8117929897	-0.9408781074	-0.1200966765
H	-5.1861106891	-1.5282599535	-0.9633461578
H	-5.3006272287	-1.3048082295	0.7871694140
H	-3.7392697412	-1.1269491997	-0.0282909936
C	0.6936243091	-0.7951891322	-2.2286951923
H	0.5317654669	-1.6727183001	-2.8581453372
H	1.7238618800	-0.4557936006	-2.3852208133
C	-0.2821575152	0.3480312765	-2.5160712078
H	-1.2968134314	-0.0480342678	-2.6363414637
H	-0.0356028100	0.9148614133	-3.4163173344

Cyanine-like S₁ minimum

H	8.8374019483	-0.5097944766	2.8248571490
C	8.5482131574	-0.2702379337	1.8080813653
C	7.8297944575	0.3647040051	-0.8476738840
C	7.2182491157	-0.1289990760	1.4261845268
C	9.5179620708	-0.0863110235	0.8280735732
C	9.1704544243	0.2269151713	-0.4852725226
C	6.8553635169	0.1868104907	0.1150418108
H	10.5644217741	-0.1881056638	1.0957779978
H	9.9472108627	0.3652763862	-1.2295788674
H	7.5634023623	0.6097922272	-1.8716355648
N	6.0582602125	-0.2551308154	2.1962240555

C	4.9347825438	-0.0204013581	1.4567377230
C	5.3471919244	0.2716196938	0.0150155688
H	5.6360019579	0.2535925846	4.1916252625
C	6.0424290292	-0.5787882323	3.6075686177
H	5.4316562893	-1.4689892059	3.7862844586
H	7.0562245789	-0.7798585412	3.9464233217
C	3.6696098614	-0.0357648344	2.0249063777
H	3.6206158832	-0.2179988699	3.0924834124
C	2.4534833850	0.1831121343	1.3571681459
H	2.4612205258	0.3044896686	0.2812052773
C	1.2105759254	0.3164498837	1.9818278932
C	0.0435786596	0.5130816281	1.1909007601
C	-1.1533933080	1.0431423509	1.7730389931
C	-2.3549498861	0.9783936238	1.0768288975
H	-2.3234877047	0.4273218513	0.1447683821
C	1.1281499319	0.3450841280	3.4919321865
H	1.7612147809	1.1661743458	3.8556915662
H	1.5623254897	-0.5725752687	3.9086903296
C	-1.0470236811	1.5604599091	3.1832970452
H	-0.5111803963	2.5195862696	3.2066226664
H	-2.0338010867	1.7385224179	3.6146136846
C	-0.2898486894	0.5324959304	4.0264382198
H	-0.2519384811	0.8456746127	5.0740561491
H	-0.8341887635	-0.4177809630	3.9949642436
H	-8.7041695105	2.6991461059	1.4960086277
C	-8.3842623861	2.0304327307	0.7053540514
C	-7.5868366643	0.2781268400	-1.3598131847
C	-7.0572392635	1.6397690071	0.5524383681
C	-9.3092352636	1.5239165161	-0.2011603548
C	-8.9228611859	0.6578892811	-1.2234983578
C	-6.6564010810	0.7720767967	-0.4665575222
H	-10.3517326560	1.8089005800	-0.1061959319
H	-9.6654535497	0.2768509535	-1.9161742253
H	-7.2900725121	-0.3973836223	-2.1566993826
C	-5.1631475343	0.5392168753	-0.3743768539
C	-4.8044916086	1.3783616897	0.8515910463
C	-3.5835826948	1.5398522206	1.4821109675
H	-3.5753825198	2.1614519428	2.3698896671
N	-5.9393506077	1.9893199212	1.3118430148
N	0.0705458554	0.2184550706	-0.1688348531
C	-0.1429510372	1.2192912181	-1.2192012987
H	-1.0300342772	1.8296709141	-1.0286614176
C	0.4104048484	-1.0976814845	-0.7221665441
H	-0.4332060784	-1.7919074295	-0.5941658433
H	1.2748314317	-1.5460048861	-0.2248562004
H	0.7151761391	1.9068825917	-1.2761892535
C	-5.9692625794	2.8792151243	2.4529978318
H	-6.9726265988	3.2807204000	2.5759846042
H	-5.2763276178	3.7131970680	2.3040291135
H	-5.6907317908	2.3459390472	3.3680894723
C	4.8201351208	-0.7993295458	-0.9619435559
H	3.7294844595	-0.7918198984	-1.0220587657
H	5.1404325935	-1.7998171572	-0.6602386153

