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Triphenylene Containing Blue-Light Emitting Semi-fluorinated Aryl Ether Polymers with Excellent Thermal and Photostability

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General Procedures

All reagents and solvents were purified according to the established procedure.[1] Anhydrous dimethylformamide (DMF) was further dried by storing over molecular sieves (4 Å). All reactions were carried out in oven-dried glassware (at 120 °C) under argon atmosphere unless otherwise noted.

Materials

4-Methoxyphenylacetic acid, 9,10-phenanthrenequinone, phenylacetylene, diphenylacetylene, dimethyl acetylenedicarboxylate, trimethylsilylacetylene, potassium acetate (KOAc), methanesulfonic acid and bis(pinacolato)diboron were purchased from Oakwood chemicals, SC, USA. Sodium hydride (NaH), *p*-toluenesulfonic acid (*p*TsOH), tetrakis (triphenylphosphine) palladium(0) $Pd(pph_3)_4$, 1,1'-bis(diphenylphosphino)ferrocene $Pd(dppf)Cl_2$, cesium carbonate (Cs_2CO_3), ethanol, diphenyl oxide, anhydrous toluene, anhydrous DMF, 1,4-dioxane and dry DCM were purchased from Acros organics. 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) was purchased from Fischer Scientific. 1-Bromo-4-(trifluorovinyloxy)benzene was generously donated by Tetramer Technologies, LLC, Pendleton, SC. De-ionized water was obtained from in-house water purification system based on a reverse osmosis process.

Instrumentation

Nuclear magnetic resonance (NMR) spectroscopy

The ^{1}H, ^{19}F and ^{13}C-NMR were measured on a Bruker AVANCE III 500 MHz instrument. Chloroform-d ($CDCl_3$) was used as a solvent for NMR experiments, and all chemical shifts are reported in parts per million (δ ppm). ^{1}H-NMR spectra were internally referenced to tetramethylsilane (δ = 0.0).

Fourier transform infrared (FTIR) spectroscopy

Experiments were conducted using an Agilent Cary 630 spectrophotometer with a diamond crystal ATR sample head between the wavelengths 4000 to 400 cm^{-1}. The experiments were carried at a resolution of 2 cm^{-1}, and one hundred twenty-eight scans were carried out for each sample.

Differential scanning calorimetric (DSC)

The thermal order-disorder events of the homo- and co-polymers using a TA Q20 V4. DSC instrument was studied. Approximately, 5 to 9 mg of the monomer or polymer was placed in TA low-mass aluminum pan, sealed, and a heat–cool-heat cycle (4 heating and 4 cooling cycles) was employed between the temperatures of 0–400 °C at a scanning rate of 10 °C/min. Between the cycles, the pans were isothermally held at 300 °C and at 0 °C for 3 minutes. Polymer glass transition temperatures (T_g's) were obtained on the fourth heat-cool-heat cycle of DSC analysis. The raw data was extracted using TA universal analysis software V4.5a, and the plots were created using OriginPro 2018.

Thermogravimetric analyzer (TGA)

For TGA, small samples (5 to 10 mg) were measured using a TA Q50 V20 TGA instrument over the temperature range 50–1000 °C, at a heating rate of 10 °C/min. The experiments were carried out under both nitrogen and air with a flow rate of 50 mL/min, and TA universal analyses software

was used to analyze the thermal degradation patterns of the polymers, and the data was exported for further processing using OriginPro 2018.

Gel permeation chromatography (GPC)

Molecular weight measurements based on data were collected using a TOSOH EcoSEC HLC-8320 gel permeation chromatograph at 30 °C, equipped with TSK gel super H-RC columns (6 mm internal diameter, 15 cm long, particle size 4 μm). HPLC grade tetrahydrofuran (THF) was used as the eluting solvent at a flow rate of 0.7 mL/min. The molecular weights (Mn, Mw, and Mz) were obtained by calibrating against polystyrene standards (PS090705) based on the retention times monitored by a UV detector (λ= 254 nm).

Photoluminescence (PL)

The UV-vis extinction spectra were acquired using the Thermo Scientific Evolution 300 UV-vis spectrophotometer with a slit width of 2 nm. All Stokes-Shifted fluorescence (SSF) spectra were obtained with the Horiba Fluoromax-4-spectrofluorometer. All SSF spectra were acquired with 4 mL fluorescence cuvettes with a pathlength of 1 cm. The spectral integration time was 0.3 s and slit widths of both excitation and detection monochromator slits were kept 2 nm in all SSF spectral acquisitions. The SSF spectra were obtained by normalizing the signal from the sample detector from the reference detector (S1/R1) to eliminate any spectral variation due to wavelength or time-dependent intensity variation in the xenon lamp.

Atomic force microscopy (AFM) and water angle contact

Triphenylene-enchained FAVE polymers were dissolved in THF and spin-coated on stainless steel (SS) substrate using Laurell model MW-650MZ-23 NPPB for AFM and water angle contact investigation. AFM was used to investigate the surface morphology, the average surface roughness (R_a) and the root mean square roughness (R_q) of the spin coated films using Bruker dimension icon with SCANASYST air chip in tapping mode. Static water contact angle (CA) measurements were performed on a Tantec contact angle meter with a macro-lens-equipped smartphone, while ImageJ was used for the droplet analysis and CA calculation.

Wide angle X-ray scattering (WAXS)

All 2D-frames were recorded at room temperature (T = 293K), using a three circles goniometer Kappa geometry with a fixed Kappa angle at = 54.74 deg Bruker AXS D8 Venture, equipped with a Photon 100 CMOS active pixel sensor detector. A monochromatized Cu X-ray radiation (λ = 1.54184 Å) was selected for the measurement. Using the following measurement conditions: **Frame 1**: Irradiation time = 90.00 s, Goniometer radius = 34.0 mm, theta = 350.00 deg; **Frame 2**: Irradiation time = 90.00 s, Goniometer radius = 34.0 mm, theta = 323.00 deg; and **Frame 3**: Irradiation time = 120.00 s, Goniometer radius = 34.0 mm, theta = 296.00 deg. 2D Frames were integrated using the software: DIFFRAC.EVA.V5.2 from AXS BRUKER; Bruker: Version 5.2 0.5 (32 Bit).

Polarized optical microscopy (POM)

