Supplementary Material (ESI) for Chemical Science

[Supporting Information]

Symmetry and Polar-π Effects on the Dynamics of Enshrouded Aryl-Alkyne Molecular Rotors

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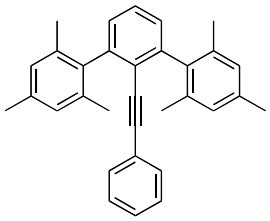
Experimental Details	Page 2-20
Computational Details	
B3LYP	Page 20-38
B97-D	Page 39-55
M-06	Page 56-72
Crystallographic ORTEP Plots	Page 73-82

Experimental Methods. General.

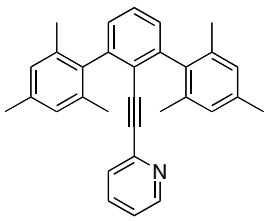
Data were collected on the following instruments: ^{1}H and ^{13}C NMR: Bruker AV 300 (300 and 75.5 MHz), Bruker AV2 400 (300 and 100 MHz). EI-MS: Finnegan MAT 95 spectrometer (70 eV). Crystallographic data were recorded using a Kappa CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å). Chromatography was performed using Merck silica gel 60 (230-400 mesh) or Fluka neutral alumina (Brockmann I, Activity II). Other compounds not mentioned in the experimental section are commercially available.



1-(2,6-bis-(2,4,6-trimethylphenyl)-2-phenylethyne (1a).

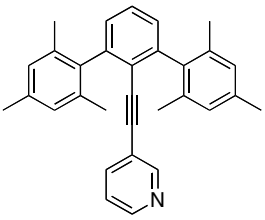
To an anhydrous solution of 2-bromomesitylene (700 mg, 3.6 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this mixture was added a solution of anhydrous zinc chloride (485 mg, 3.6 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **6a** (300 mg, 0.9 mmol) and palladium tetrakis(triphenylphosphine) (103 mg, 0.09 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 16 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with an aqueous saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (hexanes on silica) to give 250 mg (68%) of a yellow solid: mp = 168-170 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (t, *J* = 8 Hz, 1H), 7.16 (d, *J* = 8 Hz, 2H), 7.05 (m, 3H), 6.94 (s, 4H), 6.64 (d, *J* = 8 Hz, 2H), 2.38 (s, 6H), 2.06(s, 12H); ^{13}C NMR (150

MHz, $CDCl_3$) δ 144.48, 138.21, 136.70, 136.31, 131.54, 128.42, 128.08, 128.07, 127.96, 127.76, 123.90, 123.51, 94.47, 87.49, 21.33, 20.55; MS (EI) 414.1



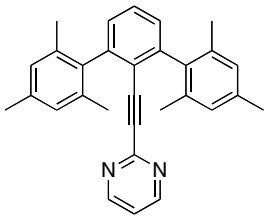
2-(2,6-di(2,4,6-trimethylphenyl)phenyl)-1-(pyridin-2-yl)ethyne (1b).

To an anhydrous solution of 2-bromomesitylene (1.4 g, 7.1 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this was added a solution of anhydrous zinc chloride (970 mg, 7.1 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **6b** (600 mg, 1.8 mmol) and palladium tetrakis(triphenylphosphine) (205 mg, 0.18 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 16 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (2:1 hexanes: methylene chloride on alumina) to give 100 mg (13%) of a white solid: mp = 193-195 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 3 Hz, 1H), 7.49 (t, *J*= 8 Hz, 1H), 7.37 (ddd, *J1* = *J2* = 1 Hz, *J3* = 5 Hz, 1H), 7.18 (d, *J* = 8 Hz, 2H), 7.01 (ddd, *J1* = *J2* =1 Hz, *J3*= 5 Hz, 1H), 6.97 (s, 4H), 6.42 (d, *J* = 8 Hz, 1H), 2.37 (s, 6H), 2.11 (s, 12H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.38, 144.91, 143.72, 137.67, 136.61, 135.93, 135.52, 129.04, 128.14, 128.11, 127.91, 122.20, 121.92, 93.47, 87.82, 21.09, 20.33; MS (EI) 415.1



2-(2,6-di(2,4,6-trimethylphenyl)phenyl)-1-(pyridin-3-yl)ethyne (1c).

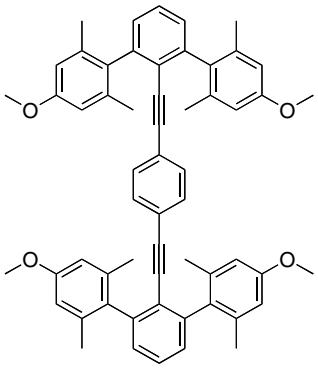
To an anhydrous solution of 2-bromomesitylene (955 mg, 4.8 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this was added a solution of anhydrous zinc chloride (650 mg, 4.8 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **6c** (400 mg, 1.2 mmol) and palladium tetrakis(triphenylphosphine) (140 mg, 0.12 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 16 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (methylene chloride on silica) to yield 120 mg (24%) of a white solid: mp = 306-308 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 (m, 1H), 7.84 (m, 1H), 7.49 (t, *J* = 7 Hz, 1H), 7.21 (d, *J* = 7 Hz, 2H), 7.06 (m, 1H), 6.98 (s, 4H), 6.95 (d, *J* = 8 Hz, 1H) 2.45 (s, 6H), 2.10 (s, 12H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 151.94, 147.63, 144.54, 138.02, 137.69, 136.77, 136.02, 128.88, 128.07, 127.98, 127.82, 122.57, 90.72, 90.63, 21.16, 20.39; MS (Hi-res EI) found: 415.2291 calcd: 415.2300



2-(2,6-di(2,4,6-trimethylphenyl))-1-(pyrimidin-2-yl)ethyne (1d).

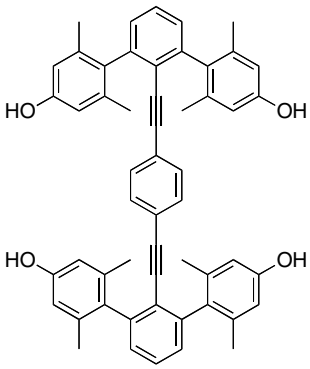
To an anhydrous solution of 2-bromomesitylene (870 mg, 4.4 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this was added a solution of anhydrous zinc chloride (600 mg, 4.4 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **6d** (370 mg,

1.1 mmol) and palladium tetrakis(triphenylphosphine) (126 mg, 0.11 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 16 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (methylene chloride on silica) to give 105 mg (23%) of a white solid: mp = 204-206 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5 Hz, 2H), 7.49 (t, *J* = 8 Hz, 1H), 7.18 (d, *J* = 8 Hz, 2H), 7.00 (t, *J* = 5 Hz, 1 H), 6.92 (s, 4H), 2.31 (s, 6H), 2.10 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.79, 153.04, 145.17, 137.21, 136.53, 135.76, 129.32, 128.30, 127.92, 121.52, 119.00, 92.10, 85.20, 21.07, 20.37 ; MS: EI: 416.2

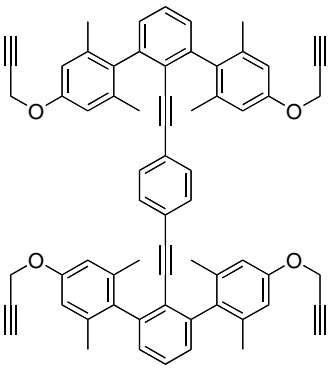


1,4-di(2,6-di(4-methoxy-2,6-dimethylphenyl)phenylethynyl)benzene (2a-Me). A solution of 1,4-diiodobenzene (54 mg, 0.16 mmol), **7-H/Me** (150 mg 0.4 mmol), copper iodide (3 mg, 0.02 mmol), and trans-dichlorobis(triphenylphosphine)palladium(II) (11 mg, 0.02 mmol) in triethylamine was heated to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (2:1 hexanes: methylene chloride) to yield 50 mg (38%) of a white solid: mp = 304-306 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 (t, *J* = 8 Hz, 2H), 7.17 (d, *J* = 8 Hz, 4H) 6.68 (s, 8H), 6.43 (s, 4H), 3.87 (s, 12H), 2.05 (s, 24H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.70,

144.22, 137.79, 133.68, 131.05, 128.49, 124.04, 122.97, 112.58, 112.54, 94.41, 89.13, 55.41, 20.87; MS: MALDI: 814.3

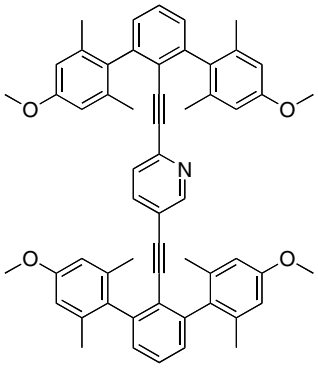


1,4-di[2,6-di(4-hydroxy-2,6-dimethylphenyl)phenylethynyl]benzene (2a-H). A solution of 1,4-diiodobenzene (96 mg, 0.29 mmol), **7-H/H** (200 mg 0.58 mmol), copper iodide (6 mg, 0.029 mmol), and palladium tetrakis(triphenylphosphine) (34 mg, 0.029 mmol) in triethylamine was heated to 80 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with ethyl acetate. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (2:1 hexane:ethyl acetate on silica) to yield 90 mg (41%) of a white solid: mp > 350 °C; ^{1}H NMR (300 MHz, acetone) δ 8.11 (s, 4H), 7.53 (t, *J* = 8 Hz, 2H), 7.18 (d, *J* = 8 Hz, 4H), 6.69 (s, 8H), 6.49 (s, 4H), 2.82 (s, 24H) ^{13}C NMR (100 MHz, acetone) δ 157.04, 144.84, 137.42, 132.19, 129.81, 129.27, 123.89, 123.29, 114.73, 114.68, 93.71, 90.69, 21.14; MS: MALDI: 758.7

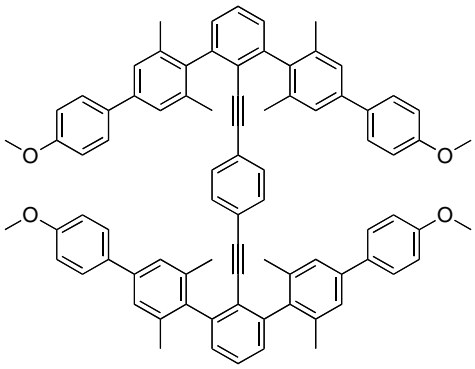


1,4-di[2,6-di(2,6-dimethyl-4-(prop-2-ynoxy)phenyl)phenylethynyl]-benzene (2a-CH_2CCH). To a solution of **2a-H** (90 mg, 0.12 mmol) and cesium carbonate (390 mg, 1.2 mmol) in N,N-dimethylformamide was added propargyl bromide (113 mg of a 80% solution in toluene). The reaction mixture was heated to 50 °C and stirred at this temperature for 20 h. Methylene chloride was added and the mixture was transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The product was purified by column chromatography

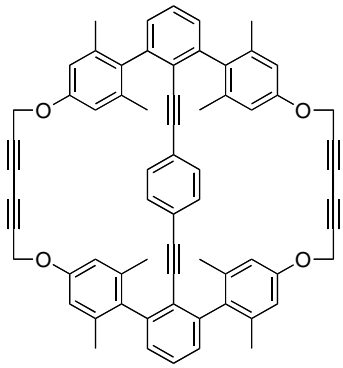
(2:1 hexanes: methylene chloride on silica) to yield 20 mg (18%) of a white solid: mp > 350 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (t, *J* = 8, 2H), 7.15 (d, *J* = 8, 4H), 6.73 (s, 8H), 6.40 (s, 4H), 4.74 (d, *J* = 2, 8H), 2.51(t, *J* = 2, 4H), 2.01 (s, 24H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.58, 144.03, 137.89, 134.46, 131.09, 128.57, 128.41, 123.84, 122.87, 113.49, 94.51, 88.94, 79.17, 75.53, 55.88, 20.89; MS: MALDI: 910.4



2,5-di(2,6-di(4-methoxy-2,6-dimethylphenyl)phenylethynyl)pyridine (2b-Me). A solution of 2-bromo-5-iodopyridine (30 mg, 0.11 mmol), **7-H/Me** (80 mg, 0.22 mmol), palladium tetrakis(triphenylphosphine) (12 mg, 0.011 mmol), and copper iodide (2 mg, 0.011 mmol) in triethylamine (5 mL) was heated to 80°C and stirred at this temperature for 36 h. The reaction mixture was allowed to cool to room temperature, methylene chloride was added, and the mixture was transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (6:1 methylene chloride: hexanes on silica) to yield 34 mg (38%) of a white solid. mp = 310-312°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 1, 2 Hz, 1H), 7.47 (t, *J* = 7 Hz, 1H), 7.46 (t, *J* = 7 Hz, 1H), 7.16 (d, *J* = 7 Hz, 2H), 7.15 (d, *J* = 7 Hz, 2H), 6.70 (dd, *J* = 2, 8 Hz, 1H), 6.65 (s, 4H), 6.64 (s, 4H), 6.29 (dd, *J* = 1, 8 Hz), 3.84 (s, 6H), 3.82 (s, 6H), 2.07 (s, 12H), 2.04 (s, 12H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.09, 159.02, 145.22, 144.79, 138.24, 137.97, 133.59, 129.67, 129.39, 129.06, 128.88, 127.55, 123.69, 123.29, 119.47, 113.07, 112.89, 55.67, 55.63, 21.21, 21.17 ; MS: MALDI: 816.4

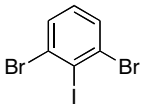


1,4-di(2,6-di[4-(4-methoxyphenyl)-2,6-dimethylphenyl]-phenylethynyl)benzene (2d). A solution of 1,4-diiodobenzene (13 mg, 0.076 mmol), **8-H** (40 mg 0.038 mmol), copper iodide (1 mg, 0.007 mmol), and palladium tetrakis(triphenylphosphine) (4 mg, 0.007 mmol) in triethylamine was heated to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (1:1 hexanes:methylene chloride) to yield 17 mg (42%) of a white solid: mp = 292-294 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7Hz, 8H), 7.46 (t, *J* = 8 Hz, 2H), 7.27 (s, 8H), 7.21 (d, *J* = 8 Hz, 4H), 6.97 (d, *J* = 7 Hz, 8H), 6.32 (s, 4H), 3.87 (s, 12H), 2.10 (s, 24H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.99, 144.05, 139.62, 139.18, 136.54, 133.94, 130.75, 128.45, 128.08, 127.86, 125.43, 122.88, 122.60, 114.10, 94.50, 88.67, 55.34, 20.55; MS: MALDI: 1118.4

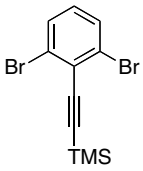


Alkyne Cyclophane (3). To a solution of **2a-CH_2CCH** (15 mg, 0.016 mmol) in ethanol (15 mL) was added copper (II) acetate monohydrate (65 mg, 0.33 mmol). The reaction mixture was heated to 80 °C and stirred at this temperate for 36 h. After cooling to room temperature, methylene chloride was added and the mixture was transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (1:1 hexanes: methylene chloride on silica) to yield 6 mg (40%) of a white solid. m.p. > 350 °C ; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (t, *J* = 8 Hz, 2H), 7.18 (d, *J* = 8 Hz, 4H), 6.72

(s, 8H), 6.43 (s, 4H), 4.82 (s, 8H), 2.01 (s, 24H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.82, 144.06, 138.04, 135.05, 131.10, 128.58, 127.99, 124.11, 122.76, 114.27, 94.57, 88.16, 75.51, 70.78, 57.20, 20.84; MS: MALDI: 906.3

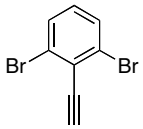


2,6-Dibromoiodobenzene (4). To a solution of 2,6-dibromoaniline (10.0 g, 40 mmol) in concentrated HCl (40 mL) at 0 °C was added dropwise an aqueous solution of sodium nitrite (3.0 g, 44 mmol) over 45 min. Stirring was continued for an additional 30 min. The resulting solution was added dropwise over 30 min to a vigorously stirred aqueous solution of potassium iodide (66.4 g, 0.4 mol) at 0 °C. Stirring was continued for an additional 3 h and the crude product was collected by filtration. The solid was then dissolved in methylene chloride and the solution was transferred to a separatory funnel. The organic phase was washed twice with a 10% aqueous sodium bisulfite solution and once with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The product was dry loaded onto silica and passed through a silica plug with hexanes to yield 12.0 g (83%) of a white solid: mp = 98-99 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8 Hz, 2H), 7.06 (t, *J*=8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 131.27, 131.04, 130.30, 109.36; MS: GC/MS: 360:362:364 (1:2:1)

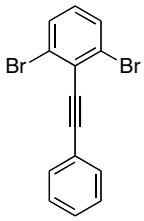


2-(2,6-dibromophenyl)-1-(trimethylsilyl)ethyne (5-TMS). A solution of **4** (2.0 g, 5.5 mmol), (trimethysilyl)acetylene (1.6 g, 16.5 mmol), copper iodide (0.28 mmol 52 mg), and palladium tetrakis(triphenylphosphine) (320 mg, 0.55 mmol) in triethylamine (20 mL) was heated in a sealed flask to 75 ˚C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column

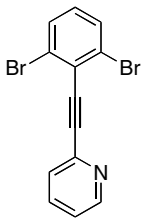
chromatography (hexanes on silica) to yield 1.4 g (76%) of a yellow liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8 Hz, 2H), 7.00 (t, *J* = 8 Hz, 1H), 0.30 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 131.38, 130.50, 127.25, 126.77, 105.55, 101.95, 0.00; MS: GC/MS: 330:332:334 (1:2:1)



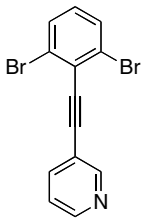
2,6-Dibromoethynylbenzene (5-H). To a solution of **5-TMS** (1.3 g, 3.9 mmol) in methanol was added potassium carbonate (2.7 g, 19 mmol) and the mixture was stirred at room temperature for 16 h. Methylene chloride was added to the reaction mixture, which was then transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield 650 mg (64%) of a white solid: mp = 93-95 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8 Hz, 2H), 7.04 (t, *J* = 8 Hz, 1H), 3.69 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 131.32, 130.23, 126.74, 126.04, 86.64, 80.84; MS: GC/MS: 258:260:262 (1:2:1)



1-(2,6-dibromophenyl)-2-phenylethyne (6a). A solution of **4** (1.0 g, 2.8 mmol), phenylacetylene (560 mg, 5.5 mmol), and trans-dichlorobis(triphenylphosphine)palladium(II) (96 mg, 0.14 mmol) in triethylamine (10 mL) was heated in a sealed flask to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, and dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (hexanes on silica) to yield 600 mg (65%) of a white solid: mp = 85-87 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8 Hz, 1H), 7.56 (d, *J* = 8 Hz, 2H), 7.38 (m, 3H), 7.03 (t, *J* = 8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 131.83, 131.36, 129.65, 127.46, 127.39, 127.24, 127.09, 121.40, 95.41, 94.68; MS: GC/MS: 334:336:338 (1:2:1)

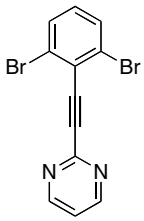


2-(2,6-dibromophenyl)-1-(pyridin-2-yl)ethyne (6b). A solution of **4** (1.0 g, 2.8 mmol), 2-ethynylpyridine (850 mg, 8.4 mmol), copper iodide (26 mg, 0.14 mmol), and trans-dichlorobis(triphenylphosphine)palladium(II) (72 mg, 0.28 mmol) in triethylamine (20 mL) was heated in a sealed flask to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (methylene chloride on silica) to yield 600 mg (65%) of a green liquid: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (dd, *J*=1,5 Hz, 1H), 7.74 (dt, *J*=2,5 Hz, 1H), 7.64 (m, 1H) 7.60 (d, *J* = 7 Hz, 2H), 7.29 (m, 1H), 7.07 (t, *J* = 7 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.21, 142.80, 136.00, 131.24, 130.23, 127.72, 126.70, 126.30, 123.22, 96.97, 86.62; MS: GC/MS: 335:337:339 (1:2:1)

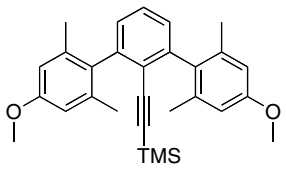


2-(2,6-dibromophenyl)-1-(pyridin-3-yl)ethyne (6c). A solution of **4** (500 mg, 1.4 mmol), 3-ethynylpyridine (280 mg, 2.8 mmol), copper iodide (5 mg, 0.07 mmol), and trans-dichlorobis(triphenylphosphine)palladium(II) (48mg, 0.07 mmol) in triethylamine (10 mL) was heated in a sealed flask to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (5:1 hexanes: ethyl acetate on silica) to yield 260 mg (56%) of a white solid: mp = 81-83 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.85(s, 1H), 8.61 (d, *J* = 5 Hz, 1H), 7.93 (dd, *J* = 2 Hz, 6 Hz, 1H), 7.60 (d, *J* = 8 Hz, 2H), 7.36 (dd, *J* = 5 Hz, 7 Hz, 1H), 7.09 (t, *J* = 8 Hz, 1H); ^{13}C NMR (150 MHz,

$CDCl_3$) δ 154.23, 150.67, 140.84, 133.93, 131.29, 129.34, 129.10, 124.63, 117.35, 94.36, 88.18; MS: GC/MS: 335:337:339 (1:2:1)

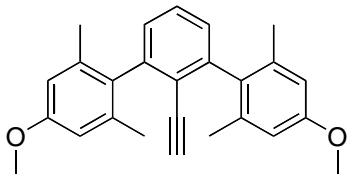


2-(2,6-dibromophenyl)-1-(pyrimidin-2-yl)ethyne (6d). A solution of **5-H** (650 mg, 2.5 mmol), 2-iodopyrimidine (770 mg, 3.8 mmol), copper iodide (24 mg, 0.13 mmol), and palladium tetrakis(triphenylphosphine) (144 mg, 0.13 mmol) in triethylamine (20 mL) was heated in a sealed flask to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (methylene chloride on silica) to yield 515 mg (61%) of a tan solid: mp = 153-155 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.83 (d, *J* = 7 Hz, 2H), 7.64 (d, *J* = 8 Hz, 2H), 7.28 (t, *J* = 7 Hz, 1H), 7.11 (t, *J* = 8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.37, 153.49, 131.86, 131.39, 127.72, 126.12, 120.55, 96.43, 85.91; MS: GC/MS: 336:338:340

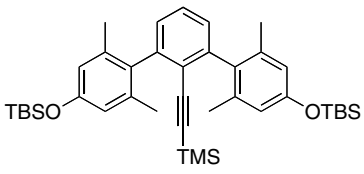


2-(2,6-di(4-methoxy-2,6-dimethylphenyl)phenyl)-1-(trimethylsilyl)ethyne (7-TMS/Me). To an anhydrous solution of **10** (970 mg, 4.5 mmol) in THF at -78°C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this was added a solution of anhydrous zinc chloride (614 mg, 4.5 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **5-TMS** (500 mg, 1.5 mmol) and palladium tetrakis(triphenylphosphine) (173 mg, 0.15 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 16 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic

phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (6:1 hexanes:methylene chloride on silica) to give 430 mg (65%) of a yellow oil : ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (t, *J* = 8 Hz, 1H), 7.12 (d, *J* = 8 Hz, 2H), 6.65 (s, 4H), 3.83 (s, 6H), 2.05 (s, 12H), -0.20 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.01, 144.97, 137.91, 134.08, 128.71, 124.61, 113.18, 112.91, 102.89, 99.89, 55.73, 21.66, 0.00; MS: EI: 442.2

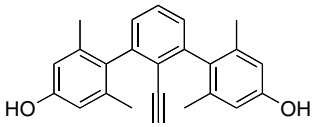


2,6-di(4-methoxy-2,6-dimethyl)ethynylbenzene (7-H/Me). To a solution of **7-TMS/Me** (400 mg, 0.91 mmol) in methanol / THF was added potassium carbonate (625 mg, 4.5 mmol) and the mixture was stirred at room temperature for 16 h. Methylene chloride was added to the reaction mixture, which was then transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield 310 mg (92%) of a white solid: mp = 152-154°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (t, *J* = 8 Hz, 1H), 7.13 (d, *J* = 8 Hz, 2H), 6.68 (s, 4H), 3.83 (s, 6H), 2.05 (s, 12H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.98, 144.05, 136.54, 133.17, 130.75, 128.08, 125.43, 114.10, 94.50, 88.67, 55.34, 20.55; MS: EI: 370.2

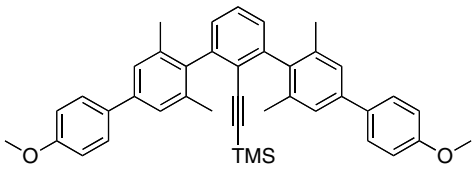


2-[(2,6-di(4-*tert*butyldimethylsilyloxy-2,6-dimethylphenyl)phenyl]-1-(TMS)ethyne (7-TMS/TBDMS). To an anhydrous solution of **14** (830 mg, 2.6 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this was added a solution of anhydrous zinc chloride (360 mg, 2.6 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **5-TMS** (350 mg, 1.1 mmol) and palladium tetrakis(triphenylphosphine) (60 mg, 0.11 mmol) in THF.