H	5.2153925652	-0.6053496226	-1.9634326200
C	4.9142417602	1.6828822184	-0.4274397897
H	5.2904811120	2.4424976400	0.2623696200
H	3.8272079357	1.7753345758	-0.4779990283
H	5.3195980510	1.8970254952	-1.4205747952
C	-4.4699878952	1.0588778485	-1.6508735956
H	-4.6770660250	2.1206580345	-1.8073871517
H	-4.8463399953	0.5100820634	-2.5191593874
H	-3.3869648693	0.9220905716	-1.6093769370
C	-4.8630538763	-0.9562136006	-0.1557440287
H	-5.2307503319	-1.5321577703	-1.0098661604
H	-5.3604740835	-1.3288742287	0.7431842409
H	-3.7915882944	-1.1435663178	-0.0571958939
C	0.6611721698	-0.8112084023	-2.2026331970
H	0.4586425702	-1.6777532198	-2.8359816510
H	1.7062520351	-0.5204187263	-2.3601485257
C	-0.2576695349	0.3802202542	-2.4901528875
H	-1.2892038177	0.0332947283	-2.6199059950
H	0.0219464418	0.9384865266	-3.3863456529

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Bis-dipole Franck-Condon Point

H	0.3185552181	8.4650419556	-0.9912417798
C	0.5761978977	7.9989264164	-0.0470323213
C	1.2584657723	6.8235201963	2.4195157007
C	0.3229424465	6.6614759404	0.2120407489
C	1.1838491590	8.7469797336	0.9610217381
C	1.5237640013	8.1729953935	2.1808001183
C	0.6562801588	6.0733451311	1.4279085560
H	1.3930064399	9.7968428829	0.7840347778
H	1.9959709358	8.7752645584	2.9491869960
H	1.5241330894	6.3759703458	3.3731054906
N	-0.2731750850	5.6930432600	-0.6157600295
C	-0.3502937656	4.4760140142	0.0049358467
C	0.2506131303	4.6116365528	1.4128757524
H	-0.5752706639	6.9785797467	-2.2206282009
C	-0.7472794082	5.9367025456	-1.9584294401
H	-0.2160454627	5.3054857848	-2.6786573074
H	-1.8203867469	5.7324167423	-2.0338776929
C	-0.8900054350	3.3797187666	-0.6111031377
H	-1.2572650063	3.5138978701	-1.6204673590
C	-1.0228081855	2.0816818858	-0.0323387214
H	-0.6927823693	1.9823184073	0.9965297999
C	-1.4787150144	0.9493068105	-0.6374573641
C	-1.4327739432	-0.3240170311	0.0957597865
C	-0.7457176596	-1.4197989274	-0.5837200522
C	0.1708621639	-2.2022604725	0.0668260349
H	0.3530484402	-1.9815989559	1.1102497657
C	-1.8119430070	0.8490107875	-2.1075487539
H	-1.7093747879	1.8228263400	-2.5876741231
H	-2.8604329247	0.5479709625	-2.2371889313
C	-0.9942761316	-1.5213348205	-2.0788837867
H	-0.2816931555	-2.2130328461	-2.5290228170

