Supporting Information for:

The Importance of Direct Metal-π Bonding in Electronic Transport Through Conjugated Single-molecule Junctions

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General Information

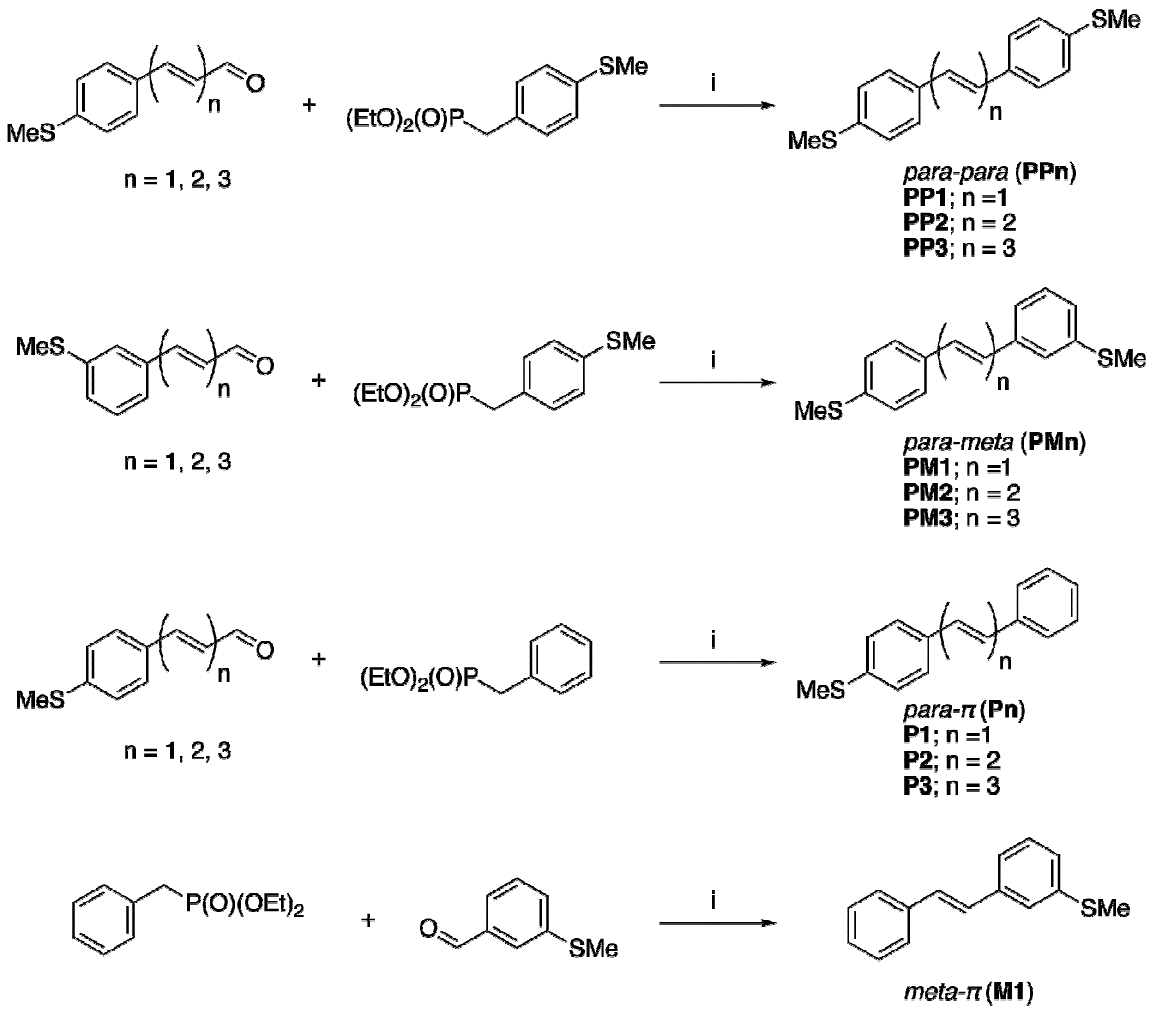
(*E*)-4-nitrostilbene, diethyl benzylphosphonate and (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide were purchased from TCI America and the latter was stored in a desiccator. 3-nitrobenzaldehyde, 4-nitrobenzaldehyde, 3-nitrobenzyl bromide, 4-nitrobenzyltriphenylphosphonium bromide, (*E*)-4,4'-diaminostilbene (**PP1A**), 4-nitrostilbene, 4-(methylthio)benzaldehyde, 4-(methylthio)benzyl bromide, 3-(methylthio)benzyl bromide, n-butyl lithium (1.6 M) in hexanes and all other reagents were purchased from Sigma-Aldrich. All reactions were carried out under nitrogen unless otherwise noted.

Compounds were prepared by the reported procedures: 3-(methylthio)benzaldehyde;[i] (*E*)-4-(methylthio)cinnamaldehyde and (2*E*,4*E*)-5-(4-(methylthio)phenyl)penta-2,4-dienal;[ii] (*E*)-4,4'-di-(methylthio)stilbene (**PP1**);[i] 3-(dimethylamino)benzaldehyde;[iii] (*E*)-methyl(4-styrylphenyl)sulfane (**P1**);[iv] dimethyl 4-(methylthio)benzylphosphonate;[v] and (*E*)-4-aminostilbene (**P1A**).[vi]

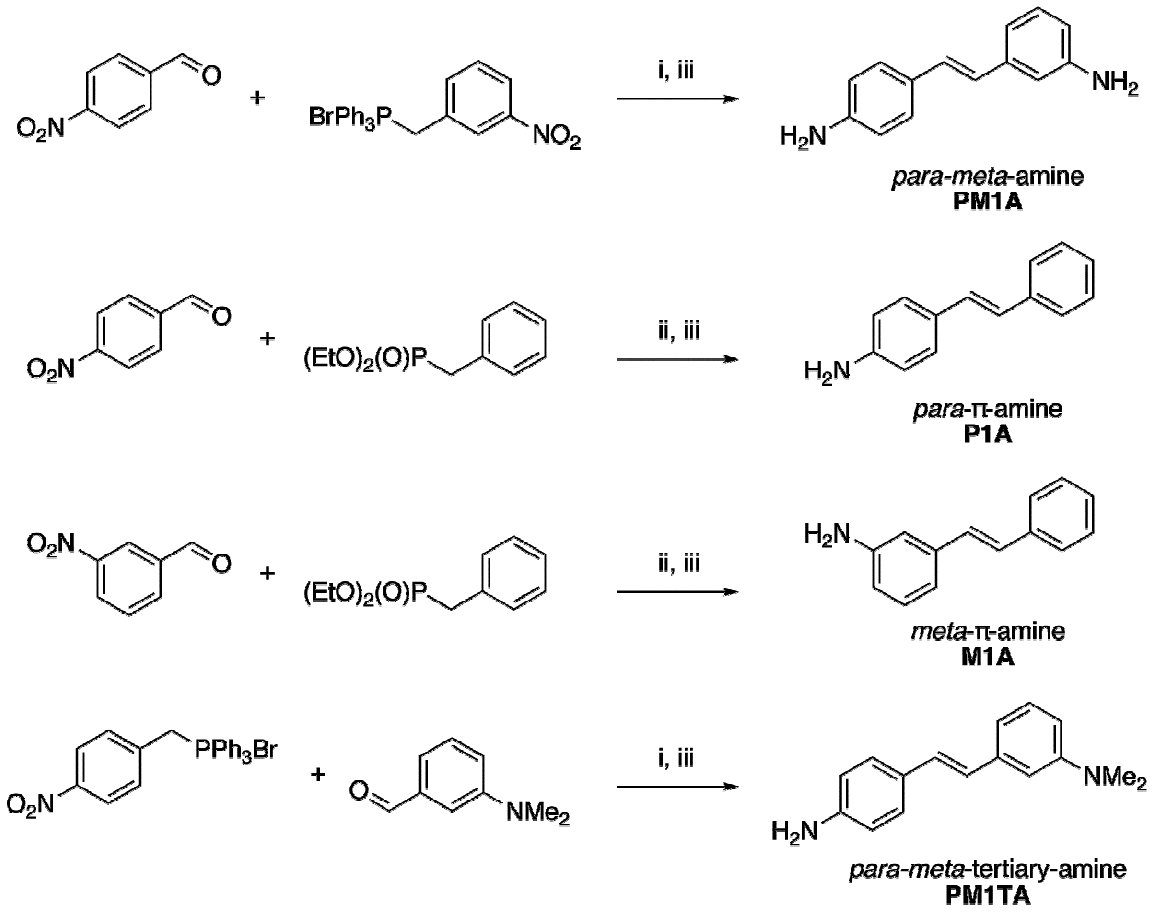
Chromatography was performed on a Teledyne ISCO Combiflash RF using Redisep RF silica columns. ^{1}H, ^{13}C and ^{31}P NMR spectra were taken on a Bruker DRX300 (300MHz), DRX400 (400MHz) and DMX500 (500MHz).

High resolution mass spectrometry (HR-MS) were obtained for all target molecules on a double focusing mass spectrometer (JMS-HX110A; JEOL, ltd.; Tokyo, Japan); Ionization method: FAB, High energy Xe* beam (3 kV); Matix: *meta*-nitrobenzyl alcohol (m-NBA); MS Acceleration-Voltage: 10 kJ; Resolution: 3,000/10,000 (Low-Res/High-Res).

Synthetic Experimentals

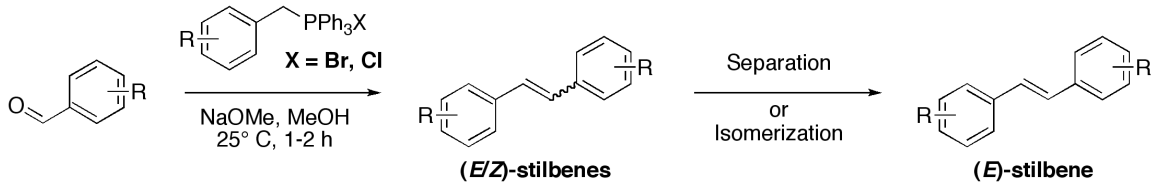


Scheme S1. Synthesis of *trans*-α,ω-diphenyl-μ,ν-oligoenes, where n = 1-3; (i) General H.W.E. reaction: General H.W.E. reaction: ^{t}BuOK (1.1 eq.), THF, 0° C, 1 h, let warm to room temperature overnight.

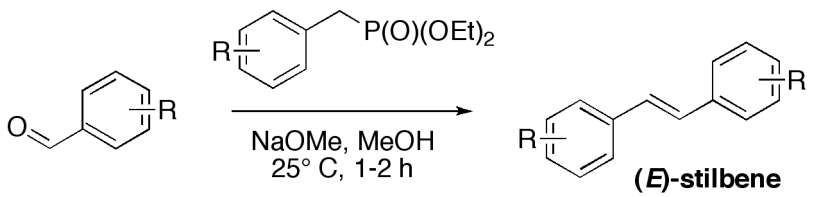


Scheme S2. Amine-functionalized stilbene derivative through Wittig Reaction or H.W.E. and $SnCl_2$ reduction. Compound **M1A** was prepared as a control molecule to verify conductance trends found in the methylsulfide molecular wires; (i) NaOMe (1.2 eq.), MeOH, 1 h, produces a mixture of (E/Z)-stereoisomers that may be separated by flash column chromatography or by isomerization using I_2, acetone, reflux, 12 h; (ii) General H.W.E. reaction: ^{t}BuOK (1.1 eq.), THF, 0˚ C, 1 h, let warm to room temperature overnight; (iii) $SnCl_2 \bullet 2H_2O$, EtOH (anhydrous), 70˚ C, 2 h (50-90%).

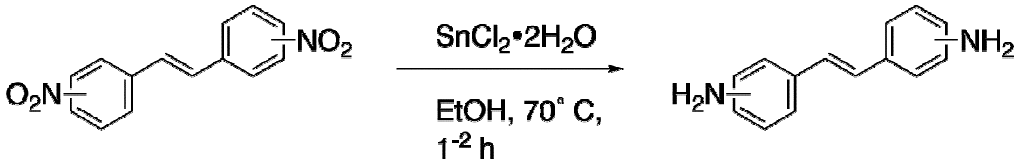
General Procedures



General Wittig Procedure: Adapted from the reported procedure.[vii] In a 100-mL round-bottom flask, 3-nitrobenzaldehyde (0.100 g, 6.62 mmol) and 3-nitrobenzyltriphenyl-phosphonium bromide (3.20 g, 6.62 mmol) were dissolved in 50 mL of anhydrous methanol under nitrogen. Sodium methoxide (13.2 mmol) was added to the solution slowly over 15 min. A colorful (usually yellow) precipitate forms while the reaction was stirred for an additional 1-2 hours at room temperature. The resultant *E*/*Z* mixture of isomers was collected by filtration as a light yellow solid that was dried in air. The stereoisomers were separated (by chromatography or recrystallization) or where isomerized completely to the (*E)*-isomer.