This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 16 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (10:1 hexanes: methylene chloride) to give 200 mg (30%) of a clear film: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (t, *J* = 8 Hz, 1H), 7.13 (d, *J* = 8 Hz, 2H), 6.60 (s, 4H), 2.01 (s, 12H), 1.05 (s, 18H), -0.15 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.79, 145.04, 137.65, 134.52, 129.01, 128.60, 124.35, 118.84, 102.90, 99.51, 26.26, 20.88, 18.71, 0.00, -3.86; MS: EI: 643.4

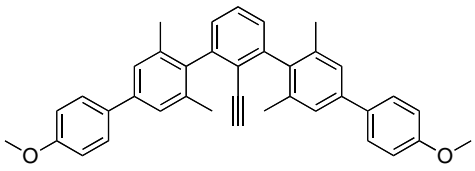


2,6-di(4-hydroxy-2,6-dimethylphenyl)ethynylbenzene (7-H/H). To a solution of **7-TMS/TBDMS** (300 mg, 0.47 mmol) in methanol / THF was added potassium carbonate (650 mg, 4.7 mmol) and the mixture was stirred at room temperature for 16 h. Methylene chloride was added to the reaction mixture, which was then transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield 130 mg (81%) of a white solid. mp = 256-258 °C; ^{1}H NMR (300 MHz, Acetone) δ 8.06 (s, 2H), 7.51 (t, *J* = 8 Hz, 1H), 7.11 (d, *J* = 8 Hz, 2H), 6.60 (s, 4H), 3.03 (s, 1H), 1.96 (s, 12H); ^{13}C NMR (75 MHz, Acetone) δ 157.03, 145.86, 137.57, 132.98, 129.45, 129.20, 123.84, 114.69, 83.00, 81.41, 20.52; MS: EI: 342.1



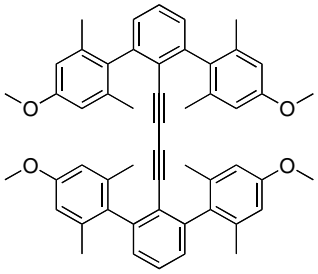
2-(2,6-di[(4-methoxyphenyl)-2,6-dimethylphenyl]phenyl)-1-(trimethylsilyl)ethyne (8-TMS). To an anhydrous solution of **13** (620 mg, 2.1 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equivalents of a 2.4 molar solution in hexane) by syringe. To this was added a

solution of anhydrous zinc chloride (290 mg, 2.1 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **5-TMS** (300 mg, 0.9 mmol) and palladium tetrakis(triphenylphosphine) (104 mg, 0.09 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 36 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (2:1 hexanes: methylene chloride) to give 230 mg (30%) of a white solid. mp: 170-172 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8 Hz, 4H), 7.45 (t, *J* = 7 Hz, 1H), 7.27 (s, 4H), 7.18 (d, *J* = 7 Hz, 2H), 6.98 (d, 4H, *J* = 8 Hz, 4H), 3.84 (s, 6H), 2.11 (s, 12H), -0.27 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.61, 145.15, 140.23, 139.90, 137.02, 134.78, 128.72, 128.41, 126.42, 126.10, 123.83, 114.75, 102.73, 100.54, 55.94, 21.38, 0.00; MS: EI: 594.2

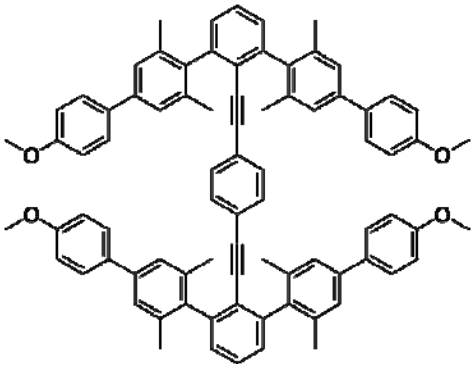


2,6-di[(4-methoxyphenyl)-2,6-dimethylphenyl]ethynyl-benzene (8-H). To a solution of **8-TMS** (220 mg, 0.37 mmol) in methanol / THF was added potassium carbonate (255 mg, 1.85 mmol) and the mixture was stirred at room temperature for 18 h. Methylene chloride was added to the reaction mixture, which was then transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield 310 mg (92%) of a white solid: mp = 229-231 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7 Hz, 4H), 7.52 (t, *J* = 7 Hz, 1H), 7.36 (s, 4H), 7.23 (d, *J* = 7 Hz, 2H), 7.01 (d, *J* = 7 Hz, 4H), 3.84 (s,

6H), 2.18 (s, 12H), 2.66 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) 158.96, 144.81, 139.47, 139.01, 136.27, 133.65, 130.15, 128.81, 127.97, 125.39, 121.76, 114.03, 82.10, 80.13, 55.23, 20.45; MS: EI: 522.1

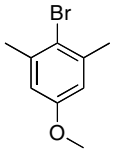


1,4-di(2,6-di(4-methoxy-2,6-dimethylphenyl)phenyl)buta-1,3-diyne (9). A solution of **7-H/Me** (100 mg, 0.27 mmol) and copper acetate monohydrate (540 mg, 2.7 mmol) in ethanol (10 mL) was heated to reflux. The reaction mixture was stirred at this temperature for 48 h, then allowed to cool and diluted with methylene chloride. The mixture was transferred into a separatory funnel and washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure. The product was purified by column chromatography (2:1 methylene chloride: hexanes) to yield 80 mg (80%) of a white solid. mp = 255-257 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (t, *J* = 8 Hz, 2H), 7.08 (d, *J* = 8 Hz, 4H), 6.63 (s, 8H), 3.85 (s, 12H), 2.01 (s, 24H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.34, 144.93, 137.17, 132.56, 128.33, 122.97, 112.35, 112.32, 79.80, 78.50, 54.92, 20.35; MS (EI) 738.4

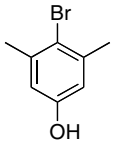


1,4-di(2,6-di[4-(4-methoxyphenyl)-2,6-dimethylphenyl]-phenylethynyl)benzene (2c).A solution of 1,4-diiodobenzene (13 mg, 0.076 mmol), 2,6-di[(4-methoxyphenyl)-2,6-dimethylphenyl]ethynylbenzene, (40 mg 0.038 mmol), copper iodide (1 mg, 0.007 mmol), and palladium tetrakis(triphenylphosphine) (4 mg, 0.007 mmol) in triethylamine was heated to 75 °C and stirred at this temperature for 18 h. The reaction mixture was allowed to cool to room temperature, then diluted with methylene chloride. The mixture was transferred to a separatory funnel, washed twice with water, then dried over magnesium sulfate.

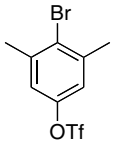
Solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (1:1 hexanes:methylene chloride) to yield 17 mg (42%) of a white solid: mp = 292-294 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7Hz, 8H), 7.46 (t, *J* = 8 Hz, 2H), 7.27 (s, 8H), 7.21 (d, *J* = 8 Hz, 4H), 6.97 (d, *J* = 7 Hz, 8H), 6.32 (s, 4H), 3.87 (s, 12H), 2.10 (s, 24H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.99, 144.05, 139.62, 139.18, 136.54, 133.94, 130.75, 128.45, 128.08, 127.86, 125.43, 122.88, 122.60, 114.10, 94.50, 88.67, 55.34, 20.55; MS: MALDI: 1118.4



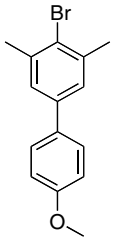
4-methoxy-2,6-(dimethyl)bromobenzene (10). To a solution of 3,5-dimethylanisole in acetonitrile was added dropwise over 1 h a solution of N-bromosuccinimide in acetonitrile. Stirring was continued for 2 h after the addition was complete. Water was added to the reaction mixture, which was then transferred to a separatory funnel. Hexanes was added and the phases were separated. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield a clear liquid. Spectral data matches literature values: ^{1}H NMR (300 MHz, $CDCl_3$) 6.63 (s, 2H), 3.74 (s, 3H), 2.36 (s, 6H); MS: GC/MS: 214:216 (1:1)



4-hydroxy-2,6-dimethylbromobenzene (11). To a solution of **10** (5.0 g, 23.3 mmol) in methylene chloride at –78 °C was slowly added boron tribromide (4.4 mL, 46.6 mmol) by syringe. The reaction mixture was stirred for 16 h. Water was very slowly added to the reaction mixture at 0 °C and the contents were transferred to a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield 4.4 g (94%) of a white solid. mp = 112-114 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (s, 1H), 6.65 (s, 2H), 2.32 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.96, 139.51, 116.88, 116.25, 23.72; MS: GC/MS: 201:203 (1:1)

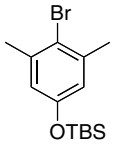


4-Bromo-3,5-dimethylphenyltrifluoromethanesulfonate (12). To a solution of **11** (2.6 g, 12.9 mmol) and pyridine (5 mL) in methylene chloride at –78°C was slowly added triflic anhydride (7.3 g, 25.8 mmol) by syringe. The reaction mixture was stirred for 18 h, then water was added. The solution was transferred to a separatory funnel, methylene chloride was added, and the phases were separated. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure and the product was purified by column chromatography (hexanes on silica) to yield 3.4 g (79%) of a clear liquid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.01 (s, 2H), 2.46 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.61, 140.72, 126.87, 124.98 (q, $J_{C\text{-}F}$ = 318 Hz, 1C); MS: GC/MS: 332:334 (1:1)



4-(4-methoxyphenyl)-2,6-dimethylbromobenzene (13). To an anhydrous solution of 4-bromoanisole (1.0 g, 5.3 mmol) in THF at -78 °C was slowly added n-butyllithium (1.05 equiv of 2.4 M hexane) by syringe. To this was added a solution of anhydrous zinc chloride (730 mg, 5.3 mmol) in THF via cannula. The cold bath was removed after the addition was complete. Upon warming to room temperature, this solution was transferred via cannula to an anhydrous solution of **21** (1.6 g, 4.9 mmol) and palladium tetrakis(triphenylphosphine) (283 mg, 0.49 mmol) in THF. This flask was equipped with a condenser and the reaction mixture was heated to reflux. Stirring was continued at this temperature for 18 h. The solvent was evaporated under reduced pressure and methylene chloride was added to the mixture. The contents of the flask were transferred to a separatory funnel and the organic phase was washed once with a saturated EDTA solution and twice with water, then dried over magnesium sulfate. Solvent was removed under reduced pressure. The crude product was purified by column chromatography (10:1 hexanes: methylene chloride) to give 700 mg (45%) of a white solid. mp = 103-105 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, J = 8 Hz, 2H),

7.26 (s, 2H), 6.99 (d, J = 8 Hz, 2H), 3.86 (s, 3H), 2.48 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.17, 139.24, 138.37, 132.75, 127.90, 126.44, 125.92, 114.13, 55.24, 23.88; MS: GC/MS: 290:292 (1:1)



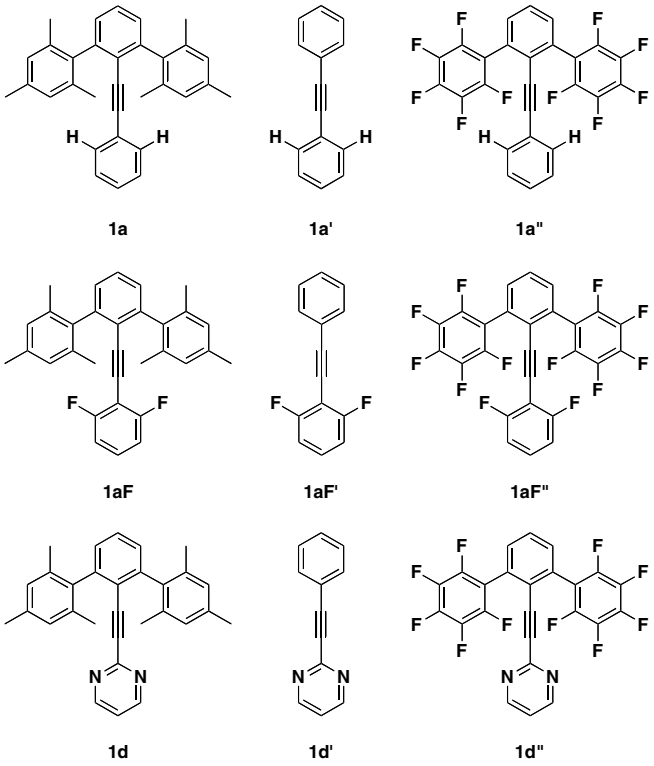
(4-Bromo-3,5-dimethylphenoxy)(*tert*-butyl)dimethylsilane (14). To a solution of **11** (2.0 g, 9.9 mmol) in methylene chloride (25 mL) was added triethylamine (1.5 mL, 10.9 mmol) and *tert*-butylchlorodimethylsilane (1.6 g, 10.4 mmol). The reaction mixture was stirred at room temperature for 16 h. Water was added and the mixture was transferred into a separatory funnel. The organic phase was washed twice with water, then dried over magnesium sulfate. Solvent was evaporated under reduced pressure to yield 1.85 g (84%) of a clear liquid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.57 (s, 2H), 2.35 (s, 6H), 0.97 (s, 9H), 0.18 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.06, 138.90, 119.82, 118.88, 25.58, 23.77, 18.08, -4.15; MS: GC/MS: 314:316 (1:1)

Computational Methods:

The conformational analyses of the molecular systems described in this study, including structural and orbital arrangements as well as property calculations, were carried out using the GAMESS[57] software package. Structural computations of all compounds were performed using the B97-D,[54] M06,[58] and B3LYP[59-61] density functional methods, with a subset additionally computed using conventional perturbation theory methods, MP2.[62] The Dunning double-z polarized basis set, DZ(2d,p), was employed.[63] Full geometry optimizations were performed and uniquely characterized via second derivatives (Hessian) analysis to determine the number of imaginary frequencies (0=minima; 1=transition state). Molecular orbital contour plots, used as an aid in the analysis of results, were generated and depicted using the programs QMView[64] and WebMO.[65]

Computational Optimized Structures

B3LYP data:



1a α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2089513411	0.0000000000	-3.3986805311
C	6.0	0.0000000000	0.0000000000	-4.0998941910
C	6.0	0.0000000000	0.0000000000	-1.2971032174
C	6.0	1.2298944093	0.0000000000	-2.0010376737
C	6.0	0.0000000000	0.0000000000	0.1293604039
C	6.0	0.0000000000	0.0000000000	1.3463908960
C	6.0	0.0000000000	0.0000000000	2.7718438763
C	6.0	1.2145074648	0.0000000000	3.4864922641
C	6.0	1.2105526736	0.0000000000	4.8818340395
C	6.0	0.0000000000	0.0000000000	5.5855468840
C	6.0	2.5404337223	0.0000000000	-1.2805560243
C	6.0	5.0510157606	0.0000000000	0.0194485657
C	6.0	4.4074304092	1.1998312627	-0.3047707885
C	6.0	3.1636163731	1.2193410538	-0.9480604720
C	6.0	6.4136869745	0.0000000000	0.6722909167
C	6.0	2.5043966191	2.5432482719	-1.2617067123
H	1.0	2.1530638769	0.0000000000	-3.9370383644
H	1.0	0.0000000000	0.0000000000	-5.1866240889
H	1.0	2.1536025021	0.0000000000	5.4219817761
H	1.0	0.0000000000	0.0000000000	6.6723339662
H	1.0	4.8835650123	2.1452880556	-0.0532109321
H	1.0	7.2099316129	0.0000000000	-0.0842662269
H	1.0	6.5597850791	0.8868353239	1.2979476962
H	1.0	3.1536425601	3.3788940481	-0.9848586434
H	1.0	1.5602158621	2.6539976168	-0.7145247304
H	1.0	2.2665970117	2.6346747990	-2.3275095149
H	1.0	2.1498396632	0.0000000000	2.9355152059

1a β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2085119809	0.0000000000	-3.3925919035
C	6.0	0.0000000000	0.0000000000	-4.0937198611
C	6.0	0.0000000000	0.0000000000	-1.2907060334
C	6.0	1.2288515337	0.0000000000	-1.9941093875
C	6.0	0.0000000000	0.0000000000	0.1408216444
C	6.0	0.0000000000	0.0000000000	1.3575181056
C	6.0	0.0000000000	0.0000000000	2.7871218991
C	6.0	0.0000000000	1.2124499206	3.5029727910
C	6.0	0.0000000000	1.2096106175	4.8987483920
C	6.0	0.0000000000	0.0000000000	5.6029337608
C	6.0	2.5413954322	0.0000000000	-1.2771912771

C	6.0	5.0596051134	0.0000000000	0.0068919350
C	6.0	4.4146734827	1.1997399576	-0.3142645135
C	6.0	3.1670273506	1.2192196251	-0.9495332193
C	6.0	6.4241361907	0.0000000000	0.6555824060
C	6.0	2.5069132738	2.5428830100	-1.2627916007
H	1.0	2.1528754718	0.0000000000	-3.9304244930
H	1.0	0.0000000000	0.0000000000	-5.1805275754
H	1.0	0.0000000000	2.1532557474	5.4378304286
H	1.0	0.0000000000	0.0000000000	6.6896678171
H	1.0	4.8920649439	2.1450431201	-0.0645869052
H	1.0	7.2186698059	0.0000000000	-0.1028104299
H	1.0	6.5712522720	0.8865590242	1.2812996276
H	1.0	3.1531783561	3.3789503210	-0.9800612061
H	1.0	1.5589271319	2.6506996203	-0.7216692118
H	1.0	2.2751422482	2.6369365274	-2.3298075918
H	1.0	0.0000000000	2.1493770136	2.9548989195

1a' α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	4.8509936218
C	6.0	1.2100555091	0.0000000000	4.1469431047
C	6.0	1.2133949958	0.0000000000	2.7516833030
C	6.0	0.0000000000	0.0000000000	2.0352415496
C	6.0	0.0000000000	0.0000000000	0.6089355893
H	1.0	0.0000000000	0.0000000000	5.9376662068
H	1.0	2.1533189900	0.0000000000	4.6865751599
H	1.0	2.1501919194	0.0000000000	2.2033061481

1a' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2098903460	0.0000000000	-3.3983165885
C	6.0	0.0000000000	0.0000000000	-4.1020249723
C	6.0	0.0000000000	0.0000000000	-1.2873358040
C	6.0	1.2129683267	0.0000000000	-2.0023653054
C	6.0	0.0000000000	0.0000000000	0.1431682981
C	6.0	0.0000000000	0.0000000000	1.3602897425
C	6.0	0.0000000000	0.0000000000	2.7907953214
C	6.0	0.0000000000	1.2129722394	3.5058183985
C	6.0	0.0000000000	1.2098918033	4.9017716023
C	6.0	0.0000000000	0.0000000000	5.6054740720
H	1.0	2.1496095723	0.0000000000	-1.4537103739
H	1.0	2.1533051828	0.0000000000	-3.9376914962
H	1.0	0.0000000000	0.0000000000	-5.1887418157

H	1.0	0.0000000000	2.1496123109	2.9571635204
H	1.0	0.0000000000	2.1533150566	5.4411302656
H	1.0	0.0000000000	0.0000000000	6.6921929135

1a" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2077977769	0.0000000000	-3.4311680078
C	6.0	0.0000000000	0.0000000000	-4.1331746409
C	6.0	0.0000000000	0.0000000000	-1.3191318487
C	6.0	1.2190696007	0.0000000000	-2.0359092717
C	6.0	0.0000000000	0.0000000000	0.1047534203
C	6.0	0.0000000000	0.0000000000	1.3217473559
C	6.0	0.0000000000	0.0000000000	2.7473236000
C	6.0	1.2143360614	0.0000000000	3.4615371172
C	6.0	1.2108811171	0.0000000000	4.8564622388
C	6.0	0.0000000000	0.0000000000	5.5591932474
C	6.0	2.5202094930	0.0000000000	-1.3093524617
C	6.0	4.9958959119	0.0000000000	0.0405508242
C	6.0	4.3822988684	1.2064338261	-0.2923352387
C	6.0	3.1580584129	1.1922521557	-0.9580676849
F	9.0	6.1659505588	0.0000000000	0.6752910886
F	9.0	2.5912809345	2.3626153601	-1.2621104709
H	1.0	2.1514687000	0.0000000000	-3.9686073350
H	1.0	0.0000000000	0.0000000000	-5.2188779641
H	1.0	2.1536483179	0.0000000000	5.3964756477
H	1.0	0.0000000000	0.0000000000	6.6457805943
F	9.0	4.9694793696	2.3605394676	0.0258854654
H	1.0	2.1512983751	0.0000000000	2.9136376515

1a" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2078686848	0.0000000000	-3.4333156359
C	6.0	0.0000000000	0.0000000000	-4.1346999725
C	6.0	0.0000000000	0.0000000000	-1.3224239954
C	6.0	1.2184807734	0.0000000000	-2.0373758419
C	6.0	0.0000000000	0.0000000000	0.1060748353
C	6.0	0.0000000000	0.0000000000	1.3223105428
C	6.0	0.0000000000	0.0000000000	2.7522238705
C	6.0	0.0000000000	1.2143965038	3.4644177925
C	6.0	0.0000000000	1.2105938248	4.8600792664
C	6.0	0.0000000000	0.0000000000	5.5626515732
C	6.0	2.5196154648	0.0000000000	-1.3102729787
C	6.0	4.9956032518	0.0000000000	0.0391789855

C	6.0	4.3818676630	1.2062371188	-0.2936614539
C	6.0	3.1577038144	1.1919553292	-0.9590628500
F	9.0	6.1651339545	0.0000000000	0.6739616491
F	9.0	2.5896778032	2.3627237400	-1.2618929295
H	1.0	2.1517080716	0.0000000000	-3.9703906637
H	1.0	0.0000000000	0.0000000000	-5.2204955839
H	1.0	0.0000000000	2.1535993135	5.3997661136
H	1.0	0.0000000000	0.0000000000	6.6492716631
F	9.0	4.9683068094	2.3606631450	0.0247291009
H	1.0	0.0000000000	2.1509683084	2.9157396275

1d α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2095159874	0.0000000000	-3.3550735868
C	6.0	0.0000000000	0.0000000000	-4.0548672283
C	6.0	0.0000000000	0.0000000000	-1.2555302066
C	6.0	1.2314039953	0.0000000000	-1.9573790744
C	6.0	0.0000000000	0.0000000000	0.1711866054
C	6.0	0.0000000000	0.0000000000	1.3869261111
C	6.0	0.0000000000	0.0000000000	2.8191366643
N	7.0	1.1991096745	0.0000000000	3.4312691748
C	6.0	1.1845781552	0.0000000000	4.7638993335
C	6.0	0.0000000000	0.0000000000	5.5037441058
C	6.0	2.5456033554	0.0000000000	-1.2442471476
C	6.0	5.0708452013	0.0000000000	0.0223287482
C	6.0	4.4238990231	1.1997117560	-0.2938519114
C	6.0	3.1720365511	1.2195648777	-0.9201060390
C	6.0	6.4393739258	0.0000000000	0.6624499564
C	6.0	2.5084523613	2.5434266057	-1.2249058088
H	1.0	2.1531857623	0.0000000000	-3.8938382971
H	1.0	0.0000000000	0.0000000000	-5.1417376073
H	1.0	2.1559659740	0.0000000000	5.2572539939
H	1.0	0.0000000000	0.0000000000	6.5887550863
H	1.0	4.9018260057	2.1450429489	-0.0455376198
H	1.0	7.2295047024	0.0000000000	-0.1005496898
H	1.0	6.5896538045	0.8864467204	1.2875948324
H	1.0	3.1598155210	3.3788571947	-0.9524448968
H	1.0	1.5697946183	2.6533530502	-0.6680836626
H	1.0	2.2606402548	2.6380952835	-2.2883634733

1d β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2090141192	0.0000000000	-3.3686921970

C	6.0	0.0000000000	0.0000000000	-4.0690611856
C	6.0	0.0000000000	0.0000000000	-1.2712211800
C	6.0	1.2302236393	0.0000000000	-1.9704180097
C	6.0	0.0000000000	0.0000000000	0.1596149027
C	6.0	0.0000000000	0.0000000000	1.3744176129
C	6.0	0.0000000000	0.0000000000	2.8098011217
N	7.0	0.0000000000	1.1982595947	3.4204172753
C	6.0	0.0000000000	1.1845658955	4.7537810987
C	6.0	0.0000000000	0.0000000000	5.4928523533
C	6.0	2.5410968345	0.0000000000	-1.2504955599
C	6.0	5.0563907093	0.0000000000	0.0371890896
C	6.0	4.4116245558	1.1998933483	-0.2837389805
C	6.0	3.1647293212	1.2198114276	-0.9204535106
C	6.0	6.4210002430	0.0000000000	0.6857767284
C	6.0	2.5028394152	2.5436900883	-1.2286876622
H	1.0	2.1533928568	0.0000000000	-3.9063983427
H	1.0	0.0000000000	0.0000000000	-5.1558426069
H	1.0	0.0000000000	2.1558691903	5.2470531179
H	1.0	0.0000000000	0.0000000000	6.5778584014
H	1.0	4.8881323405	2.1452212059	-0.0326029824
H	1.0	7.2152917600	0.0000000000	-0.0728142578
H	1.0	6.5680548275	0.8866083365	1.3115021920
H	1.0	3.1555626957	3.3790045415	-0.9591730638
H	1.0	1.5654164470	2.6561559358	-0.6703331633
H	1.0	2.2538919644	2.6348443429	-2.2920556464