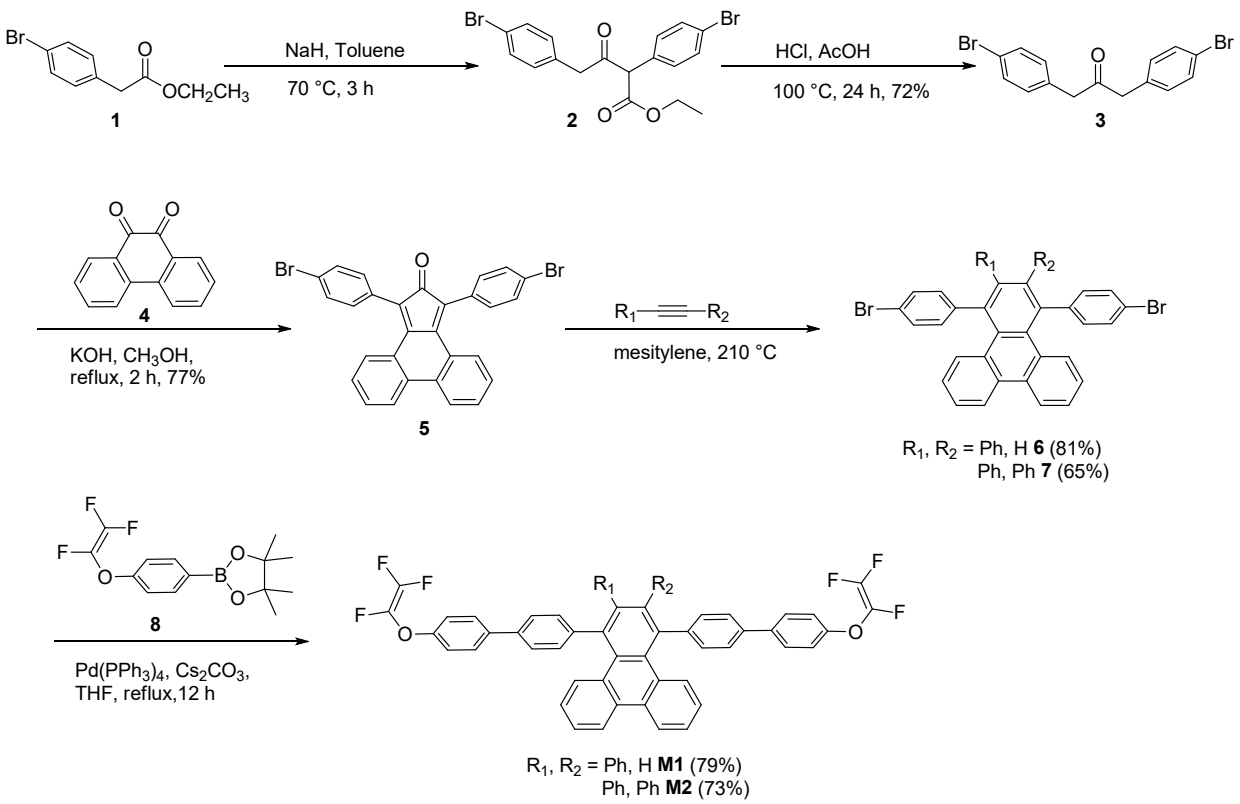
Pictures were recorded using an Olympus SZX9 high resolution research grade stereo microscope The dual position nosepiece has a DF PLAPO 1X-2 auxiliary lense. The magnification range is 6.3x - 57x. The microscope was equipped with a AmScope digital camera, frames were processed

using the software: AmScope Version X64 for Windows. The cross-polarizer was 'ON' during the POM experiment.

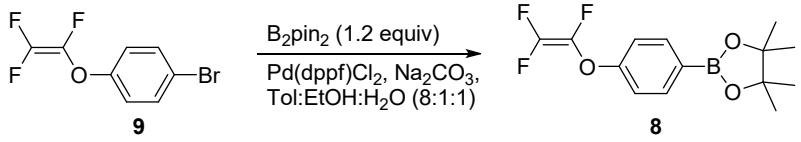
Computational method

All density functional theory (DFT) computations were carried out using Gaussian 16 Revision C.01.[2] Default integration grids were used for all computations (99 radial shells with 590 points per shell (99,590) and a pruned SG1 grid using 50 radial shells with 194 points per shell (50,194) for Hessians). To reduce the computational cost, the polymer structures with one and two units were selected. All geometry optimizations and corresponding vibrational frequencies were computed at the SMD(dichloromethane)-ωB97XD/BS1 level theory (BS1 = 6-31G(d')[3–5] for C, H, O and F). The single point TD-DFT (time dependent density functional theory) calculation is performed on optimized ground state geometries to generate the absorption spectra calculation. The emission simulation spectra, on the other hand were obtained from exited state optimization process also at SMD (dichloromethane)-ωB97XD/BS1 level theory. In addition, the NTO (natural transition orbital) analyst[6] is used to study the electronic structure changes due to the Scholl coupling reaction.

Preparation of monomers



Scheme S1. Synthesis of triphenylene-enchained monomers M1-M2.



Scheme S2. Synthesis of boronic ester intermediate 8 from commercially available 4-bromotrifluorovinyloxybenzene 9.

Preparation of 1,3-bis(4-bromophenyl)acetone 3. To a suspension of NaH (60 wt% in mineral oil, 4.80 g, 0.20 mol) and anhydrous toluene (150 mL), solution of ethyl 4-bromophenylacetate (1, 30.0 g, 0.123 mol in 50 mL anhydrous toluene) was added slowly dropwise for an hour at room temperature. After complete addition, the temperature of the reaction was slowly raised to 50 °C for next 1 hour and then, with subsequent increase in heating to 70 °C for another 2 hours. The reaction mixture was cooled to rt, poured into aqueous 10% HCl at 0 °C, and extracted with

dichloromethane (3 × 150 mL), dried over sodium sulfate, and concentrated to afford crude 2 as a yellow solid. In 250 mL RBF, the crude solid was dissolved in 50 mL acetic acid and 10 mL HCl (37%) and heated to reflux for 24h before allowing it to cool at rt. The reaction mixture was dissolved in 200 mL dichloromethane and extracted with distilled water (3 × 100 mL), and saturated sodium bicarbonate (2 × 100 mL), dried over sodium sulfate, and concentrated. The crude product was recrystallized from heptane to obtain (**3**, 14.9 g, 40.5 mmol, 72% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) 7.46 (4 H, d, J = 8.2 Hz), 7.16 (4 H, d, J = 8.5 Hz), 3.61 (4 H, s). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) 177.0, 132.1, 131.8, 131.1, 121.5, 40.3.

Preparation of 5,10-dibromo-1,3-diphenyl-2H-cyclopenta[l]phenanthren-2-one 5. Solution of 1,3-bis(4-bromophenyl)acetone (3, 3.33 g, 9.05 mmol) and phenanthrene-9,10-dione (4, 1.88 g, 9.05 mmol) in methanol (60 mL) was heated to 60 °C. The solution of KOH (0.25 g in 5 mL methanol) was added dropwise. The reaction mixture was heated to reflux for next 2 h before allowing it to cool at rt. The precipitate was filtered and washed with methanol and dried overnight in vacuum oven to obtain (**5**, 4.2 g 7.77 mmol, 77% yield) dark green sold. ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) 7.82 (2 H, d, J = 7.9 Hz), 7.56 (4 H, d, J = 8.2 Hz), 7.52 (2 H, d, J = 8.2 Hz), 7.31 (3 H, t, J = 7.6 Hz), 7.28 (6 H, s), 6.99 (2 H, t, J = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) 199.2, 148.7, 1336, 131.9, 131.8, 131.6, 131.0, 129.0, 128.4, 128.0, 124.6, 122.5, 122.0.

Preparation of 1,4-bis(4-bromophenyl)-2-phenyltriphenylene 6. To a flame dried 50 mL, 2-neck pressure tube cyclopentadienone (**5**, 2.1 g, 3.89 mmol), phenylacetylene (0.48 g, 4.7 mmol), and 5 mL mesitylene were added. The pressure tube was caped, and the mixture was heated to reflux (210 °C) for 3 h before allowing it to cool at rt. The reaction mixture was diluted with the 30 mL methanol and the obtained precipitate was filtered and washed with methanol (100 mL) and dried overnight in vacuum oven to obtain (**6**, 2.13 g, 3.46 mmol, 81% yield) as white solid. ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) 8.44 (2 H, d, J = 7.9 Hz), 7.70 (1 H, d, J = 8.2 Hz), 7.59 (1 H, s), 7.54 (2 H, d, J = 8.5 Hz), 7.48 (2 H, t, J = 8.2 Hz), 7.44 (1 H, t, J = 7.7 Hz), 7.38 (2 H, d, J = 8.5 Hz), 7.31 (2 H, d, J = 8.5 Hz), 7.25–7.21 (3 H, m), 7.17 (1 H, t, J = 7.6 Hz), 7.10–7.02 (3 H, m), 6.98 (2 H, m, J = 8.2 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) 143.1, 141.1, 140.9, 140.1, 137.0, 135.4, 133.6, 132.3, 132.2, 131.9, 131.65, 131.63, 131.36, 131.2, 130.2, 130.0, 129.8, 129.7, 129.65, 129.63, 127.9, 127.0, 126.7, 126.5, 125.8, 125.5, 123.4, 123.3, 121.6, 121.0.