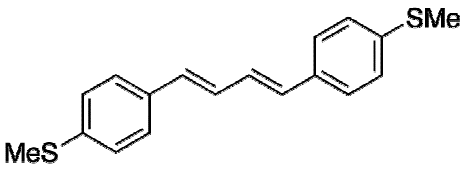


General Hoerner-Wadsworth-Emmons (H.W.E.) Procedure: Inside a flame-dried flask, aldehyde (0.150 g, 1.0 eq.) and phosphonate (1.1 eq.) were dissolved in 25 mL of dry THF. After being cooled to 0° C, a solution of tBuOK (1.1 eq.) in 5 mL of THF was slowly added to the stirred reaction solution. The reaction was stirred overnight while ice bath melted and reaction slowly warmed to room temperature. A large portion of water was added (~100). Dichloromethane was added and the organic layer was extracted. The organic layers were combined and washed with brine and dried over magnesium sulfate, and the organic solvent was removed under reduced pressure. The product was isolated by column chromatography (usually 10% ethyl acetate in hexanes).

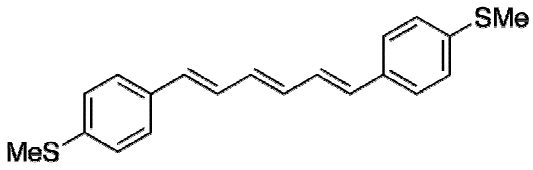


General Reduction of Aryl-NO_2 to Aryl-NH_2 Group: Dinitrostilbene (0.100 g, 0.370 mmol, 1.0 eq.), tin(II) chloride dihydrate (0.835 g, 3.70 mmol, 10.0 eq.), and 10 mL of anhydrous ethanol were added to a 25-mL RBF with stir bar and sealed with a septum. The suspension was purged with nitrogen for 10 minutes before heating to 75° C under an inert atmosphere. After 2-3 hours all solids dissolved and the reaction, which was monitored by TLC, was complete. The reaction solution was cooled to room temperature and water and then basified be the addition of 1 M sodium hydroxide. The aqueous layer was extracted with ethyl acetate (3 times). The organic layers were combined, washed with aqueous brine solution and dried over magnesium sulfate. The product was isolated by column chromatography on silica gel (usually in 50% ethyl acetate in hexanes).

Specific Procedures

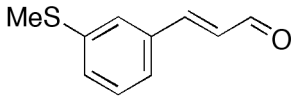


(1E,3E)-1,4-bis(4-(methylthio)phenyl)buta-1,3-diene (**PP2**): General H.W.E. Procedure. The product was prepared from (*E*)-3-(4-(methylthio)phenyl)acrylaldehyde[ii] and dimethyl 4-(methylthio)benzylphosphonate and was isolated by column chromatography (10% ethyl acetate in hexanes) as a pale yellow solid in 67.7% yield. ^{1}H NMR (400MHz, $C_2D_2C1_4$): δ 7.38 (d, *J* = 8.4 Hz, 4H), 7.22 (d, *J* = 8.4 Hz, 4H), 6.97-6.87 (m, 2H), 6.68-6.52 (m, 2H), 2.51 (s, 6H); ^{13}C NMR (400MHz, $C_2D_2C1_4$): δ 137.18, 133.64, 131.43, 128.15, 126.28, 125.93, 15.17; HR-MS: m/z calcd for ($C_{18}H_{18}S_2$): 298.0850, found: 298.0841.

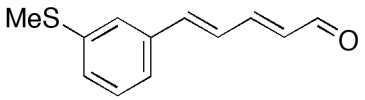


(1E,3E,5E)-1,6-bis(4-(methylthio)phenyl)hexa-1,3,5-triene (**PP3**): General H.W.E. Procedure. The product was prepared from (2*E*,4*E*)-5-(4-(methylthio)phenyl)penta-2,4-dienal[ii] and *dimethyl 4-(methylthio)benzylphosphonate* and was isolated by column chromatography (10% ethyl acetate in hexanes) as a yellowish-green solid in 54.0% yield. This compound was previously prepared by Spangler and coworkers.[viii] Our NMR characterization data agrees with their report. ^{1}H NMR (400MHz, 350K, $C_2D_2C1_4$): δ 7.36 (bs, 4H), 7.26 (bs, 4H), 7.35 (t, *J* = 7.5 Hz, 2H), 6.85 (bm, 2H), 6.72-6.33 (m, 4H),

2.53 (bs, 6H), note: spectral shifts appeared broad; ^{13}C NMR (400MHz, 350K, $C_2D_2C1_4$): δ 137.30, 137.04, 132.83, 131.43, 128.24, 126.56, 126.25, 15.46; HR-MS: m/z calcd for ($C_{20}H_{20}S_2$): 324.1006, found: 324.1011.

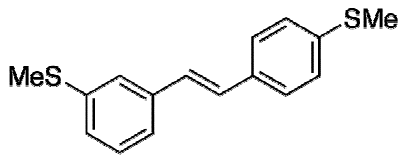


(E)-3-(methylthio)cinnamaldehyde: General Wittig homologation procedure. Product was prepared from 3-(methylthio)benzaldehyde and (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide and isolated as a pale yellow solid (yield: 0.456 g, 38.9%). ^{1}H NMR (300MHz, $CDCl_3$): δ 9.70 (d, *J* = 7.8 Hz, 1H), 7.44-7.30 (m, 5H), 6.70 (dd, *J* = 7.8 Hz, *J* = 16.2 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (300MHz, $CDCl_3$): δ 194.0, 152.5, 140.4, 135.0, 129.8, 129.4, 129.3, 126.3, 125.4, 15.9; HR-MS: m/z calcd for ($C_{10}H_{10}OS$): 178.0452, found: 178.0460.

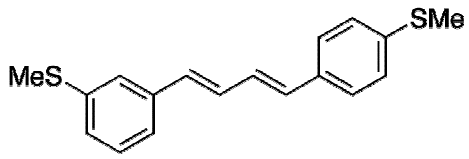


(2E,4E)-5-(3-(methylthio)phenyl)penta-2,4-dienal: General Wittig homologation procedure. Product was prepared from (*E*)-3-(methylthio)cinnamaldehyde and (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide and isolated as a yellow solid (yield: 0.501 g, 96.2%). ^{1}H NMR (300MHz, $CDCl_3$): δ 9.59 (d, *J* = 8.1 Hz, 1H), 7.32 (s, 1H), 7.28-7.14 (m, 4H), 6.98-6.86 (m, 2H), 6.23 (dd, *J* = 7.8 Hz, J = 15.3 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (300MHz, $CDCl_3$): δ 194.0, 152.2, 142.2, 139.9, 136.6, 132.2, 129.7,

127.8, 127.1, 125.7, 124.6, 16.1; HR-MS: m/z calcd for ($C_{12}H_{12}OS$): 204.0609, found: 204.0636.

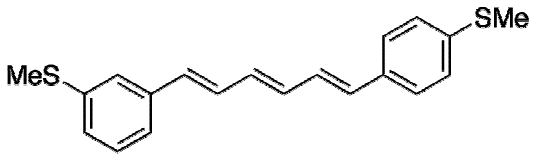


(E)-3,4'-di-(methylthio)stilbene (**PM1**): General Wittig Procedure. The product was prepared from 3-(methylthio)benzaldehyde and dimethyl 4-(methylthio)benzyl-phosphonate. Pure product as collected by filtration from the reaction suspension as a white solid (43.0%). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.36 (bs, 1H), 7.30-7.20 (m, 5H), 7.20-7.09 (m, 1H), 7.04 (d, *J* = 16.4 Hz, 1H), 7.03 (d, *J* = 16.4 Hz, 1H), 2.52 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 138.9, 138.1, 138.0, 134.1, 129.1, 128.7, 127.5, 127.0, 126.7, 125.7, 124.6, 123.3, 15.9, 15.7; HR-MS: m/z calcd for ($C_{16}H_{16}S_2$): 272.0693, found: 272.0686.

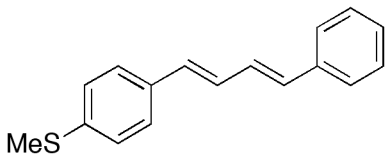


(1E,3E)-1-(3-(methylthio)phenyl)-4-(4-methylthio)phenyl)-buta-1,3-diene (**PM2**): General H.W.E. Procedure. The product was prepared from (*E*)-3-(methylthio)cinnamaldehyde and dimethyl 4-(methylthio)benzylphosphonate and isolated by column chromatography (10% ethyl acetate in hexanes) as an off-white solid in 86.5% yield. ^{1}H NMR (500MHz, $CDC1_3$): δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 1.6 Hz, 1H), 7.29-7.15 (m, 4H), 7.13 (dt, *J* = 1.6 Hz, 7.5 Hz, 1H), 7.00-6.84 (m, 2H), 6.68-

6.53 (m, 2H), 2.51 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (500MHz, $CDCl_3$): δ 138.97, 138.16, 138.12, 134.34, 132.78, 32.09, 130.02, 129.19, 128.60, 126.94, 126.78, 125.78, 124.58, 123.34, 16.02, 15.91; HR-MS: m/z calcd for ($C_{18}H_{18}S_2$): 298.0850, found: 298.0848.

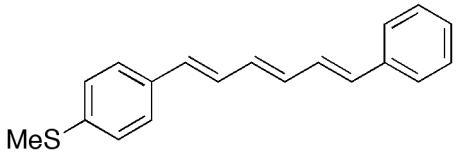


(1E,3E,5E)-1-(3-(methylthio)phenyl)-6-(4-methylthio)phenyl)-hexa-1,3,5-triene (**PM3**): General H.W.E. Procedure. The product was prepared from (2*E*,4*E*)-5-(3-(methylthio)phenyl)penta-2,4-dienal and dimethyl 4-(methylthio)benzylphosphonate and isolated by column chromatography (10% ethyl acetate in hexanes) as a yellow solid in 40.5% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.34 (d, *J* = 8.4 Hz, 2H), 7.30 (t, J = 1.5 Hz, 1H), 7.24-7.18 (m, 4H), 7.12 (dt, *J* = 1.5 Hz, 7.5 Hz, 1H), 6.91-6.81 (m, 2H), 6.75-6.40 (m, 4H), 2.51 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (500MHz, $CDCl_3$): δ 138.96, 138.20, 138.07, 134.47, 134.17, 133.30, 132.49, 132.08, 129.93, 129.18, 128.63, 126.92, 126.82, 125.84, 124.66, 123.37, 16.05, 15.94; HR-MS: m/z calcd for ($C_{20}H_{20}S_2$): 324.1006, found: 324.0997.

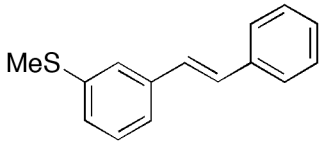


(1E,3E)-1-(4-(methylthio)phenyl)-4-phenyl-buta-1,3-diene (**3b**): General H.W.E. Procedure. The product was previously prepared from cyclopropyl carbinols through indium triflate catalyzed rearrangements by Ranu and Banerjee.[ix] Our ^{1}H and ^{13}C NMR

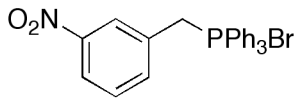
data agrees with their findings. We prepared the product from (*E*)-4-(methylthio)cinnamaldehyde[ii] and diethyl benzylphosphonate and isolated it as a white solid in 45.0% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.51 (d, *J* = 7.5 Hz, 2H), 7.44-7.35 (m, 4H), 7.30-7.24 (m, 3H), 7.07-6.94 (m, 2H), 6.74-6.66 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (300MHz, CD_2Cl_2): δ 138.5, 137.8, 134.6, 132.9, 132.5, 130.8, 129.6, 129.0, 127.9, 127.1, 126.9, 126.7, 15.8; HR-MS: m/z calcd for ($C_{17}H_{16}S$): 252.0973, found: 252.0979.



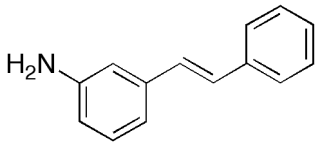
(1E,3E,5E)-1-(4-(methylthio)phenyl)-6-phenyl-hexaa-1,3,5-triene (**3c**): General H.W.E. Procedure. The product was prepared from (2*E*,4*E*)-5-(4-(methylthio)phenyl)penta-2,4-dienal[ii] and diethyl benzylphosphonate and isolated as a yellow solid in 31.3% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.48 (d, *J* = 7.5 Hz, 2H), 7.41-7.33 (m, 4H), 7.28-7.23 (m, 3H), 7.00-6.88 (m, 2H), 6.7-6.56 (m, 4H), 2.53 (s, 3H); ^{13}C NMR (500MHz, $C_2D_2Cl_4$): δ 137.36, 136.85, 133.81, 133.24, 133.02, 132.18, 131.66, 128.78, 128.35, 128.18, 127.27 , 126.42, 126.10, 126.01, 15.32; HR-MS: m/z calcd for ($C_{19}H_{18}S$): 278.1129, found: 278.1134.



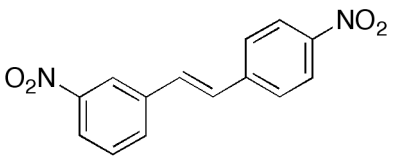
(E)-3-(methtylthio)stilbene (**4**): The compound is known in the literature and was initially synthesized by cationic cycloaromatization of the respective styryl *ß,ß*-bis(methylthio)vinyl ketones.[x] General H.W.E. Procedure. The product was prepared from 3-(methylthio)benzaldehyde and diethyl benzylphosphonate and isolated by column chromatography (5% ethyl acetate in hexanes) as a white solid in 98% yield. ^{1}H NMR (400MHz, $CDC1_3$): δ 7.52 (d, *J* = 7.6 Hz, 2H), 7.40 (bs, 1H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.30-7.24 (m, 3H), 7.15 (m, 1H), 7.09 (d, *J* = 16.0 Hz, 1H), 7.07 (d, *J* = 16.4 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (400MHz, $CDC1_3$): δ 138.9, 138.0, 137.1, 129.3, 129.1, 128.7, 128.1, 127.8, 126.6, 125.7, 124.6, 123.4, 15.9; HR-MS: m/z calcd for ($C_{15}H_{14}S$): 226.0816, found: 226.0808.