H	-1.9903118174	-1.9517508519	-2.2525262578
C	-0.9051866653	-0.1726794009	-2.7900075649
H	0.1290620616	0.1879114866	-2.7644553464
H	-1.1852463779	-0.2883680625	-3.8419510443
H	4.5796307096	-7.0174703704	-0.8212779299
C	4.5166946200	-6.5231589781	0.1413608324
C	4.3807725544	-5.2627156018	2.6570314899
C	3.6142745937	-5.5026219179	0.3928919450
C	5.3609035727	-6.9066010598	1.1829409290
C	5.2987435605	-6.2884156978	2.4269305630
C	3.5397923427	-4.8748378349	1.6315425630
H	6.0776392817	-7.7033156369	1.0137199815
H	5.9661133325	-6.6043979044	3.2212149414
H	4.3336970828	-4.7807210204	3.6294024003
C	2.4620652055	-3.8086800017	1.5950498948
C	1.9515245023	-3.9391216930	0.1520553150
C	0.9671006526	-3.2369851330	-0.4974412711
H	0.7759142944	-3.5086018005	-1.5269904022
N	2.6597340211	-4.9269336906	-0.4680391605
N	-1.9940329615	-0.4496993363	1.2985198744
C	-2.9083473324	0.5658890463	1.8848611378
H	-3.9287159449	0.2726582133	1.6133339659
C	-1.9630300827	-1.7142792297	2.0709126691
H	-1.0449431149	-1.7409227707	2.6680984001
H	-1.9198189651	-2.5424884661	1.3625263522
H	-2.7247675456	1.5315469351	1.4359426541
C	2.4504604853	-5.3215922561	-1.8430772055
H	2.6236109502	-4.4772592977	-2.5181327958
H	1.4298981360	-5.6894252807	-1.9902611166
H	3.1448800521	-6.1180759845	-2.1019000580
C	-0.7959514742	4.3522334423	2.5115520214
H	-1.1030775452	3.3036559595	2.5481071990
H	-1.6865545469	4.9665935389	2.3567996155
H	-0.3748953428	4.6093425339	3.4877696680
C	1.4867520080	3.7148457895	1.5972842346
H	2.2247263493	3.8998611168	0.8126117281
H	1.2289175926	2.6529817999	1.5773485626
H	1.9581331861	3.9300393527	2.5607423296
C	3.0770221170	-2.4232188873	1.8593952319
H	3.8544446939	-2.1944089247	1.1260900555
H	3.5354360775	-2.4075551248	2.8524786303
H	2.3284764194	-1.6277973618	1.8209853601
C	1.3651192721	-4.1387387950	2.6229164554
H	1.7999694439	-4.1758626912	3.6257867457
H	0.9118261322	-5.1117000786	2.4163354168
H	0.5727279131	-3.3868372952	2.6290415442
C	-3.1575635454	-1.8465548983	3.0074092901
H	-3.0896740673	-2.8227721143	3.4957508703
H	-4.0836567465	-1.8634711040	2.4236874025
C	-2.7631618621	0.6166158125	3.4002888035
H	-3.3714911296	1.4437276017	3.7762602141
H	-1.7234303814	0.8606377438	3.6460548226
C	-3.1823978929	-0.7194021124	4.0463885487

H	-4.1844743212	-0.6418232555	4.4768213969
H	-2.5078936546	-0.9599384283	4.8736388024
Bis-dipole S₁ minimum			
H	-0.5463447582	8.7038273515	-1.2206936985
C	0.0577703054	8.3167858327	-0.4086459438
C	1.6599761808	7.3339431429	1.7010782268
C	0.0330631774	6.9829753280	-0.0281780977
C	0.9096306849	9.1606198422	0.2970834640
C	1.7015109936	8.6798011645	1.3384196805
C	0.8185171206	6.4853979918	1.0067785182
H	0.9571693255	10.2097939194	0.0271346556
H	2.3587557714	9.3592458871	1.8695896739
H	2.2816237790	6.9654296607	2.5111229201
N	-0.7246685433	5.9214590908	-0.5652963301
C	-0.4511111196	4.7538809418	0.0538679253
C	0.5705767394	5.0015481001	1.1631054155
H	-1.8039212184	7.1299554577	-1.8734137145
C	-1.6602319330	6.0722752491	-1.6668916955
H	-1.2764433308	5.5836216011	-2.5667705038
H	-2.6263965092	5.6380918762	-1.4012044137
C	-1.0352909922	3.5569120599	-0.3511111815
H	-1.7155940913	3.6024713388	-1.1928212444
C	-0.8012048349	2.2943464033	0.2219587245
H	-0.1671419948	2.2311825983	1.0978023806
C	-1.3476893649	1.1079272046	-0.2189010566
C	-1.0317778898	-0.1804774460	0.4468258354
C	-0.1371548067	-1.0139082649	-0.2511210985
C	0.5689207226	-2.0315291156	0.3800806042
H	0.5197950198	-2.0419044224	1.4622480997
C	-1.9665929300	0.9041386466	-1.5574100308
H	-2.3677478368	1.8043705920	-2.0318505323
H	-2.7644708149	0.1571430863	-1.4997177203
C	-0.0836600264	-0.8772173717	-1.7715594921
H	0.9532549413	-0.9039019440	-2.1231623370
H	-0.5554691922	-1.7788682186	-2.1849323642
C	-0.7739755387	0.3537701975	-2.3899328192
H	-0.0511743841	1.1693135212	-2.4975436832
H	-1.1256660179	0.1113038804	-3.3974017625
H	4.6484109593	-7.0583814975	-0.9039017168
C	4.4404944450	-6.7854177742	0.1245237163
C	3.9199811534	-6.1101067473	2.8075764498
C	3.5839241559	-5.7454103239	0.4543288418
C	5.0384305533	-7.4877812278	1.1702924691
C	4.7860151746	-7.1606875223	2.4978116625
C	3.3226137940	-5.4060377464	1.7806009013
H	5.7128798604	-8.3054138726	0.9373331353
H	5.2617735172	-7.7226795297	3.2941251683
H	3.7222464074	-5.8539466512	3.8447705876
C	2.3548272156	-4.2390216461	1.8249082852
C	2.1216869122	-3.9791521310	0.3328594427
C	1.3439626820	-3.0231302995	-0.2695665365
H	1.3343225146	-3.0186082374	-1.3539875332
N	2.8610456890	-4.8895345220	-0.3877538853