Preparation of 1,4-bis(4-bromophenyl)-2,3-diphenyltriphenylene 7. To a flame dried 50 mL, 2-neck pressure tube fitted with rubber septa, and magnetic stir bar, the cyclopentadienone (**5**, 2.45 g, 4.54 mmol), diphenylacetylene (0.97 g, 5.44 mmol), and 10 mL mesitylene were added and flushed with argon for 5 min. The pressure tube was caped, and the mixture was heated at 210 °C for 48 h before allowing it to cool at rt. The reaction mixture was diluted with the 30 ml methanol and the precipitate was filtered and wash with excess methanol and dried. The residue was purified by flash column chromatography (silica gel, dichloromethane: hexanes = 1:5 to 1:4) to produce (**7**, 1.75 g, 2.54 mmol, 65% yield) as white solid. ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) 8.43 (2 H, d, J = 8.2 Hz), 7.54 (2 H, d, J = 8.5 Hz), 7.43 (2 H, t, J = 7.6 Hz), 7.22 (4 H, d, J = 8.2 Hz), 7.09 (2 H, t, J = 7.8 Hz), 7.00–6.87 (10 H, m), 6.67 (4 H, d, J = 7.0 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) 141.6, 140.3, 139.7, 136.0, 133.6, 131.6, 131.4, 131.2, 130.3, 129.9, 126.9, 126.6, 125.7, 125.6, 123.3, 120.6.

Preparation of monomer 2-phenyl-1,4-bis(4'-((1,2,2-trifluorovinyl)oxy)-[1,1'-biphenyl]-4 yl)triphenylene M1. To a 100 mL two-neck flask fitted with a condenser, a rubber septum, and magnetic stir bar were added (**8**, 1.40 g, 2.28 mmol), 4,4,5,5-Tetramethyl-2-(4-trifluorovinyloxy-phenyl)1,3,2-dioxaborolane (**7**, 2.00 g, 6.67 mmol), cesium carbonate (3.00 g, 8.88 mmol), and $Pd(PPh_3)_4$ (256 mg, 0.22 mmol). The flask was flushed with argon, and anhydrous THF (50 mL) was introduced via cannula. The reaction mixture was heated at reflux for 12 h before it was cooled to rt. The reaction mixture was then passed through a short silica gel column, and the column was further eluted with dichloromethane (3 × 100 mL). The combined eluates were concentrated in vacuo. The solid residue was further purified by flash column chromatography (silica gel/dichloromethane:hexanes = 1:20 to 1:10) to produce **M1** (1.44 g, 1.80 mmol, 79% yield) as a white solid. ν_{max}/cm^{-1} 1932, 1603, 1492, 1270, 1136 and 822. ^1H NMR ($CDCl_3$, 500 MHz) δ (ppm) 8.46 (1 H, d, J = 8.3 Hz), 8.45 (1 H, d, J = 8.3), 7.82 (1 H, d, J = 8.6 Hz), 7.71 (1 H, s), 7.68 (2 H, d, J = 8.5 Hz), 7.64–7.57 (6 H, m), 7.47 (2 H, t, J = 7.5 Hz), 7.44–7.38 (3 H, m), 7.24–7.08 (11 H, m), 7.03 (1 H, t, J = 7.8 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) 154.6 (m), 146.9 (ddd, J = 334, 272, 62 Hz), 143.5, 141.5, 141.3, 140.2, 138.7, 137.8, 137.6, 137.5, 136.1, 133.7 (ddd, J = 42, 49, 263), 133.7, 132.6, 132.4, 132.0, 131.7, 131.4, 130.7, 130.2, 130.1, 130.0, 128.5, 128.4, 127.8, 127.5, 126.8, 126.7, 126.5, 126.3, 125.7, 125.4, 123.3. ^{19}F NMR ($CDCl_3$, 125 MHz) δ (ppm) -119.49 (1 F, dd, J = 59, 26 Hz), -119.69 (1 F, dd, J = 59, 26 Hz), -126.40 (1 F, dd, J = 97, 49 Hz), -126.63 (1 F, dd, J = 97, 49 Hz), -133.80 (1 F, dd, J = 109, 57 Hz).

Preparation of monomer 2,3-diphenyl-1,4-bis(4'-((1,2,2-trifluorovinyl)oxy)-[1,1'-biphenyl]-4-yl)triphenylene M2. To a 250 mL two-neck flask fitted with a condenser, a rubber septum, and magnetic stir bar were added **9** (4.03 g, 5.83 mmol), 4,4,5,5-Tetramethyl-2-(4-trifluorovinyloxy-phenyl)1,3,2-dioxaborolane (**7**, 5.25 g, 17.49 mmol), cesium carbonate (8.24 g, 23.36 mmol), and $Pd(PPh_3)_4$ (674 mg, 0.58 mmol). The flask was flushed with argon, and anhydrous THF (100 mL) was introduced via cannula. The reaction mixture was heated at reflux for 18 h before it was cooled to rt. The reaction mixture was then passed through a short silica gel column, and the column was further eluted with dichloromethane (3 × 100 mL). The combined eluates were concentrated in vacuo. The solid residue was further purified by flash column chromatography (silica gel/dichloromethane:hexanes = 1:20 to 1:10) to produce **M2** (3.75 g, 4.28 mmol, 73% yield) as a white soli. ν_{max}/cm^{-1} 1832, 1603, 1272, 1137, 1005 and 699. ^1H NMR ($CDCl_3$, 500 MHz) δ (ppm) 8.44 (2 H, d, J = 7.6 Hz), 7.67 (2 H, dd, J = 8.5, 0.9 Hz), 7.56 (4 H, d, J = 8.9 Hz), 7.41 (2 H, td, J = 7.0, 5.8 Hz), 7.31 (4 H, d, J = 8.3 Hz), 7.14 (4 H, d, J = 6.7 Hz), 7.12 (4 H, d, J = 6.8 Hz), 7.04 (2 H, ddd, J = 8.3, 7.1, 1.1 Hz), 6.95–6.87 (6 H, m) 6.76–6.67 (4 H, m). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) 154.5-154.4 (m), 146 (ddd, J = 334, 272, 62 Hz), 142.1, 140.4, 140.2, 137.6, 137.3, 136.6, 133.74 (ddd, J = 42, 49, 263), 132.6, 131.6, 131.5, 131.3, 130.7, 130.0, 128.3, 126.7, 126.5, 126.3, 125.6, 125.4, 123.3, 116.1; ^{19}F NMR ($CDCl_3$, 125 MHz) δ -120.4 (2 F, dd, J = 94.0, 65.4 Hz), -127.3 (2 F, dd, J = 108.1, 98.7 Hz), -134.5 (2 F, dd, J = 112.8, 61.1 Hz).

Preparation of polymers

Synthesis of polymer P1. To a suspension of NaH (11.98 mg, 4.0 mmol) in DMF (0.5 mL), a solution of bisphenol A (28.5 mg, 1 mmol) in DMF (0.5 mL) was added at room temperature. To

this mixture, solution of monomer **M1** (100 mg, 1.0 mmol) dissolved in anhydrous DMF (0.5 mL) was transferred via syringe. This mixture was stirred for 1 h at room temperature, then heated to 45 °C for 2 h, with subsequent increase in heat to 80 °C for 15 h. An increase in viscosity was observed (by gel/solid formation) for the first few hours of heating and additional DMF was added as needed to maintain a constant stirring rate. After regular intervals, aliquots of polymerization mixture were taken for gel permeation chromatography (GPC) to study the change in molecular weight with respect to time and temperature. After achieving a unimodal molecular weight distribution in GPC for the respective polymerization, reaction was stopped and cooled to room temperature. The polymer was precipitated in MeOH/H_2O (1:1), filtered, and washed sequentially with deionized water (20 mL x 3), methanol (10 mL x 3), and hexane (10 mL x 3). The solid polymer was then dried in a vacuum oven at 50 °C for 48 h. Additional purification was performed by dissolving dried polymer in a minimal amount of THF and precipitated in deionized water, filtered, and washed sequentially with methanol (10 mL x 3), and hexane (10 mL x 3). The solid polymer was then dried in a vacuum oven at 60 °C for 24 h to afford **P1** as fibrous white solid (93% yield). ν_{max}/cm^{-1} 2969-2858, 1674, 1602, 1495, 1220, 1176, 1098, 1004, 822, 760, 728 and 700. ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 7.45 - 7.55 (br), 7.61 - 7.70 (br). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -84.43 and -85.19 (AB pattern, J = 141.2 Hz, CHFC$\underline{F}_2$), -121.22 and -121.91 (d, J = 37.54 Hz, (*Z*) CF=CF), -128.40 (d, J = 31.41Hz, (*E*) CF=CF), -141.44 (d, J = 149.5 Hz, CH$\underline{F}$CF$_2$).