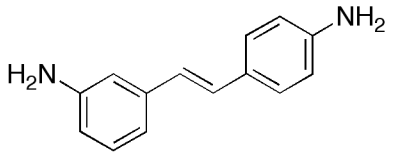
3-nitrobenzyltriphenylphosphonium bromide: This compound is known in the literature,[xi] however detailed characterization was not given. General Synthesis of triphenylphosphonium Halide Salts (above). Product was prepared from 3-nitrobenzyl bromide and triphenylphosphine and isolated as a white powder in quantitative yields. ^{1}H NMR (300MHz, DMSO-d_6): δ 8.16 (d, *J* = 7.2 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 3H), 7.79-7.65 (m, 14H), 7.55 (t, *J* = 8.1 Hz, 1H), 7.47 (bd, *J* = 7.8 Hz, 2H), 5.36 (d, *J* = 15.9 Hz, 2H); ^{13}C NMR (300MHz, DMSO-d_6): δ 138.2, 136.2, 135.0, 134.9, 131.2, 131.0, 126.4, 126.4, 124.1, 118.7, 117.5, 28.8, 28.2; HR-MS: m/z calcd for triphenylphosphonium cation ($C_{25}H_{21}NO_2P$): 398.1310, found: 398.1301.



(E)-3-aminostilbene (**7**): This compound is known[xii] and was synthesized as a control molecule to verify the trends in conductance found within the methylsulfide molecular wires. It was prepared by the General Reduction of Aryl-NO_2 to Aryl-NH_2 Group. (*E*)-3-dinitrostilbene[xiii] (0.100 g, 0.370 mmol), tin(II) chloride dihydrate (0.835 g), and 12 mL of anhydrous ethanol were added to a flame dried, 25-mL round-bottomed flask with stir bar and sealed with a septum. The suspension was purged with nitrogen for 10 minutes before heating to 70° C under an inert atmosphere. After 16 h the reaction was cooled to room temperature and the ethanol was removed under reduced pressure. Water was added followed by sat. aqueous $NaHCO_3$. The aqueous layer was extracted three times with dichloromethane. The solvent was remove and leaving a off-white solid (0.059 g, 68%). ^{1}H NMR (400MHz, $CDC1_3$): δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 8.4 Hz, 2H), 7.29 (td, *J* = 1.6 Hz, 7.2 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 16.4 Hz, 1H), 7,07 (d, *J* = 16.4 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.87 (s, 1H), 6.64 (dd, *J* = 2.0 Hz, 8.0 Hz, 1H), 3.70 (bs, 2H); ^{13}C NMR (400MHz, $CDC1_3$): δ 146.7, 138.4, 137.4, 129.6, 128.9, 128.7, 128.5, 127.6, 126.5, 117.3, 114.7, 112.9; HR-MS: m/z calcd for ($C_{14}H_{13}N$): 195.1048, found: 195.0461.

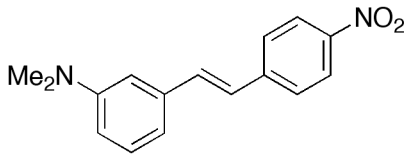


(E)-3,4'-dinitrostilbene: This compound is known in the literature,[xiv] however HR-MS, ^{1}H and ^{13}C NMR data was not provided. General Wittig Procedure. The product was prepared from 4-nitrobenzyltriphosphonium bromide and 3-nitrobenzaldehyde. A mixture of E/Z isomers was collected by vacuum filtration from the reaction suspension as a pale yellow precipitate. The E/Z mixture was placed in a 50-mL round-bottom flask with 20 mL of acetone and a crystal of iodine. The mixture was heated at reflux under a nitrogen atmosphere for 12 hours. The solution was cooled, and the product was collected by filtration to give yellow needles in overall 29% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 8.43 (t, *J* = 1.9 Hz, 1H), 8.27 (d, *J* = 8.9 Hz, 2H), 8.18 (d, *J* = 6.9 Hz, 1H), 7.88-7.81 (m, 1H), 7.69 (d, *J* = 8.9 Hz, 2H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.29 (s, 2H); ^{13}C NMR (300MHz, $CDC1_3$): δ 148.5, 147.4, 142.6, 138.0, 132.7, 130.5, 129.9, 129.3, 127.3, 124.3, 123.1, 121.3; HR-MS: m/z calcd for ($C_{14}H_{10}N_2O_4$): 270.0641, found: 270.0636.

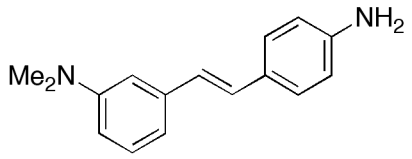


(E)-3,4'-diaminostilbene (**5**): This compound is known in the literature.[xv] General Reduction of Aryl-NO_2 to Aryl-NH_2 Group. The product was prepared from (*E)*-3,4'-dinitrostilbene and stannous chloride dihydrate and isolated by column chromatography (50% ethyl acetate in hexanes) as an off-white solid in 23.6% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.32 (d, *J* = 8.4 Hz, 2H), 7.11 (t, *J* = 7.8 Hz, 1H), 6.99 (d, *J* = 16.2 Hz, 1H),

6.89 (d, *J* = 7.8 Hz, 1H), 6.84 (d, *J* = 15.9 Hz, 1H), 6.79 (s, 1H), 6.67 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 7.5 Hz, 1H), 3.71 (bs, 4H); ^{13}C NMR (CDC13): δ 147.0, 146.5, 139.4, 129.8, 128.9, 128.5, 128.1, 125.7, 117.3, 115.6, 114.4, 112.9; HR-MS: m/z calcd for ($C_{14}H_{14}N_2$): 210.1157, found: 210.1152.



(E)-3-dimethylamino-4'-nitrostilbene: The product was prepared from 3-dimethylaminobenzaldehyde and 4-nitrobenzyltriphenylphosphonium bromide using the General Wittig Procedure. Pure product was isolated by column chromatography (10% ethyl acetate in hexanes) as an orange solid in 20.0% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 8.22 (d, *J* = 8.7 Hz, 2H), 7.63 (d, *J* = 8.7 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 16.2 Hz, 1H), 7.13 (d, *J* = 16.2 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.85 (bs, 1H), 6.74 (dd, *J* = 2.4 Hz, 8.1 Hz, 1H), 3.00 (s, 6H); ^{13}C NMR (300MHz, $CDCl_3$): δ 151.4, 147.1, 144.6, 137.3, 134.8, 129.9, 127.2, 126.2, 124.5, 115.7, 113.7, 111.5, 40.9; HR-MS: m/z calcd for ($C_{16}H_{16}N_2O_2$): 268.1212, found: 268.1225.



(E)-3-dimethylamino-4'-aminostilbene (**8**): General Reduction of Aryl-NO_2 to Aryl-NH_2 Group. The product was prepared from (*E*)-3-dimethylamino-4'-nitrostilbene and tin(II) chloride dihydrate isolated by column chromatography (25% ethyl acetate in hexanes) as

a off-white solid in 5.3% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.35 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.03 (d, *J* = 16.2 Hz, 1H), 6.92 (d, *J* = 16.2 Hz, 1H), 6.89 (d, *J* = 7.2 Hz, 1H), 6.82 (bs, 1H), 6.67 (d, *J* = 8.4 Hz, 2H), 6.62 (dd, *J* = 2.4 Hz, 8.4 Hz, 1H), 3.62 (bs, 2H), 2.97 (s, 6H); ^{13}C NMR (300MHz, $CDCl_3$): δ 151.3, 146.4, 139.1, 129.6, 128.7, 128.6, 128.1, 126.5, 115.6, 115.2, 112.1, 111.0, 41.1; HR-MS: m/z calcd for ($C_{16}H_{18}N_2$): 238.1470, found: 238.1480.

UV-vis Absorption Spectroscopy

The HOMO-LUMO gap of all our molecular wires was estimated using solution-phase UV-vis absorption spectroscopy. Absorption spectra were taken on an Agilent Technologies 8453 UV-Vis spectrophotometer using a quartz cuvette with path length equal to 1.0 cm. Solutions of molecular wires were prepared in CH_2Cl_2 at concentrations of ~1 mM. All spectra were normalized to 1.0 Abs for clarity.

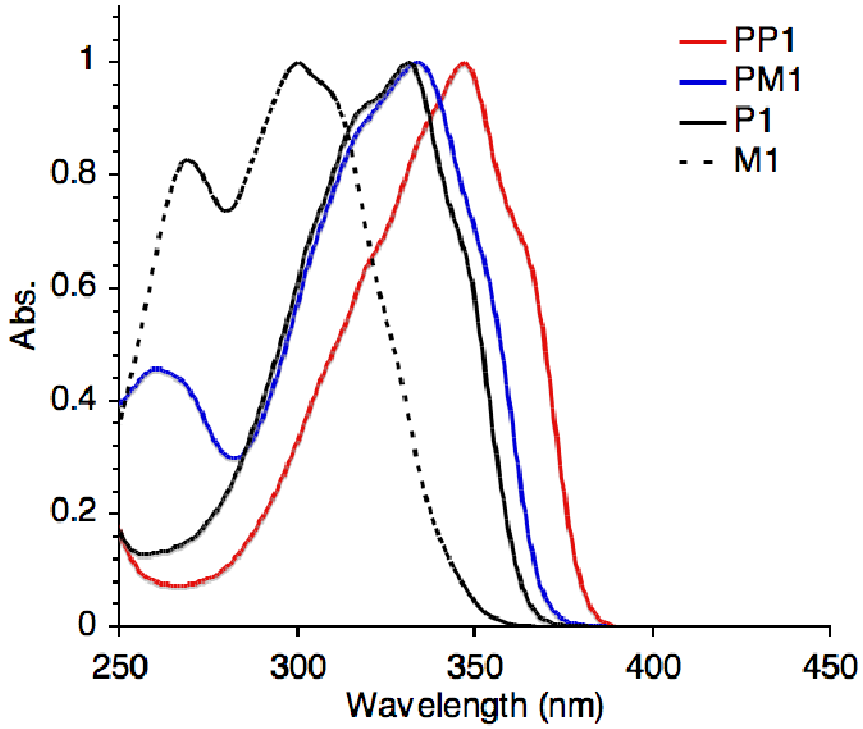


Figure S1. Optical absorption spectra of the methylsulfide-functionalized stilbenes.

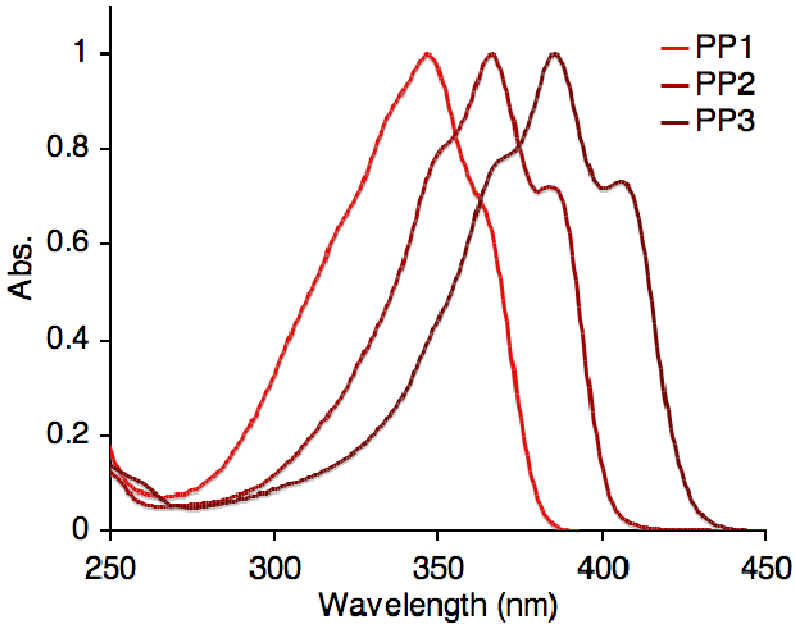


Figure S2. Optical absorption spectra of the *para-para* series (**PPn**).