1d' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2113897763	0.0000000000	-3.3359656855
C	6.0	0.0000000000	0.0000000000	-4.0380589059
C	6.0	0.0000000000	0.0000000000	-1.2282037029
C	6.0	1.2150321185	0.0000000000	-1.9409430572
C	6.0	0.0000000000	0.0000000000	0.1972410223
C	6.0	0.0000000000	0.0000000000	1.4133080142
C	6.0	0.0000000000	0.0000000000	2.8455466917
N	7.0	1.1994035098	0.0000000000	3.4569306068
C	6.0	1.1846813243	0.0000000000	4.7899390047
C	6.0	0.0000000000	0.0000000000	5.5292726288
H	1.0	2.1501014077	0.0000000000	-1.3899034777
H	1.0	2.1537666570	0.0000000000	-3.8768072160
H	1.0	0.0000000000	0.0000000000	-5.1247832447
H	1.0	2.1557320148	0.0000000000	5.2837449352
H	1.0	0.0000000000	0.0000000000	6.6142511123

1d' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2101652795	0.0000000000	-3.3393624591
C	6.0	0.0000000000	0.0000000000	-4.0424494456
C	6.0	0.0000000000	0.0000000000	-1.2316480544
C	6.0	1.2140593471	0.0000000000	-1.9436468982
C	6.0	0.0000000000	0.0000000000	0.1980371229
C	6.0	0.0000000000	0.0000000000	1.4133346062
C	6.0	0.0000000000	0.0000000000	2.8505027330
N	7.0	0.0000000000	1.1981371714	3.4607666836
C	6.0	0.0000000000	1.1845183461	4.7944923152
C	6.0	0.0000000000	0.0000000000	5.5333610563
H	1.0	2.1504460331	0.0000000000	-1.3948658829
H	1.0	2.1533866172	0.0000000000	-3.8788467504
H	1.0	0.0000000000	0.0000000000	-5.1291018659
H	1.0	0.0000000000	2.1558738465	5.2875234575
H	1.0	0.0000000000	0.0000000000	6.6184067524

1d" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2095709098	0.0000000000	-3.4078352452
C	6.0	0.0000000000	0.0000000000	-4.1074975121
C	6.0	0.0000000000	0.0000000000	-1.3015893224
C	6.0	1.2213470597	0.0000000000	-2.0128239246
C	6.0	0.0000000000	0.0000000000	0.1225832262
C	6.0	0.0000000000	0.0000000000	1.3370229498
C	6.0	0.0000000000	0.0000000000	2.7707665943
N	7.0	1.1995933155	0.0000000000	3.3778886894
C	6.0	1.1858176157	0.0000000000	4.7115285691
C	6.0	0.0000000000	0.0000000000	5.4492204907
C	6.0	2.5180922378	0.0000000000	-1.2783609184
C	6.0	4.9690277067	0.0000000000	0.1127643977
C	6.0	4.3619018056	1.2063825351	-0.2307963538
C	6.0	3.1493881326	1.1922959095	-0.9167085967
F	9.0	6.1274186265	0.0000000000	0.7678203513
F	9.0	2.5848944702	2.3624239330	-1.2284451253
H	1.0	2.1523915572	0.0000000000	-3.9464909547
H	1.0	0.0000000000	0.0000000000	-5.1933407086
H	1.0	2.1565486242	0.0000000000	5.2051845944
H	1.0	0.0000000000	0.0000000000	6.5341166834
F	9.0	4.9427716215	2.3604915453	0.0980259540

1d" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2080968640	0.0000000000	-3.3942426593
C	6.0	0.0000000000	0.0000000000	-4.0951647906
C	6.0	0.0000000000	0.0000000000	-1.2869106596
C	6.0	1.2197500063	0.0000000000	-1.9984671027
C	6.0	0.0000000000	0.0000000000	0.1418334094
C	6.0	0.0000000000	0.0000000000	1.3559139795
C	6.0	0.0000000000	0.0000000000	2.7948894119
N	7.0	0.0000000000	1.1983737512	3.4006222462
C	6.0	0.0000000000	1.1856509275	4.7347884907
C	6.0	0.0000000000	0.0000000000	5.4722711867
C	6.0	2.5203789775	0.0000000000	-1.2705050916
C	6.0	4.9939218725	0.0000000000	0.0808041986
C	6.0	4.3812733213	1.2066330178	-0.2529191611
C	6.0	3.1577700624	1.1927041841	-0.9196500270
F	9.0	6.1629622863	0.0000000000	0.7167083669
F	9.0	2.5911167156	2.3624136042	-1.2259512800
H	1.0	2.1519764972	0.0000000000	-3.9311484467
H	1.0	0.0000000000	0.0000000000	-5.1809311859
H	1.0	0.0000000000	2.1568028773	5.2275163807
H	1.0	0.0000000000	0.0000000000	6.5572291493
F	9.0	4.9683769193	2.3604240131	0.0654339097

1aF α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2096080517	0.0000000000	-3.4013233801
C	6.0	0.0000000000	0.0000000000	-4.1016002408
C	6.0	0.0000000000	0.0000000000	-1.3026205996
C	6.0	1.2314041094	0.0000000000	-2.0038116961
C	6.0	0.0000000000	0.0000000000	0.1232212196
C	6.0	0.0000000000	0.0000000000	1.3388234386
C	6.0	0.0000000000	0.0000000000	2.7562040688
C	6.0	1.1920621911	0.0000000000	3.5046763196
C	6.0	1.2159127282	0.0000000000	4.8915644996
C	6.0	0.0000000000	0.0000000000	5.5839754553
C	6.0	2.5407583682	0.0000000000	-1.2816316458
C	6.0	5.0440192012	0.0000000000	0.0293226860
C	6.0	4.4030418772	1.1996473461	-0.2989943387
C	6.0	3.1622675051	1.2193687224	-0.9471296683
C	6.0	6.4015144071	0.0000000000	0.6924857473
C	6.0	2.5042313473	2.5434147504	-1.2630927128
H	1.0	2.1533826324	0.0000000000	-3.9400619391
H	1.0	0.0000000000	0.0000000000	-5.1884066868
H	1.0	2.1705323553	0.0000000000	5.4056609138
H	1.0	0.0000000000	0.0000000000	6.6696573951

H	1.0	4.8771776706	2.1449915472	-0.0433681892
H	1.0	7.2039494040	0.0000000000	-0.0578215650
H	1.0	6.5418707849	0.8865985068	1.3197069891
H	1.0	3.1536435630	3.3787233331	-0.9855123773
H	1.0	1.5592411114	2.6561481615	-0.7175732097
H	1.0	2.2683916210	2.6349878013	-2.3294626692
F	9.0	2.3512241419	0.0000000000	2.8356884051

1aF β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2091838169	0.0000000000	-3.3941333256
C	6.0	0.0000000000	0.0000000000	-4.0943020089
C	6.0	0.0000000000	0.0000000000	-1.2954268644
C	6.0	1.2301327886	0.0000000000	-1.9958550557
C	6.0	0.0000000000	0.0000000000	0.1347488660
C	6.0	0.0000000000	0.0000000000	1.3495760767
C	6.0	0.0000000000	0.0000000000	2.7707488558
C	6.0	0.0000000000	1.1899796609	3.5193889246
C	6.0	0.0000000000	1.2153690201	4.9065220334
C	6.0	0.0000000000	0.0000000000	5.5989789732
C	6.0	2.5414091689	0.0000000000	-1.2764838292
C	6.0	5.0574121982	0.0000000000	0.0107813655
C	6.0	4.4125568744	1.1998025849	-0.3102994760
C	6.0	3.1654686277	1.2196917109	-0.9467328087
C	6.0	6.4221076067	0.0000000000	0.6591302819
C	6.0	2.5037059509	2.5438303425	-1.2541992640
H	1.0	2.1533884790	0.0000000000	-3.9320764541
H	1.0	0.0000000000	0.0000000000	-5.1811319324
H	1.0	0.0000000000	2.1703036046	5.4200010445
H	1.0	0.0000000000	0.0000000000	6.6846474154
H	1.0	4.8893640914	2.1451642587	-0.0598619525
H	1.0	7.2161839362	0.0000000000	-0.0997272234
H	1.0	6.5693973642	0.8866695970	1.2846513641
H	1.0	3.1604587301	3.3788006526	-0.9934591964
H	1.0	1.5709864375	2.6604961218	-0.6888451078
H	1.0	2.2462489134	2.6316690512	-2.3157885758
F	9.0	0.0000000000	2.3515699465	2.8511255996

1aF' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2107077246	0.0000000000	-3.3868621447
C	6.0	0.0000000000	0.0000000000	-4.0899336839
C	6.0	0.0000000000	0.0000000000	-1.2780567234

C	6.0	1.2146990819	0.0000000000	-1.9917250251
C	6.0	0.0000000000	0.0000000000	0.1471988503
C	6.0	0.0000000000	0.0000000000	1.3632886134
C	6.0	0.0000000000	0.0000000000	2.7815327377
C	6.0	1.1910224669	0.0000000000	3.5309447240
C	6.0	1.2156339126	0.0000000000	4.9174204937
C	6.0	0.0000000000	0.0000000000	5.6100452517
H	1.0	2.1505524823	0.0000000000	-1.4419386453
H	1.0	2.1535232787	0.0000000000	-3.9270893137
H	1.0	0.0000000000	0.0000000000	-5.1766184569
F	9.0	2.3518487260	0.0000000000	2.8619465513
H	1.0	2.1702591677	0.0000000000	5.4314694569
H	1.0	0.0000000000	0.0000000000	6.6956290177

1aF' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2103328560	0.0000000000	-3.3907367436
C	6.0	0.0000000000	0.0000000000	-4.0936355460
C	6.0	0.0000000000	0.0000000000	-1.2819265236
C	6.0	1.2137792981	0.0000000000	-1.9949519626
C	6.0	0.0000000000	0.0000000000	0.1477363746
C	6.0	0.0000000000	0.0000000000	1.3632064639
C	6.0	0.0000000000	0.0000000000	2.7856703812
C	6.0	0.0000000000	1.1905942775	3.5339991156
C	6.0	0.0000000000	1.2155736700	4.9212637088
C	6.0	0.0000000000	0.0000000000	5.6132965879
H	1.0	2.1500729424	0.0000000000	-1.4459194959
H	1.0	2.1533858008	0.0000000000	-3.9305488862
H	1.0	0.0000000000	0.0000000000	-5.1803473354
F	9.0	0.0000000000	2.3512691281	2.8659425646
H	1.0	0.0000000000	2.1702509215	5.4351825866
H	1.0	0.0000000000	0.0000000000	6.6989556239

1aF" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2093539471	0.0000000000	-3.4479054774
C	6.0	0.0000000000	0.0000000000	-4.1482159229
C	6.0	0.0000000000	0.0000000000	-1.3414411110
C	6.0	1.2213866464	0.0000000000	-2.0529825869
C	6.0	0.0000000000	0.0000000000	0.0813714761
C	6.0	0.0000000000	0.0000000000	1.2961189166
C	6.0	0.0000000000	0.0000000000	2.7128614067
C	6.0	1.1925352405	0.0000000000	3.4590930041

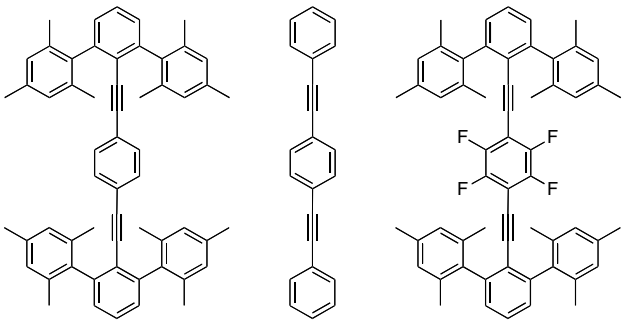
C	6.0	1.2172441628	0.0000000000	4.8448525117
C	6.0	0.0000000000	0.0000000000	5.5354559799
C	6.0	2.5162720002	0.0000000000	-1.3151015275
C	6.0	4.9583163386	0.0000000000	0.0931366438
C	6.0	4.3534681276	1.2061610316	-0.2547723794
C	6.0	3.1457048993	1.1920484717	-0.9490447103
F	9.0	6.1122295121	0.0000000000	0.7561262534
F	9.0	2.5835345525	2.3625992537	-1.2637240320
H	1.0	2.1523474189	0.0000000000	-3.9863557918
H	1.0	0.0000000000	0.0000000000	-5.2339972765
H	1.0	2.1709469167	0.0000000000	5.3603505354
H	1.0	0.0000000000	0.0000000000	6.6209959306
F	9.0	4.9317508416	2.3605057731	0.0783581778
F	9.0	2.3512607577	0.0000000000	2.7850461387

1aF" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2082097792	0.0000000000	-3.4286025138
C	6.0	0.0000000000	0.0000000000	-4.1293534561
C	6.0	0.0000000000	0.0000000000	-1.3198855983
C	6.0	1.2194193015	0.0000000000	-2.0327598258
C	6.0	0.0000000000	0.0000000000	0.1081160795
C	6.0	0.0000000000	0.0000000000	1.3226142624
C	6.0	0.0000000000	0.0000000000	2.7447109810
C	6.0	0.0000000000	1.1922826614	3.4903297165
C	6.0	0.0000000000	1.2165097295	4.8772665101
C	6.0	0.0000000000	0.0000000000	5.5679096164
C	6.0	2.5201693854	0.0000000000	-1.3051259815
C	6.0	4.9957180969	0.0000000000	0.0428817383
C	6.0	4.3824085023	1.2065467695	-0.2898969677
C	6.0	3.1580723216	1.1925308566	-0.9550674251
F	9.0	6.1654331791	0.0000000000	0.6774624536
F	9.0	2.5906578975	2.3624022552	-1.2600373115
H	1.0	2.1518695791	0.0000000000	-3.9658966744
H	1.0	0.0000000000	0.0000000000	-5.2151515532
H	1.0	0.0000000000	2.1706909629	5.3918994782
H	1.0	0.0000000000	0.0000000000	6.6535487033
F	9.0	4.9695333110	2.3605094858	0.0280256269
F	9.0	0.0000000000	2.3501320420	2.8197112517



2 **2'** **2F**

2 ⊥α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2090673311	0.0000000000	-7.5920519883
C	6.0	0.0000000000	0.0000000000	-8.2932144509
C	6.0	0.0000000000	0.0000000000	-5.4906323958
C	6.0	1.2301741113	0.0000000000	-6.1945294849
C	6.0	0.0000000000	0.0000000000	-4.0646099010
C	6.0	0.0000000000	0.0000000000	-2.8471492213
C	6.0	0.0000000000	0.0000000000	-1.4240297705
C	6.0	1.2125262984	0.0000000000	-0.7047080729
C	6.0	2.5403096363	0.0000000000	-5.4735806017
C	6.0	5.0520397242	0.0000000000	-4.1761219436
C	6.0	4.4079167629	1.1998569789	-4.4992342049
C	6.0	3.1635390515	1.2194115375	-5.1413981821
C	6.0	6.4159280023	0.0000000000	-3.5258709878
C	6.0	2.5043850732	2.5432916796	-5.4553809260
C	6.0	1.2113486696	0.0000000000	0.6863861597
C	6.0	0.0000000000	0.0000000000	1.4065953034
C	6.0	0.0000000000	0.0000000000	2.8339477248
C	6.0	0.0000000000	0.0000000000	4.0511254447
C	6.0	0.0000000000	0.0000000000	5.4826677875
C	6.0	0.0000000000	1.2084456102	7.5844214898
C	6.0	0.0000000000	1.2290130936	6.1859699090
C	6.0	0.0000000000	0.0000000000	8.2855943932
C	6.0	0.0000000000	2.5419654989	5.4698806069
C	6.0	0.0000000000	5.0605139558	4.1863784683
C	6.0	1.1997082202	4.4155297737	4.5075649967
C	6.0	1.2192625586	3.1678600002	5.1427585630
C	6.0	0.0000000000	6.4248329857	3.5372526958
C	6.0	2.5431253040	2.5080856403	5.4559760012
H	1.0	2.1531209029	0.0000000000	-8.1304356274
H	1.0	0.0000000000	0.0000000000	-9.3799359586
H	1.0	2.1498739098	0.0000000000	-1.2518573231
H	1.0	4.8845198784	2.1452792219	-4.2485159887

H	1.0	7.2106682898	0.0000000000	-4.2838952268
H	1.0	6.5628765082	0.8866612543	-2.9001581815
H	1.0	3.1544012520	3.3789194140	-5.1803087604
H	1.0	1.5608858432	2.6549078628	-4.9072607157
H	1.0	2.2654967978	2.6338545753	-6.5210248944
H	1.0	0.0000000000	0.0000000000	9.3723817694
H	1.0	2.1496565821	0.0000000000	1.2317084575
H	1.0	0.0000000000	2.1530119384	8.1218829355
H	1.0	2.1450356581	4.8927551792	4.2577314701
H	1.0	0.0000000000	7.2195042066	4.2955745193
H	1.0	0.8865732503	6.5716725774	2.9115650310
H	1.0	3.3788277558	3.1553462360	5.1745801306
H	1.0	2.6515503286	1.5607005890	4.9139092365
H	1.0	2.6372475208	2.2754224657	6.5228092503

2 ⊥γ C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.9622606887	0.7322991405	-7.5865683521
C	6.0	0.0000000000	0.0000000000	-8.2876437994
C	6.0	0.0000000000	0.0000000000	-5.4853405675
C	6.0	0.9797212846	0.7438185614	-6.1890015643
C	6.0	0.0000000000	0.0000000000	-4.0573212917
C	6.0	0.0000000000	0.0000000000	-2.8398457073
C	6.0	0.0000000000	0.0000000000	-1.4153035152
C	6.0	1.2120855077	0.0043199250	-0.6953958586
C	6.0	2.0192427806	1.5404653082	-5.4669188022
C	6.0	4.0022204256	3.0630583541	-4.1462644076
C	6.0	2.7582167966	3.6201071800	-4.4636872591
C	6.0	4.2306012630	1.7261883055	-4.4913560027
C	6.0	1.7637540528	2.8814517116	-5.1162345625
C	6.0	3.2602669815	0.9561170765	-5.1449286536
C	6.0	5.0752278326	3.8882355945	-3.4754926466
C	6.0	0.4298852311	3.5263818419	-5.4179621924
C	6.0	3.5530352182	-0.4900712000	-5.4770507503
H	1.0	1.7121835162	1.3061495449	-8.1246744497
H	1.0	0.0000000000	0.0000000000	-9.3743417620
H	1.0	2.1496428792	0.0123878358	-1.2418660845
H	1.0	2.5518441176	4.6538389125	-4.1938319889
H	1.0	5.1871431008	1.2682137649	-4.2476348482
H	1.0	5.6943922001	4.4071751945	-4.2195213892
H	1.0	4.6432469419	4.6523537816	-2.8204203175
H	1.0	5.7438160565	3.2634643886	-2.8739356452
H	1.0	0.4196343003	4.5718538047	-5.0963190760
H	1.0	4.5822357423	-0.7507105734	-5.2142162189
H	1.0	0.1979291213	3.4977316610	-6.4887372422
H	1.0	3.4100939715	-0.6986158446	-6.5433466241

H	1.0	-0.3857217255	3.0070855904	-4.9004889059
H	1.0	2.8829219071	-1.1644634773	-4.9295907977

2 ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2092516541	0.0000000000	-7.5817143485
C	6.0	0.0000000000	0.0000000000	-8.2827391771
C	6.0	0.0000000000	0.0000000000	-5.4803175955
C	6.0	1.2302900510	0.0000000000	-6.1841782645
C	6.0	0.0000000000	0.0000000000	-4.0545647348
C	6.0	0.0000000000	0.0000000000	-2.8368834895
C	6.0	0.0000000000	0.0000000000	-1.4143300592
C	6.0	1.2136603351	0.0000000000	-0.6952464024
C	6.0	2.5398055663	0.0000000000	-5.4619486522
C	6.0	5.0473333700	0.0000000000	-4.1560007933
C	6.0	4.4047010174	1.1998795122	-4.4821516542
C	6.0	3.1622317706	1.2193948379	-5.1280421556
C	6.0	6.4077261998	0.0000000000	-3.4983829970
C	6.0	2.5036527100	2.5434004539	-5.4430435548
H	1.0	2.1531915017	0.0000000000	-8.1202781271
H	1.0	0.0000000000	0.0000000000	-9.3694934335
H	1.0	2.1503060771	0.0000000000	-1.2436487713
H	1.0	4.8800848263	2.1452656986	-4.2290977123
H	1.0	7.2068242434	0.0000000000	-4.2518653136
H	1.0	6.5514722767	0.8868271765	-2.8721248905
H	1.0	3.1529528791	3.3789313116	-5.1660166694
H	1.0	1.5588767624	2.6547013285	-4.8970973275
H	1.0	2.2672572675	2.6343902590	-6.5092050534

2 ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2085152883	0.0000000000	-7.5943264249
C	6.0	0.0000000000	0.0000000000	-8.2953770758
C	6.0	0.0000000000	0.0000000000	-5.4926455070
C	6.0	1.2289836807	0.0000000000	-6.1958793505
C	6.0	0.0000000000	0.0000000000	-4.0610915124
C	6.0	0.0000000000	0.0000000000	-2.8440696394
C	6.0	0.0000000000	0.0000000000	-1.4163489153
C	6.0	0.0000000000	1.2102306995	-0.6958167067
C	6.0	2.5416750341	0.0000000000	-5.4792642775
C	6.0	5.0599562672	0.0000000000	-4.1955496149
C	6.0	4.4150341389	1.1997035467	-4.5167003047
C	6.0	3.1674418664	1.2192712687	-5.1519964453

C	6.0	6.4243782552	0.0000000000	-3.5467114028
C	6.0	2.5076834653	2.5430670473	-5.4653172801
H	1.0	2.1529063625	0.0000000000	-8.1321048228
H	1.0	0.0000000000	0.0000000000	-9.3821862937
H	1.0	0.0000000000	2.1491874711	-1.2400110585
H	1.0	4.8924546783	2.1450287585	-4.2671744894
H	1.0	7.2188438320	0.0000000000	-4.3051919861
H	1.0	6.5711308908	0.8865217373	-2.9208867400
H	1.0	3.1540639126	3.3789019807	-5.1822623922
H	1.0	1.5595301175	2.6511867110	-4.9245282376
H	1.0	2.2763967946	2.6374257395	-6.5324214573

2' ⊥α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.2102570288	0.0000000000	-7.6015189569
C	6.0	0.0000000000	0.0000000000	-8.3053378416
C	6.0	0.0000000000	0.0000000000	-5.4902543064
C	6.0	-1.2137532948	0.0000000000	-6.2063695902
C	6.0	0.0000000000	0.0000000000	-4.0644264354
C	6.0	0.0000000000	0.0000000000	-2.8462143482
C	6.0	0.0000000000	0.0000000000	-1.4222994654
C	6.0	-1.2114857636	0.0000000000	-0.7013069841
H	1.0	-2.1504905047	0.0000000000	-5.6579073880
C	6.0	-1.2111624444	0.0000000000	0.6898498070
C	6.0	0.0000000000	0.0000000000	1.4099192894
C	6.0	0.0000000000	0.0000000000	2.8379669414
C	6.0	0.0000000000	0.0000000000	4.0554449111
C	6.0	0.0000000000	0.0000000000	5.4858415496
C	6.0	0.0000000000	-1.2099911706	7.5963619163
C	6.0	0.0000000000	-1.2132277329	6.2004414228
C	6.0	0.0000000000	0.0000000000	8.2998954998
H	1.0	0.0000000000	-2.1498587744	5.6517800640
H	1.0	-2.1534132344	0.0000000000	-8.1412658721
H	1.0	0.0000000000	0.0000000000	-9.3919909027
H	1.0	-2.1502417200	0.0000000000	-1.2458790858
H	1.0	0.0000000000	0.0000000000	9.3865936394
H	1.0	-2.1496095198	0.0000000000	1.2349971941
H	1.0	0.0000000000	-2.1533642095	8.1357474427

2' ⊥γ C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.8815789839	-0.8292406884	-7.5983251123
C	6.0	0.0000000000	0.0000000000	8.3020107405

C	6.0	0.0000000000	0.0000000000	5.4877954601
C	6.0	-0.8856257568	-0.8299578331	-6.2031004644
C	6.0	0.0000000000	0.0000000000	4.0599412270
C	6.0	0.0000000000	0.0000000000	2.8420218027
C	6.0	0.0000000000	0.0000000000	1.4162284119
C	6.0	-1.2113541332	-0.0020682866	-0.6955455258
H	1.0	-1.5666492500	-1.4718969314	-5.6533001700
H	1.0	-1.5666900738	-1.4766058483	-8.1390175691
H	1.0	0.0000000000	0.0000000000	9.3886231336
H	1.0	-2.1499717618	-0.0030008529	-1.2404109084

2' ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	8.2993068642
C	6.0	1.2102654846	0.0000000000	7.5954840254
C	6.0	1.2137625980	0.0000000000	6.2003738407
C	6.0	0.0000000000	0.0000000000	5.4841564887
C	6.0	0.0000000000	0.0000000000	4.0585418689
C	6.0	0.0000000000	0.0000000000	2.8401041376
C	6.0	0.0000000000	0.0000000000	1.4168110057
C	6.0	1.2117352367	0.0000000000	0.6951379708
H	1.0	0.0000000000	0.0000000000	9.3859638051
H	1.0	2.1505069724	0.0000000000	5.6519459350
H	1.0	2.1534048136	0.0000000000	8.1352592530
H	1.0	2.1503398685	0.0000000000	1.2400107015

2' ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	8.3058387235
C	6.0	1.2099939859	0.0000000000	7.6023315815
C	6.0	1.2132107558	0.0000000000	6.2064198945
C	6.0	0.0000000000	0.0000000000	5.4918745045
C	6.0	0.0000000000	0.0000000000	4.0614670279
C	6.0	0.0000000000	0.0000000000	2.8440846902
C	6.0	0.0000000000	0.0000000000	1.4155283883
C	6.0	0.0000000000	1.2109441376	0.6959937231
H	1.0	0.0000000000	0.0000000000	9.3925409259
H	1.0	2.1498348968	0.0000000000	5.6577773189
H	1.0	2.1533526453	0.0000000000	8.1417343212
H	1.0	0.0000000000	2.1495323475	1.2408946236

2F ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2101862653	0.0000000000	-7.5825087185
C	6.0	0.0000000000	0.0000000000	-8.2820618091
C	6.0	0.0000000000	0.0000000000	-5.4852820513
C	6.0	1.2326292559	0.0000000000	-6.1852861564
C	6.0	0.0000000000	0.0000000000	-4.0603993238
C	6.0	0.0000000000	0.0000000000	-2.8444769313
C	6.0	0.0000000000	0.0000000000	-1.4306210460
C	6.0	1.1983567670	0.0000000000	-0.6928884515
C	6.0	2.5405163728	0.0000000000	-5.4605931426
C	6.0	5.0367617554	0.0000000000	-4.1365724908
C	6.0	4.3978665291	1.1996154936	-4.4691164797
C	6.0	3.1606588231	1.2196295995	-5.1239243997
C	6.0	6.3897948358	0.0000000000	-3.4647839555
C	6.0	2.5058602011	2.5442484250	-5.4446932113
H	1.0	2.1536416569	0.0000000000	-8.1216624348
H	1.0	0.0000000000	0.0000000000	-9.3688766210
F	9.0	2.3655553688	0.0000000000	-1.3384364501
H	1.0	4.8706429441	2.1448810315	-4.2109032234
H	1.0	7.1965990071	0.0000000000	-4.2103022832
H	1.0	6.5258306237	0.8864719482	-2.8366057486
H	1.0	3.1573193577	3.3786472096	-5.1694673707
H	1.0	1.5611390456	2.6621608775	-4.8997270460
H	1.0	2.2708861074	2.6330718798	-6.5114302363

2F ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2096258632	0.0000000000	-7.5911843712
C	6.0	0.0000000000	0.0000000000	-8.2906724260
C	6.0	0.0000000000	0.0000000000	-5.4944175481
C	6.0	1.2310065494	0.0000000000	-6.1930092159
C	6.0	0.0000000000	0.0000000000	-4.0644358959
C	6.0	0.0000000000	0.0000000000	-2.8496439767
C	6.0	0.0000000000	0.0000000000	-1.4310521215
C	6.0	0.0000000000	1.1956011680	-0.6934937672
C	6.0	2.5405583942	0.0000000000	-5.4709153893
C	6.0	5.0513503957	0.0000000000	-4.1746359953
C	6.0	4.4078889807	1.1999308417	-4.4982095778
C	6.0	3.1632622671	1.2199658787	-5.1393653448
C	6.0	6.4133612490	0.0000000000	-3.5207471156
C	6.0	2.5033821918	2.5442474798	-5.4505851599
H	1.0	2.1535060548	0.0000000000	-8.1296010523
H	1.0	0.0000000000	0.0000000000	-9.3774884833

F	9.0	0.0000000000	2.3656427186	-1.3363654646
H	1.0	4.8838103590	2.1452129247	-4.2459879077
H	1.0	7.2101461118	0.0000000000	-4.2767105943
H	1.0	6.5581827140	0.8865742256	-2.8945679326
H	1.0	3.1575669228	3.3790611159	-5.1833858824
H	1.0	1.5660302097	2.6606248834	-4.8928450019
H	1.0	2.2545651490	2.6335195849	-6.5140910362

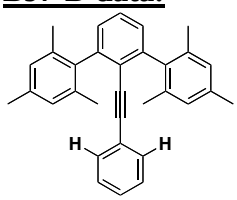
HESSIAN ANALYSIS SUMMARY @ B3LYP

Molecule	Character	ZPE
1a α C_2v	TS	0.517790
1a β C_2v	TS	0.517634
1a' α D_2h	PD	0.190736
1a' β C_2v	PD	0.190855
1a" α C_2v	MNE	0.270224
1a" β C_2v	MNE	0.270139
1d α C_2v	TS	0.494039
1d β C2V	TS	0.494044
1d' α C_2v	PD	0.167371
1d' β C_2v	TS	0.167208
1d" α C_2v	MNE	0.246601
1d" β C_2v	MNE	0.246523
1aF α C_2v	PD	0.501608
1aF β C_2v	TS	0.501622
1aF' α C_2v	PD	0.174941
1aF' β C_2v	PD	0.174844
1aF" α C_2v	MNE	0.254083
1aF" β C_2v	MNE	0.254081
2 ⊥α C_2v	TS	0.934119
2 ⊥γ D_2	MNE	0.933602
2 ‖α D_2h	TS	0.935326
2 ‖β D_2h	TNE	0.935050
2' ⊥α C_2v	TS	0.282127
2' ⊥γ D_2	TS	0.282247
2' ‖α D_2h	PD	0.281472
2' ‖β D_2h	TNE	0.281246
2F ‖α D_2h	TS	0.902813
2F ‖β D_2h	TNE	0.903184

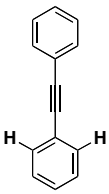
PD = 0 negative eigenvalues; TS = 1 negative eigenvalues; TNE = 2 negative eigenvalues; MNE > 2 negative eigenvalues.

The potential energy surface around these stationary points is very flat and the analysis of curvature is sensitive to function and level used. The symmetry forms chosen are all stationary points, which do not deviate substantially in energy if at all from the local PD structure. For purposes of comparing conformational forms, these energies are presumed to be representative of the conformational dynamics.

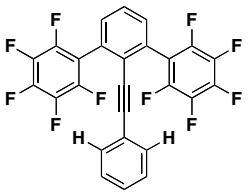
B97-D data:



1a



1a'



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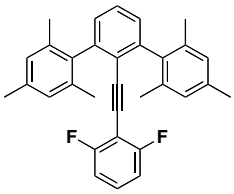

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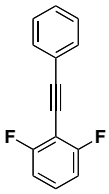

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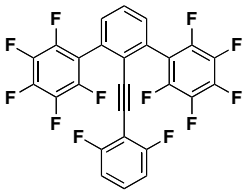

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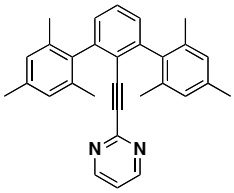
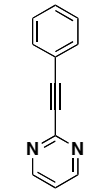
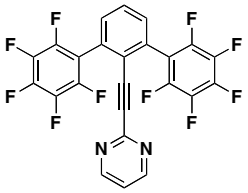


1d



1d'



1d"

1a α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2165114403	0.0000000000	-3.4692959499
C	6.0	0.0000000000	0.0000000000	-4.1735942182
C	6.0	0.0000000000	0.0000000000	-1.3600873081
C	6.0	1.2345370303	0.0000000000	-2.0667298836
C	6.0	0.0000000000	0.0000000000	0.0629280058
C	6.0	0.0000000000	0.0000000000	1.2886141263
C	6.0	0.0000000000	0.0000000000	2.7116330732
C	6.0	1.2231574480	0.0000000000	3.4295709933
C	6.0	1.2176738622	0.0000000000	4.8314271661
C	6.0	0.0000000000	0.0000000000	5.5383290143
C	6.0	2.5289318953	0.0000000000	-1.3208443724
C	6.0	4.9812981292	0.0000000000	0.0992459699
C	6.0	4.3510190487	1.2071400767	-0.2533664849
C	6.0	3.1317870683	1.2253899017	-0.9544543745
C	6.0	6.3184875077	0.0000000000	0.8125448794
C	6.0	2.4630774428	2.5444098083	-1.2860508976
H	1.0	2.1658920353	0.0000000000	-4.0066678169
H	1.0	0.0000000000	0.0000000000	-5.2646085436
H	1.0	2.1640416933	0.0000000000	5.3744740418
H	1.0	0.0000000000	0.0000000000	6.6294312597

H	1.0	4.8155612401	2.1560862491	0.0243066802
H	1.0	7.1477196467	0.0000000000	0.0849061562
H	1.0	6.4367753921	0.8924705512	1.4442719329
H	1.0	3.1024862019	3.3923107360	-1.0051624007
H	1.0	1.5064968976	2.6402254261	-0.7478742937
H	1.0	2.2322613055	2.6183266663	-2.3593191055
H	1.0	2.1609115836	0.0000000000	2.8738670170

1a β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2151214138	0.0000000000	-3.4395121453
C	6.0	0.0000000000	0.0000000000	-4.1444603861
C	6.0	0.0000000000	0.0000000000	-1.3287041269
C	6.0	1.2328379588	0.0000000000	-2.0358889038
C	6.0	0.0000000000	0.0000000000	0.1003264302
C	6.0	0.0000000000	0.0000000000	1.3258951189
C	6.0	0.0000000000	0.0000000000	2.7537770394
C	6.0	0.0000000000	1.2202529413	3.4735724163
C	6.0	0.0000000000	1.2162824457	4.8759090092
C	6.0	0.0000000000	0.0000000000	5.5835327720
C	6.0	2.5346416052	0.0000000000	-1.3027472609
C	6.0	5.0234684445	0.0000000000	0.0510700185
C	6.0	4.3843603091	1.2071309769	-0.2848804349
C	6.0	3.1473007152	1.2253600354	-0.9535806778
C	6.0	6.3773500765	0.0000000000	0.7324382783
C	6.0	2.4723723867	2.5439783039	-1.2747304552
H	1.0	2.1655528155	0.0000000000	-3.9749672015
H	1.0	0.0000000000	0.0000000000	-5.2355152357
H	1.0	0.0000000000	2.1635229034	5.4173240281
H	1.0	0.0000000000	0.0000000000	6.6745438286
H	1.0	4.8559531011	2.1559460189	-0.0190127965
H	1.0	7.1896490857	0.0000000000	-0.0138974576
H	1.0	6.5092302824	0.8920577417	1.3620187400
H	1.0	3.1095302520	3.3926722710	-0.9909741601
H	1.0	1.5159991256	2.6327378328	-0.7348548365
H	1.0	2.2387283163	2.6241457543	-2.3470897532
H	1.0	0.0000000000	2.1599839781	2.9217332651

1a' α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	4.8701642932
C	6.0	1.2167724642	0.0000000000	4.1624718062
C	6.0	1.2212026166	0.0000000000	2.7605988083

C	6.0	0.0000000000	0.0000000000	2.0391285645
C	6.0	0.0000000000	0.0000000000	0.6137715113
H	1.0	0.0000000000	0.0000000000	5.9611551536
H	1.0	2.1637442990	0.0000000000	4.7043140275
H	1.0	2.1612050741	0.0000000000	2.2092246036

1a' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2164474145	0.0000000000	-3.4141658091
C	6.0	0.0000000000	0.0000000000	-4.1215726140
C	6.0	0.0000000000	0.0000000000	-1.2916356281
C	6.0	1.2205519493	0.0000000000	-2.0114717932
C	6.0	0.0000000000	0.0000000000	0.1383552178
C	6.0	0.0000000000	0.0000000000	1.3650984781
C	6.0	0.0000000000	0.0000000000	2.7950906695
C	6.0	0.0000000000	1.2205536049	3.5149238483
C	6.0	0.0000000000	1.2164486835	4.9176180239
C	6.0	0.0000000000	0.0000000000	5.6250234830
H	1.0	2.1604536226	0.0000000000	-1.4599489718
H	1.0	2.1636599531	0.0000000000	-3.9555988329
H	1.0	0.0000000000	0.0000000000	-5.2126026920
H	1.0	0.0000000000	2.1604551731	2.9634037733
H	1.0	0.0000000000	2.1636655895	5.4590418062
H	1.0	0.0000000000	0.0000000000	6.7160567975

1a" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2154932233	0.0000000000	-3.4908913581
C	6.0	0.0000000000	0.0000000000	-4.1956138667
C	6.0	0.0000000000	0.0000000000	-1.3698178694
C	6.0	1.2251115323	0.0000000000	-2.0904381649
C	6.0	0.0000000000	0.0000000000	0.0514165876
C	6.0	0.0000000000	0.0000000000	1.2773471041
C	6.0	0.0000000000	0.0000000000	2.7006449956
C	6.0	1.2227332515	0.0000000000	3.4184386893
C	6.0	1.2178868216	0.0000000000	4.8198103839
C	6.0	0.0000000000	0.0000000000	5.5256816478
C	6.0	2.5149194770	0.0000000000	-1.3417301071
C	6.0	4.9294483924	0.0000000000	0.1398950902
C	6.0	4.3303455591	1.2157835770	-0.2251288689
C	6.0	3.1330571907	1.2001645569	-0.9560815113
F	9.0	6.0728629449	0.0000000000	0.8354735262
F	9.0	2.5689078153	2.3736346092	-1.2826988287

H	1.0	2.1641422217	0.0000000000	-4.0278012569
H	1.0	0.0000000000	0.0000000000	-5.2855380409
H	1.0	2.1640707021	0.0000000000	5.3624037371
H	1.0	0.0000000000	0.0000000000	6.6165352441
F	9.0	4.9031402622	2.3748790476	0.1278111139
H	1.0	2.1622629673	0.0000000000	2.8661762650

1a" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2149234329	0.0000000000	-3.4790391332
C	6.0	0.0000000000	0.0000000000	-4.1836183525
C	6.0	0.0000000000	0.0000000000	-1.3581470389
C	6.0	1.2239291434	0.0000000000	-2.0775936689
C	6.0	0.0000000000	0.0000000000	0.0684961039
C	6.0	0.0000000000	0.0000000000	1.2938327414
C	6.0	0.0000000000	0.0000000000	2.7223291008
C	6.0	0.0000000000	1.2220499728	3.4387731464
C	6.0	0.0000000000	1.2171122741	4.8410246913
C	6.0	0.0000000000	0.0000000000	5.5471858908
C	6.0	2.5173372121	0.0000000000	-1.3344358556
C	6.0	4.9568236253	0.0000000000	0.1057641167
C	6.0	4.3510694426	1.2155129560	-0.2484461033
C	6.0	3.1416640697	1.1999351825	-0.9587150615
F	9.0	6.1113897884	0.0000000000	0.7818421575
F	9.0	2.5719688417	2.3738513375	-1.2769562169
H	1.0	2.1639290986	0.0000000000	-4.0152835155
H	1.0	0.0000000000	0.0000000000	-5.2736247715
H	1.0	0.0000000000	2.1637875700	5.3828745198
H	1.0	0.0000000000	0.0000000000	6.6380571043
F	9.0	4.9289369091	2.3750223354	0.0949158997
H	1.0	0.0000000000	2.1615204050	2.8866896321

1d α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2157920495	0.0000000000	-3.4191705080
C	6.0	0.0000000000	0.0000000000	-4.1231900618
C	6.0	0.0000000000	0.0000000000	-1.3132295232
C	6.0	1.2343409196	0.0000000000	-2.0157098138
C	6.0	0.0000000000	0.0000000000	0.1150874437
C	6.0	0.0000000000	0.0000000000	1.3390568627
C	6.0	0.0000000000	0.0000000000	2.7737741046
N	7.0	0.0000000000	1.2107664878	3.3826647999
C	6.0	0.0000000000	1.1913985802	4.7233769270

C	6.0	0.0000000000	0.0000000000	5.4663528302
C	6.0	2.5335561019	0.0000000000	-1.2782188661
C	6.0	5.0156392069	0.0000000000	0.0854655493
C	6.0	4.3775917302	1.2072654622	-0.2518296715
C	6.0	3.1430926885	1.2259861633	-0.9250561246
C	6.0	6.3680397127	0.0000000000	0.7695206118
C	6.0	2.4674644656	2.5447837530	-1.2432930071
H	1.0	2.1658961038	0.0000000000	-3.9550657909
H	1.0	0.0000000000	0.0000000000	-5.2142346549
H	1.0	0.0000000000	2.1658173308	5.2213723541
H	1.0	0.0000000000	0.0000000000	6.5560081314
H	1.0	4.8474433886	2.1560825182	0.0169030535
H	1.0	7.1814875165	0.0000000000	0.0243525892
H	1.0	6.4990575310	0.8922364099	1.3989703594
H	1.0	3.1122785620	3.3926127831	-0.9749552068
H	1.0	1.5220595517	2.6416076973	-0.6860517426
H	1.0	2.2164008866	2.6192137992	-2.3121263608

1d β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2166522419	0.0000000000	-3.4119118268
C	6.0	0.0000000000	0.0000000000	-4.1150388690
C	6.0	0.0000000000	0.0000000000	-1.3039600065
C	6.0	1.2360078937	0.0000000000	-2.0091616827
C	6.0	0.0000000000	0.0000000000	0.1195900125
C	6.0	0.0000000000	0.0000000000	1.3442889204
C	6.0	0.0000000000	0.0000000000	2.7751905468
N	7.0	1.2121320174	0.0000000000	3.3858202462
C	6.0	1.1915906709	0.0000000000	4.7256484267
C	6.0	0.0000000000	0.0000000000	5.4694071155
C	6.0	2.5375109771	0.0000000000	-1.2766066743
C	6.0	5.0221848341	0.0000000000	0.0809369065
C	6.0	4.3842212667	1.2070059748	-0.2562532967
C	6.0	3.1483565710	1.2257163848	-0.9262640791
C	6.0	6.3742399863	0.0000000000	0.7653019735
C	6.0	2.4728025323	2.5446326640	-1.2443931861
H	1.0	2.1657694853	0.0000000000	-3.9493828322
H	1.0	0.0000000000	0.0000000000	-5.2061723737
H	1.0	2.1659742651	0.0000000000	5.2239839738
H	1.0	0.0000000000	0.0000000000	6.5590913822
H	1.0	4.8540929258	2.1557963811	0.0124033248
H	1.0	7.1884443013	0.0000000000	0.0208796202
H	1.0	6.5043929039	0.8921626750	1.3949462582
H	1.0	3.1163176170	3.3924036044	-0.9727141533
H	1.0	1.5252042664	2.6402466233	-0.6904750372
H	1.0	2.2248453008	2.6216158404	-2.3138415693

1d' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2180883685	0.0000000000	-3.3495991311
C	6.0	0.0000000000	0.0000000000	-4.0552591063
C	6.0	0.0000000000	0.0000000000	-1.2304001856
C	6.0	1.2229406753	0.0000000000	-1.9480267287
C	6.0	0.0000000000	0.0000000000	0.1941531581
C	6.0	0.0000000000	0.0000000000	1.4200625464
C	6.0	0.0000000000	0.0000000000	2.8523846351
N	7.0	1.2120136877	0.0000000000	3.4627274562
C	6.0	1.1915685536	0.0000000000	4.8029749086
C	6.0	0.0000000000	0.0000000000	5.5463112547
H	1.0	2.1611884845	0.0000000000	-1.3940497170
H	1.0	2.1640975507	0.0000000000	-3.8927054355
H	1.0	0.0000000000	0.0000000000	-5.1462720702
H	1.0	2.1657423945	0.0000000000	5.3014968631
H	1.0	0.0000000000	0.0000000000	6.6359471732

1d' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2166524221	0.0000000000	-3.3532491718
C	6.0	0.0000000000	0.0000000000	-4.0600361064
C	6.0	0.0000000000	0.0000000000	-1.2341478073
C	6.0	1.2217650404	0.0000000000	-1.9508559646
C	6.0	0.0000000000	0.0000000000	0.1949619055
C	6.0	0.0000000000	0.0000000000	1.4201237472
C	6.0	0.0000000000	0.0000000000	2.8578562758
N	7.0	0.0000000000	1.2104128122	3.4666906534
C	6.0	0.0000000000	1.1913087930	4.8078300853
C	6.0	0.0000000000	0.0000000000	5.5506633266
H	1.0	2.1614219201	0.0000000000	-1.3993048471
H	1.0	2.1636900331	0.0000000000	-3.8946823144
H	1.0	0.0000000000	0.0000000000	-5.1509672620
H	1.0	0.0000000000	2.1658287727	5.3054448107
H	1.0	0.0000000000	0.0000000000	6.6403632543

1d" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z

C	6.0	1.2170033586	0.0000000000	-3.4618505576
C	6.0	0.0000000000	0.0000000000	-4.1643811781
C	6.0	0.0000000000	0.0000000000	-1.3460853979
C	6.0	1.2274603921	0.0000000000	-2.0615657872
C	6.0	0.0000000000	0.0000000000	0.0758619281
C	6.0	0.0000000000	0.0000000000	1.2995393989
C	6.0	0.0000000000	0.0000000000	2.7321215942
N	7.0	1.2124258674	0.0000000000	3.3378378667
C	6.0	1.1927368111	0.0000000000	4.6786735904
C	6.0	0.0000000000	0.0000000000	5.4202904825
C	6.0	2.5149556701	0.0000000000	-1.3087834674
C	6.0	4.9135343324	0.0000000000	0.1954725329
C	6.0	4.3184826644	1.2156069890	-0.1753399756
C	6.0	3.1287148258	1.2002708108	-0.9174525362
F	9.0	6.0494002856	0.0000000000	0.9023900920
F	9.0	2.5652008890	2.3735011718	-1.2488391905
H	1.0	2.1649147249	0.0000000000	-3.9997289966
H	1.0	0.0000000000	0.0000000000	-5.2544841619
H	1.0	2.1664782762	0.0000000000	5.1771836343
H	1.0	0.0000000000	0.0000000000	6.5098027727
F	9.0	4.8869770981	2.3747976222	0.1833851469

1d" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2152548758	0.0000000000	-3.4407304963
C	6.0	0.0000000000	0.0000000000	-4.1446747709
C	6.0	0.0000000000	0.0000000000	-1.3238435638
C	6.0	1.2252622097	0.0000000000	-2.0393995806
C	6.0	0.0000000000	0.0000000000	0.1029765904
C	6.0	0.0000000000	0.0000000000	1.3263615511
C	6.0	0.0000000000	0.0000000000	2.7649043491
N	7.0	0.0000000000	1.2106991107	3.3689719596
C	6.0	0.0000000000	1.1923718536	4.7105048404
C	6.0	0.0000000000	0.0000000000	5.4519713148
C	6.0	2.5178630285	0.0000000000	-1.2951803512
C	6.0	4.9546589176	0.0000000000	0.1467853379
C	6.0	4.3499978291	1.2159373934	-0.2082109035
C	6.0	3.1413975656	1.2007570102	-0.9198907101
F	9.0	6.1084020428	0.0000000000	0.8243074691
F	9.0	2.5729224469	2.3734951333	-1.2413460029
H	1.0	2.1641711788	0.0000000000	-3.9769955787
H	1.0	0.0000000000	0.0000000000	-5.2346722600
H	1.0	0.0000000000	2.1666159179	5.2078982161
H	1.0	0.0000000000	0.0000000000	6.5415259214
F	9.0	4.9284441738	2.3747957418	0.1349636836

1aF α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2166605579	0.0000000000	-3.4572759377
C	6.0	0.0000000000	0.0000000000	-4.1610181735
C	6.0	0.0000000000	0.0000000000	-1.3502852492
C	6.0	1.2358429108	0.0000000000	-2.0547574973
C	6.0	0.0000000000	0.0000000000	0.0721278363
C	6.0	0.0000000000	0.0000000000	1.2965090520
C	6.0	0.0000000000	0.0000000000	2.7117222523
C	6.0	1.2007914745	0.0000000000	3.4664284385
C	6.0	1.2229475191	0.0000000000	4.8607977748
C	6.0	0.0000000000	0.0000000000	5.5555874049
C	6.0	2.5325054264	0.0000000000	-1.3131485434
C	6.0	4.9961724817	0.0000000000	0.0837979204
C	6.0	4.3636496330	1.2069206238	-0.2636475380
C	6.0	3.1381836130	1.2253733520	-0.9526871579
C	6.0	6.3363937631	0.0000000000	0.7911599660
C	6.0	2.4657828659	2.5438703587	-1.2788258796
H	1.0	2.1659947570	0.0000000000	-3.9944937237
H	1.0	0.0000000000	0.0000000000	-5.2520855284
H	1.0	2.1803075265	0.0000000000	5.3782554918
H	1.0	0.0000000000	0.0000000000	6.6454717329
H	1.0	4.8294776258	2.1557214152	0.0122539745
H	1.0	7.1633553697	0.0000000000	0.0608389176
H	1.0	6.4558301996	0.8921008699	1.4230972817
H	1.0	3.1062096517	3.3924219884	-1.0022079087
H	1.0	1.5129778476	2.6393160270	-0.7337788481
H	1.0	2.2269455310	2.6186920540	-2.3503764805
F	9.0	2.3670821336	0.0000000000	2.7952506608

1aF β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2162223838	0.0000000000	-3.4520554801
C	6.0	0.0000000000	0.0000000000	-4.1556426085
C	6.0	0.0000000000	0.0000000000	-1.3455196376
C	6.0	1.2342883421	0.0000000000	-2.0486050856
C	6.0	0.0000000000	0.0000000000	0.0816269874
C	6.0	0.0000000000	0.0000000000	1.3051646874
C	6.0	0.0000000000	0.0000000000	2.7244579114
C	6.0	0.0000000000	1.1981979017	3.4791759028
C	6.0	0.0000000000	1.2222252822	4.8738291407
C	6.0	0.0000000000	0.0000000000	5.5688356711