Synthesis of polymer P1'. A mixture of bisphenol A (28.5 mg, 1 mmol) and Cs_2CO_3 (162.75 mg, 4.0 mmol) in DMF (0.5 mL) was stirred at room temperature. To this mixture, solution of monomer **M1** (100 mg, 1.0 mmol) dissolved in anhydrous DMF (0.5 mL) was transferred via syringe. This mixture was stirred for 1 h at room temperature, then heated to 45 °C for 2 h, with subsequent increase in heat to 80 °C for 15 h. An increase in viscosity was observed (by gel/solid formation) for the first few hours of heating and additional DMF was added as needed to maintain a constant stirring rate. After regular intervals, aliquots of polymerization mixture were taken for gel permeation chromatography (GPC) to study the change in molecular weight with respect to time and temperature. After achieving a unimodal molecular weight distribution in GPC for the respective polymerization, reaction was stopped and cooled to room temperature. The polymer was precipitated in MeOH/H_2O (1:1), filtered, and washed sequentially with deionized water (20 mL x 3), methanol (10 mL x 3), and hexane (10 mL x 3). The solid polymer was then dried in a vacuum oven at 50 °C for 48 h. Additional purification was performed by dissolving dried polymer in a minimal amount of THF and precipitated in deionized water, filtered, and washed sequentially with water (10 mL x 3), methanol (10 mL x 3), and hexane (10 mL x 3). The solid polymer was then dried in a vacuum oven at 60 °C for 24 h to afford **P1'** as fibrous white solid (92% yield). ν_{max}/cm^{-1} 2969, 1603, 1495, 1274, 1213, 1176, 1099, 1004, 821, 759, 728 and 699. ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 7.12 - 7.40 (br) 7.43 - 7.63 (br). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) –90.91 (AB pattern, J = 149.6 Hz, CHFC$\underline{F}_2$), -144.16 (d, J = 57.4 Hz, CH$\underline{F}$CF$_2$).

Synthesis of polymer P2. A solution of monomer **M1** (100 mg, 1 mmol), bisphenol AF (42 mg, 1 mmol), and NaH (11.98 mg, 4.0 mmol) were used following the procedure outlined for the preparation of **P1** to afford fibrous white solid **P2** (89% yield). ν_{max}/cm^{-1} 2938, 2850, 1670, 1607, 1512, 1495, 1219, 1170, 1099, 1004, 968, 929, 822, 760, 728 and 700. ^{1}H NMR (500 MHz,

DMSO-d_6) δ (ppm) 6.81 - 6.84 (br), 7.07 - 7.14 (br), 7.41 - 7.51 (br). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -63.4 (s, C(C$\underline{F}_3$)$_2$), -85.5 and -86.6 (AB pattern, J = 145.0 Hz, CHFC$\underline{F}_2$), -121.25 (d, J = 42.3 Hz, (Z) CF=CF), -127.1 (d, J=- 33.1 Hz, (E) CF=CF), -141.25 (d, J = 48 Hz, CH$\underline{F}$CF$_2$).

Synthesis of polymer P2'. A solution of monomer **M1** (100 mg, 1 mmol), bisphenol AF (42 mg, 1 mmol), and Cs_2CO_3 (162.75 mg, 4.0 mmol) were used following the procedure outlined for the preparation of **P1** to afford fibrous white solid **P2** (95% yield). ν_{max}/cm^{-1} 2946, 2918, 2855, 1669, 1609, 1511, 1497, 1219, 1170, 1104, 1004, 968, 928, 822, 760, 728 and 700. ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 7.16 - 7.32 (br), 7.43 - 7.54 (br), 7.61 - 7.71 (br), 7.71 - 7.78 (br). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -64.05 (s, C(C$\underline{F}_3$)$_2$), -84.54 and -87.50 (d, J = 145.7 Hz, CHFC$\underline{F}_2$), -141.37 and -141.5 (d, J = 56.05 Hz, CH$\underline{F}$CF$_2$).

Synthesis of polymer P3. A solution of monomer **M2** (100 mg, 1 mmol), bisphenol A (26 mg, 1 mmol), and NaH (10.9 mg, 4.0 mmol) were used following the procedure outlined for the preparation of **P1** to afford fibrous white solid **P3** (78% yield). ν_{max}/cm^{-1} 3035, 2970, 2928, 1599, 1495, 1219, 1176, 1096, 1004, 824, 758, 727 and 699. ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 6.62 - 7.07 (m,), 7.10 - 7.38 (br), 7.41 - 7.53 (br), 7.55 - 7.90 (br). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -84.54 and -85.25 (AB pattern, J = 141 Hz, CHFC$\underline{F}_2$), -121.26 and -121.95 (d, J=37.6 Hz, (Z) CF=CF), -128.42 (d, J=31.4 Hz, (E) CF=CF), -141.2 (d, J = 49.8 Hz, CH$\underline{F}$CF$_2$).