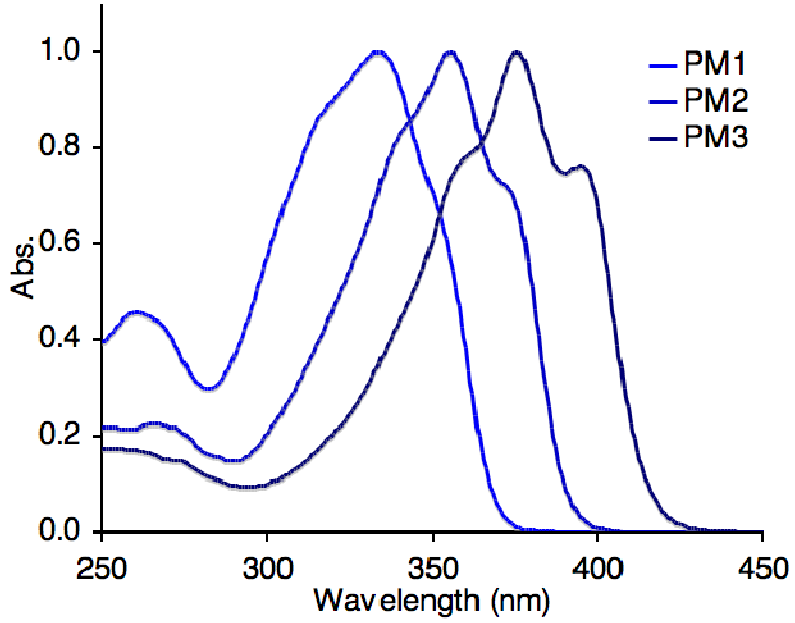


Figure S3. Optical absorption spectra of the *para-meta* series (**PMn**).

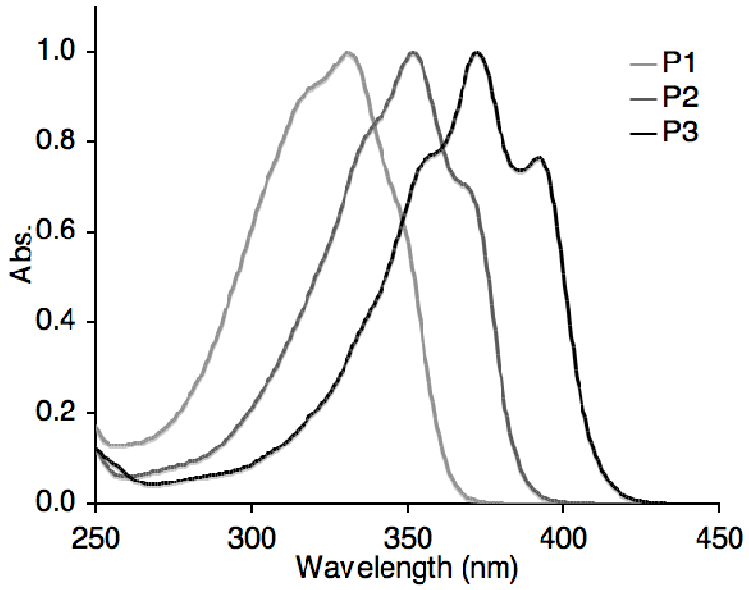


Figure S4. Optical absorption spectra of the *para*-π series (**Pn**).

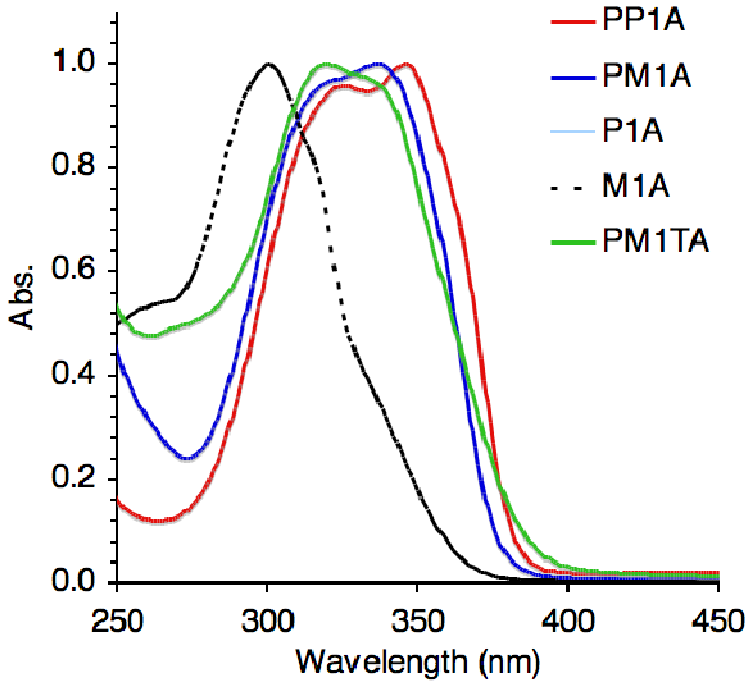


Figure S5. Optical absorption spectra of the amine-functionalized stilbene derivatives.

Molecule	E_{OP} (nm)	E_{OP} (eV)
PP1	389	3.19
PP2	416	2.98
PP3	435	2.85
PM1	380	3.26
PM2	403	3.08
PM3	430	2.88
P1	373	3.32
P2	395	3.14
P3	428	2.90
M1	358	3.46
PM1A	395	3.14
P1A	389	3.19
PM1TA	411	3.02

Table S1. Solution optical band gaps (E_{OP}) for target molecules range from 2.88-3.46 eV.

Conductance and Force Measurement and Analysis

STM Break Junction Conductance Measurement. Gold substrates were prepared by evaporating 100 nm of gold on freshly cleaved mica. A freshly cut gold wire was used as the STM tip. The junctions were repeatedly formed and broken in dilute solution of stilbene derivatives (1 ± 0.1 mM in 1,2,4-trichlorobenzene). The junction conductance (current/voltage) was measured at a constant bias of 500 mV. Over 5000 traces were used to construct 2D conductance-displacement (Figures S6 and S7) and 1D (Figure S8) conductance histograms.

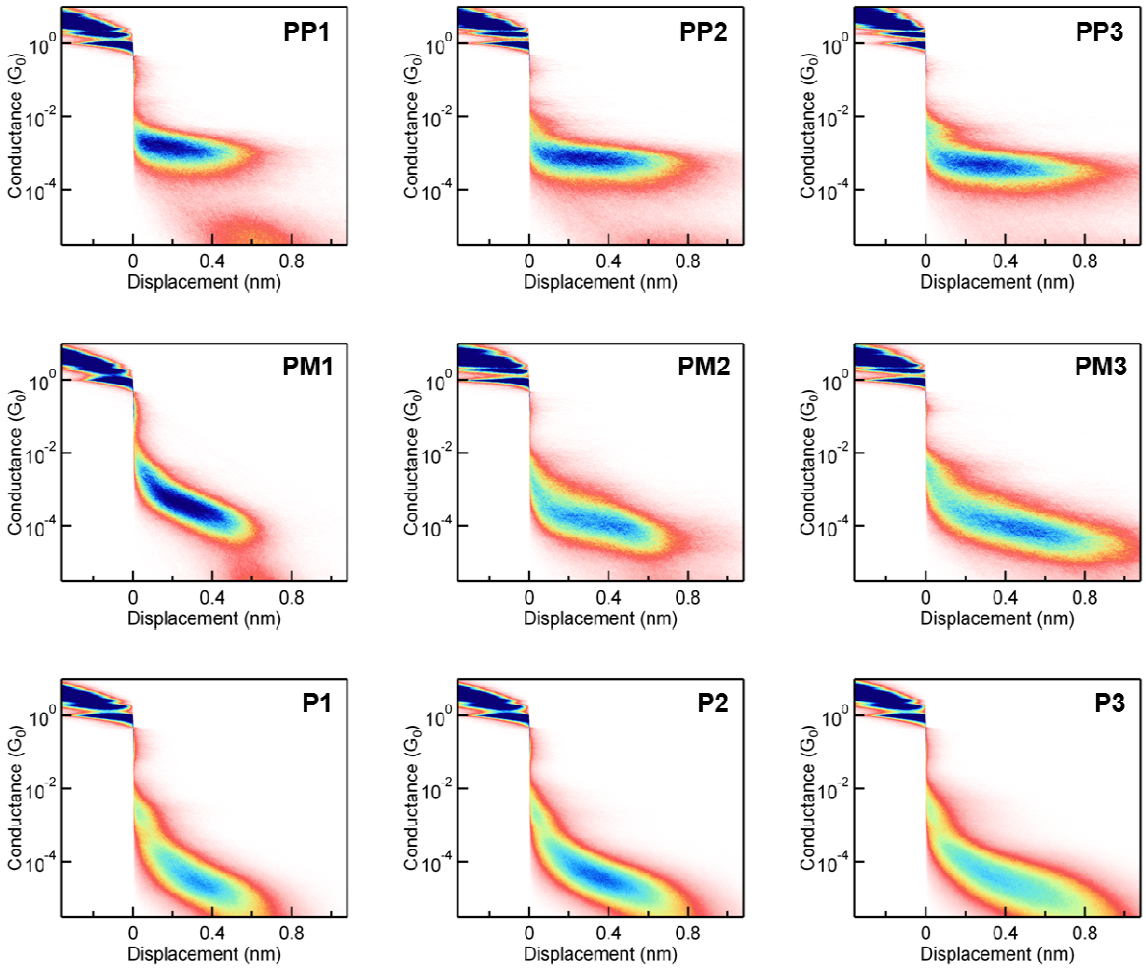


Figure S6. 2D conductance-displacement histograms for **PPn**, **PMn** and **Pn** molecular junctions.

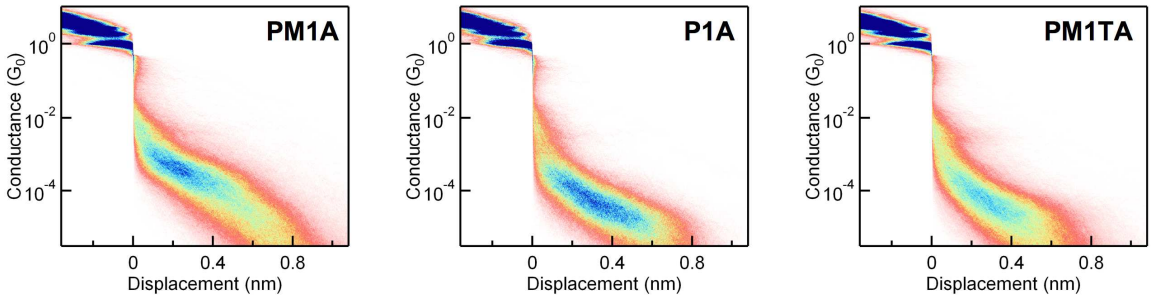


Figure S7. 2D conductance-displacement histograms for molecular junctions of amine-terminated molecular wires.

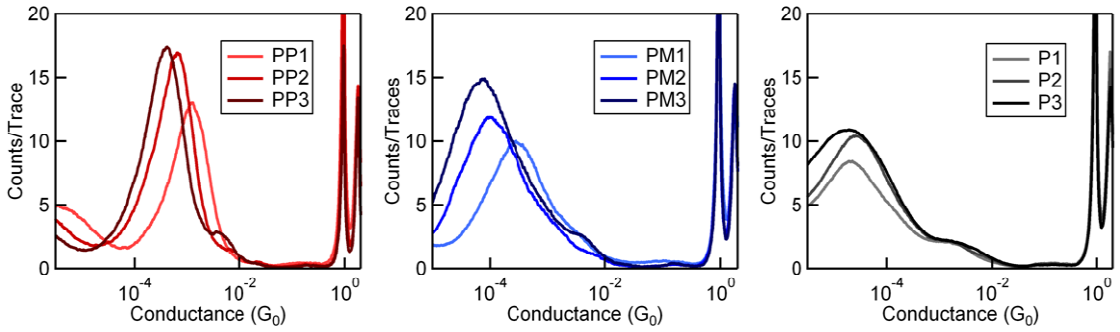


Figure S8. 1D conductance histograms of molecular junctions of **PPn**, **PMn** and **Pn** series of molecular wires.

Junction Variation Analysis. The variability of the mono-substituted series, **Pn**, is quantified in two steps. First, we construct separate (logarithmically binned) 1D histograms, 1000 traces at a time, for each molecule. The peak position of each of these

histograms is well defined, and is extracted using a Gaussian fit in the neighborhood of the molecular conductance feature. Then, peak values from these individual histograms are compiled from at least three separate experiments with different tip-sample combinations, totaling more than 30,000 individual measurements. The arithmetic mean as well as the 10^{th}, 25^{th}, 75^{th} and 90^{th} percentiles are computed from these peak positions, and are used to construct Figure 2 in the manuscript. Table S2 provides a summary of these statistics, along with the variation– defined as (75^{th} – 25^{th} percentile)/(mean value) for **Pn** series. The largest variation among the difunctionalized compounds was observed in **PM3**, and is given in the table for comparison.

Table S2. Comparison of Conductance Variation in STM-BJ's.

Molecule	Mean	25th %ile	75th %ile	% variation
P1	1.95×10^{-5}	1.71×10^{-5}	2.56×10^{-5}	44
P2	2.74×10^{-5}	1.56×10^{-5}	3.39×10^{-5}	67
P3	1.31×10^{-5}	8.25×10^{-6}	3.65×10^{-5}	216
PM3	8.74×10^{-5}	7.28×10^{-5}	9.47×10^{-5}	25

AFM Simultaneous Force and Conductance Measurement. A home-built conducting atomic force microscope (AFM) is used to simultaneously measure conductance and force across single molecule junctions. Au-coated (100 nm) mica substrates and Au-coated (100 nm) commercial AFM cantilevers (~50 N/m, NanoAndMore Inc.) are used as the two electrodes. Dilute solutions of the molecules (~ 1mM in 1,2,4-trichlorobenzene) are deposited on the substrates to perform single-molecule measurements. A constant voltage bias of 75 mV is used to obtain conductance measurements, while minimizing electrostatic tip-substrate interactions. The details of the experimental setup[xvi] and analysis technique[i] have both been described in detail previously.