C	6.0	2.5319481230	0.0000000000	-1.3081362500
C	6.0	5.0083191312	0.0000000000	0.0670433833
C	6.0	4.3713482167	1.2071812431	-0.2726551212
C	6.0	3.1395408227	1.2258331739	-0.9510322646
C	6.0	6.3583106000	0.0000000000	0.7562145738
C	6.0	2.4634897012	2.5448459469	-1.2677776799
H	1.0	2.1659018857	0.0000000000	-3.9886902851
H	1.0	0.0000000000	0.0000000000	-5.2467158621
H	1.0	0.0000000000	2.1800169229	5.3904603850
H	1.0	0.0000000000	0.0000000000	6.6586855624
H	1.0	4.8398347323	2.1560506958	-0.0015927168
H	1.0	7.1743652631	0.0000000000	0.0138269868
H	1.0	6.4870150349	0.8922182035	1.3861794073
H	1.0	3.1088023923	3.3926151111	-1.0003858098
H	1.0	1.5191575117	2.6414455773	-0.7084467336
H	1.0	2.2098894509	2.6197320403	-2.3359084845
F	9.0	0.0000000000	2.3669947354	2.8082521971

1aF' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2173826802	0.0000000000	-3.4037453683
C	6.0	0.0000000000	0.0000000000	-4.1105422742
C	6.0	0.0000000000	0.0000000000	-1.2833793403
C	6.0	1.2225016441	0.0000000000	-2.0020069332
C	6.0	0.0000000000	0.0000000000	0.1407051995
C	6.0	0.0000000000	0.0000000000	1.3665149466
C	6.0	0.0000000000	0.0000000000	2.7838281799
C	6.0	1.1991382255	0.0000000000	3.5409140966
C	6.0	1.2223365089	0.0000000000	4.9349687619
C	6.0	0.0000000000	0.0000000000	5.6304022851
H	1.0	2.1614909598	0.0000000000	-1.4491536631
H	1.0	2.1639092582	0.0000000000	-3.9461900951
H	1.0	0.0000000000	0.0000000000	-5.2015392916
F	9.0	2.3679192765	0.0000000000	2.8711975595
H	1.0	2.1801363774	0.0000000000	5.4516193875
H	1.0	0.0000000000	0.0000000000	6.7202206042

1aF' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2168691720	0.0000000000	-3.4080313721
C	6.0	0.0000000000	0.0000000000	-4.1146711011

C	6.0	0.0000000000	0.0000000000	-1.2876961862
C	6.0	1.2213330391	0.0000000000	-2.0055018324
C	6.0	0.0000000000	0.0000000000	0.1413041311
C	6.0	0.0000000000	0.0000000000	1.3664537563
C	6.0	0.0000000000	0.0000000000	2.7884790048
C	6.0	0.0000000000	1.1984486188	3.5442484857
C	6.0	0.0000000000	1.2221363247	4.9392171537
C	6.0	0.0000000000	0.0000000000	5.6341113540
H	1.0	2.1608276484	0.0000000000	-1.4535157988
H	1.0	2.1637173307	0.0000000000	-3.9499073884
H	1.0	0.0000000000	0.0000000000	-5.2056952900
F	9.0	0.0000000000	2.3671414182	2.8754542609
H	1.0	0.0000000000	2.1800678572	5.4555997707
H	1.0	0.0000000000	0.0000000000	6.7240055737

1aF" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

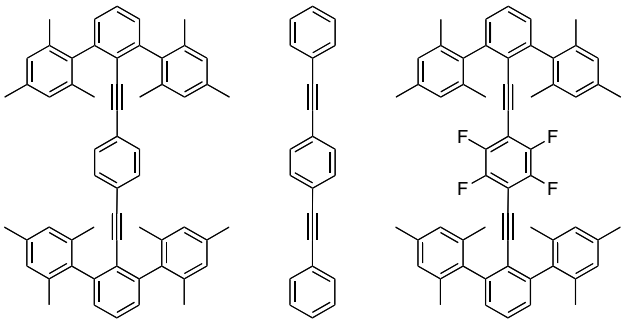
ATOM	CHARGE	X	Y	Z
C	6.0	1.2174559816	0.0000000000	-3.5203079074
C	6.0	0.0000000000	0.0000000000	-4.2229265050
C	6.0	0.0000000000	0.0000000000	-1.4057572604
C	6.0	1.2278761904	0.0000000000	-2.1202506770
C	6.0	0.0000000000	0.0000000000	0.0140118291
C	6.0	0.0000000000	0.0000000000	1.2376115716
C	6.0	0.0000000000	0.0000000000	2.6520118609
C	6.0	1.2013079312	0.0000000000	3.4042527924
C	6.0	1.2244071143	0.0000000000	4.7974603477
C	6.0	0.0000000000	0.0000000000	5.4902735664
C	6.0	2.5083127531	0.0000000000	-1.3551548522
C	6.0	4.8643244568	0.0000000000	0.2166365348
C	6.0	4.2802472118	1.2152253051	-0.1713912596
C	6.0	3.1119541256	1.1998321942	-0.9465102113
F	9.0	5.9785607652	0.0000000000	0.9571372389
F	9.0	2.5557991410	2.3736378315	-1.2883842409
H	1.0	2.1651100624	0.0000000000	-4.0587747850
H	1.0	0.0000000000	0.0000000000	-5.3129475242
H	1.0	2.1808651258	0.0000000000	5.3162354798
H	1.0	0.0000000000	0.0000000000	6.5799781338
F	9.0	4.8370538022	2.3745083950	0.2054802178
F	9.0	2.3669855376	0.0000000000	2.7277174956

1aF" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2153987742	0.0000000000	-3.4767851257

C	6.0	0.0000000000	0.0000000000	-4.1806337730
C	6.0	0.0000000000	0.0000000000	-1.3582455280
C	6.0	1.2249190891	0.0000000000	-2.0754636677
C	6.0	0.0000000000	0.0000000000	0.0678295436
C	6.0	0.0000000000	0.0000000000	1.2914215667
C	6.0	0.0000000000	0.0000000000	2.7121806894
C	6.0	0.0000000000	1.2002357616	3.4646842455
C	6.0	0.0000000000	1.2230460506	4.8591788141
C	6.0	0.0000000000	0.0000000000	5.5526547921
C	6.0	2.5175563408	0.0000000000	-1.3312243639
C	6.0	4.9539193466	0.0000000000	0.1121973739
C	6.0	4.3491852897	1.2158132149	-0.2430811975
C	6.0	3.1409382273	1.2005240721	-0.9553617869
F	9.0	6.1073025054	0.0000000000	0.7902648524
F	9.0	2.5721929035	2.3735157455	-1.2761572207
H	1.0	2.1642319888	0.0000000000	-4.0131621214
H	1.0	0.0000000000	0.0000000000	-5.2706844111
H	1.0	0.0000000000	2.1803942612	5.3763875303
H	1.0	0.0000000000	0.0000000000	6.6424124500
F	9.0	4.9271693292	2.3748406355	0.1007024568
F	9.0	0.0000000000	2.3657939423	2.7927188102



2 **2'** **2F**

2 ⊥α C_{2v}

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2166379534	0.0000000000	-7.6183835954
C	6.0	0.0000000000	0.0000000000	-8.3226551493
C	6.0	0.0000000000	0.0000000000	-5.5093943835
C	6.0	1.2348637338	0.0000000000	-6.2159906336
C	6.0	0.0000000000	0.0000000000	-4.0871307603
C	6.0	0.0000000000	0.0000000000	-2.8609100292
C	6.0	0.0000000000	0.0000000000	-1.4408445765
C	6.0	1.2216455876	0.0000000000	-0.7184176269
C	6.0	2.5290305974	0.0000000000	-5.4699888301
C	6.0	4.9801317902	0.0000000000	-4.0479742517

C	6.0	4.3501504395	1.2072631259	-4.4010584346
C	6.0	3.1315202313	1.2254543938	-5.1032809614
C	6.0	6.3169470788	0.0000000000	-3.3335958011
C	6.0	2.4624426125	2.5439562482	-5.4360094795
C	6.0	1.2201931910	0.0000000000	0.6780934483
C	6.0	0.0000000000	0.0000000000	1.4017308122
C	6.0	0.0000000000	0.0000000000	2.8266914214
C	6.0	0.0000000000	0.0000000000	4.0528628936
C	6.0	0.0000000000	0.0000000000	5.4815554618
C	6.0	0.0000000000	1.2154073898	7.5915659547
C	6.0	0.0000000000	1.2330460778	6.1879686979
C	6.0	0.0000000000	0.0000000000	8.2962603677
C	6.0	0.0000000000	2.5328926340	5.4518385401
C	6.0	0.0000000000	5.0135482999	4.0836615304
C	6.0	1.2071598193	4.3764876576	4.4232938582
C	6.0	1.2253564705	3.1433104082	5.0989174949
C	6.0	0.0000000000	6.3634844739	3.3948935761
C	6.0	2.5437920563	2.4693175078	5.4223730958
H	1.0	2.1659450926	0.0000000000	-8.1558841735
H	1.0	0.0000000000	0.0000000000	-9.4136580239
H	1.0	2.1610356907	0.0000000000	-1.2709413113
H	1.0	4.8145433609	2.1561725796	-4.1229251896
H	1.0	7.1466078505	0.0000000000	-4.0607819691
H	1.0	6.4349766697	0.8925195605	-2.7018820866
H	1.0	3.1011602163	3.3925172452	-5.1554139045
H	1.0	1.5055322845	2.6396288327	-4.8983751082
H	1.0	2.2320963992	2.6168562372	-6.5094059529
H	1.0	0.0000000000	0.0000000000	9.3873232429
H	1.0	2.1606808325	0.0000000000	1.2283163804
H	1.0	0.0000000000	2.1656023657	8.1275131264
H	1.0	2.1559732494	4.8463276694	4.1543253134
H	1.0	0.0000000000	7.1795247972	4.1372805027
H	1.0	0.8920422720	6.4921257180	2.7647554745
H	1.0	3.3925502054	3.1065040147	5.1387408559
H	1.0	2.6341327614	1.5125924974	4.8833465073
H	1.0	2.6224554172	2.2367381066	6.4950539153

2' $\perp\gamma$ D_2

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.9700735356	0.7324917183	-7.6087260663
C	6.0	0.0000000000	0.0000000000	-8.3138270405
C	6.0	0.0000000000	0.0000000000	-5.4975270511
C	6.0	0.9855592035	0.7426480454	-6.2060135874
C	6.0	0.0000000000	0.0000000000	-4.0720735794
C	6.0	0.0000000000	0.0000000000	-2.8452935081
C	6.0	0.0000000000	0.0000000000	-1.4226320764

C	6.0	1.2207361447	0.0057310579	-0.6982618279
C	6.0	2.0198718148	1.5331167783	-5.4731701082
C	6.0	3.9934349485	3.0446509973	-4.1120572605
C	6.0	2.7481759297	3.6109426910	-4.4396817217
C	6.0	4.2237071717	1.7010320934	-4.4583067797
C	6.0	1.7560569531	2.8743685654	-5.1108725897
C	6.0	3.2544578913	0.9351421053	-5.1309351130
C	6.0	5.0674381133	3.8674351563	-3.4293454875
C	6.0	0.4121535750	3.5068951520	-5.4134714841
C	6.0	3.5270971851	-0.5200805634	-5.4586268709
H	1.0	1.7260990046	1.3078867627	-8.1448552428
H	1.0	0.0000000000	0.0000000000	-9.4047798095
H	1.0	2.1609111135	0.0160291423	-1.2489985798
H	1.0	2.5385544331	4.6466107842	-4.1623795678
H	1.0	5.1785499737	1.2363501013	-4.2015988319
H	1.0	5.6926962310	4.3888427883	-4.1736090409
H	1.0	4.6297172927	4.6340012877	-2.7731476242
H	1.0	5.7337054551	3.2337514624	-2.8260232595
H	1.0	0.3932576906	4.5596607932	-5.1002136450
H	1.0	4.5538344585	-0.7986364255	-5.1857122665
H	1.0	0.1749979549	3.4561698787	-6.4870440698
H	1.0	3.3810356091	-0.7254336918	-6.5299362954
H	1.0	-0.3934791196	2.9749728344	-4.8833175775
H	1.0	2.8317234589	-1.1770500857	-4.9122739638

2 ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2169738050	0.0000000000	-7.5955113655
C	6.0	0.0000000000	0.0000000000	-8.2995055906
C	6.0	0.0000000000	0.0000000000	-5.4869623996
C	6.0	1.2351168291	0.0000000000	-6.1932679000
C	6.0	0.0000000000	0.0000000000	-4.0651621096
C	6.0	0.0000000000	0.0000000000	-2.8387317095
C	6.0	0.0000000000	0.0000000000	-1.4195020586
C	6.0	1.2233945302	0.0000000000	-0.6978274940
C	6.0	2.5269808113	0.0000000000	-5.4432941976
C	6.0	4.9640242364	0.0000000000	-3.9972698403
C	6.0	4.3380692773	1.2071818275	-4.3575774029
C	6.0	3.1262702072	1.2253988709	-5.0713025768
C	6.0	6.2920860294	0.0000000000	-3.2670356925
C	6.0	2.4597402097	2.5439846615	-5.4085653998
H	1.0	2.1661600375	0.0000000000	-8.1331857113
H	1.0	0.0000000000	0.0000000000	-9.3905261580
H	1.0	2.1616994326	0.0000000000	-1.2522856941
H	1.0	4.7994608925	2.1560674122	-4.0744805438
H	1.0	7.1303420594	0.0000000000	-3.9842291005

H	1.0	6.4021817234	0.8924659147	-2.6338554984
H	1.0	3.0981352078	3.3923749482	-5.1268359888
H	1.0	1.5011071667	2.6410921768	-4.8742033099
H	1.0	2.2327619600	2.6154564350	-6.4827546054

2 ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2153735340	0.0000000000	-7.6135880174
C	6.0	0.0000000000	0.0000000000	-8.3182670036
C	6.0	0.0000000000	0.0000000000	-5.5033021648
C	6.0	1.2331605086	0.0000000000	-6.2099760817
C	6.0	0.0000000000	0.0000000000	-4.0743842142
C	6.0	0.0000000000	0.0000000000	-2.8483676494
C	6.0	0.0000000000	0.0000000000	-1.4228822371
C	6.0	0.0000000000	1.2185720669	-0.6986099008
C	6.0	2.5340150422	0.0000000000	-5.4749990249
C	6.0	5.0172801124	0.0000000000	-4.1109687689
C	6.0	4.3797113536	1.2070644057	-4.4498120112
C	6.0	3.1454637279	1.2253832050	-5.1235022865
C	6.0	6.3682752187	0.0000000000	-3.4240926653
C	6.0	2.4727515700	2.5444953633	-5.4474036251
H	1.0	2.1655048733	0.0000000000	-8.1495652069
H	1.0	0.0000000000	0.0000000000	-9.4093381903
H	1.0	0.0000000000	2.1600176857	-1.2470869436
H	1.0	4.8500416638	2.1559340635	-4.1819651235
H	1.0	7.1834684627	0.0000000000	-4.1673806988
H	1.0	6.4976451711	0.8920522393	-2.7941338391
H	1.0	3.1101340501	3.3925664671	-5.1623369994
H	1.0	1.5150628721	2.6356552469	-4.9104062575
H	1.0	2.2425584200	2.6238230904	-6.5205910991

2' ⊥α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.2168921653	0.0000000000	-7.6288655066
C	6.0	0.0000000000	0.0000000000	-8.3363404108
C	6.0	0.0000000000	0.0000000000	-5.5059479264
C	6.0	-1.2215803261	0.0000000000	-6.2272061511
C	6.0	0.0000000000	0.0000000000	-4.0811809302
C	6.0	0.0000000000	0.0000000000	-2.8530417292
C	6.0	0.0000000000	0.0000000000	-1.4304641275
C	6.0	-1.2195454792	0.0000000000	-0.7042723910
H	1.0	-2.1615957180	0.0000000000	-5.6758781962
C	6.0	-1.2191652524	0.0000000000	0.6925103334

C	6.0	0.0000000000	0.0000000000	1.4175338015
C	6.0	0.0000000000	0.0000000000	2.8446276341
C	6.0	0.0000000000	0.0000000000	4.0720054146
C	6.0	0.0000000000	0.0000000000	5.5018930640
C	6.0	0.0000000000	-1.2164569215	7.6239525754
C	6.0	0.0000000000	-1.2207958353	6.2213624837
C	6.0	0.0000000000	0.0000000000	8.3311764800
H	1.0	0.0000000000	-2.1607581395	5.6699620576
H	1.0	-2.1637012826	0.0000000000	-8.1708640081
H	1.0	0.0000000000	0.0000000000	-9.4272729936
H	1.0	-2.1614550151	0.0000000000	-1.2519099784
H	1.0	0.0000000000	0.0000000000	9.4221518390
H	1.0	-2.1607412693	0.0000000000	1.2407246110
H	1.0	0.0000000000	-2.1635840019	8.1654133481

2' ⊥γ D_2

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.9029154283	-0.8158213453	-7.6255390347
C	6.0	0.0000000000	0.0000000000	8.3329019718
C	6.0	0.0000000000	0.0000000000	5.5033598689
C	6.0	-0.9082487502	-0.8167532285	-6.2238023477
C	6.0	0.0000000000	0.0000000000	4.0764707677
C	6.0	0.0000000000	0.0000000000	2.8486116426
C	6.0	0.0000000000	0.0000000000	1.4241314822
C	6.0	-1.2194267511	-0.0032904429	-0.6983479220
H	1.0	-1.6043173887	-1.4470373460	-5.6709410707
H	1.0	-1.6037892373	-1.4515708771	-8.1684529575
H	1.0	0.0000000000	0.0000000000	9.4238053565
H	1.0	-2.1612403552	-0.0061710890	-1.2461675183

2' ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	8.3298034928
C	6.0	1.2169502725	0.0000000000	7.6223056117
C	6.0	1.2216378625	0.0000000000	6.2206769122
C	6.0	0.0000000000	0.0000000000	5.4992822116
C	6.0	0.0000000000	0.0000000000	4.0748485184
C	6.0	0.0000000000	0.0000000000	2.8464506805
C	6.0	0.0000000000	0.0000000000	1.4247296237
C	6.0	1.2199966513	0.0000000000	0.6978468845
H	1.0	0.0000000000	0.0000000000	9.4207484549
H	1.0	2.1616099137	0.0000000000	5.6693000192
H	1.0	2.1637670390	0.0000000000	8.1643084881

H	1.0	2.1616344967	0.0000000000	1.2459915502

2' ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	8.3373917623
C	6.0	1.2164929452	0.0000000000	7.6301699691
C	6.0	1.2207815522	0.0000000000	6.2275628731
C	6.0	0.0000000000	0.0000000000	5.5081287835
C	6.0	0.0000000000	0.0000000000	4.0782542932
C	6.0	0.0000000000	0.0000000000	2.8510651074
C	6.0	0.0000000000	0.0000000000	1.4233772924
C	6.0	0.0000000000	1.2187703513	0.6988991567
H	1.0	0.0000000000	0.0000000000	9.4283817511
H	1.0	2.1606892849	0.0000000000	5.6760965960
H	1.0	2.1636301646	0.0000000000	8.1716270364
H	1.0	0.0000000000	2.1605373143	1.2467904351

2F ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2173261626	0.0000000000	-7.6001175471
C	6.0	0.0000000000	0.0000000000	-8.3030958037
C	6.0	0.0000000000	0.0000000000	-5.4948161648
C	6.0	1.2371535196	0.0000000000	-6.1979065872
C	6.0	0.0000000000	0.0000000000	-4.0737453556
C	6.0	0.0000000000	0.0000000000	-2.8489032091
C	6.0	0.0000000000	0.0000000000	-1.4376002226
C	6.0	1.2094595387	0.0000000000	-0.6968492911
C	6.0	2.5314666582	0.0000000000	-5.4524242598
C	6.0	4.9821933934	0.0000000000	-4.0330688455
C	6.0	4.3534830180	1.2068570072	-4.3876207149
C	6.0	3.1343826149	1.2255638460	-5.0876391242
C	6.0	6.3134513497	0.0000000000	-3.3095439510
C	6.0	2.4656808767	2.5444929725	-5.4198176238
H	1.0	2.1662420410	0.0000000000	-8.1380045993
H	1.0	0.0000000000	0.0000000000	-9.3941401443
F	9.0	2.3796128770	0.0000000000	-1.3511570084
H	1.0	4.8165590882	2.1555482940	-4.1069858210
H	1.0	7.1489768519	0.0000000000	-4.0300145826
H	1.0	6.4248685624	0.8920078917	-2.6762531022
H	1.0	3.1070243882	3.3923263880	-5.1434334534
H	1.0	1.5112329138	2.6441408516	-4.8782468440
H	1.0	2.2306144790	2.6171217589	-6.4923234625

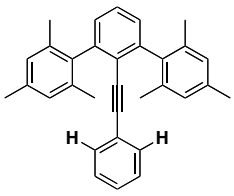
2F ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

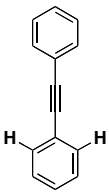
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2169402356	0.0000000000	-7.6085184162
C	6.0	0.0000000000	0.0000000000	-8.3112655114
C	6.0	0.0000000000	0.0000000000	-5.5043596529
C	6.0	1.2352615826	0.0000000000	-6.2053589488
C	6.0	0.0000000000	0.0000000000	-4.0775874664
C	6.0	0.0000000000	0.0000000000	-2.8540374674
C	6.0	0.0000000000	0.0000000000	-1.4377867622
C	6.0	0.0000000000	1.2059809021	-0.6974726670
C	6.0	2.5296134570	0.0000000000	-5.4592994926
C	6.0	4.9890867174	0.0000000000	-4.0547784016
C	6.0	4.3568605643	1.2072666961	-4.4030782679
C	6.0	3.1332258502	1.2260894397	-5.0960723343
C	6.0	6.3293596834	0.0000000000	-3.3470577189
C	6.0	2.4609156876	2.5450851600	-5.4208013732
H	1.0	2.1661394648	0.0000000000	-8.1457381526
H	1.0	0.0000000000	0.0000000000	-9.4023442308
F	9.0	0.0000000000	2.3788929037	-1.3498173647
H	1.0	4.8221730795	2.1559705820	-4.1262258665
H	1.0	7.1551729362	0.0000000000	-4.0786456329
H	1.0	6.4494105851	0.8921198744	-2.7153899986
H	1.0	3.1051932450	3.3927989517	-5.1511035469
H	1.0	1.5129168186	2.6448111099	-4.8682759732
H	1.0	2.2145893612	2.6175303228	-6.4907529349

M06 data:



1a



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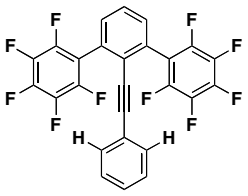

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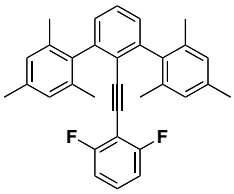

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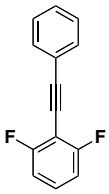

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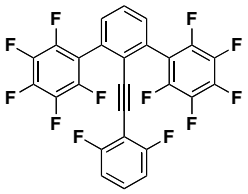

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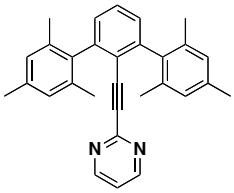

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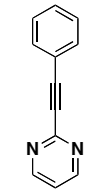

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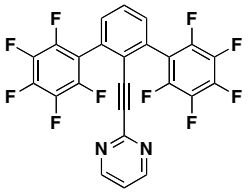


1d"

1a α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2037184332	0.0000000000	-3.3815423800
C	6.0	0.0000000000	0.0000000000	-4.0799404261
C	6.0	0.0000000000	0.0000000000	-1.2911826501
C	6.0	1.2203952031	0.0000000000	-1.9897052153
C	6.0	0.0000000000	0.0000000000	0.1315704949
C	6.0	0.0000000000	0.0000000000	1.3460151829
C	6.0	0.0000000000	0.0000000000	2.7675343464
C	6.0	1.2089177188	0.0000000000	3.4743191826
C	6.0	1.2061346598	0.0000000000	4.8631601350
C	6.0	0.0000000000	0.0000000000	5.5611885583
C	6.0	2.5167950380	0.0000000000	-1.2698575652
C	6.0	5.0167220417	0.0000000000	0.0049942533
C	6.0	4.3741093912	1.1965667666	-0.3074426223
C	6.0	3.1310026702	1.2144340584	-0.9379471073
C	6.0	6.3746334849	0.0000000000	0.6398222381
C	6.0	2.4539437219	2.5168391506	-1.2434662918
H	1.0	2.1526868909	0.0000000000	-3.9137594359
H	1.0	0.0000000000	0.0000000000	-5.1659918540
H	1.0	2.1471384113	0.0000000000	5.4052816646
H	1.0	0.0000000000	0.0000000000	6.6473147486