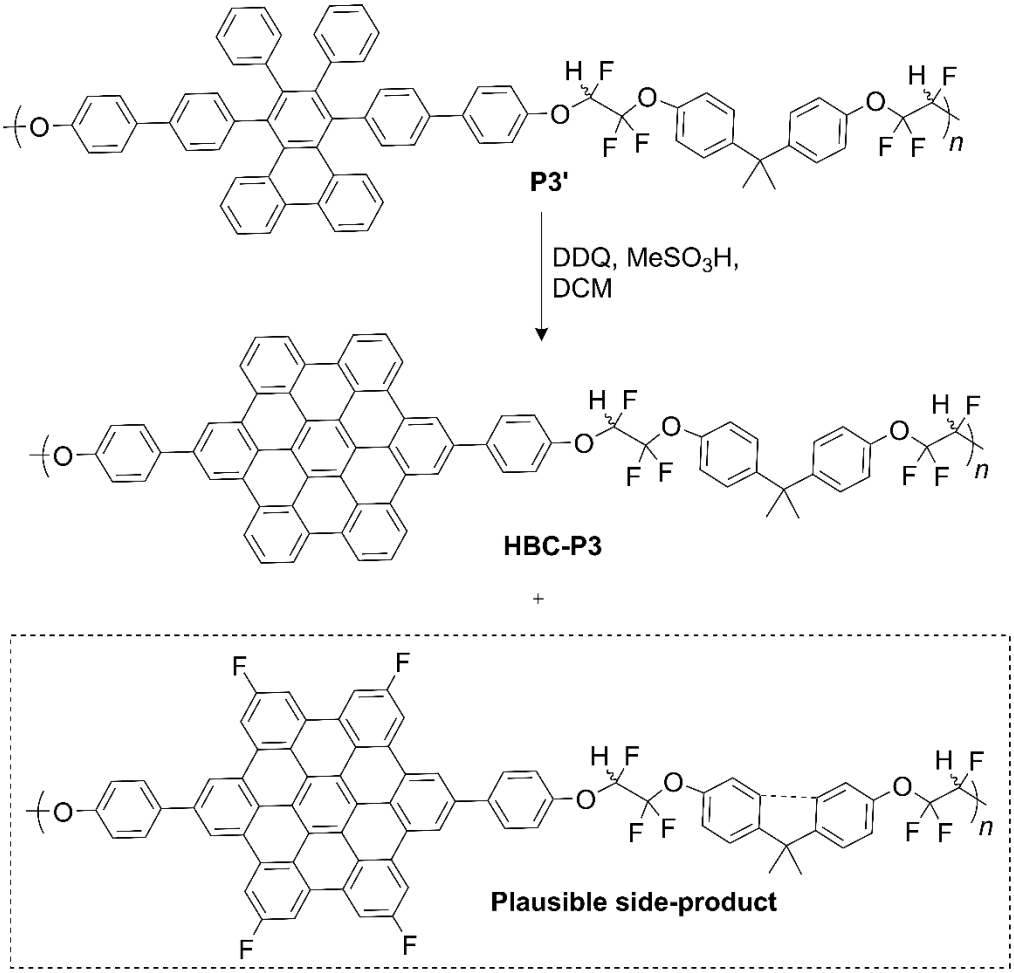
Synthesis of polymer P3'. A solution of monomer **M2** (100 mg, 1 mmol),bisphenol A (26 mg, 1 mmol), and Cs_2CO_3 (148.6 mg, 4.0 mmol) were used following the procedure outlined for the preparation of **P1** to afford fibrous white solid **P3** (82% yield). ν_{max}/cm^{-1} 3059, 2967, 1602, 1495, 1218, 1177, 1096, 1005, 826, 759, 727 and 700. ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 6.60 - 6.82 (br), 6.84 - 6.93 (br), 6.95 - 7.37 (br), 7.38 - 7.51 (br), 7.58 - 7.73 (br), 8.47 - 8.65 (br). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -85.6 (AB pattern, J=171.7 Hz, CHFC$\underline{F}_2$), -142.01 (d, J = 106.1 Hz, CH$\underline{F}$CF$_2$). ^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) 101.77-104.21 (dt, J = 37.8, 231.84 Hz), 114.91, 115.14, 117.75, 118.13, 118.37, 121.35, 121.55, 123.93, 125.83, 125.99, 126.17, 127.00, 127.18, 127.64, 127.72, 128.26, 128.35, 128.47, 129.74, 130.47, 130.99, 131.50, 132.72, 135.94, 136.81, 137.01, 140.20, 140.46, 140.80, 141.50, 141.95, 146.77, 147.05, 148.69, 149.74, 154.60, 155.40, 155.72.

Synthesis of polymer P4. A solution of monomer **M2** (100 mg, 1 mmol), bisphenol AF (38 mg, 1 mmol), and NaH (10.9 mg, 4.0 mmol) were used following the procedure outlined for the preparation of **P1** to afford fibrous white solid **P4** (86% yield). ν_{max}/cm^{-1} 3023, 29220, 1604, 1510, 1495, 1219, 1172, 1100, 1004, 968, 929, 828, 759, 728 and 700. ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 6.60 - 6.73 (m), 6.72 - 6.82 (m), 6.84 - 6.93 (m), 6.92 - 7.37 (m), 7.38 - 7.51 (m), 7.58 - 7.73 (m), 8.47 - 8.65 (m). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -63.4 (s, C(C$\underline{F}_3$)$_2$), -85.53 and -86.4 (AB pattern, J = 143.7 Hz, CHFC$\underline{F}_2$), -121.23 (d, J = 32.8 Hz, (Z) CF=CF), -128.27 (d, J=- 35.6 Hz, (E) CF=CF), -141.18 (d, J = 50.2 Hz, CH$\underline{F}$CF$_2$).

Synthesis of polymer P4'. A solution of monomer **M2** (100 mg, 1 mmol), bisphenol AF (38 mg, 1 mmol), and Cs_2CO_3 (148.6 mg, 4.0 mmol) were used following the procedure outlined for the preparation of **P1** to afford fibrous white solid **P4** (81% yield). ν_{max}/cm^{-1} 3026, 1776, 1605, 1510, 1495, 1209, 1170, 1102, 1004, 967, 926, 825, 759, 727 and 700. ^{1}H NMR (500 MHz, DMSO-d_6)

δ (ppm) 6.60 - 6.73 (m), 6.72 - 6.82 (m), 6.84 - 6.93 (m), 6.92 - 7.37 (m), 7.38 - 7.51 (m), 7.58 - 7.73 (m), 8.47 - 8.65 (m). ^{19}F NMR (470 MHz, DMSO-d_6) δ (ppm) -64.15 (s, C(C$\underline{F}_3$)$_2$), -85.6 (AB pattern, J=180.7 Hz, CHFC$\underline{F}_2$), -141.96 (d, J = 103.9 Hz, CH$\underline{F}$CF$_2$).

Post-polymerization Scholl coupling



Scheme S3. A model Scholl coupling reaction of polymer P3' to obtain a semi-fluorinated polymer containing the hexabenzocoronene core, HBC-P3 with overall yield 86%.

Synthesis of polymer HBC-P3. In an oven-dried and argon-purged Schlenk flask, 0.084 mL of methanesulfonic acid was added to a solution of polymer **P3'** (9.7 mg, 0.0086 mmol) in 0.76 mL

dry DCM, and DDQ (14.64 mg, 0.0645 mmol) was added in one portion under ice-bath cooling. This reaction mixture was allowed to stir at room temperature. The instantaneous green color appears in the reaction indicating formation of cation radical. After 20 min of stirring at room temperature, the reaction mixture was poured into 20 mL of a saturated $NaHCO_3$ solution, which was stirred vigorously for another 15 min. The organic layer was separated, and the aqueous phase was extracted with DCM (3 × 20 mL). The combined organic extract was washed with water (2 × 15 mL) and brine (10 mL). The solution obtained after workup was dried over sodium sulfate, filtered, and evaporated under reduced pressure. The obtained residue was passed through silica gel flash column chromatography, and the column was further eluted with dichloromethane (100 mL). The combined eluates were concentrated in vacuo to give the brownish solid **HBC-P3** (86% yield). ν_{max}/cm^{-1} 2922, 2853, 1718, 1675, 1456, 1377, 1264, 1091 and 735. ^1H NMR (500 MHz, DCM-d_2) δ (ppm) 9.73 (s), 8.09 (s), 7.96 (br. s.), 7.82 - 7.92 (m), 7.64 - 7.73 (m), 7.53 - 7.63 (m), 7.48 (d, J=7.9345 Hz), 7.37 - 7.45 (m), 7.16 (d, J=8.8502 Hz). ^{19}F NMR (470 MHz, CD_2Cl_2) δ (ppm) -64.16, -64.21, -64.35, -71.73, -73.42, -73.58, -73.61, -79.01 and -79.29 (AB pattern, J = 144.6 Hz, CHFC$\underline{F}_2$), -86.27, -87.29, -108.82, -115.51, -116.26, -123.29, -133.68, -133.71, -139.20 (d, J = 58.5 Hz, CH$\underline{F}CF_2$), 139.43.