Briefly, we use an automated algorithm to search for the last significant force fluctuation (of 0.3 nN or above, which is ~ 2× the noise floor of the force measurement) up to 1 nm beyond the rupture from Au point contact. If such an event is found, the force data is offset laterally such that this location becomes the origin (zero displacement), as demonstrated in Figure S10a. Every such measurement is accumulated to construct a 2D force histogram (Figure S10B).

A statistically averaged force profile is then obtained, corresponding to the location of the maximum counts in force at each displacement value, as shown in Figure S10b (blue trace overlaid). The drop in force at zero displacement is then representative of the statistically averaged value of the junction rupture force. For junctions of **PP1** and **PM1**, the algorithm finds significant force fluctuations due to molecular junctions in more than 90% of the measured traces, in contrast to **P1** where only 12% of the measurements have such events. The rupture force for **PP1** and **PM1** are found to be 0.5

nN, whereas for **P1**, we obtain 0.3 nN, which is same as the threshold used to detect the force events (inset of Figure S10B). Together, the low probability of molecular force events, and the null value of the rupture force imply that the rupture force for **P1** is smaller than 0.3 nN.

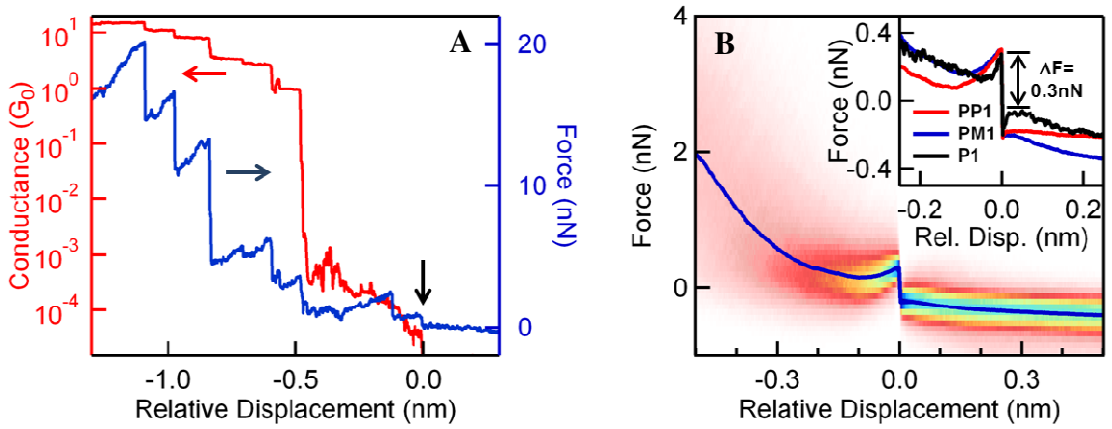


Figure S10. (A) A sample simultaneous measurement of conductance (red, left axis) and force (blue, right axis) with **PM1** molecule. The downward arrow indicates the rupture of the **PM1** molecular junction in force; a highly correlated drop in conductance is also observed in the conductance at the same location (zero of the displacement axis). (B) 2D force histogram for **PM1** constructed from 8242 traces. The averaged force profile is overlaid. Inset: Comparison of averaged force profiles for **PP1**, **PM1** and **P1**.

Theoretical Methods and Details

All electronic structure calculations used Jaguar (version 7.8, Schrodinger LLC, New York, NY, 2011) using the B3LYP hybrid functional and the 6-31G** basis sets. Final geometries and energies, as well as orbital energies are given below.

Molecule	E_{HOMO} **(eV)**	E_{LUMO} **(eV)**	E_{DFT} **(eV)**
PP1	-5.03	-1.34	3.69
PP2	-4.89	-1.58	3.31
PP3	-4.79	-1.79	3.00
PM1	-5.22	-1.41	3.81
PM2	-5.06	-1.66	3.40
PM3	-4.93	-1.86	3.07
P1	-5.21	-1.35	3.85
P2	-5.04	-1.62	3.42
P3	-4.90	-1.82	3.08
M1	-5.47	-1.44	4.04
PM1A	-4.82	-0.93	3.89
P1A	-4.93	-1.05	3.88
M1A	-5.11	-1.17	3.94
PM1TA	-4.98	-1.19	3.79

Table S3. Summary of DFT calculations. Energy of the HOMO (E_{HOMO}) and LUMO (E_{LUMO}) and the HOMO-LUMO energy gap (E_{DFT}) energies of all derivatives.

PP1

Final total energy: -1415.73607449062 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-3.8434657906	-1.8489488923	-0.0120387531
C2	-4.5597978043	-0.6660921203	-0.2805624712
C3	-5.9467255545	-0.6325681374	-0.2796433503
C4	-6.6855502592	-1.7937947552	-0.0064348986
C5	-5.9902287827	-2.9808488469	0.2650085261
C6	-4.5991963175	-3.0026449136	0.2621135588
H8	-4.0097134678	0.2469096457	-0.4949240973
H9	-6.4629515231	0.2996396986	-0.4916892543
H11	-6.5258516266	-3.8979328936	0.4823056343
H12	-4.0982714329	-3.9407699265	0.4812263322
C12	-1.5316801901	-2.8421871117	0.1511900371
C13	-2.3802636501	-1.8091183580	-0.0312521643
H15	-1.9652880229	-0.8205089096	-0.2198575523
H16	-1.9486865576	-3.8323927158	0.3259489543
C16	2.7734875957	-2.8774915889	0.1311408256
C17	2.0277379167	-4.0554884837	0.2888181918
C18	0.6411749301	-4.0140393968	0.2921141524
C19	-0.0682757996	-2.8065055585	0.1381972998
C20	0.6946137979	-1.6350753330	-0.0162369530
C21	2.0856456257	-1.6651369891	-0.0209750767
H23	2.5383213377	-5.0068558627	0.4096633569
H24	0.0856855673	-4.9404056715	0.4159550123
H25	0.1994174010	-0.6754224880	-0.1305297622
H26	2.6273682700	-0.7339753005	-0.1424063707
S26	-8.4609420801	-1.6384944700	-0.0311872223
C27	-9.0457398363	-3.3122035795	0.3862641249
H28	-10.1358266120	-3.2488756365	0.3880750438
H29	-8.7357642632	-4.0449031320	-0.3622958347
H30	-8.7077887729	-3.6191342554	1.3787457348
S30	4.5474530372	-3.0472519226	0.1422375258
C31	5.1465915681	-1.3400388869	-0.0658394496
H32	6.2362572697	-1.4100408636	-0.0593391970
H33	4.8255885854	-0.9149795515	-1.0193301512
H34	4.8286735152	-0.6998453415	0.7601083900

HOMO energy: -0.18483 hartrees

LUMO energy: -0.04928 hartrees

Orbital energies (hartrees):

-88.88533	-88.88533	-10.22391	-10.22390	-10.22024	-10.22022
-10.19744	-10.19727	-10.19490	-10.19484	-10.19299	-10.19283
-10.19270	-10.19270	-10.19168	-10.19162	-10.19059	-10.18982
-7.94627	-7.94626	-5.91154	-5.91154	-5.90741	-5.90741
-5.90116	-5.90115	-0.86678	-0.86337	-0.81690	-0.80337
-0.77646	-0.74930	-0.74811	-0.74693	-0.71289	-0.66634
-0.64406	-0.62146	-0.61013	-0.59317	-0.57536	-0.55401
-0.50733	-0.50164	-0.46834	-0.46315	-0.45534	-0.44748
-0.44163	-0.43725	-0.43718	-0.43554	-0.42303	-0.41971
-0.40553	-0.40003	-0.38175	-0.37464	-0.36866	-0.36828
-0.35153	-0.34528	-0.33545	-0.32320	-0.32060	-0.31940
-0.29357	-0.25459	-0.25419	-0.25029	-0.21622	-0.18483
-0.04928	-0.00270	-0.00263	0.01549	0.03558	0.03569
0.07273	0.07408	0.07412	0.09542		

PP2

Final total energy: -1493.14718671261 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-2.3426775229	0.3995095608	0.2271635527
C2	-3.0478500144	1.6139813026	0.1671225268
C3	-4.4559283131	1.5375564676	0.2236024395
C4	-5.1094032871	0.3209868684	0.3336649073
C5	-4.3867386852	-0.8851527425	0.3925295337
C6	-2.9896899681	-0.8288809901	0.3374113222
H7	-1.2562442673	0.4182435637	0.1862575986
H9	-5.0508083675	2.4449004000	0.1812964131
H10	-6.1949642165	0.2986233620	0.3751764357
H12	-2.3939219123	-1.7334528963	0.3790083062
C12	-2.7918756553	4.1254521647	-0.0162133438
C13	-2.3021963745	2.8637794382	0.0524918686
H15	-1.2187522020	2.7464803418	0.0200902986
H16	-3.8676876486	4.2937979399	0.0125048882
C16	-2.4443747228	6.5643786043	-0.1968484366
C17	-1.9629571924	5.2996381087	-0.1280939073
H19	-0.8877721980	5.1271682639	-0.1565392351
H20	-3.5265966465	6.6919774791	-0.1654450995
C20	-0.3049851916	10.2844717219	-0.5322354923
C21	-1.7029789238	10.2492150939	-0.4815755756
C22	-2.3696077966	9.0306797560	-0.3725988926
C23	-1.6836926068	7.8052647531	-0.3103159240
C24	-0.2741033785	7.8611504965	-0.3626713669
C25	0.3985830592	9.0672098383	-0.4705632110
H27	-2.2844765369	11.1629551894	-0.5259612429
H28	-3.4563184210	9.0293368098	-0.3350256829
H29	0.3075175889	6.9454721734	-0.3173875929
H30	1.4845883058	9.0726916977	-0.5071149586
S30	0.6745435159	11.7661241977	-0.6714303558
S31	-5.3407273913	-2.3829791615	0.5323163287
C32	-0.5657889538	13.0994612142	-0.7048297948
H33	0.0037994124	14.0278260094	-0.7824793883
H34	-1.2232856043	13.0144143901	-1.5730491862
H35	-1.1548726080	13.1215346676	0.2148660257
C35	-4.0751165783	-3.6914743480	0.5912039609
H36	-4.6268065871	-4.6293897572	0.6814976262
H37	-3.4816895207	-3.7170720836	-0.3256451807
H38	-3.4230535777	-3.5792297134	1.4604472093

HOMO energy: -0.17989 hartrees
LUMO energy: -0.05819 hartrees

Orbital energies (hartrees):

-88.88601	-88.88588	-10.22447	-10.22425	-10.22057	-10.22050
-10.19725	-10.19723	-10.19413	-10.19405	-10.19398	-10.19375
-10.19270	-10.19268	-10.19246	-10.19226	-10.19081	-10.19078
-10.18983	-10.18946	-7.94694	-7.94681	-5.91220	-5.91207
-5.90808	-5.90794	-5.90186	-5.90172	-0.86558	-0.86476
-0.82047	-0.80901	-0.79180	-0.76513	-0.74978	-0.74851
-0.73865	-0.70716	-0.66780	-0.64956	-0.61125	-0.61004
-0.60663	-0.58150	-0.56194	-0.54973	-0.51334	-0.49343
-0.47655	-0.46312	-0.45779	-0.45268	-0.44704	-0.44006
-0.43752	-0.43742	-0.42570	-0.42117	-0.41798	-0.40503
-0.38873	-0.38726	-0.37988	-0.37744	-0.36963	-0.35834
-0.34567	-0.34181	-0.33736	-0.33359	-0.32096	-0.32057
-0.30755	-0.27847	-0.25434	-0.25395	-0.23881	-0.21178
-0.17989	-0.05819	-0.00481	-0.00258	0.00028	0.03521
0.03540	0.04919	0.07278	0.07419	0.09198	

PP3

Final total energy: -1570.55777722054 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-3.1551496645	-0.6879559967	0.0298618562
C2	-3.8331293924	0.5370730239	-0.0962281767
C3	-5.2228585531	0.6212940323	-0.0665630512
C4	-5.9934697400	-0.5356753780	0.0926084957
C5	-5.3320694910	-1.7712854312	0.2194653054
C6	-3.9494693277	-1.8440539426	0.1886412849
H8	-3.2545191227	1.4492428745	-0.2207461730
H9	-5.6921724636	1.5930939161	-0.1683384951
H11	-5.9135644082	-2.6807345772	0.3438048701
H12	-3.4783510527	-2.8169266177	0.2899312979
C12	-0.8723064740	-1.7732230234	0.1020687380
C13	-1.6969243605	-0.7019811848	-0.0077536449
H15	-1.2325168067	0.2754924195	-0.1391683053
H16	-1.2928066323	-2.7688387784	0.2351041179
C16	1.3962637767	-2.7598903379	0.1684609068
C17	0.5624780039	-1.6911897147	0.0564464166
H19	0.9972679888	-0.7000366234	-0.0767287034
H20	0.9581320534	-3.7497195073	0.3016018597
C20	3.6408452228	-3.7704801249	0.2427604174
C21	2.8316557782	-2.6880505007	0.1264906468
H23	3.2646124641	-1.6973844820	-0.0064163587
H24	3.1597096911	-4.7398825885	0.3743251359
C24	7.9335142822	-4.0201546780	0.1792768013
C25	7.1327097530	-5.1617697156	0.3418825608
C26	5.7503478782	-5.0538382762	0.3586689862
C27	5.0987091406	-3.8116301104	0.2154009235
C28	5.9166104051	-2.6782479235	0.0530805644
C29	7.3037137505	-2.7754150869	0.0348220496
H31	7.5981676516	-6.1369399235	0.4553998180
H32	5.1512769576	-5.9520865853	0.4860159106
H33	5.4664591196	-1.6972202701	-0.0620145632
H34	7.8884172616	-1.8716544615	-0.0931652146
S34	-7.7736393134	-0.5751673799	0.1480717571
S35	9.6970797157	-4.2727603815	0.1731346389
C36	10.3718983264	-2.5972341185	-0.0609335293
H37	11.4570840218	-2.7178796934	-0.0713936708
H38	10.0548913316	-2.1663199301	-1.0133891647
H39	10.0978857909	-1.9351469426	0.7636288567