H	1.0	4.8535140736	2.1420551551	-0.0550114961
H	1.0	7.1621659657	0.0000000000	-0.1232700771
H	1.0	6.5267857634	0.8870120488	1.2629322746
H	1.0	3.0857428622	3.3660105361	-0.9683055569
H	1.0	1.5083862447	2.6067136870	-0.6928471934
H	1.0	2.2075185901	2.6028300660	-2.3081623815
H	1.0	2.1412432158	0.0000000000	2.9163267668

1a β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2031013011	0.0000000000	-3.3807822083
C	6.0	0.0000000000	0.0000000000	-4.0793674699
C	6.0	0.0000000000	0.0000000000	-1.2893157776
C	6.0	1.2193229519	0.0000000000	-1.9883037284
C	6.0	0.0000000000	0.0000000000	0.1384780571
C	6.0	0.0000000000	0.0000000000	1.3527729210
C	6.0	0.0000000000	0.0000000000	2.7784973388
C	6.0	0.0000000000	1.2070915683	3.4868051278
C	6.0	0.0000000000	1.2050947800	4.8760421202
C	6.0	0.0000000000	0.0000000000	5.5747658147
C	6.0	2.5176547000	0.0000000000	-1.2721209861
C	6.0	5.0180334014	0.0000000000	0.0003045541
C	6.0	4.3764423212	1.1964494482	-0.3137293386
C	6.0	3.1331631691	1.2143259790	-0.9431392029
C	6.0	6.3738902363	0.0000000000	0.6391788410
C	6.0	2.4561082043	2.5167151297	-1.2489480672
H	1.0	2.1526420658	0.0000000000	-3.9119802292
H	1.0	0.0000000000	0.0000000000	-5.1654684444
H	1.0	0.0000000000	2.1467386418	5.4170845314
H	1.0	0.0000000000	0.0000000000	6.6608309756
H	1.0	4.8559122123	2.1417309449	-0.0607251381
H	1.0	7.1640442059	0.0000000000	-0.1213407623
H	1.0	6.5234144055	0.8867785546	1.2631115730
H	1.0	3.0881566417	3.3659033389	-0.9742687503
H	1.0	1.5101213143	2.6068227009	-0.6987478114
H	1.0	2.2091691467	2.6029495896	-2.3135260096
H	1.0	0.0000000000	2.1409971712	2.9329845402

1a' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	4.8279110216
C	6.0	1.2052858102	0.0000000000	4.1288245410
C	6.0	1.2074526403	0.0000000000	2.7399169779

C	6.0	0.0000000000	0.0000000000	2.0304538008
C	6.0	0.0000000000	0.0000000000	0.6072475808
H	1.0	0.0000000000	0.0000000000	5.9138701363
H	1.0	2.1471347485	0.0000000000	4.6693844754
H	1.0	2.1413309127	0.0000000000	2.1863795922

1a' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2051470227	0.0000000000	-3.3802759742
C	6.0	0.0000000000	0.0000000000	-4.0789152844
C	6.0	0.0000000000	0.0000000000	-1.2823522932
C	6.0	1.2072738548	0.0000000000	-1.9908168575
C	6.0	0.0000000000	0.0000000000	0.1447238921
C	6.0	0.0000000000	0.0000000000	1.3585907723
C	6.0	0.0000000000	0.0000000000	2.7856648273
C	6.0	0.0000000000	1.2072631405	3.4942083970
C	6.0	0.0000000000	1.2051198514	4.8836359443
C	6.0	0.0000000000	0.0000000000	5.5822584480
H	1.0	2.1411950037	0.0000000000	-1.4373775106
H	1.0	2.1469545341	0.0000000000	-3.9209403948
H	1.0	0.0000000000	0.0000000000	-5.1649227210
H	1.0	0.0000000000	2.1413563195	2.9410469406
H	1.0	0.0000000000	2.1467755275	5.4245642254
H	1.0	0.0000000000	0.0000000000	6.6682806196

1a" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2026223740	0.0000000000	-3.4139524845
C	6.0	0.0000000000	0.0000000000	-4.1128020826
C	6.0	0.0000000000	0.0000000000	-1.3149357506
C	6.0	1.2108667442	0.0000000000	-2.0248628857
C	6.0	0.0000000000	0.0000000000	0.1047484776
C	6.0	0.0000000000	0.0000000000	1.3186521171
C	6.0	0.0000000000	0.0000000000	2.7396155746
C	6.0	1.2092370764	0.0000000000	3.4451301494
C	6.0	1.2067298871	0.0000000000	4.8335518775
C	6.0	0.0000000000	0.0000000000	5.5302932717
C	6.0	2.4994629133	0.0000000000	-1.2959078611
C	6.0	4.9654893376	0.0000000000	0.0331368098
C	6.0	4.3523357145	1.2036297735	-0.2908914947
C	6.0	3.1268708362	1.1898422226	-0.9444217399
F	9.0	6.1276974258	0.0000000000	0.6501977254
F	9.0	2.5550140824	2.3423675985	-1.2374684173

H	1.0	2.1493934866	0.0000000000	-3.9470411541
H	1.0	0.0000000000	0.0000000000	-5.1977913611
H	1.0	2.1472251723	0.0000000000	5.3759065013
H	1.0	0.0000000000	0.0000000000	6.6161892847
F	9.0	4.9376370603	2.3429774308	0.0191823316
H	1.0	2.1424705715	0.0000000000	2.8885237131

1a" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2019090936	0.0000000000	-3.4029801555
C	6.0	0.0000000000	0.0000000000	-4.1019031685
C	6.0	0.0000000000	0.0000000000	-1.3026304472
C	6.0	1.2096247091	0.0000000000	-2.0130927483
C	6.0	0.0000000000	0.0000000000	0.1221690827
C	6.0	0.0000000000	0.0000000000	1.3358753329
C	6.0	0.0000000000	0.0000000000	2.7620804380
C	6.0	0.0000000000	1.2087777303	3.4675477718
C	6.0	0.0000000000	1.2058872982	4.8566836947
C	6.0	0.0000000000	0.0000000000	5.5540067971
C	6.0	2.5027130064	0.0000000000	-1.2919504860
C	6.0	4.9879541464	0.0000000000	0.0003668254
C	6.0	4.3699576468	1.2033895189	-0.3147026010
C	6.0	3.1354618917	1.1895676382	-0.9502288282
F	9.0	6.1588476112	0.0000000000	0.5999252442
F	9.0	2.5588099007	2.3425560812	-1.2350510434
H	1.0	2.1491740609	0.0000000000	-3.9352156290
H	1.0	0.0000000000	0.0000000000	-5.1869478978
H	1.0	0.0000000000	2.1469772509	5.3981786138
H	1.0	0.0000000000	0.0000000000	6.6399303530
F	9.0	4.9590500715	2.3430567830	-0.0127906279
H	1.0	0.0000000000	2.1426692414	2.9142613413

1d α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2046700183	0.0000000000	-3.3649388718
C	6.0	0.0000000000	0.0000000000	-4.0616103153
C	6.0	0.0000000000	0.0000000000	-1.2769806467
C	6.0	1.2219935926	0.0000000000	-1.9732681134
C	6.0	0.0000000000	0.0000000000	0.1461780743
C	6.0	0.0000000000	0.0000000000	1.3590383072
C	6.0	0.0000000000	0.0000000000	2.7882414117
N	7.0	1.1949459104	0.0000000000	3.3932616391
C	6.0	1.1783306331	0.0000000000	4.7205522727

C	6.0	0.0000000000	0.0000000000	5.4570940156
C	6.0	2.5175179587	0.0000000000	-1.2527205961
C	6.0	5.0025225152	0.0000000000	0.0460536443
C	6.0	4.3653438383	1.1964840078	-0.2757669174
C	6.0	3.1285756880	1.2146728670	-0.9174759381
C	6.0	6.3506674607	0.0000000000	0.7009279978
C	6.0	2.4531060818	2.5170002525	-1.2266474162
H	1.0	2.1530792680	0.0000000000	-3.8978138832
H	1.0	0.0000000000	0.0000000000	-5.1477745087
H	1.0	2.1486193683	0.0000000000	5.2174443792
H	1.0	0.0000000000	0.0000000000	6.5410075671
H	1.0	4.8413617499	2.1416211401	-0.0161087144
H	1.0	7.1498515504	0.0000000000	-0.0501605404
H	1.0	6.4925261968	0.8868164557	1.3265843957
H	1.0	3.0879407177	3.3658921427	-0.9578621849
H	1.0	1.5107599231	2.6122939322	-0.6714140734
H	1.0	2.2018771034	2.5997574693	-2.2905150828

1d β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2035355045	0.0000000000	-3.3553318571
C	6.0	0.0000000000	0.0000000000	-4.0531691117
C	6.0	0.0000000000	0.0000000000	-1.2677856074
C	6.0	1.2206330851	0.0000000000	-1.9629763968
C	6.0	0.0000000000	0.0000000000	0.1593793838
C	6.0	0.0000000000	0.0000000000	1.3717308670
C	6.0	0.0000000000	0.0000000000	2.8044563750
N	7.0	0.0000000000	1.1939681747	3.4084266353
C	6.0	0.0000000000	1.1780714630	4.7362960353
C	6.0	0.0000000000	0.0000000000	5.4724394341
C	6.0	2.5179270166	0.0000000000	-1.2446238972
C	6.0	5.0177117215	0.0000000000	0.0274170439
C	6.0	4.3759361289	1.1965428557	-0.2858214565
C	6.0	3.1325278913	1.2148580028	-0.9148985522
C	6.0	6.3741185776	0.0000000000	0.6651021740
C	6.0	2.4548446434	2.5176876422	-1.2171183961
H	1.0	2.1528573769	0.0000000000	-3.8868037004
H	1.0	0.0000000000	0.0000000000	-5.1392363511
H	1.0	0.0000000000	2.1484186657	5.2329074676
H	1.0	0.0000000000	0.0000000000	6.5563141468
H	1.0	4.8549672565	2.1419122037	-0.0325070961
H	1.0	7.1635773090	0.0000000000	-0.0960390740
H	1.0	6.5243592639	0.8869794485	1.2886392916
H	1.0	3.0923782963	3.3657902462	-0.9522077109
H	1.0	1.5173963490	2.6122706272	-0.6536179844
H	1.0	2.1956099676	2.6018903448	-2.2789260860

1d' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2066421426	0.0000000000	-3.3207229020
C	6.0	0.0000000000	0.0000000000	-4.0176554015
C	6.0	0.0000000000	0.0000000000	-1.2258626440
C	6.0	1.2091648099	0.0000000000	-1.9320567470
C	6.0	0.0000000000	0.0000000000	0.1966434865
C	6.0	0.0000000000	0.0000000000	1.4092469657
C	6.0	0.0000000000	0.0000000000	2.8389771457
N	7.0	1.1949507417	0.0000000000	3.4440843566
C	6.0	1.1780843152	0.0000000000	4.7716784391
C	6.0	0.0000000000	0.0000000000	5.5081262524
H	1.0	2.1415248931	0.0000000000	-1.3763598323
H	1.0	2.1474395630	0.0000000000	-3.8628032126
H	1.0	0.0000000000	0.0000000000	-5.1036934984
H	1.0	2.1483032988	0.0000000000	5.2685891513
H	1.0	0.0000000000	0.0000000000	6.5919630239

1d' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2054005733	0.0000000000	-3.3237758833
C	6.0	0.0000000000	0.0000000000	-4.0218546242
C	6.0	0.0000000000	0.0000000000	-1.2288242189
C	6.0	1.2082998241	0.0000000000	-1.9345155539
C	6.0	0.0000000000	0.0000000000	0.1972942512
C	6.0	0.0000000000	0.0000000000	1.4092359647
C	6.0	0.0000000000	0.0000000000	2.8435241502
N	7.0	0.0000000000	1.1938602804	3.4476923387
C	6.0	0.0000000000	1.1779744572	4.7758883918
C	6.0	0.0000000000	0.0000000000	5.5118921816
H	1.0	2.1421068314	0.0000000000	-1.3812646074
H	1.0	2.1470516684	0.0000000000	-3.8645041998
H	1.0	0.0000000000	0.0000000000	-5.1078079544
H	1.0	0.0000000000	2.1484390214	5.2721401196
H	1.0	0.0000000000	0.0000000000	6.5957828751

1d" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z

C	6.0	1.2045603045	0.0000000000	-3.4050977884
C	6.0	0.0000000000	0.0000000000	-4.1012763782
C	6.0	0.0000000000	0.0000000000	-1.3111700815
C	6.0	1.2130743235	0.0000000000	-2.0163740343
C	6.0	0.0000000000	0.0000000000	0.1092999227
C	6.0	0.0000000000	0.0000000000	1.3206346497
C	6.0	0.0000000000	0.0000000000	2.7509464555
N	7.0	1.1957060078	0.0000000000	3.3509016435
C	6.0	1.1795700140	0.0000000000	4.6792592065
C	6.0	0.0000000000	0.0000000000	5.4135708889
C	6.0	2.4951809293	0.0000000000	-1.2763387250
C	6.0	4.9172504401	0.0000000000	0.1276523197
C	6.0	4.3155505754	1.2035701150	-0.2161569730
C	6.0	3.1114185122	1.1898233673	-0.9070452380
F	9.0	6.0581797793	0.0000000000	0.7827515666
F	9.0	2.5450830713	2.3421559494	-1.2142391548
H	1.0	2.1502582433	0.0000000000	-3.9396345007
H	1.0	0.0000000000	0.0000000000	-5.1864254961
H	1.0	2.1491018260	0.0000000000	5.1768669356
H	1.0	0.0000000000	0.0000000000	6.4973466911
F	9.0	4.8893915137	2.3430054244	0.1139506493

1d" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2021457581	0.0000000000	-3.3632080159
C	6.0	0.0000000000	0.0000000000	-4.0616408995
C	6.0	0.0000000000	0.0000000000	-1.2662816154
C	6.0	1.2108115186	0.0000000000	-1.9734261312
C	6.0	0.0000000000	0.0000000000	0.1585931360
C	6.0	0.0000000000	0.0000000000	1.3699827195
C	6.0	0.0000000000	0.0000000000	2.8061219832
N	7.0	0.0000000000	1.1941629914	3.4055632702
C	6.0	0.0000000000	1.1790785517	4.7342521586
C	6.0	0.0000000000	0.0000000000	5.4688798910
C	6.0	2.5036384201	0.0000000000	-1.2519072785
C	6.0	4.9882934188	0.0000000000	0.0388879840
C	6.0	4.3709622270	1.2037468437	-0.2762775597
C	6.0	3.1363880967	1.1902807364	-0.9116652268
F	9.0	6.1592290494	0.0000000000	0.6386307281
F	9.0	2.5607449598	2.3422597806	-1.1992842903
H	1.0	2.1492310425	0.0000000000	-3.8956236212
H	1.0	0.0000000000	0.0000000000	-5.1466711884
H	1.0	0.0000000000	2.1492712254	5.2302947568
H	1.0	0.0000000000	0.0000000000	6.5526729745
F	9.0	4.9610349174	2.3428849858	0.0248151592

1aF α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2062096624	0.0000000000	-3.4182135123
C	6.0	0.0000000000	0.0000000000	-4.1139739054
C	6.0	0.0000000000	0.0000000000	-1.3359876085
C	6.0	1.2230499359	0.0000000000	-2.0268394602
C	6.0	0.0000000000	0.0000000000	0.0831711305
C	6.0	0.0000000000	0.0000000000	1.2949836341
C	6.0	0.0000000000	0.0000000000	2.7066131084
C	6.0	1.1895457553	0.0000000000	3.4414180012
C	6.0	1.2126127688	0.0000000000	4.8227831130
C	6.0	0.0000000000	0.0000000000	5.5083974493
C	6.0	2.5068368058	0.0000000000	-1.2846045739
C	6.0	4.9690823632	0.0000000000	0.0591646131
C	6.0	4.3340462160	1.1963758996	-0.2676354316
C	6.0	3.1081008289	1.2141322724	-0.9299762503
C	6.0	6.3092736864	0.0000000000	0.7299528958
C	6.0	2.4359623428	2.5164234267	-1.2471461175
H	1.0	2.1537135130	0.0000000000	-3.9527509049
H	1.0	0.0000000000	0.0000000000	-5.2000982985
H	1.0	2.1661012557	0.0000000000	5.3380658805
H	1.0	0.0000000000	0.0000000000	6.5934715493
H	1.0	4.8048908672	2.1416510609	0.0008948414
H	1.0	7.1170250050	0.0000000000	-0.0120121042
H	1.0	6.4439669100	0.8868986641	1.3570658618
H	1.0	3.0645774585	3.3655746688	-0.9648438597
H	1.0	1.4831613264	2.6084809703	-0.7088118748
H	1.0	2.2032084513	2.6014325481	-2.3149604629
F	9.0	2.3291915458	0.0000000000	2.7690971279

1aF β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2042672654	0.0000000000	-3.3906629997
C	6.0	0.0000000000	0.0000000000	-4.0878134311
C	6.0	0.0000000000	0.0000000000	-1.3036668728
C	6.0	1.2207643130	0.0000000000	-1.9984083538
C	6.0	0.0000000000	0.0000000000	0.1218703848
C	6.0	0.0000000000	0.0000000000	1.3339216832
C	6.0	0.0000000000	0.0000000000	2.7512166483
C	6.0	0.0000000000	1.1860873624	3.4903802913
C	6.0	0.0000000000	1.2107365130	4.8719793131
C	6.0	0.0000000000	0.0000000000	5.5591014017

C	6.0	2.5156488572	0.0000000000	-1.2757506919
C	6.0	5.0106139847	0.0000000000	0.0060807415
C	6.0	4.3689081025	1.1965187659	-0.3073833928
C	6.0	3.1271725367	1.2147343071	-0.9399870965
C	6.0	6.3659642674	0.0000000000	0.6459165286
C	6.0	2.4444441760	2.5171903995	-1.2323843539
H	1.0	2.1531023424	0.0000000000	-3.9228511727
H	1.0	0.0000000000	0.0000000000	-5.1739418066
H	1.0	0.0000000000	2.1656527968	5.3845958959
H	1.0	0.0000000000	0.0000000000	6.6441283496
H	1.0	4.8464211472	2.1417493970	-0.0506608731
H	1.0	7.1563858705	0.0000000000	-0.1142849976
H	1.0	6.5153838607	0.8869373751	1.2696722366
H	1.0	3.0858617393	3.3660746933	-0.9795598150
H	1.0	1.5173228409	2.6115062613	-0.6512232252
H	1.0	2.1649830352	2.6005238877	-2.2890192990
F	9.0	0.0000000000	2.3314026614	2.8252119226

1aF' α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2058889861	0.0000000000	-3.3700280074
C	6.0	0.0000000000	0.0000000000	-4.0680355996
C	6.0	0.0000000000	0.0000000000	-1.2742240901
C	6.0	1.2088220449	0.0000000000	-1.9812690194
C	6.0	0.0000000000	0.0000000000	0.1480603409
C	6.0	0.0000000000	0.0000000000	1.3608853839
C	6.0	0.0000000000	0.0000000000	2.7768401797
C	6.0	1.1861553098	0.0000000000	3.5186739279
C	6.0	1.2103332090	0.0000000000	4.8997851895
C	6.0	0.0000000000	0.0000000000	5.5876866975
H	1.0	2.1420320973	0.0000000000	-1.4269086329
H	1.0	2.1470821265	0.0000000000	-3.9115411090
H	1.0	0.0000000000	0.0000000000	-5.1540105480
F	9.0	2.3319539699	0.0000000000	2.8553772308
H	1.0	2.1656184696	0.0000000000	5.4117058862
H	1.0	0.0000000000	0.0000000000	6.6726245050

1aF' β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2055717600	0.0000000000	-3.3737614566
C	6.0	0.0000000000	0.0000000000	-4.0716125836

C	6.0	0.0000000000	0.0000000000	-1.2777909394
C	6.0	1.2080106865	0.0000000000	-1.9844618011
C	6.0	0.0000000000	0.0000000000	0.1485417867
C	6.0	0.0000000000	0.0000000000	1.3608707383
C	6.0	0.0000000000	0.0000000000	2.7806944310
C	6.0	0.0000000000	1.1858590861	3.5216878050
C	6.0	0.0000000000	1.2102985170	4.9034831941
C	6.0	0.0000000000	0.0000000000	5.5908661982
H	1.0	2.1416839419	0.0000000000	-1.4308536308
H	1.0	2.1469778266	0.0000000000	-3.9149091946
H	1.0	0.0000000000	0.0000000000	-5.1576033669
F	9.0	0.0000000000	2.3315136626	2.8593027868
H	1.0	0.0000000000	2.1656250911	5.4153041690
H	1.0	0.0000000000	0.0000000000	6.6758677933

1aF" α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

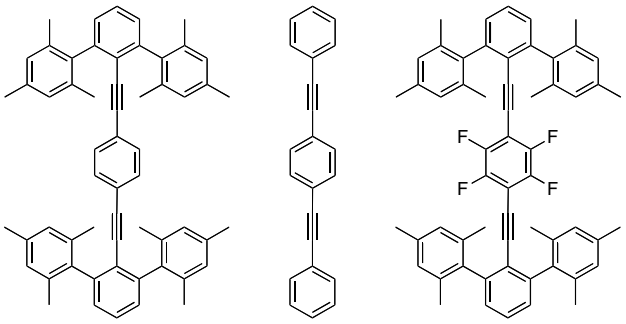
ATOM	CHARGE	X	Y	Z
C	6.0	1.2055939601	0.0000000000	-3.4773757738
C	6.0	0.0000000000	0.0000000000	-4.1730535942
C	6.0	0.0000000000	0.0000000000	-1.3862182227
C	6.0	1.2143693155	0.0000000000	-2.0891035715
C	6.0	0.0000000000	0.0000000000	0.0320426361
C	6.0	0.0000000000	0.0000000000	1.2436793371
C	6.0	0.0000000000	0.0000000000	2.6563475708
C	6.0	1.1888193518	0.0000000000	3.3924971428
C	6.0	1.2128446160	0.0000000000	4.7727369695
C	6.0	0.0000000000	0.0000000000	5.4576226062
C	6.0	2.4850582084	0.0000000000	-1.3290480908
C	6.0	4.8413204317	0.0000000000	0.1859686576
C	6.0	4.2565985426	1.2032345657	-0.1868400129
C	6.0	3.0861807267	1.1894150451	-0.9333970940
F	9.0	5.9504291120	0.0000000000	0.8937513354
F	9.0	2.5338233576	2.3423406360	-1.2633466496
H	1.0	2.1506155877	0.0000000000	-4.0130470036
H	1.0	0.0000000000	0.0000000000	-5.2581550783
H	1.0	2.1661762202	0.0000000000	5.2879068541
H	1.0	0.0000000000	0.0000000000	6.5425102200
F	9.0	4.8122998688	2.3430721757	0.1722976428
F	9.0	2.3307465536	0.0000000000	2.7203664859

1aF" β C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2021373279	0.0000000000	-3.3957655720

C	6.0	0.0000000000	0.0000000000	-4.0941401966
C	6.0	0.0000000000	0.0000000000	-1.2972967992
C	6.0	1.2104366919	0.0000000000	-2.0059991969
C	6.0	0.0000000000	0.0000000000	0.1272098348
C	6.0	0.0000000000	0.0000000000	1.3392096267
C	6.0	0.0000000000	0.0000000000	2.7583991181
C	6.0	0.0000000000	1.1876050001	3.4966993696
C	6.0	0.0000000000	1.2111751896	4.8780934091
C	6.0	0.0000000000	0.0000000000	5.5640629564
C	6.0	2.5040880081	0.0000000000	-1.2861365329
C	6.0	4.9928492558	0.0000000000	-0.0028708060
C	6.0	4.3742908637	1.2037127723	-0.3158625021
C	6.0	3.1377608622	1.1901103940	-0.9475708340
F	9.0	6.1657236345	0.0000000000	0.5928666051
F	9.0	2.5609268166	2.3422555614	-1.2328154315
H	1.0	2.1491492852	0.0000000000	-3.9282720388
H	1.0	0.0000000000	0.0000000000	-5.1791833740
H	1.0	0.0000000000	2.1659076401	5.3907368279
H	1.0	0.0000000000	0.0000000000	6.6490131887
F	9.0	4.9650597192	2.3429597469	-0.0163829884
F	9.0	0.0000000000	2.3303475198	2.8317427854



2 **2'** **2F**

2 ⊥α C_{2v}

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2038881332	0.0000000000	-7.5565745982
C	6.0	0.0000000000	0.0000000000	-8.2547859707
C	6.0	0.0000000000	0.0000000000	-5.4666270821
C	6.0	1.2206725851	0.0000000000	-6.1648219526
C	6.0	0.0000000000	0.0000000000	-4.0443728143
C	6.0	0.0000000000	0.0000000000	-2.8296385528
C	6.0	0.0000000000	0.0000000000	-1.4101500121
C	6.0	1.2079045953	0.0000000000	-0.6998754756
C	6.0	2.5162880501	0.0000000000	-5.4437630578
C	6.0	5.0138210157	0.0000000000	-4.1646159739