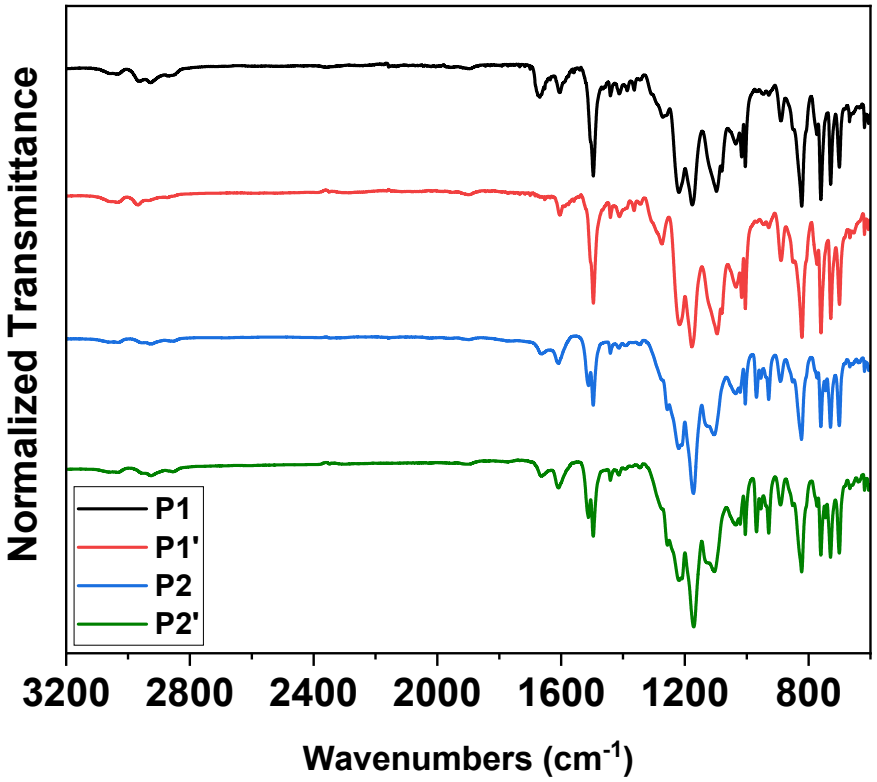


Figure S1. ATR-FTIR spectrum of polymers P1, P1′, P2 and P2′.

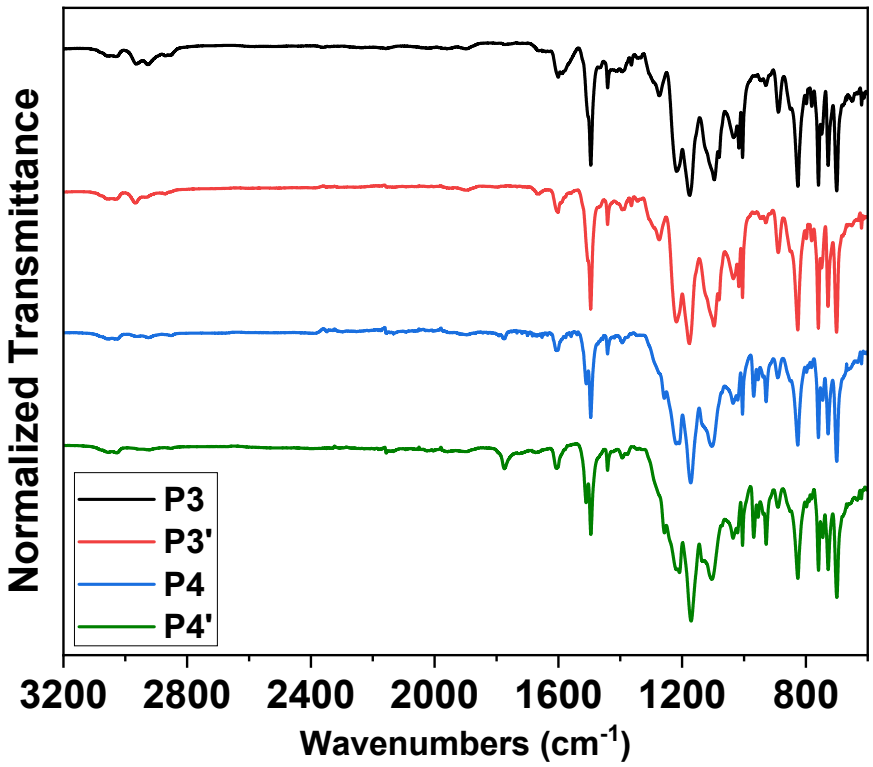


Figure S2. ATR-FTIR spectrum of polymers P3, P3′, P4 and P4′.

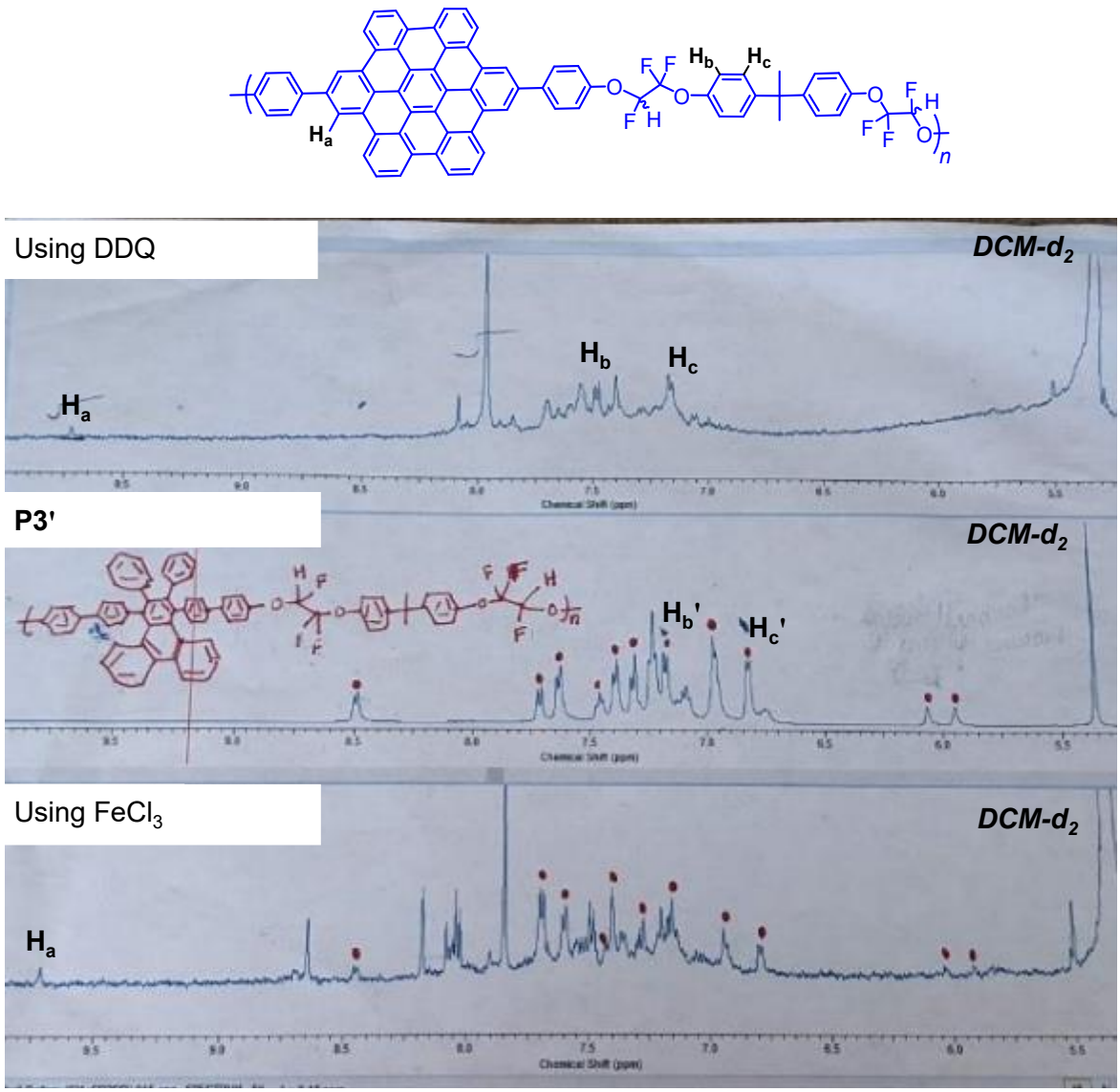


Figure S3. A comparison of ^{1}H-NMR (CD_2Cl_2 as a solvent): Scholl coupling reaction product using DDQ reaction conditions (HBC-P3, top), P3 (middle), and Scholl coupling reaction product using $FeCl_3$ reaction conditions (bottom). The red circles on top of peak resembles peak of starting material (polymer **P3**).