C39	-8.2481010201	1.1731158198	-0.0402055755
H40	-9.3394650905	1.1862091481	-0.0087950934
H41	-7.8633221428	1.7833973846	0.7799505496
H42	-7.9170999999	1.5772378425	-0.9994620603

HOMO energy: -0.17597 hartrees
LUMO energy: -0.06587 hartrees

Orbital energies (hartrees):

-88.88634	-88.88628	-10.22501	-10.22480	-10.22090	-10.22087
-10.19776	-10.19755	-10.19555	-10.19457	-10.19420	-10.19363
-10.19339	-10.19328	-10.19277	-10.19231	-10.19152	-10.19150
-10.19055	-10.19003	-10.18975	-10.18953	-7.94727	-7.94721
-5.91253	-5.91248	-5.90840	-5.90834	-5.90219	-5.90212
-0.86588	-0.86569	-0.82335	-0.81312	-0.80103	-0.78040
-0.75762	-0.74938	-0.74891	-0.73375	-0.70373	-0.66695
-0.65086	-0.61964	-0.61114	-0.60818	-0.58537	-0.56898
-0.55545	-0.54884	-0.50969	-0.49922	-0.47893	-0.46574
-0.46033	-0.45538	-0.45073	-0.44285	-0.43786	-0.43786
-0.43428	-0.42655	-0.42086	-0.41497	-0.40402	-0.39260
-0.38555	-0.37971	-0.37888	-0.37037	-0.35954	-0.35813
-0.34697	-0.34081	-0.33968	-0.33928	-0.32118	-0.32075
-0.31813	-0.29534	-0.26489	-0.25488	-0.25449	-0.23099
-0.20760	-0.17597	-0.06587	-0.01572	-0.00322	-0.00218
0.03069	0.03496	0.03504	0.07243	0.07311	0.07326

PM1

Final total energy: -1415.73537949533 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-4.1841626791	1.5569152376	0.1876405253
H2	-4.8681849692	2.1476792536	0.8002559953
H4	-3.5310557600	2.2345545285	-0.3669654053
H5	-3.5926357479	0.9112819201	0.8407662029
S5	-5.2447620944	0.5862788618	-0.9305507327
C6	-2.3823785809	-1.9177229951	-3.5570237809
C7	-3.7844491201	-1.9666890719	-3.6834427426
C8	-4.6197022234	-1.2029753234	-2.8809826322
C9	-4.0829755879	-0.3486244001	-1.9053112009
C10	-2.6889818901	-0.2887247417	-1.7631528553
C11	-1.8610176290	-1.0591520904	-2.5731102603
H13	-4.2245698321	-2.6208744022	-4.4320987891
H14	-5.6965058426	-1.2683829515	-3.0096548134
H15	-2.2361014097	0.3563953038	-1.0191008976
H16	-0.7872595727	-0.9878255599	-2.4280142244
C16	-0.2166891382	-2.8021124764	-4.4961546441
C17	-1.5629807732	-2.7490076915	-4.4409475680
H19	-2.1367771807	-3.3756844631	-5.1215955134
H20	0.3582907936	-2.1623091605	-3.8287710090
C20	2.2951312176	-5.1603142055	-7.0404801091
C21	0.9139641993	-5.3366790344	-7.0833230429
C22	0.0675872953	-4.5900090945	-6.2688007359
C23	0.6001639505	-3.6354947902	-5.3846752709
C24	1.9986199116	-3.4671145401	-5.3448578342
C25	2.8479013190	-4.2165362547	-6.1615582525
H26	2.9419420299	-5.7526805353	-7.6810011348
H27	0.4938780097	-6.0732378099	-7.7625410961
H28	-1.0032460330	-4.7569812191	-6.3168710225
H29	2.4050003077	-2.7312507175	-4.6593427007
S30	4.6277835112	-4.0636045686	-6.1743032869
C31	4.9616803185	-2.7851081655	-4.9205730380
H32	6.0476767973	-2.6723956119	-4.9002796841
H33	4.5125037958	-1.8272913686	-5.1931900786
H34	4.6202373396	-3.0942580685	-3.9298415359

HOMO energy: -0.19201 hartrees
LUMO energy: -0.05198 hartrees

Orbital energies (hartrees):

-88.88746	-88.88300	-10.22661	-10.22306	-10.22202	-10.21902
-10.20222	-10.19962	-10.19723	-10.19551	-10.19498	-10.19406
-10.19377	-10.19234	-10.19214	-10.19182	-10.19105	-10.18648
-7.94839	-7.94393	-5.91366	-5.90953	-5.90924	-5.90511
-5.90329	-5.89874	-0.86837	-0.86348	-0.81707	-0.80198
-0.78236	-0.75441	-0.75061	-0.73640	-0.71449	-0.66063
-0.65402	-0.62388	-0.60948	-0.59341	-0.57814	-0.54317
-0.51293	-0.50491	-0.47107	-0.46640	-0.45517	-0.44585
-0.44386	-0.43904	-0.43713	-0.43586	-0.42558	-0.41866
-0.40479	-0.39467	-0.38316	-0.37503	-0.37209	-0.36662
-0.35597	-0.34634	-0.33625	-0.32313	-0.32257	-0.31755
-0.29178	-0.27053	-0.25646	-0.23700	-0.21015	-0.19201
-0.05198	-0.00496	0.00104	0.01355	0.03367	0.03727
0.07153	0.07222	0.07460	0.09410		

PM2

Final total energy: -1493.14628820380 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	3.4309097782	-2.6742507232	-0.0445427170
C2	2.5858524868	-1.6221888849	0.0730163638
H3	3.0285750210	-0.6350856798	0.2075180118
H4	3.0323966266	-3.6783857411	-0.1798668317
C5	5.7072258229	-3.6165548353	-0.1211760795
C6	4.8672005688	-2.5614230687	-0.0029803294
H7	5.2693188189	-1.5585090740	0.1306008651
H8	5.2582754989	-4.6005685628	-0.2570214150
C9	9.9835303964	-3.7265535331	-0.0571460621
C10	9.2403428278	-4.9023263880	-0.2421129830
C11	7.8461417671	-4.8313837265	-0.2569875890
C12	7.1698681221	-3.6052080974	-0.0929508361
C13	7.9348211422	-2.4397050911	0.0908049013
C14	9.3242046084	-2.5106970002	0.1073491009
H15	11.0689058255	-3.7655739556	-0.0415250075
H16	7.2516000592	-5.7276615182	-0.3972100526
H17	7.4474516624	-1.4797181811	0.2249292723
H18	9.9072374063	-1.6052765001	0.2507602410
S19	10.1789174143	-6.4096989895	-0.4391533848
C20	8.9033085215	-7.6904505167	-0.6618136303
H21	9.4494681120	-8.6275149673	-0.7884150734
H22	8.2588917337	-7.7732585189	0.2163770056
H23	8.3024934736	-7.5084615313	-1.5558648984
C24	-1.7142516165	-1.5642160130	-0.0101675885
C25	-1.0213289917	-2.7807127837	-0.1512348766
C26	0.3624864690	-2.8167710817	-0.1258793556
C27	1.1265067181	-1.6421870324	0.0410959452
C28	0.4182519244	-0.4366410456	0.1809809238
C29	-0.9737426442	-0.3889636394	0.1573772335
H30	-1.5787877651	-3.7039888423	-0.2830047986
H31	0.8584053613	-3.7754774787	-0.2393656009
H32	0.9731481005	0.4892386087	0.3121587236
H33	-1.4680648502	0.5689931485	0.2707910000
S34	-3.4925301763	-1.6522694111	-0.0581361428
C35	-4.0137918152	0.0811330683	0.1413373017
H36	-5.1050381604	0.0648937336	0.1096878573
H37	-3.6938141556	0.4876739165	1.1032856899

H38	-3.6453074801	0.7064700900	-0.6748589477

HOMO energy: -0.18603 hartrees
LUMO energy: -0.06110 hartrees

Orbital energies (hartrees):

-88.88766	-88.88260	-10.22648	-10.22270	-10.22195	-10.21846
-10.20187	-10.19941	-10.19614	-10.19587	-10.19501	-10.19453
-10.19401	-10.19344	-10.19261	-10.19208	-10.19202	-10.19176
-10.19093	-10.18662	-7.94861	-7.94353	-5.91386	-5.90973
-5.90884	-5.90471	-5.90353	-5.89834	-0.86763	-0.86430
-0.82173	-0.80760	-0.79356	-0.77168	-0.75197	-0.74474
-0.73585	-0.70852	-0.66304	-0.65368	-0.62425	-0.61289
-0.59445	-0.58687	-0.55923	-0.54472	-0.51379	-0.50050
-0.48069	-0.46451	-0.45931	-0.45168	-0.44456	-0.44324
-0.43901	-0.43533	-0.42895	-0.42279	-0.41729	-0.39707
-0.39346	-0.38668	-0.38155	-0.37759	-0.36674	-0.36074
-0.35206	-0.34196	-0.33836	-0.33488	-0.32264	-0.31764
-0.30621	-0.28098	-0.26283	-0.25616	-0.22770	-0.20869
-0.18603	-0.06110	-0.00628	-0.00268	0.00190	0.03379
0.03776	0.04783	0.07179	0.07510	0.08987	

PM3

Final total energy: -1570.55698523588 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-1.1214174131	-0.5496530163	-0.1421607584
C2	-1.9001919380	-1.7258257742	-0.1936817260
C3	-3.2834508741	-1.6741721547	-0.2293588137
C4	-3.9607073966	-0.4406197988	-0.2151470989
C5	-3.2054229588	0.7361770033	-0.1636312596
C6	-1.8147633186	0.6731104147	-0.1281622186
H8	-1.4163744755	-2.6976184912	-0.2061226513
H9	-3.8530224789	-2.5986170235	-0.2688857519
H11	-3.6874124894	1.7069506489	-0.1506857277
H12	-1.2478555418	1.6001010588	-0.0885594658
S12	-5.7395675213	-0.5083250317	-0.2654271733
C13	-6.2362483257	1.2435577975	-0.2344455922
H14	-7.3276436229	1.2395804495	-0.2646318884
H15	-5.9094981105	1.7365168155	0.6838635087
H16	-5.8602332270	1.7821032315	-1.1071461148
C16	1.1738665274	-1.6085319089	-0.1099699765
C17	0.3365626975	-0.5417718681	-0.1041437221
H19	0.7891279905	0.4492863493	-0.0673123014
H20	0.7664547045	-2.6175886665	-0.1457429997
C20	3.4565476790	-2.5642195597	-0.0772933417
C21	2.6070923235	-1.5026593544	-0.0715352384
H23	3.0277071992	-0.4971960234	-0.0356951856
H24	3.0359175572	-3.5696464281	-0.1127364341
C24	5.7237014967	-3.5284870603	-0.0454439044
C25	4.8902679352	-2.4599237635	-0.0396985916
H27	5.3007783018	-1.4521846187	-0.0052862828
H28	5.2673327592	-4.5177756381	-0.0808368635
C28	9.9985608557	-3.6650738906	0.0544182194
C29	9.2449052948	-4.8481614661	0.0049838393
C30	7.8516394427	-4.7671879714	-0.0266147217
C31	7.1852568012	-3.5244732234	-0.0100516582
C32	7.9600816236	-2.3514923509	0.0397254081
C33	9.3488468432	-2.4327556513	0.0712834146
H34	11.0833252990	-3.7111547758	0.0798298231
H36	7.2494542945	-5.6684899257	-0.0650609156
H37	7.4808841818	-1.3783068197	0.0544626917
H38	9.9396869824	-1.5219005612	0.1101052170
S38	10.1671572344	-6.3780466925	-0.0131781070

C39	8.8764800127	-7.6616286812	-0.0775953370
H40	9.4116810129	-8.6134289617	-0.0887541255
H41	8.2323539104	-7.6291314697	0.8042028085
H42	8.2763354500	-7.5834368827	-0.9871154871

HOMO energy: -0.18110 hartrees
LUMO energy: -0.06838 hartrees

Orbital energies (hartrees):