N	-1.7424440935	-0.5682741396	1.5697082281
C	-2.3482657838	0.4300501314	2.4497031151
H	-3.1859068637	0.9482077010	1.9573339992
C	-2.2433091712	-1.9437735716	1.7100822429
H	-1.6706219134	-2.4941311195	2.4684389546
H	-2.0825764754	-2.4563778433	0.7609965198
H	-1.5980954286	1.1913670507	2.6871927576
C	2.8901432982	-4.9302881359	-1.8288059052
H	3.2473772910	-3.9784320489	-2.2375022134
H	1.8923765822	-5.1312147688	-2.2346698500
H	3.5624142765	-5.7201062707	-2.1585391420
C	-0.0228934501	4.7041691663	2.5549229835
H	-0.2343689558	3.6415883961	2.6895287268
H	-0.9475275148	5.2638327679	2.7171382285
H	0.6925646899	5.0052135697	3.3246360599
C	1.8750036644	4.2161367901	0.9278769231
H	2.2878782855	4.4228808447	-0.0629166019
H	1.7264454558	3.1389429280	1.0197493593
H	2.6171599084	4.5184558649	1.6712775911
C	3.0066822190	-3.0319062880	2.5220883236
H	3.9258880641	-2.7355175027	2.0100169343
H	3.2632433475	-3.2937754134	3.5529581450
H	2.3377818852	-2.1686867874	2.5475593380
C	1.0580719035	-4.6542314940	2.5433573522
H	1.2812393432	-4.9368104845	3.5764414243
H	0.5970037945	-5.5131228158	2.0492725950
H	0.3304306552	-3.8398436480	2.5640328583
C	-3.7209912600	-1.9387759346	2.0898100957
H	-4.0970316015	-2.9663963571	2.0998146359
H	-4.2764598054	-1.4109925410	1.3060495119
C	-2.8448933560	-0.2234910057	3.7351036953
H	-3.2071272478	0.5525128540	4.4157530735
H	-1.9915001441	-0.6997479065	4.2298340844
C	-3.9442231284	-1.2605890689	3.4532768604
H	-4.9286037564	-0.7824873832	3.4698232136
H	-3.9494267672	-2.0065310035	4.2537779902

Cyanine-like Franck-Condon Point

H	-0.2234359147	7.9225059394	-4.3912593911
C	-0.9130857608	7.7603076986	-3.5708820058
C	-2.7185097432	7.3767786772	-1.4402897117
C	-0.9717935218	6.5649240167	-2.8735969833
C	-1.7866237334	8.7736817190	-3.1789375489
C	-2.6804391639	8.5895560946	-2.1292052161
C	-1.8561680318	6.3658064970	-1.8200605123
H	-1.7639456209	9.7216158501	-3.7060834135
H	-3.3515509800	9.3924917726	-1.8444408427
H	-3.4177919338	7.2363760618	-0.6212742150
N	-0.2161222636	5.3866151358	-3.0582006437
C	-0.5650515535	4.4221456418	-2.1709074249
C	-1.6723043698	4.9688836073	-1.2617047735
H	0.8675723477	6.1241793357	-4.6747482342
C	0.7972353410	5.2168007238	-4.0790796111
H	1.7730715182	5.0196535897	-3.6252868209