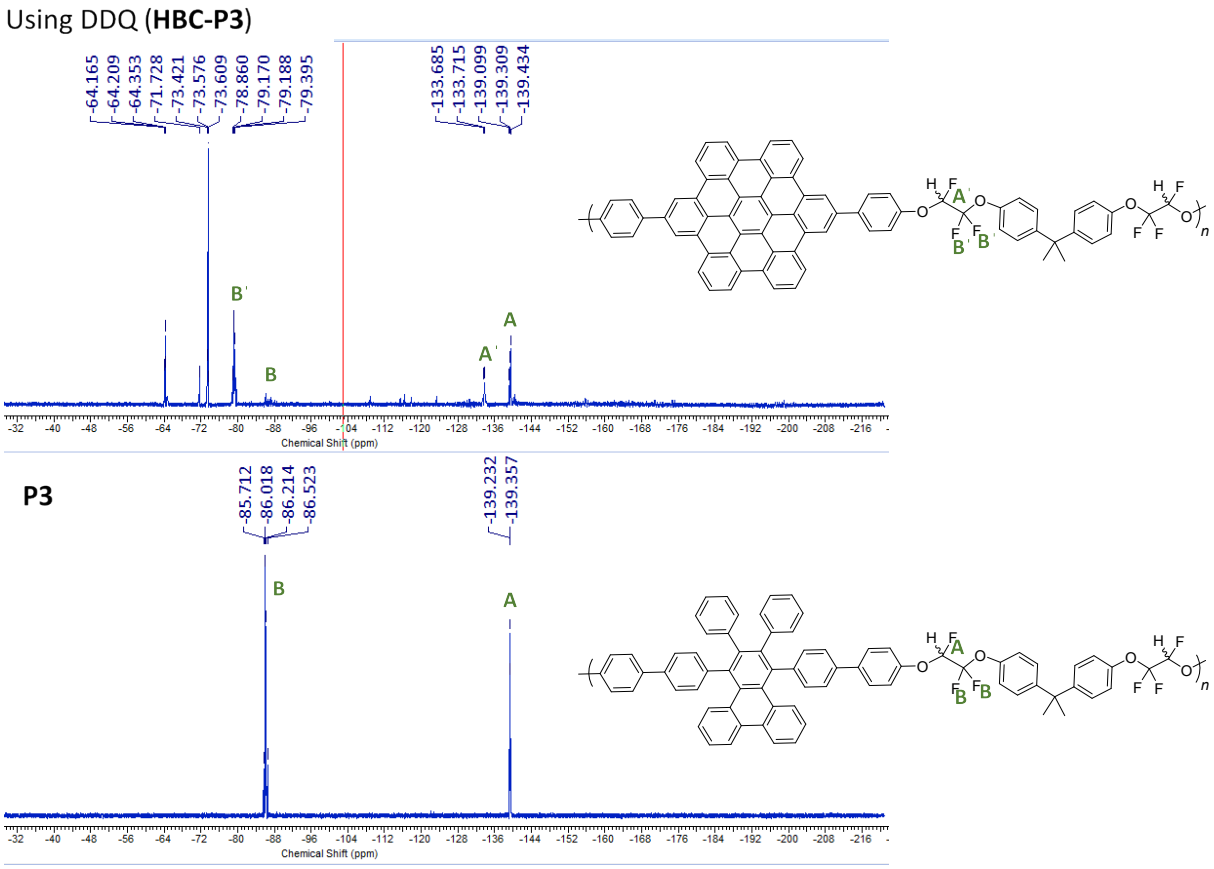


Figure S4. A comparison of ^{19}F-NMR spectra (CD_2Cl_2 as a solvent) for polymer P3 and HBC-P3 (after Scholl coupling using DDQ as an oxidant).

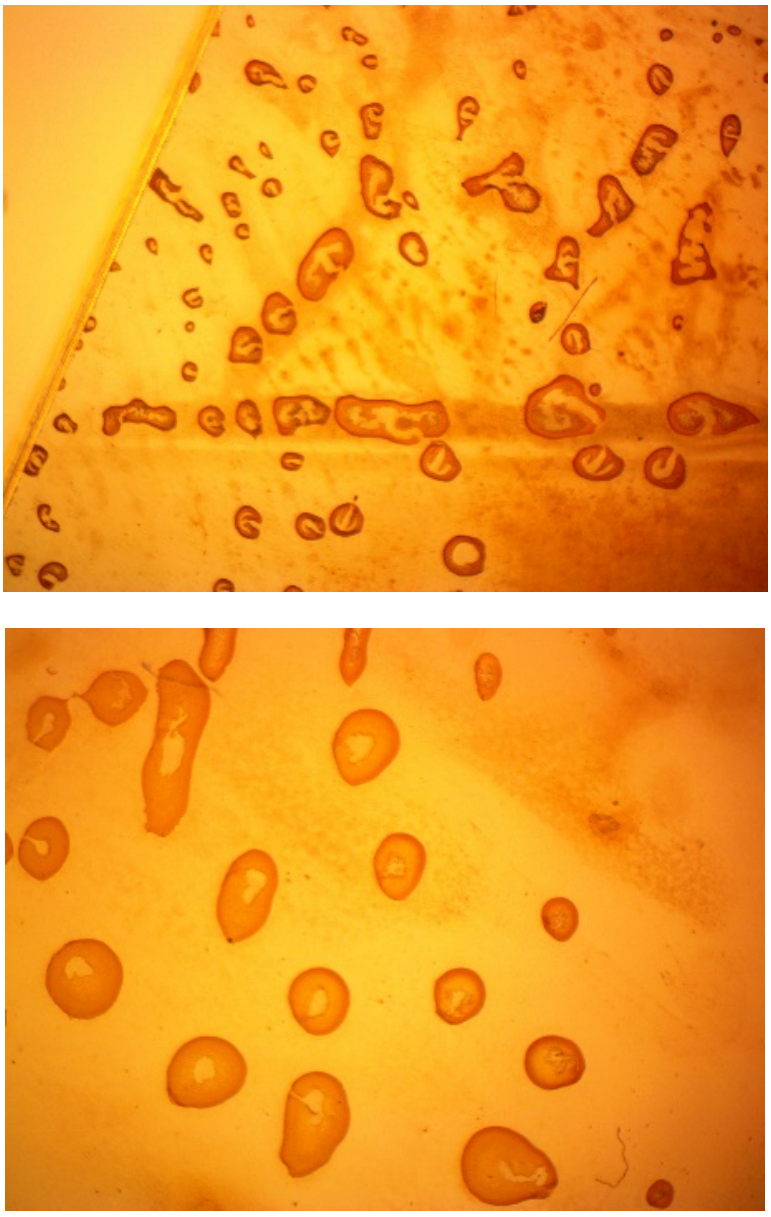
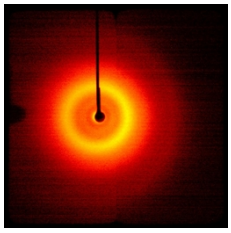


Figure S5. Polarized optical microscopy (POM) of polymer HBC-P3 after heating at 190 °C for 1 h.