-88.88788	-88.88275	-10.22678	-10.22303	-10.22203	-10.21863
-10.20205	-10.19954	-10.19631	-10.19605	-10.19512	-10.19475
-10.19413	-10.19347	-10.19336	-10.19278	-10.19218	-10.19215
-10.19195	-10.19177	-10.19129	-10.18675	-7.94882	-7.94368
-5.91407	-5.90994	-5.90899	-5.90486	-5.90375	-5.89849
-0.86769	-0.86447	-0.82497	-0.81250	-0.80028	-0.78455
-0.76331	-0.75141	-0.73904	-0.73475	-0.70442	-0.66362
-0.65390	-0.62980	-0.61297	-0.59650	-0.59224	-0.56831
-0.55723	-0.53965	-0.51326	-0.50457	-0.47979	-0.47022
-0.46122	-0.45589	-0.44789	-0.44419	-0.43914	-0.43544
-0.43506	-0.43149	-0.42133	-0.41000	-0.39854	-0.39277
-0.38735	-0.38126	-0.37826	-0.37313	-0.36001	-0.35965
-0.35008	-0.34249	-0.34164	-0.33865	-0.32276	-0.31784
-0.31782	-0.29387	-0.27437	-0.25688	-0.25258	-0.22107
-0.20764	-0.18110	-0.06838	-0.01702	-0.00480	0.00133
0.02933	0.03363	0.03757	0.07122	0.07177	0.07498

P1

Final total energy: -978.23224126891 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	2.0459081377	0.4276365722	-0.0033426950
C2	1.3357180151	1.6440195419	-0.0032010887
C3	-0.0509626423	1.6827516209	-0.0043976047
C4	-0.7949471235	0.4930725167	-0.0057504205
C5	-0.1054134668	-0.7279813582	-0.0058315340
C6	1.2853240827	-0.7547205650	-0.0047644557
H8	1.8906094781	2.5790452759	-0.0021160369
H9	-0.5626683380	2.6411109630	-0.0042185370
H11	-0.6448710554	-1.6681824002	-0.0067592443
H12	1.7820003632	-1.7199402003	-0.0049731160
C12	4.3565611442	-0.5836143713	-0.0031851937
C13	3.5091188302	0.4651646844	-0.0019358149
H15	3.9261363203	1.4704971079	0.0003770118
H16	3.9426085933	-1.5902623916	-0.0059349083
C16	8.6461496155	-0.5837977461	0.0026889973
C17	7.9253881781	-1.7773089379	-0.0017504087
C18	6.5331388321	-1.7519178731	-0.0036753571
C19	5.8216071913	-0.5376343723	-0.0012014785
C20	6.5674223129	0.6575897095	0.0031382380
C21	7.9575194646	0.6324310976	0.0050957687
H22	9.7321370603	-0.5981631253	0.0043013150
H23	8.4472423474	-2.7301744527	-0.0036965366
H24	5.9784854030	-2.6871478172	-0.0071477200
H25	6.0575640714	1.6160273577	0.0050404350
H26	8.5102615451	1.5677966082	0.0085199717
S26	-2.5692484006	0.6578768678	-0.0073705386
C27	-3.1620558017	-1.0642160476	0.0066487642
H28	-4.2519946798	-0.9987417114	0.0092229984
H29	-2.8427859704	-1.6057339193	-0.8866139095
H30	-2.8375598464	-1.5928114655	0.9057416875

HOMO energy: -0.19140 hartrees
LUMO energy: -0.04978 hartrees

Orbital energies (hartrees):
-88.88605 -10.22510 -10.22073 -10.19829 -10.19791 -10.19560
-10.19370 -10.19348 -10.19245 -10.19143 -10.18997 -10.18924
-10.18880 -10.18807 -10.18794 -10.18777 -7.94699 -5.91226

-5.90812 -5.90188 -0.86639 -0.85434 -0.81273 -0.78538
-0.75183 -0.74903 -0.74254 -0.71061 -0.65808 -0.62398
-0.60859 -0.60066 -0.57900 -0.55231 -0.51218 -0.50381
-0.46992 -0.46098 -0.45569 -0.44382 -0.43779 -0.43495
-0.42517 -0.41757 -0.41477 -0.40152 -0.38078 -0.36983
-0.36882 -0.36377 -0.34479 -0.34107 -0.33284 -0.32059
-0.31770 -0.27920 -0.25495 -0.24926 -0.23260 -0.19140
-0.04978 -0.00337 0.00157 0.01631 0.03503 0.07321
0.07500 0.09514 0.09722 0.10780

P2

Final total energy: -1055.64297608260 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	2.8973854205	-0.4443906152	-0.1831191150
H2	2.1970329203	0.1579681372	0.3989276309
H4	3.5114362165	0.2204662576	-0.7948510606
H5	3.5267705594	-1.0165161671	0.5023183332
S5	1.8644758597	-1.5374438418	-1.2111918286
C6	4.7999241016	-4.1456015661	-3.6511417726
C7	3.3992281022	-4.2782860333	-3.7351491977
C8	2.5419533889	-3.4816912974	-2.9900771823
C9	3.0523015305	-2.5062489895	-2.1187563074
C10	4.4437506303	-2.3589915839	-2.0223349818
C11	5.2939417983	-3.1632213857	-2.7732566971
H13	2.9790440950	-5.0269831043	-4.4022237057
H14	1.4677589366	-3.6160828947	-3.0814617644
H15	4.8772719135	-1.6172547051	-1.3615056586
H16	6.3647112429	-3.0185615614	-2.6692786264
C16	7.0013969925	-5.0313840855	-4.5188869564
C17	5.6483797033	-5.0154281452	-4.4602167591
H19	5.1105003154	-5.7294557356	-5.0841794250
H20	7.5793866300	-4.3344543659	-3.9140130575
C20	9.1127623910	-5.9437484210	-5.4039763198
C21	7.7600831444	-5.9320135220	-5.3493989552
H23	7.1848576830	-6.6309883102	-5.9544538115
H24	9.6455241721	-5.2264740881	-4.7794887427
C24	11.7293982254	-8.4357731511	-7.7080428338
C25	10.3458184511	-8.5964101881	-7.8237255724
C26	9.4784234639	-7.7989931974	-7.0861572139
C27	9.9706063371	-6.8133435733	-6.2072903554
C28	11.3672679908	-6.6665382750	-6.1053234127
C29	12.2357494690	-7.4652975610	-6.8438792508
H30	12.4032313170	-9.0609799261	-8.2863648288
H31	9.9419125411	-9.3492254975	-8.4948693297
H32	8.4080152396	-7.9420409230	-7.1944555221
H33	11.7694786509	-5.9120831771	-5.4336771646
H34	13.3090166275	-7.3296322298	-6.7446284783

HOMO energy: -0.18521 hartrees
LUMO energy: -0.05953 hartrees

Orbital energies (hartrees):

-88.88657	-10.22529	-10.22116	-10.19829	-10.19815	-10.19577
-10.19402	-10.19384	-10.19293	-10.19241	-10.19156	-10.19081
-10.19061	-10.18952	-10.18907	-10.18848	-10.18834	-10.18812
-7.94749	-5.91276	-5.90863	-5.90240	-0.86626	-0.85526
-0.81868	-0.80021	-0.77172	-0.74949	-0.74407	-0.74169
-0.70563	-0.65924	-0.62474	-0.61445	-0.60273	-0.58502
-0.56214	-0.54984	-0.51716	-0.49874	-0.47693	-0.46217
-0.45748	-0.45183	-0.43976	-0.43811	-0.43153	-0.42378
-0.41703	-0.41020	-0.39958	-0.38000	-0.37984	-0.37141
-0.36220	-0.35855	-0.34280	-0.33986	-0.33478	-0.33130
-0.32103	-0.29967	-0.26358	-0.25511	-0.24961	-0.22364
-0.18521	-0.05953	-0.00602	-0.00055	0.00305	0.03462
0.05007	0.07292	0.09114	0.09391	0.09629	

P3

Final total energy: -1133.05366167212 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-1.0698586648	2.1599637374	0.6695269374
H2	-1.8175361083	2.6015366693	1.3314113209
H4	-0.3339965142	2.9236838039	0.4079257627
H5	-0.5852566007	1.3292716903	1.1876646061
S5	-1.9908574827	1.5888324925	-0.7943259717
C6	1.1356252020	-0.3088822037	-3.6157988250
C7	-0.2390748395	-0.2447349763	-3.9213569268
C8	-1.1547952013	0.3320731935	-3.0548180697
C9	-0.7309406481	0.8751932235	-1.8316170211
C10	0.6332691168	0.8204321149	-1.5098262489
C11	1.5437782995	0.2400786071	-2.3860730676
H13	-0.5896129526	-0.6591269932	-4.8633469430
H14	-2.2066172740	0.3631751435	-3.3250485412
H15	0.9969667255	1.2286948988	-0.5738795252
H16	2.5911447770	0.2146165946	-2.1022017493
C16	3.3863725785	-1.0819427407	-4.4730796369
C17	2.0426602878	-0.9310210281	-4.5726489431
H19	1.5635581306	-1.3167731946	-5.4726854704
H20	3.9129159188	-0.7122485867	-3.5946824855
C20	5.5355100701	-1.8861293380	-5.4100089716
C21	4.1885764005	-1.7184344025	-5.4808218196
H23	3.6647102056	-2.0906768177	-6.3615791014
H24	6.0666624958	-1.5167344543	-4.5323777263
C24	7.6621111493	-2.6973203201	-6.3615524555
C25	6.3197093365	-2.5284338518	-6.4290881232
H27	5.7723220073	-2.8915284435	-7.2973913803
H28	8.1732332106	-2.3179259120	-5.4767153983
C28	10.3031827474	-4.5495930945	-9.1802564836
C29	8.9333816406	-4.4925851242	-9.4534648870
C30	8.0573712795	-3.8966378024	-8.5535216593
C31	8.5289099888	-3.3373048524	-7.3481763529
C32	9.9118569438	-3.4051393650	-7.0909529020
C33	10.7881291877	-4.0020630737	-7.9927142924
H34	10.9830803070	-5.0164784144	-9.8867791907
H35	8.5473810589	-4.9173414135	-10.3758883145
H36	6.9979789213	-3.8656061704	-8.7881527355
H37	10.2963869402	-2.9799883481	-6.1670738855
H38	11.8503309505	-4.0396795834	-7.7679459868

HOMO energy: -0.18009 hartrees
LUMO energy: -0.06687 hartrees

Orbital energies (hartrees):

-88.88700	-10.22598	-10.22145	-10.19843	-10.19825	-10.19648
-10.19474	-10.19425	-10.19327	-10.19284	-10.19172	-10.19129
-10.19089	-10.19072	-10.19042	-10.18957	-10.18909	-10.18853
-10.18841	-10.18811	-7.94794	-5.91320	-5.90907	-5.90285
-0.86688	-0.85527	-0.82293	-0.80842	-0.78740	-0.76206
-0.75016	-0.74318	-0.73537	-0.70171	-0.66041	-0.62883
-0.61596	-0.60444	-0.59077	-0.57028	-0.55649	-0.54740
-0.51387	-0.50383	-0.47753	-0.46843	-0.45777	-0.45518
-0.44779	-0.43850	-0.43451	-0.42968	-0.42184	-0.41693
-0.40891	-0.39453	-0.38622	-0.38040	-0.37184	-0.36646
-0.36026	-0.35364	-0.34278	-0.34010	-0.34009	-0.33480
-0.32164	-0.31361	-0.28521	-0.25606	-0.25084	-0.24947
-0.21680	-0.18009	-0.06687	-0.01596	-0.00333	0.00180
0.03138	0.03425	0.07264	0.07337	0.08889	0.09623

M1

Final total energy: -978.23150103717 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	0.3642957432	0.8695936629	-0.2724815267
C2	-0.3381187969	2.0868137688	-0.2048729813
C3	-1.7284326436	2.1262271657	-0.2694616638
C4	-2.4550064930	0.9438346947	-0.4037590078
C5	-1.7749181289	-0.2752980164	-0.4717365436
C6	-0.3867561617	-0.3140860954	-0.4066117776
H8	0.2219301637	3.0129532474	-0.1005743682
H9	-2.2438677293	3.0808832409	-0.2149218739
H10	-3.5395052064	0.9690055540	-0.4545330883
H11	-2.3325348759	-1.2018725777	-0.5753061860
H12	0.1173585509	-1.2737648617	-0.4593138594
C12	2.6734725212	-0.1446155163	-0.2608163758
C13	1.8277462033	0.9025539758	-0.2001425573
H15	2.2421603871	1.9029215422	-0.0911925563
H16	2.2611696912	-1.1439588559	-0.3850426175
C16	6.9503433696	-0.1435051994	-0.0774355543
C17	6.2571340082	1.0659714963	0.1084786340
C18	4.8644337747	1.0772638636	0.0536671860
C19	4.1377404230	-0.1065255413	-0.1881644399
C20	4.8494776065	-1.3031338228	-0.3661164480
C21	6.2421032368	-1.3153577877	-0.3119856006
H22	8.0355382503	-0.1590426267	-0.0347459601
H24	4.3255761644	2.0040488248	0.2055571759
H25	4.3049859927	-2.2251287029	-0.5507944634
H26	6.7808340536	-2.2478945375	-0.4537809942
S26	7.2665089081	2.5086421731	0.4101439572
C27	6.0517307707	3.8484449315	0.6206949933
H28	6.6394484610	4.7491308494	0.8093946318
H29	5.4572603416	3.9974770632	-0.2837673200
H30	5.3983390158	3.6667585827	1.4773240499

HOMO energy: -0.20120 hartrees
LUMO energy: -0.05288 hartrees

Orbital energies (hartrees):
-88.88355 -10.22441 -10.21947 -10.20292 -10.20105 -10.19440
-10.19361 -10.19288 -10.19243 -10.19231 -10.19192 -10.19159
-10.19098 -10.19079 -10.19074 -10.18770 -7.94449 -5.90980