C	6.0	4.3718320444	1.1965696725	-4.4782322063
C	6.0	3.1298326882	1.2145065564	-5.1109103379
C	6.0	6.3703785156	0.0000000000	-3.5269798143
C	6.0	2.4531449773	2.5167991617	-5.4176121764
C	6.0	1.2070590966	0.0000000000	0.6850298103
C	6.0	0.0000000000	0.0000000000	1.3960791470
C	6.0	0.0000000000	0.0000000000	2.8197787864
C	6.0	0.0000000000	0.0000000000	4.0344124980
C	6.0	0.0000000000	0.0000000000	5.4620300460
C	6.0	0.0000000000	1.2031881114	7.5529283466
C	6.0	0.0000000000	1.2195475674	6.1605044097
C	6.0	0.0000000000	0.0000000000	8.2513817377
C	6.0	0.0000000000	2.5175264721	5.4436851094
C	6.0	0.0000000000	5.0170153513	4.1697095551
C	6.0	1.1964548293	4.3756823143	4.4842420186
C	6.0	1.2143886465	3.1328105423	5.1144098014
C	6.0	0.0000000000	6.3723603264	3.5298735892
C	6.0	2.5168688930	2.4560548296	5.4205338810
H	1.0	2.1526940159	0.0000000000	-8.0890714066
H	1.0	0.0000000000	0.0000000000	-9.3408237264
H	1.0	2.1417559931	0.0000000000	-1.2549178071
H	1.0	4.8508890266	2.1419729000	-4.2248754573
H	1.0	7.1595194101	0.0000000000	-4.2884355784
H	1.0	6.5213146461	0.8870366109	-2.9036395710
H	1.0	3.0851646276	3.3661014079	-5.1435113688
H	1.0	1.5076271949	2.6076033597	-4.8670706539
H	1.0	2.2064617033	2.6016353415	-6.4823177311
H	1.0	0.0000000000	0.0000000000	9.3374686271
H	1.0	2.1412516788	0.0000000000	1.2378760084
H	1.0	0.0000000000	2.1527070629	8.0841235070
H	1.0	2.1417021385	4.8549213879	4.2307222215
H	1.0	0.0000000000	7.1629348942	4.2899178200
H	1.0	0.8867173765	6.5214130964	2.9057853690
H	1.0	3.3659303601	3.0882030818	5.1457716688
H	1.0	2.6073893348	1.5099632507	4.8705692047
H	1.0	2.6031061394	2.2093252108	6.4851509208

2 ⊥γ D_2

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.8721287436	0.8325067801	-7.5519549363
C	6.0	0.0000000000	0.0000000000	-8.2491425256
C	6.0	0.0000000000	0.0000000000	-5.4642472904
C	6.0	0.8848745977	0.8419504233	-6.1609948586

C	6.0	0.0000000000	0.0000000000	-4.0391302366
C	6.0	0.0000000000	0.0000000000	-2.8246146258
C	6.0	0.0000000000	0.0000000000	-1.4031007587
C	6.0	1.2077602552	0.0049448138	-0.6925100516
C	6.0	1.8015737337	1.7272592303	-5.4027100323
C	6.0	3.4854001759	3.3650425948	-3.8686602543
C	6.0	2.2253246152	3.8088084210	-4.2660110919
C	6.0	3.8861309037	2.0850492558	-4.2481264870
C	6.0	1.3753241124	3.0074790768	-5.0248746218
C	6.0	3.0590524661	1.2563779568	-5.0043852278
C	6.0	4.3893800221	4.2469778535	-3.0609378451
C	6.0	0.0076361454	3.4920360469	-5.4009482396
C	6.0	3.4905942334	-0.1366339450	-5.3520149567
H	1.0	1.5557820783	1.4888201986	-8.0858210966
H	1.0	0.0000000000	0.0000000000	-9.3351020051
H	1.0	2.1416066919	0.0124791644	-1.2468860324
H	1.0	1.8929744502	4.8023594649	-3.9663497816
H	1.0	4.8637047088	1.7186901598	-3.9354695812
H	1.0	5.0168307147	4.8718668952	-3.7073820058
H	1.0	3.8135794177	4.9190094579	-2.4172529806
H	1.0	5.0591020567	3.6563757438	-2.4282871750
H	1.0	-0.1298464346	4.5432720159	-5.1328837950
H	1.0	4.5435659128	-0.3027209910	-5.1073579948
H	1.0	-0.1778778272	3.3834978475	-6.4755375657
H	1.0	3.3463872400	-0.3509037839	-6.4168172098
H	1.0	-0.7672823897	2.9082686466	-4.8865200106
H	1.0	2.8961667959	-0.8771489411	-4.7995688246

2 ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2038954962	0.0000000000	-7.5481298439
C	6.0	0.0000000000	0.0000000000	-8.2463601139
C	6.0	0.0000000000	0.0000000000	-5.4581297912
C	6.0	1.2206996070	0.0000000000	-6.1564083566
C	6.0	0.0000000000	0.0000000000	-4.0360230649
C	6.0	0.0000000000	0.0000000000	-2.8211177577
C	6.0	0.0000000000	0.0000000000	-1.4020044056
C	6.0	1.2090526879	0.0000000000	-0.6921699453
C	6.0	2.5161859892	0.0000000000	-5.4351840649
C	6.0	5.0118995638	0.0000000000	-4.1525756449
C	6.0	4.3705317051	1.1965786351	-4.4673853167
C	6.0	3.1293617076	1.2145362763	-5.1017275372
C	6.0	6.3673220104	0.0000000000	-3.5122627591
C	6.0	2.4531846756	2.5168932521	-5.4094844733
H	1.0	2.1526771128	0.0000000000	-8.0806941705
H	1.0	0.0000000000	0.0000000000	-9.3323908305

H	1.0	2.1420706976	0.0000000000	-1.2486218551
H	1.0	4.8490768615	2.1420143876	-4.2132162954
H	1.0	7.1579893223	0.0000000000	-4.2721273585
H	1.0	6.5167764228	0.8870025345	-2.8885067540
H	1.0	3.0845584005	3.3661074467	-5.1336538179
H	1.0	1.5064828867	2.6075605398	-4.8608529676
H	1.0	2.2085586763	2.6020816452	-6.4746115874

2 ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2031450479	0.0000000000	-7.5618834305
C	6.0	0.0000000000	0.0000000000	-8.2604067801
C	6.0	0.0000000000	0.0000000000	-5.4708431181
C	6.0	1.2195072582	0.0000000000	-6.1694593964
C	6.0	0.0000000000	0.0000000000	-4.0431354812
C	6.0	0.0000000000	0.0000000000	-2.8285998637
C	6.0	0.0000000000	0.0000000000	-1.4045276458
C	6.0	0.0000000000	1.2059669901	-0.6927080387
C	6.0	2.5172439768	0.0000000000	-5.4523891446
C	6.0	5.0153981171	0.0000000000	-4.1760360562
C	6.0	4.3744758854	1.1964710750	-4.4912934043
C	6.0	3.1322723444	1.2143868119	-5.1227618356
C	6.0	6.3699039479	0.0000000000	-3.5344011019
C	6.0	2.4558450366	2.5167911881	-5.4299671669
H	1.0	2.1526614078	0.0000000000	-8.0931018842
H	1.0	0.0000000000	0.0000000000	-9.3464737984
H	1.0	0.0000000000	2.1411616632	-1.2438323470
H	1.0	4.8536555553	2.1416936431	-4.2376236666
H	1.0	7.1613873467	0.0000000000	-4.2935536127
H	1.0	6.5181260739	0.8867235387	-2.9101542187
H	1.0	3.0877988840	3.3659276595	-5.1550693499
H	1.0	1.5088680225	2.6070565459	-4.8814931096
H	1.0	2.2104758811	2.6029176107	-6.4949267489

2' ⊥α C_2v

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.2054940666	0.0000000000	-7.5682545919
C	6.0	0.0000000000	0.0000000000	-8.2669180440
C	6.0	0.0000000000	0.0000000000	-5.4702365380
C	6.0	-1.2078738765	0.0000000000	-6.1794877843
C	6.0	0.0000000000	0.0000000000	-4.0474215591
C	6.0	0.0000000000	0.0000000000	-2.8326160150

C	6.0	0.0000000000	0.0000000000	-1.4114401976
C	6.0	-1.2064180339	0.0000000000	-0.6981443823
H	1.0	-2.1419023803	0.0000000000	-5.6262519818
C	6.0	-1.2061696831	0.0000000000	0.6869216668
C	6.0	0.0000000000	0.0000000000	1.3993674710
C	6.0	0.0000000000	0.0000000000	2.8242306241
C	6.0	0.0000000000	0.0000000000	4.0384086684
C	6.0	0.0000000000	0.0000000000	5.4653000476
C	6.0	0.0000000000	-1.2052167365	7.5627677231
C	6.0	0.0000000000	-1.2075016515	6.1733763313
C	6.0	0.0000000000	0.0000000000	8.2611779327
H	1.0	0.0000000000	-2.1415728208	5.6202250307
H	1.0	-2.1469985742	0.0000000000	-8.1093549486
H	1.0	0.0000000000	0.0000000000	-9.3528759042
H	1.0	-2.1422199336	0.0000000000	-1.2479269518
H	1.0	0.0000000000	0.0000000000	9.3471795237
H	1.0	-2.1413114692	0.0000000000	1.2378178564
H	1.0	0.0000000000	-2.1467981627	8.1037332632

2' $\perp\gamma$ D_2

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.8886119622	-0.8141116990	-7.5664146136
C	6.0	0.0000000000	0.0000000000	8.2657528543
C	6.0	0.0000000000	0.0000000000	5.4682671631
C	6.0	-0.8923895627	-0.8137574149	-6.1775611005
C	6.0	0.0000000000	0.0000000000	4.0435206286
C	6.0	0.0000000000	0.0000000000	2.8290381942
C	6.0	0.0000000000	0.0000000000	1.4059018995
C	6.0	-1.2062357982	-0.0017454195	-0.6925708115
H	1.0	-1.5819574682	-1.4430845183	-5.6239131983
H	1.0	-1.5816933217	-1.4507454146	-8.1079262310
H	1.0	0.0000000000	0.0000000000	9.3516051116
H	1.0	-2.1419367749	-0.0021604732	-1.2423502840

2' $\|\alpha$ D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	8.2611726423
C	6.0	1.2054907650	0.0000000000	7.5623353959
C	6.0	1.2077673270	0.0000000000	6.1735557591
C	6.0	0.0000000000	0.0000000000	5.4643349206
C	6.0	0.0000000000	0.0000000000	4.0417503127
C	6.0	0.0000000000	0.0000000000	2.8267772998
C	6.0	0.0000000000	0.0000000000	1.4060940979

C	6.0	1.2066129699	0.0000000000	0.6921568161
H	1.0	0.0000000000	0.0000000000	9.3471075385
H	1.0	2.1415933916	0.0000000000	5.6199703933
H	1.0	2.1472256746	0.0000000000	8.1030115773
H	1.0	2.1421607556	0.0000000000	1.2423843125

2' ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	8.2671950864
C	6.0	1.2052605631	0.0000000000	7.5686211869
C	6.0	1.2073927509	0.0000000000	6.1791687067
C	6.0	0.0000000000	0.0000000000	5.4713103261
C	6.0	0.0000000000	0.0000000000	4.0444745469
C	6.0	0.0000000000	0.0000000000	2.8303829460
C	6.0	0.0000000000	0.0000000000	1.4050395653
C	6.0	0.0000000000	1.2060276265	0.6928721089
H	1.0	0.0000000000	0.0000000000	9.3531704822
H	1.0	2.1411347529	0.0000000000	5.6254541191
H	1.0	2.1471879228	0.0000000000	8.1089729259
H	1.0	0.0000000000	2.1415429994	1.2431418420

2F ||α D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2066212042	0.0000000000	-7.5320495829
C	6.0	0.0000000000	0.0000000000	-8.2271796599
C	6.0	0.0000000000	0.0000000000	-5.4510217856
C	6.0	1.2240643063	0.0000000000	-6.1408875811
C	6.0	0.0000000000	0.0000000000	-4.0325949556
C	6.0	0.0000000000	0.0000000000	-2.8205381530
C	6.0	0.0000000000	0.0000000000	-1.4115494845
C	6.0	1.1986973973	0.0000000000	-0.6906047371
C	6.0	2.5079203904	0.0000000000	-5.3990849732
C	6.0	4.9703881321	0.0000000000	-4.0561444956
C	6.0	4.3353851361	1.1964086841	-4.3831713689
C	6.0	3.1093516978	1.2143765882	-5.0452879126
C	6.0	6.3097560404	0.0000000000	-3.3840606245
C	6.0	2.4376804563	2.5166710483	-5.3636571647
H	1.0	2.1538527577	0.0000000000	-8.0668912435
H	1.0	0.0000000000	0.0000000000	-9.3134022631
F	9.0	2.3450363813	0.0000000000	-1.3427910435
H	1.0	4.8063140018	2.1415042373	-4.1143499756
H	1.0	7.1180066566	0.0000000000	-4.1254001055
H	1.0	6.4436299073	0.8867231087	-2.7566872860

H	1.0	3.0671931594	3.3658833300	-5.0838004104
H	1.0	1.4856985135	2.6112674767	-4.8243256728
H	1.0	2.2033884881	2.5999330054	-6.4312776236

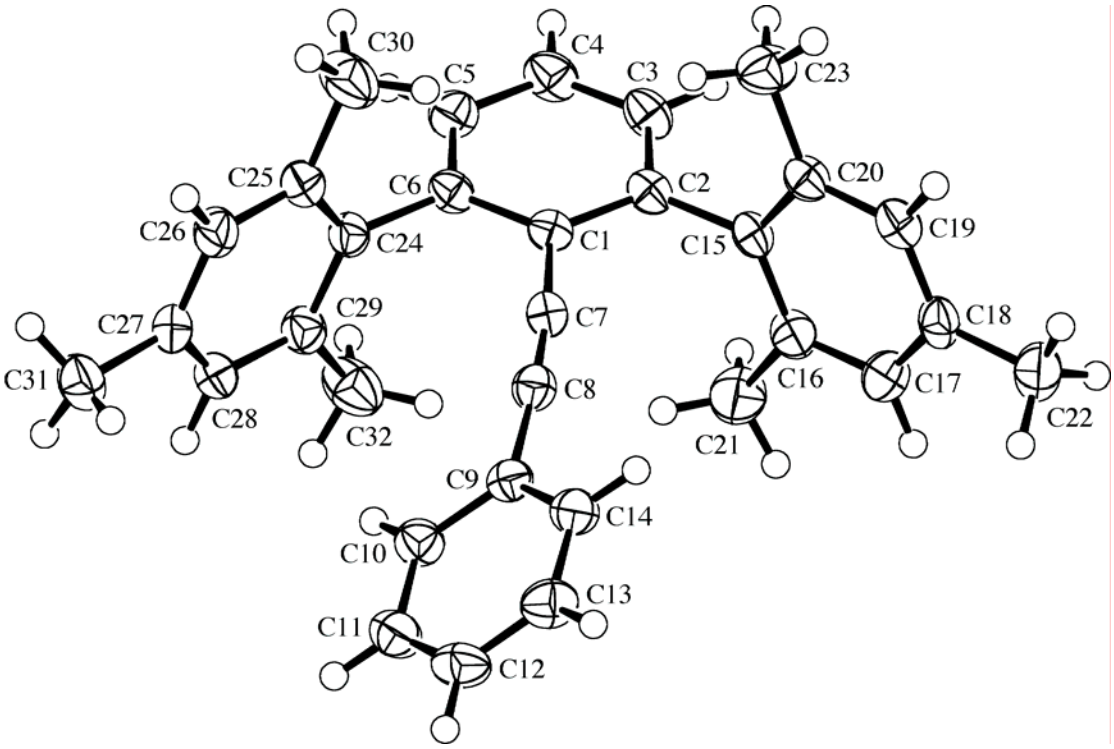
2F ||β D_2h

***** EQUILIBRIUM GEOMETRY LOCATED *****

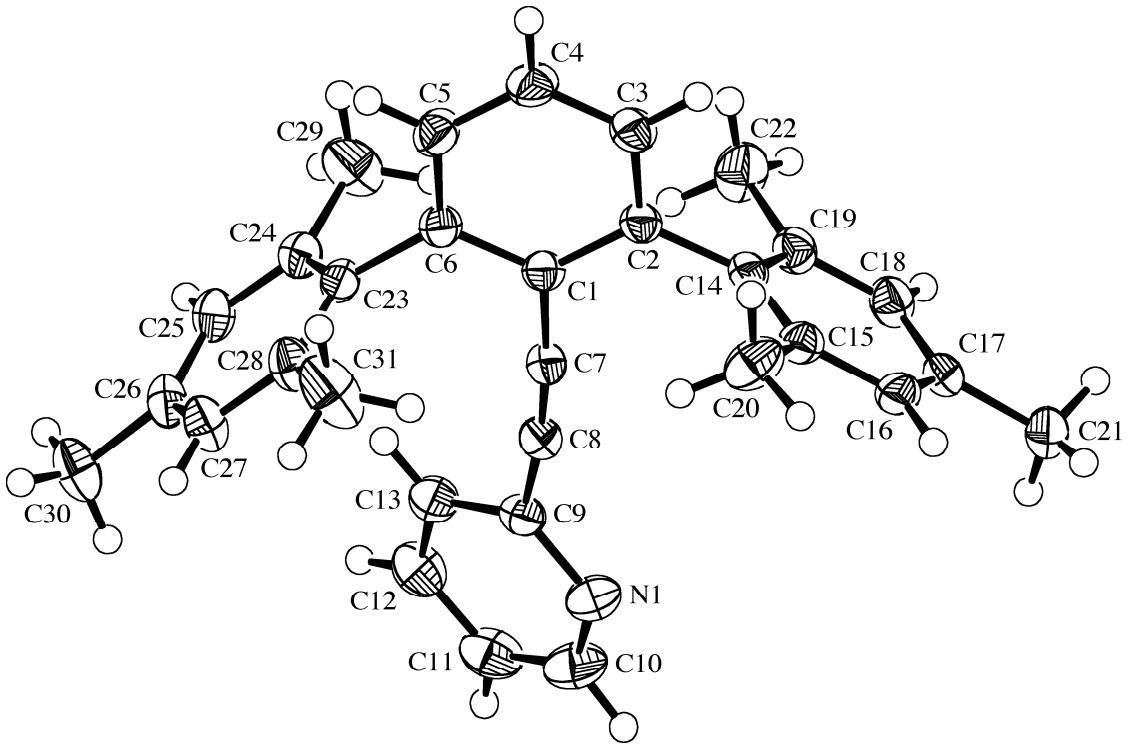
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	1.2047079088	0.0000000000	-7.5551400461
C	6.0	0.0000000000	0.0000000000	-8.2516367060
C	6.0	0.0000000000	0.0000000000	-5.4699362084
C	6.0	1.2216684768	0.0000000000	-6.1630563966
C	6.0	0.0000000000	0.0000000000	-4.0445648140
C	6.0	0.0000000000	0.0000000000	-2.8326018134
C	6.0	0.0000000000	0.0000000000	-1.4174809265
C	6.0	0.0000000000	1.1933318840	-0.6911690648
C	6.0	2.5150829911	0.0000000000	-5.4380698517
C	6.0	5.0060652385	0.0000000000	-4.1493241293
C	6.0	4.3654684737	1.1965501870	-4.4651390600
C	6.0	3.1256238990	1.2150410939	-5.1013435413
C	6.0	6.3591476651	0.0000000000	-3.5049882013
C	6.0	2.4448840198	2.5177106413	-5.3976848214
H	1.0	2.1533145484	0.0000000000	-8.0875146155
H	1.0	0.0000000000	0.0000000000	-9.3377536759
F	9.0	0.0000000000	2.3465546631	-1.3328706633
H	1.0	4.8424987628	2.1416779239	-4.2073543270
H	1.0	7.1520650878	0.0000000000	-4.2625150995
H	1.0	6.5067054678	0.8871352775	-2.8811181147
H	1.0	3.0845840705	3.3663064164	-5.1399662147
H	1.0	1.5134586303	2.6127092000	-4.8235728137
H	1.0	2.1734050324	2.6017041791	-6.4563922876

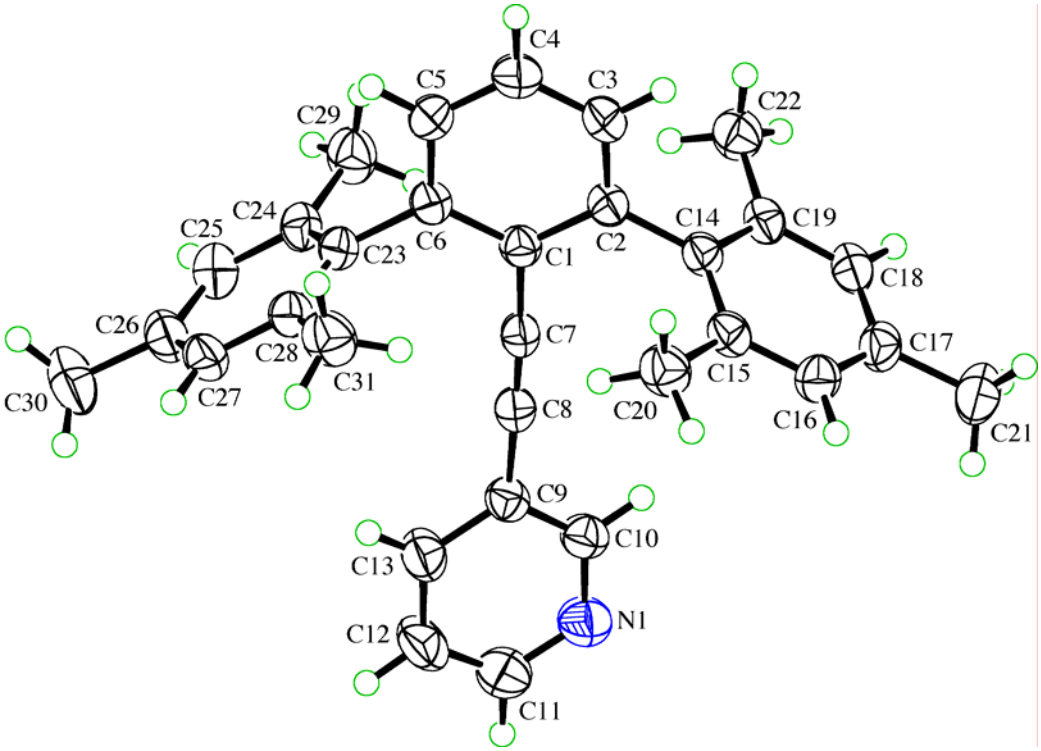
Crystallographic ORTEP Plots.



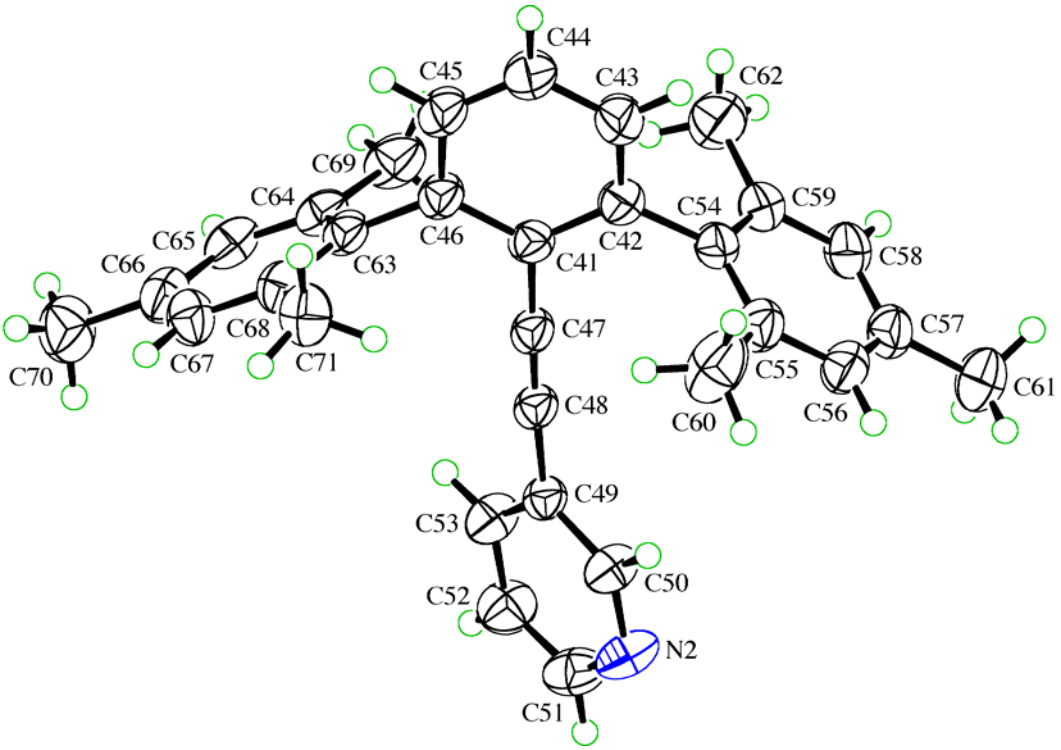
An ORTEP view of the molecular structure of **1a** (50% probability ellipsoids).