H	0.5373621617	4.3852122241	-4.7407914769
C	0.0367174903	3.1785079557	-2.1770853604
H	0.8003564854	3.0130872745	-2.9262566945
C	-0.2434912258	2.1098847285	-1.3040614710
H	-0.9591831552	2.2759027419	-0.5099735809
C	0.2825537390	0.8361190249	-1.4165213533
C	-0.0730668551	-0.1756706385	-0.4677423779
C	0.0078984991	-1.5532589242	-0.8680119966
C	0.2991850550	-2.5250171018	0.0631569421
H	0.4329473533	-2.1835901631	1.0809661275
C	1.1108968536	0.4840920428	-2.6416178959
H	2.0844744723	0.9891071521	-2.5984172942
H	0.5986456617	0.8984437916	-3.5181954362
C	0.0915236639	-1.7898992693	-2.3546735764
H	0.1864265491	-2.8509559423	-2.5873468806
H	-0.8123524576	-1.4330919123	-2.8635128178
C	1.3119649366	-1.0181603477	-2.8633834715
H	2.1957674703	-1.3761155330	-2.3248834369
H	1.4866657319	-1.2105391948	-3.9264127561
H	1.8770626329	-8.8769496660	0.7280175574
C	2.0124987742	-8.2028988916	1.5661223364
C	2.3809464988	-6.4796418549	3.7650586885
C	1.6849643704	-6.8587235007	1.4981662374
C	2.5353753405	-8.6759510415	2.7688937752
C	2.7187671963	-7.8303411852	3.8577100832
C	1.8639555829	-5.9998914882	2.5765278222
H	2.8034173066	-9.7240789529	2.8506619657
H	3.1273910529	-8.2219359676	4.7828027270
H	2.5271879139	-5.8212873935	4.6164754620
C	1.4177977867	-4.6030647764	2.1918487470
C	0.9793278764	-4.8147344361	0.7358601625
C	0.5072585820	-3.9008104142	-0.1807183351
H	0.2954342934	-4.2709067249	-1.1756068079
N	1.1489595689	-6.1262167117	0.4190817497
N	-0.4868052983	0.1546882191	0.7934999943
C	0.1358909131	1.2405255724	1.5748666065
H	-0.3937330207	2.1914709595	1.4557404825
C	-1.5754809092	-0.5753235430	1.4768319573
H	-1.2073039469	-1.4428138992	2.0338911473
H	-2.2592816301	-0.9512712771	0.7132077837
H	1.1499161017	1.3861675771	1.1984854649
C	0.8364786646	-6.6883959355	-0.8774518885
H	1.4644452940	-6.2427764254	-1.6557622246
H	-0.2146141904	-6.5151244223	-1.1263417512
H	1.0143847613	-7.7614528301	-0.8599728305
C	-2.9745323169	4.1611015624	-1.4000255216
H	-2.8647790144	3.1426130502	-1.0199205217
H	-3.2919231101	4.1033870395	-2.4442627885
H	-3.7709309554	4.6505744386	-0.8322892869
C	-1.2171998475	5.0466072202	0.2068327887
H	-0.2701743149	5.5841588920	0.2999196947
H	-1.0938939414	4.0543229215	0.6459569514
H	-1.9682615717	5.5822705847	0.7940975242

C	2.5966921021	-3.6198835739	2.2991839855
H	3.4305556613	-3.9351661949	1.6666523454
H	2.9520882958	-3.5862436792	3.3331256823
H	2.3108183296	-2.6066475554	2.0065205315
C	0.2442408690	-4.1650369903	3.0869098241
H	0.5578315056	-4.1851078715	4.1343715695
H	-0.6089770234	-4.8390949699	2.9764998348
H	-0.0881302441	-3.1496790626	2.8581460458
C	-2.2814011767	0.3555016427	2.4563553902
H	-3.1530226766	-0.1599856352	2.8695975855
H	-2.6657590663	1.2254128376	1.9119105338
C	0.1249296028	0.8723732759	3.0543586456
H	0.7028267743	1.6143864622	3.6126874792
H	0.6384067787	-0.0866070664	3.1874202690
C	-1.3213357743	0.7944828568	3.5766658617
H	-1.6355290388	1.7675211643	3.9662502655
H	-1.3731294378	0.0940934430	4.4158605683