-5.90567	-5.89931	-0.86636	-0.85701	-0.80977	-0.79098
-0.75924	-0.74554	-0.73735	-0.71167	-0.65791	-0.63563
-0.60720	-0.59741	-0.57493	-0.55060	-0.51429	-0.51140
-0.47081	-0.46602	-0.45339	-0.44550	-0.43647	-0.43445
-0.43016	-0.41809	-0.41387	-0.39575	-0.38139	-0.37292
-0.37076	-0.36304	-0.34804	-0.34259	-0.33602	-0.31824
-0.31598	-0.28292	-0.26149	-0.25203	-0.21545	-0.20120
-0.05288	-0.00121	0.00022	0.01416	0.03646	0.07307
0.07421	0.09338	0.09535	0.10465		

PM1A

Final total energy: -651.44579983956 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	0.9022076285	-0.2088632304	0.0340343948
C2	0.2103317063	1.0127703760	0.0649771006
C3	-1.1901454641	1.0739459415	0.0677182325
C4	-1.9159794967	-0.1261423215	0.0375693172
C5	-1.2384644954	-1.3442607682	0.0064085838
C6	0.1503435750	-1.3998306379	0.0043269629
H8	0.7786545271	1.9408538365	0.0841512159
H10	-3.0028199342	-0.1012362234	0.0319223919
H11	-1.8111900401	-2.2675586331	-0.0173094659
H12	0.6467918854	-2.3635176622	-0.0213235811
C12	3.2089220325	-1.2294237409	0.0398884893
C13	2.3685416501	-0.1740592938	0.0367716031
H15	2.7915570935	0.8289790533	0.0392032070
H16	2.7827908732	-2.2312182216	0.0441252324
C16	7.5205416186	-1.2877533810	0.0458864424
C17	6.8292113899	-0.0622884967	0.0265702129
C18	5.4433046847	-0.0262257033	0.0242362819
C19	4.6716835614	-1.2048576484	0.0424279065
C20	5.3777833133	-2.4219712895	0.0615939482
C21	6.7653999535	-2.4710789936	0.0631663589
H23	7.3933157273	0.8673772614	0.0168130205
H24	4.9513554702	0.9411180787	0.0045770635
H25	4.8188390341	-3.3544002289	0.0729194637
H26	7.2740368978	-3.4320170201	0.0817409004
N26	8.9128575323	-1.3229776680	0.1055042654
H27	9.3821593327	-0.5083392571	-0.2655236629
H28	9.3355592761	-2.1826225310	-0.2170010959
N28	-1.8478638654	2.3087964095	0.0419166426
H29	-2.7868380898	2.2926346861	0.4167277742
H30	-1.3130472212	3.0780154316	0.4223007057

HOMO energy: -0.17707 hartrees
LUMO energy: -0.03402 hartrees

Orbital energies (hartrees):
-14.34379 -14.33452 -10.22729 -10.21882 -10.18742 -10.18437
-10.18402 -10.18347 -10.18166 -10.18047 -10.18030 -10.17858
-10.17696 -10.17264 -10.17217 -10.16792 -0.91893 -0.91017

-0.84042	-0.82975	-0.77832	-0.74110	-0.73925	-0.71731
-0.69156	-0.62481	-0.60965	-0.59486	-0.58379	-0.54488
-0.51744	-0.51327	-0.50094	-0.49536	-0.46837	-0.46434
-0.43791	-0.43371	-0.41513	-0.41425	-0.40815	-0.40146
-0.38172	-0.37485	-0.36849	-0.35375	-0.34407	-0.33194
-0.32892	-0.32334	-0.30678	-0.27095	-0.24580	-0.23147
-0.19817	-0.17707	-0.03402	0.00547	0.02108	0.03496
0.07692	0.08462	0.09737	0.10404	0.10784	0.11434

P1A

Final total energy: -596.08770091935 hartrees

Final geometry:

		angstroms	
atom	x	y	z
N1	1.6499256042	1.3024215562	0.0759396850
H2	2.5875266164	1.5499405815	-0.2085590009
H4	1.6409178744	0.7740372203	0.9374759812
C4	-0.9048579788	-0.1141201096	-3.0001118396
C5	-1.1300291782	-0.4309674901	-1.6475705049
C6	-0.2891079537	0.0125644342	-0.6357000029
C7	0.8308969524	0.8046424790	-0.9358688524
C8	1.0688507934	1.1302016844	-2.2842420818
C9	0.2224771102	0.6810707322	-3.2859608153
H11	-1.9894574321	-1.0440322485	-1.3866891314
H12	-0.4994882283	-0.2499493487	0.3984011830
H13	1.9280729193	1.7457455486	-2.5399878084
H14	0.4467559460	0.9538154821	-4.3126489929
C14	-1.7812695632	-0.4192687079	-5.3456986335
C15	-1.8313741330	-0.6192989618	-4.0124312702
H17	-2.6442358542	-1.2212163793	-3.6085737273
H18	-0.9718210368	0.1841606089	-5.7532560950
C18	-4.4401662431	-1.8527756973	-8.3966146760
C19	-4.6765175330	-2.1908790287	-7.0609769118
C20	-3.8293614819	-1.7386172488	-6.0550703804
C21	-2.7143561888	-0.9303684403	-6.3541008097
C22	-2.4934503819	-0.6011326144	-7.7048612068
C23	-3.3415606373	-1.0538386431	-8.7123229103
H24	-5.1045023940	-2.2085224623	-9.1785313246
H25	-5.5290522117	-2.8130583826	-6.8025782472
H26	-4.0369753093	-2.0177284883	-5.0265634792
H27	-1.6396182572	0.0215715110	-7.9610089553
H28	-3.1432629305	-0.7816128383	-9.7453092903

HOMO energy: -0.18127 hartrees
LUMO energy: -0.03876 hartrees

Orbital energies (hartrees):

-14.34584 -10.22964 -10.19214 -10.18691 -10.18649 -10.18597
-10.18439 -10.18387 -10.18368 -10.18316 -10.18240 -10.18209
-10.18178 -10.18145 -10.18056 -0.92097 -0.84952 -0.83981
-0.78511 -0.74447 -0.74192 -0.73643 -0.69567 -0.62672
-0.61119 -0.59808 -0.58244 -0.54702 -0.51911 -0.51521

-0.49903 -0.47489 -0.45330 -0.44502 -0.43067 -0.42272
-0.41483 -0.41136 -0.40529 -0.38410 -0.37200 -0.36437
-0.35708 -0.33620 -0.33531 -0.32728 -0.32529 -0.28412
-0.24805 -0.24345 -0.23330 -0.18127 -0.03876 0.00323
0.00747 0.02862 0.07488 0.08964 0.10011 0.10196
0.10559 0.12581

M1A

Final total energy: -596.08503296076 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-0.2895692466	0.3590289273	-0.0932129658
C2	-0.9758155339	1.5196733895	-0.4804834983
C3	-2.3782522905	1.5942184994	-0.4606696530
C4	-3.1014732961	0.4661396360	-0.0359225663
C5	-2.4242053173	-0.6878562516	0.3522146310
C6	-1.0357932746	-0.7577054339	0.3290445405
H7	-0.4055143116	2.3872086762	-0.8067539301
H8	-4.1878056885	0.4992673269	-0.0115590031
H9	-2.9981123789	-1.5513089248	0.6776757863
H10	-0.5384096527	-1.6698535949	0.6400528411
C11	2.0153322259	-0.6341230807	0.1444437440
C12	1.1761636393	0.3779546906	-0.1502197804
H13	1.5985727958	1.3279701325	-0.4723044226
H14	1.5941438711	-1.5859748902	0.4625481972
C15	6.3034869834	-0.7001430455	0.0104189899
C16	5.6211943033	0.4671931991	-0.3427329346
C17	4.2320262224	0.5120021452	-0.3062046422
C18	3.4806837301	-0.6129945291	0.0854860142
C19	4.1857629553	-1.7788129174	0.4372752591
C20	5.5771321542	-1.8242450929	0.4012118348
H21	6.1773984575	1.3490813217	-0.6483351226
H22	3.7272259296	1.4313861870	-0.5853417944
H23	3.6269732208	-2.6601883963	0.7423518947
H24	6.0938000611	-2.7389034138	0.6781771323
N25	-3.0270859254	2.7469965583	-0.8480711070
H26	-4.0294972101	2.8060298144	-0.8344345723
H27	-2.5127276021	3.5515003032	-1.1592360387
H28	7.3887440385	-0.7305032580	-0.0196203385

HOMO energy: -0.18789 hartrees
LUMO energy: -0.04314 hartrees

Orbital energies (hartrees):

-14.34056 -10.22659 -10.19499 -10.19093 -10.18659 -10.18602
-10.18577 -10.18535 -10.18505 -10.18497 -10.18471 -10.18150
-10.17578 -10.17577 -10.16986 -0.91561 -0.85234 -0.83488
-0.78791 -0.75019 -0.73974 -0.72299 -0.70038 -0.63027
-0.60381 -0.59932 -0.58675 -0.54965 -0.51883 -0.50742

-0.50432 -0.47329 -0.45985 -0.44902 -0.43519 -0.42021
-0.41488 -0.40955 -0.40154 -0.38031 -0.36766 -0.36702
-0.35168 -0.34230 -0.33377 -0.32713 -0.32175 -0.28806
-0.25357 -0.24643 -0.20403 -0.18789 -0.04314 0.00441
0.01934 0.02852 0.07923 0.08719 0.09828 0.10294
0.11059 0.12577

PM1TA

Final total energy: -1112.20499561224 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-1.2106703531	-0.5803126647	-0.0882786851
C2	-2.5315992428	-0.7769215720	0.0968129706
H3	-0.5826405231	-1.4358836992	-0.3302271185
H5	-3.1594587183	0.0884337127	0.3008329027
C6	1.0065903020	3.1119110051	0.0652895781
C7	1.6142701591	1.9032859301	-0.3082254053
C8	0.8780954871	0.7271329729	-0.3468227401
C9	-0.4916347679	0.6941654280	-0.0200035872
C10	-1.0831444844	1.9132458634	0.3570645407
C11	-0.3554237643	3.0984380091	0.3986410873
H13	2.6687498220	1.8864039324	-0.5698243125
H14	1.3728756392	-0.1952622666	-0.6411124325
H15	-2.1329392874	1.9447093059	0.6324677552
H16	-0.8607527293	4.0098336107	0.6974845644
C16	-4.7948221688	-4.4026172427	-0.0665453956
C17	-5.4162645425	-3.1636194629	0.0382833813
C18	-4.6747386462	-1.9881042634	0.0899227764
C19	-3.2713838379	-2.0427450682	0.0357666965
C20	-2.6446638477	-3.2957385709	-0.0622981972
C21	-3.3844839253	-4.4925966102	-0.1289696412
H22	-5.4061790136	-5.2956476214	-0.0931271049
H23	-6.5010183965	-3.1202451988	0.0858130036
H24	-5.1732972093	-1.0266602541	0.1731428798
H25	-1.5633908251	-3.3348378746	-0.0687436771
S26	2.0436697153	4.5620176615	0.0819697073
C27	0.9166304275	5.8915888591	0.6110378542
H28	1.5240096460	6.7988066879	0.6320303258
H29	0.0980484972	6.0307342358	-0.0988439203
H30	0.5210598526	5.7079511923	1.6126572514
N30	-2.7513271705	-5.7274952909	-0.2558076542
C32	-1.3105489286	-5.8035709535	-0.0957018341
H33	-0.8012074257	-5.1787148549	-0.8376362887
H34	-0.9684572779	-5.4896549681	0.9035131249
H35	-0.9867032585	-6.8329371841	-0.2592487188
C35	-3.5195254187	-6.9412737351	-0.0390624690
H36	-2.8690389293	-7.8054591714	-0.1844162616
H37	-3.9535168609	-7.0039917746	0.9717578671
H38	-4.3378348475	-7.0244896689	-0.7627696868

HOMO energy: -0.18301 hartrees
LUMO energy: -0.04357 hartrees

Orbital energies (hartrees):

-88.88330	-14.34937	-10.22178	-10.22152	-10.21848	-10.21639
-10.21602	-10.19420	-10.19224	-10.19032	-10.18976	-10.18963
-10.18891	-10.18571	-10.18416	-10.18029	-10.17593	-10.17380
-10.17100	-7.94422	-5.90949	-5.90537	-5.89910	-0.94253
-0.86235	-0.84047	-0.80813	-0.77960	-0.74803	-0.74518
-0.73967	-0.72400	-0.70260	-0.65666	-0.65304	-0.61832
-0.60381	-0.58084	-0.56618	-0.54628	-0.51733	-0.50076
-0.47559	-0.46971	-0.46293	-0.46078	-0.45053	-0.44481
-0.43532	-0.43190	-0.42110	-0.41878	-0.41245	-0.40522
-0.39469	-0.39209	-0.38150	-0.37624	-0.36514	-0.36185
-0.35829	-0.34668	-0.33404	-0.32831	-0.31762	-0.31509
-0.28555	-0.26348	-0.25127	-0.22856	-0.19273	-0.18301
-0.04357	0.00011	0.01637	0.02745	0.03748	0.07575
0.08155	0.08591	0.09984	0.10937		

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