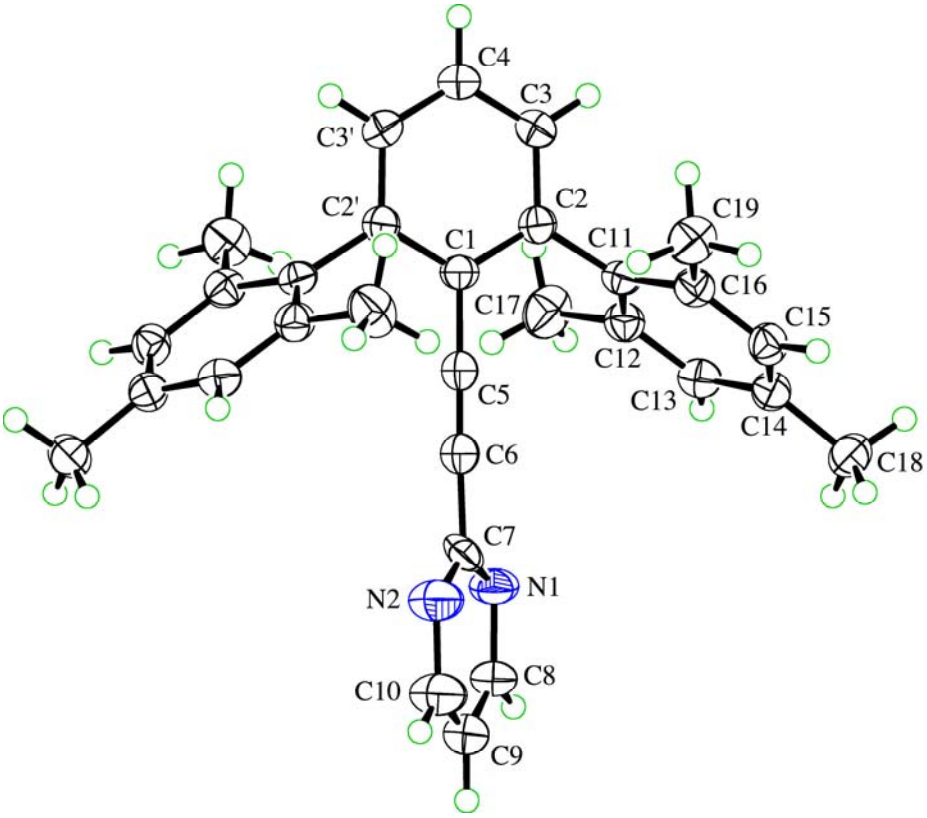
An ORTEP view of the molecular structure of **1b** (50% probability ellipsoids).



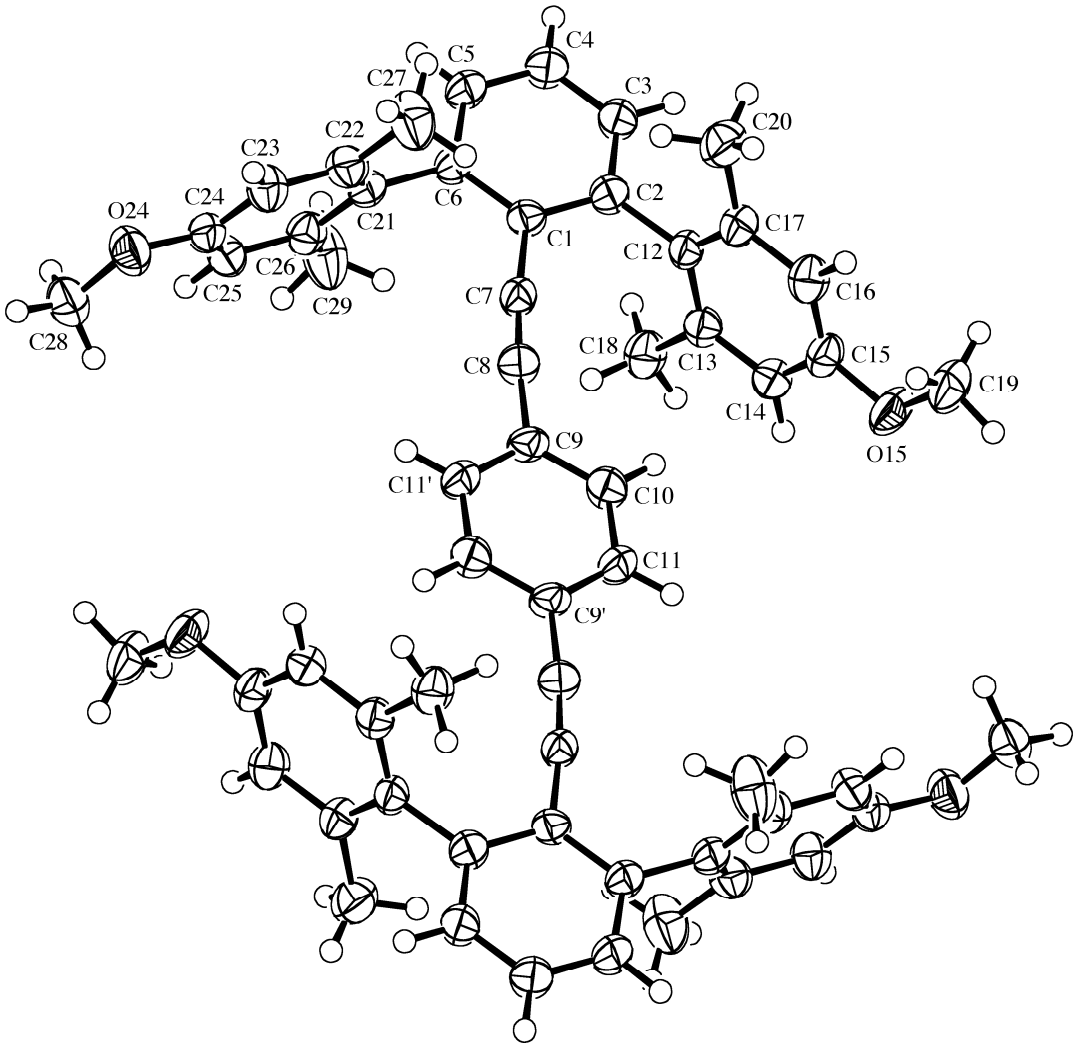
An ORTEP view of molecule A of **1c** (50% probability ellipsoids).



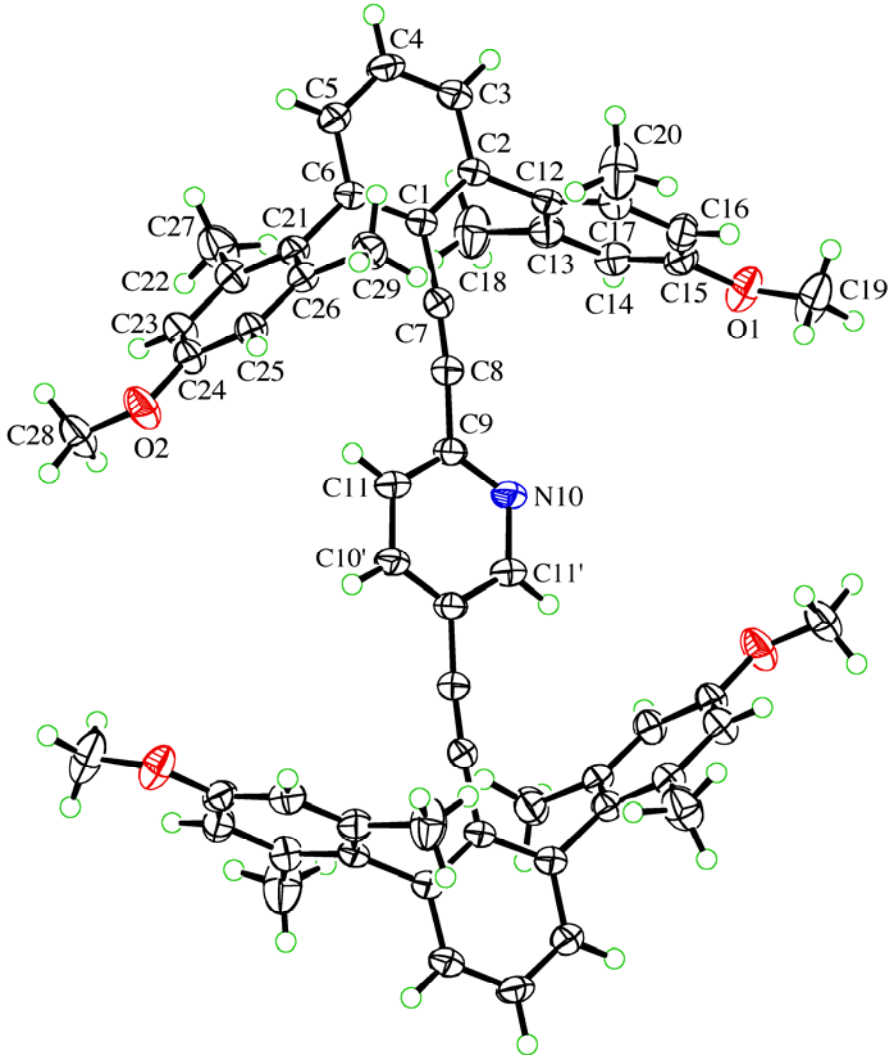
An ORTEP view of molecule B of **1c** (50% probability ellipsoids).



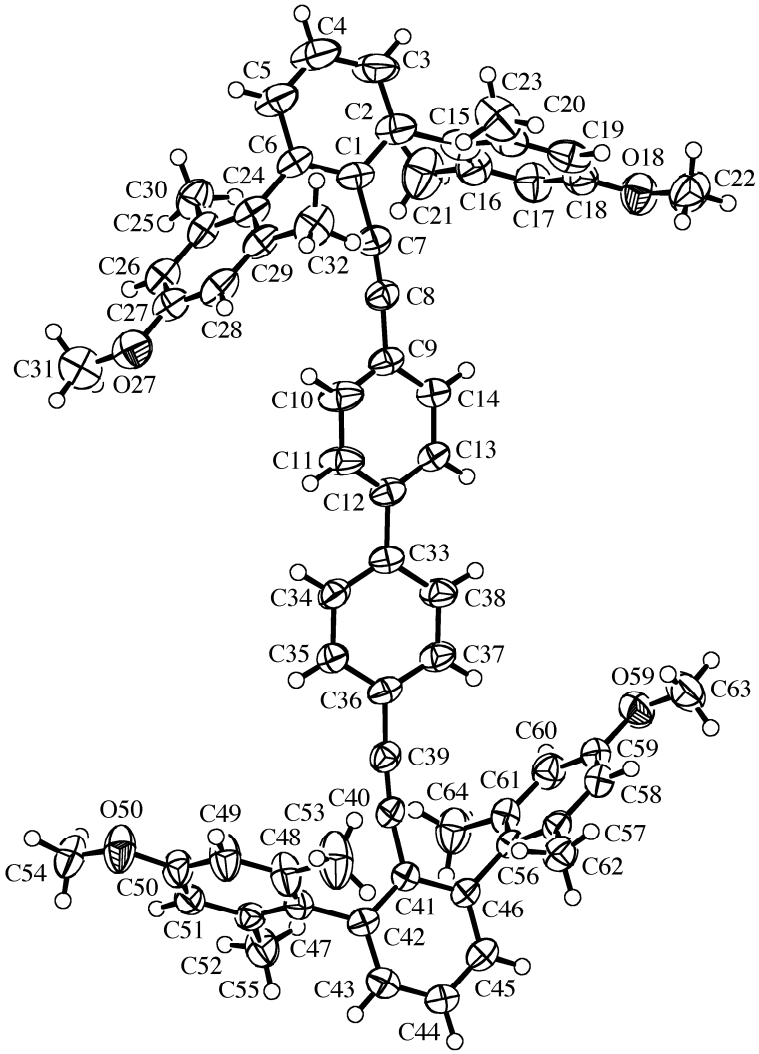
An ORTEP view of the molecular structure of **1d** (50% probability ellipsoids).



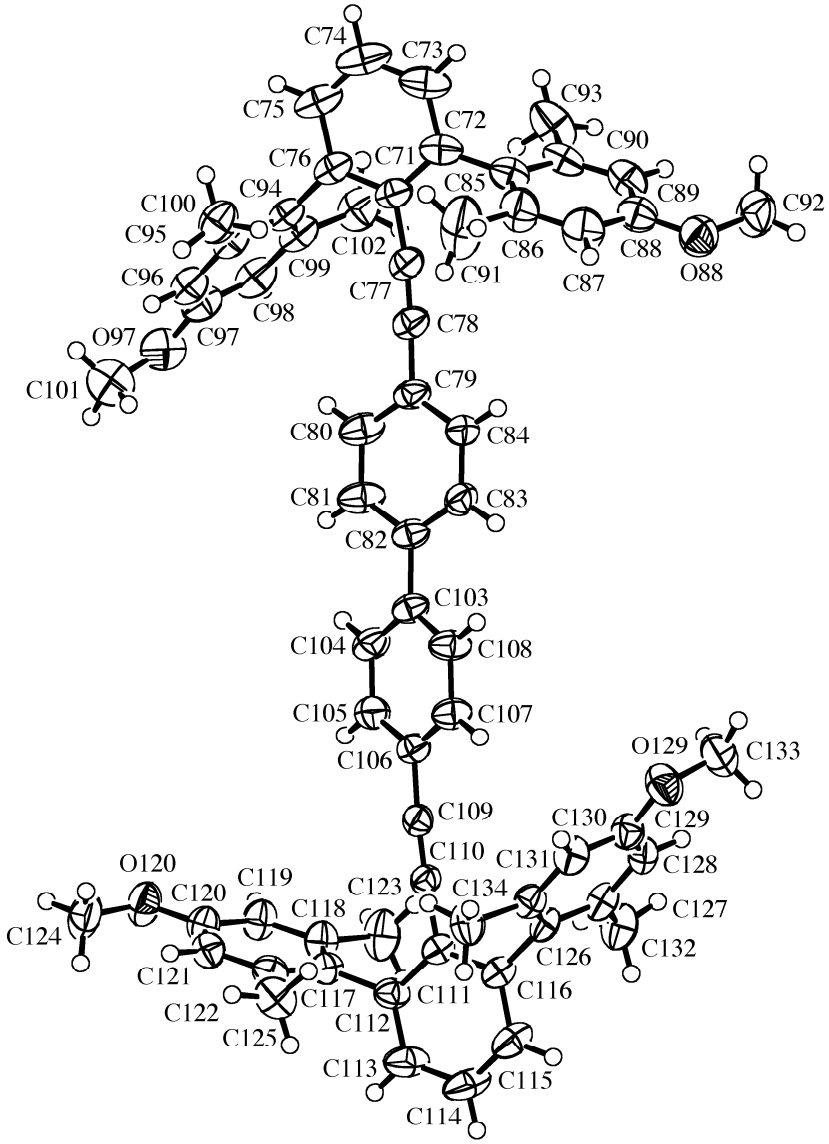
An ORTEP view of the molecular structure of **2a** (50% probability ellipsoids).



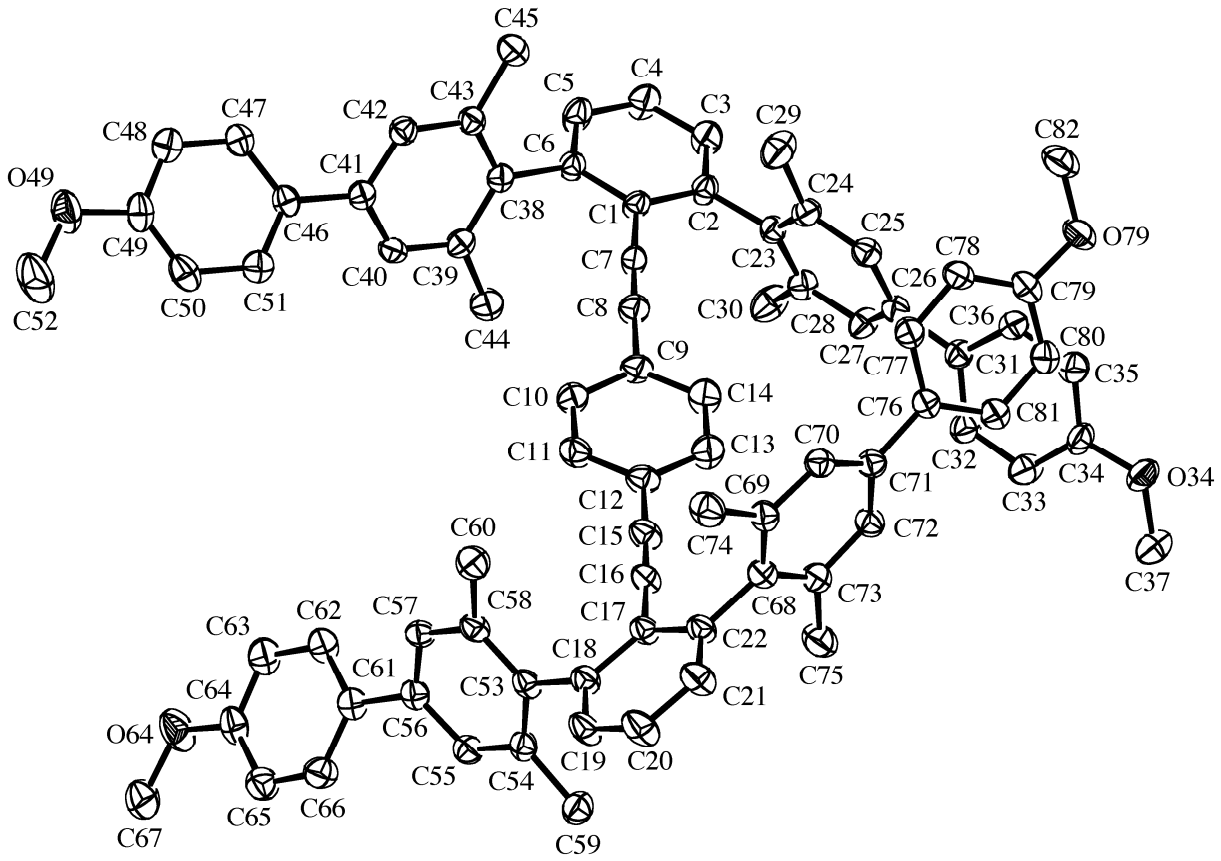
An ORTEP view of the molecular structure of **2b** (50% probability ellipsoids).



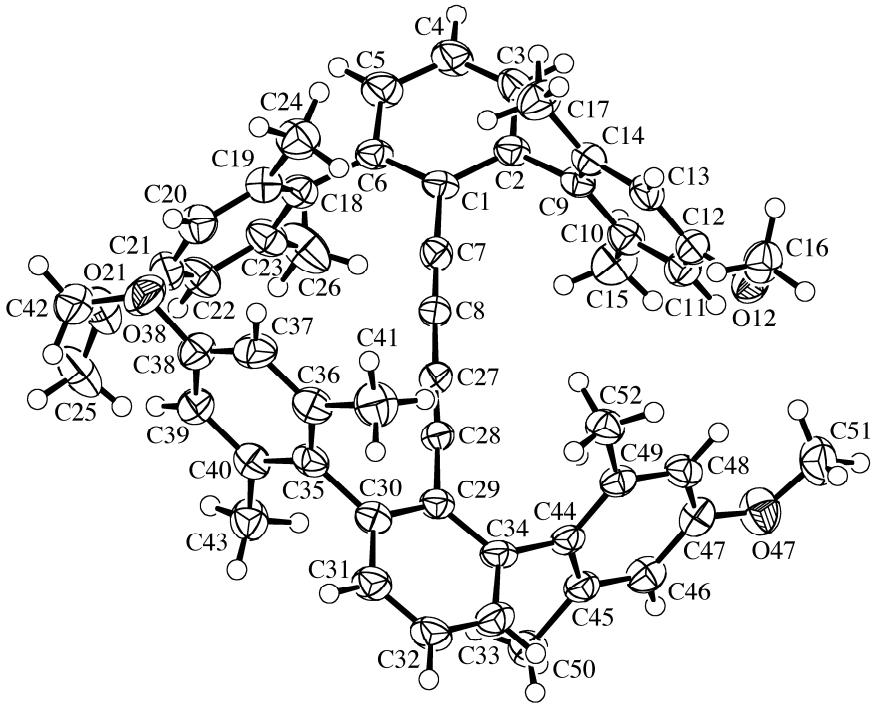
An ORTEP view of the molecular structure of **2c** molecule A (50% probability ellipsoids).



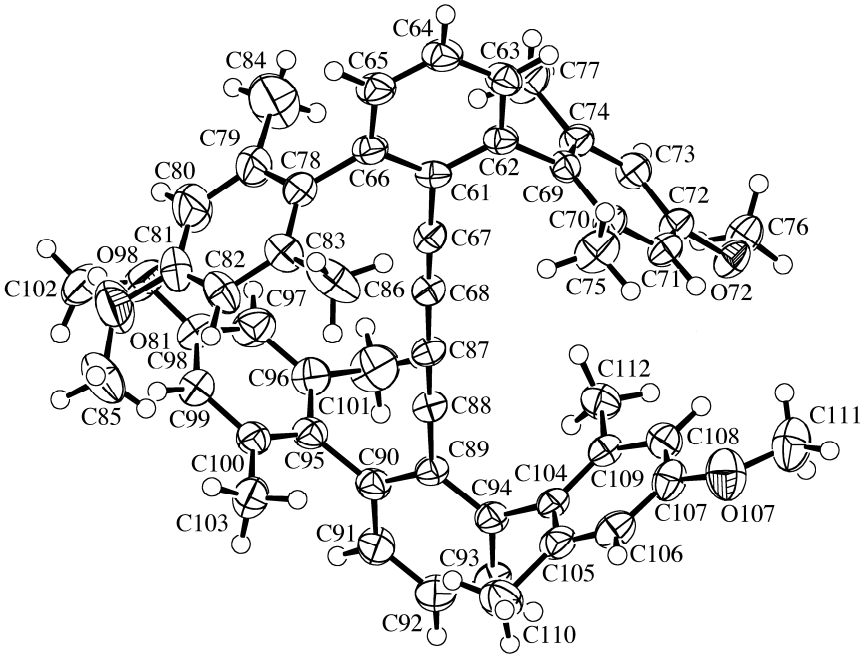
An ORTEP view of the molecular structure of **2c** molecule B (50% probability ellipsoids).



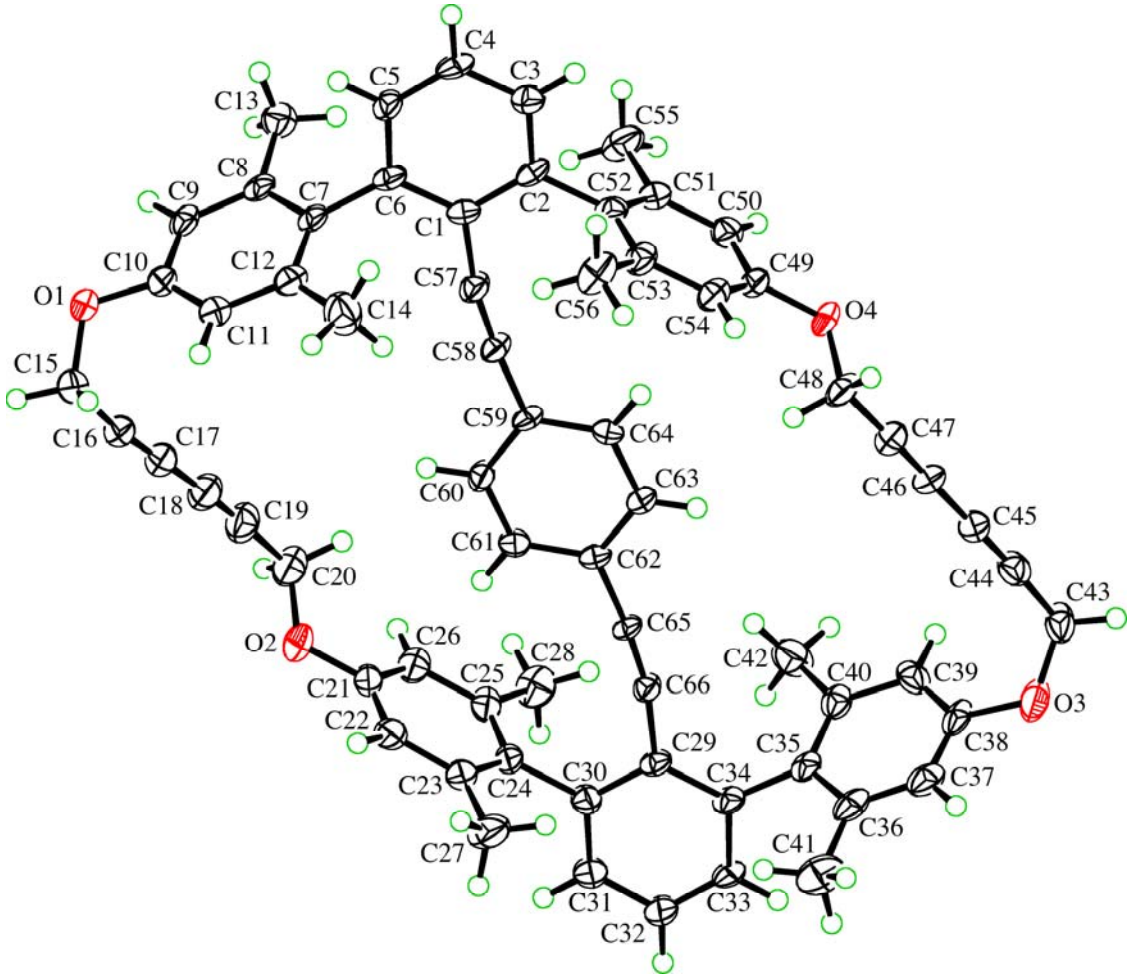
An ORTEP view of the molecular structure of **2d** (50% probability ellipsoids).



An ORTEP view of molecule A of **9** (50% probability ellipsoids).



An ORTEP view of molecule B of **9** (50% probability ellipsoids).



An ORTEP view of the molecular structure of **3** (50% probability ellipsoids).