Cyanine-like S₁ minimum

H	-0.4568018528	7.9781395612	-4.4031659099
C	-1.0832605870	7.8074433570	-3.5351533245
C	-2.7345797306	7.3963131153	-1.2824803274
C	-1.0864761558	6.6007738491	-2.8438983473
C	-1.9273816778	8.8117549104	-3.0730976159
C	-2.7456892274	8.6156288598	-1.9614177099
C	-1.8996143789	6.3899590702	-1.7282055286
H	-1.9465407007	9.7649049975	-3.5904514812
H	-3.3934559127	9.4166429227	-1.6227917231
H	-3.3750282819	7.2475690893	-0.4181769107
N	-0.3480432475	5.4392678253	-3.0880180775
C	-0.6366953434	4.4581751154	-2.1829797967
C	-1.6767936222	4.9890492954	-1.1983491148
H	0.6574346424	6.2112052452	-4.7392176233
C	0.5933543802	5.2824987539	-4.1767803597
H	1.5880168508	5.0387386258	-3.7910126013
H	0.2697962090	4.4845932893	-4.8530558689
C	-0.0388628104	3.2077244838	-2.2508311870
H	0.6575316326	3.0543414014	-3.0671871144
C	-0.2485273271	2.1226078715	-1.3848567924
H	-0.8994768444	2.2507350979	-0.5300735415
C	0.2818184531	0.8409291602	-1.5735486265
C	0.0457508095	-0.1811563794	-0.6153946646
C	0.2583233102	-1.5618502115	-0.9613365791
C	0.4667892902	-2.5068468190	0.0316394406
H	0.5186767121	-2.1196920018	1.0413117079
C	1.0347555217	0.5349320806	-2.8525488401
H	1.9065305439	1.1956750929	-2.9413356127
H	0.3818582285	0.7888981830	-3.6983208576
C	0.4079203615	-1.8596903918	-2.4289465894
H	0.6923569342	-2.8983851389	-2.6047289239
H	-0.5403211337	-1.6922195492	-2.9568895283
C	1.4790392254	-0.9208030280	-2.9896901586
H	2.4118456879	-1.0865932641	-2.4396616280
H	1.6816943272	-1.1469498612	-4.0411268287

H	1.8114210408	-8.9023419689	0.8806787081
C	1.9120921823	-8.2229357561	1.7190085293
C	2.1940790290	-6.4763809620	3.9191604618
C	1.6269809658	-6.8647475811	1.6132613318
C	2.3430012315	-8.6924533693	2.9545440749
C	2.4842404077	-7.8358605495	4.0459449308
C	1.7667257178	-5.9941075372	2.6976003247
H	2.5732172552	-9.7464125356	3.0679085501
H	2.8222313371	-8.2295860213	4.9981511177
H	2.3070386564	-5.8134208011	4.7719106800
C	1.3834038627	-4.5919449638	2.2722864772
C	1.0338667077	-4.8105156438	0.7998970300
C	0.6552718423	-3.8940912034	-0.1619639464
H	0.4967265483	-4.2791982405	-1.1624471658
N	1.1816195971	-6.1411601256	0.5074561695
N	-0.3971804501	0.1413510146	0.6626083539
C	0.3121889783	1.1057639938	1.5086524411
H	-0.0979229783	2.1225928138	1.4315281842
C	-1.6014573647	-0.4858588444	1.2250308420
H	-1.3976368993	-1.4679508276	1.6736759654
H	-2.3129881353	-0.6544083471	0.4116102886
H	1.3486431884	1.1578171535	1.1664018639
C	0.9122773029	-6.7158282114	-0.7933179012
H	1.6027778231	-6.3199892485	-1.5456988581
H	-0.1136312883	-6.4920988164	-1.1015440284
H	1.0315996096	-7.7958552702	-0.7458839200
C	-2.9863453036	4.1772693873	-1.2582639226
H	-2.8423847202	3.1531952768	-0.9062473771
H	-3.3779544419	4.1379079025	-2.2780682600
H	-3.7411501263	4.6514213941	-0.6245302348
C	-1.1285317277	5.0422969668	0.2416315505
H	-0.2019781873	5.6203096647	0.2903693217
H	-0.9292033318	4.0420641102	0.6318453619
H	-1.8625447796	5.5209516495	0.8962853223
C	2.5751471719	-3.6296614341	2.4467777494
H	3.4434970724	-3.9696802580	1.8769076623
H	2.8583048813	-3.5863868099	3.5025064004
H	2.3271751181	-2.6169839000	2.1206638485
C	0.1682126404	-4.1040769881	3.0872125763
H	0.4237650067	-4.0942057820	4.1507805313
H	-0.6907415533	-4.7658681004	2.9510175136
H	-0.1274228645	-3.0915267636	2.8030756437
C	-2.2044368927	0.4211513708	2.2924104470
H	-3.1414114707	-0.0168362055	2.6493137721
H	-2.4653873502	1.3826759469	1.8346768057
C	0.2364261497	0.6578667946	2.9653871888
H	0.8452278852	1.3234405515	3.5845962759
H	0.6853025297	-0.3394726617	3.0452678695
C	-1.2243941288	0.6313611274	3.4592065158
H	-1.4679354388	1.5655445551	3.9744286030
H	-1.3457656076	-0.1674545465	4.1980670217

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