WAXS data



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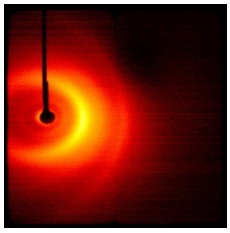
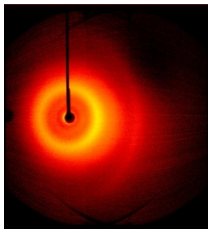
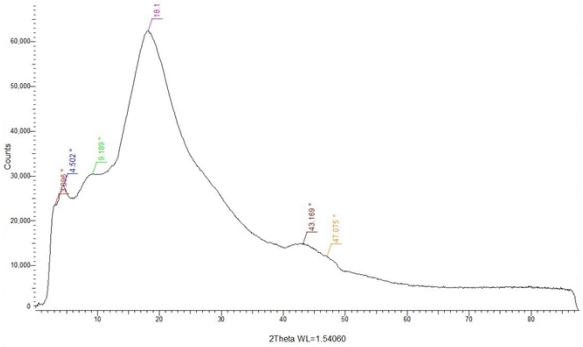


2-theta 323 °
d = 29.960 mm



Merged frames

Figure S6. 2D-WAXS of polymer P1'.



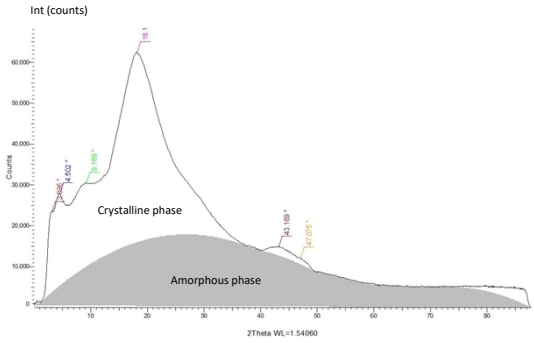
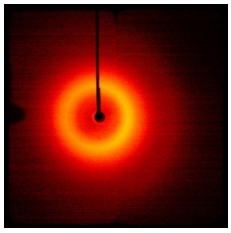


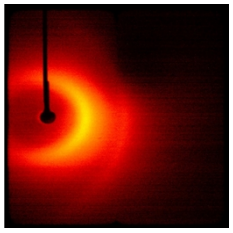
Figure S7. WAXS of polymer P1'.

Table S1. WAXS of polymer P1'.

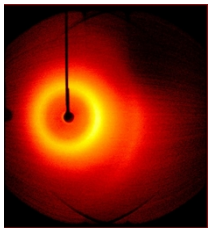
Color	Name	Angle	d Value	Net Intensity
Red	1	3.096	28.51035	19603.7
Blue	2	4.502	19.60972	22500.6
Lime	3	9.189	9.616	20380.9
Magenta	4	18.172	4.87777	46381.5
Dark Red	5	43.169	2.09394	2020.44
Dark Orange	6	47.075	1.92891	1565.52



2-theta = 350 °
d = 29.960 mm

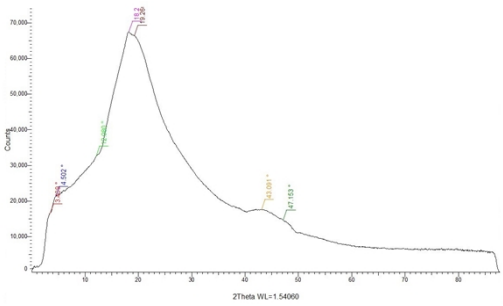


2-theta 323 °
d = 29.960 mm



Merged frames

Figure S8. 2D-WAXS of polymer P2'.



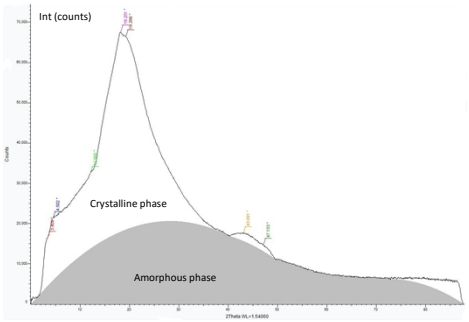
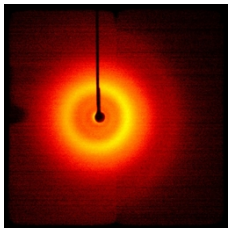


Figure S9. WAXS of polymer P2'.

Table S2. WAXS of polymer P2'.

Color	Name	Angle	d Value	Net Intensity
Red	1	3.409	28.898	11935.8
Blue	2	4.502	19.609	15426.4
Green	3	12.080	7.3209	18805.4
Magenta	4	18.251	4.8571	49647.7
Brown	5	19.266	4.6033	47969.8
Yellow	6	43.091	2.0975	1880.06
Dark Green	7	47.153	1.9259	1514.4



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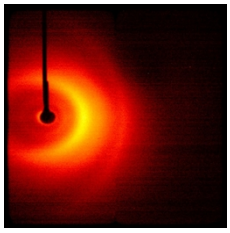

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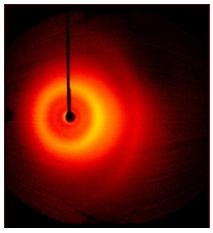


Merged frames

Figure S10. 2D-WAXS of polymer P3'.

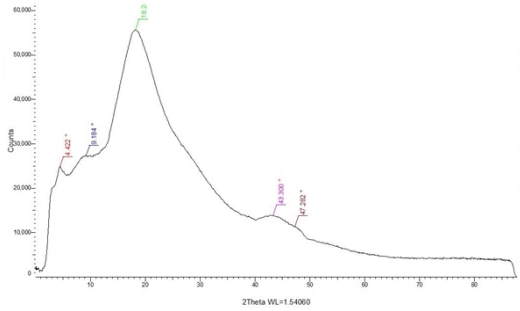
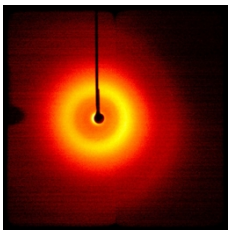


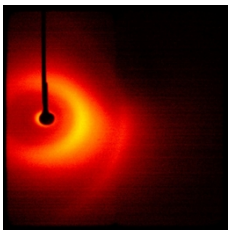
Figure S11. WAXS of polymer P3'.

Table S3. WAXS of polymer P3'.

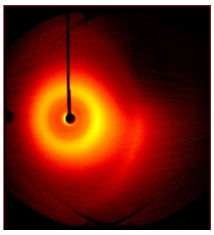
Color	Name	Angle	d Value	Net Intensity
Blue	1	4.375	20.180	10482.8
Green	2	8.748	10.0999	1299.47
Magenta	3	18.071	4.9049	26141.1
Brown	4	43.589	2.07474	1387.10
Yellow	5	47.577	1.9097	893.47



2-theta = 350 °
d = 29.960 mm



2-theta 323 °
d = 29.960 mm



Merged frames

Figure S12. 2D-WAXS of polymer P4'.

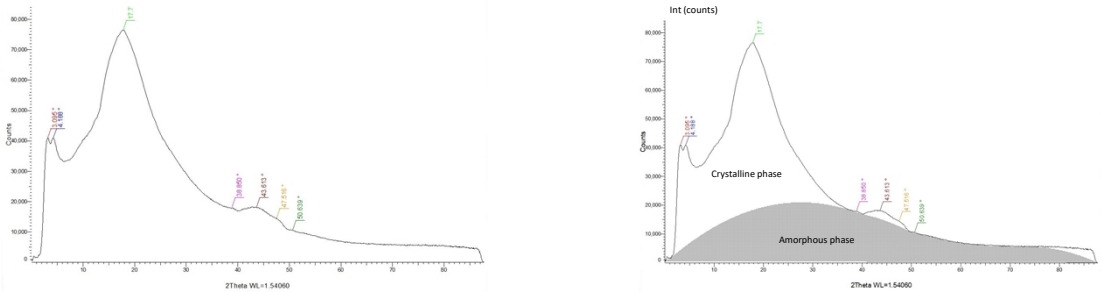


Figure S13. WAXS of polymer P4'.

Table S4. WAXS of polymer P4'.

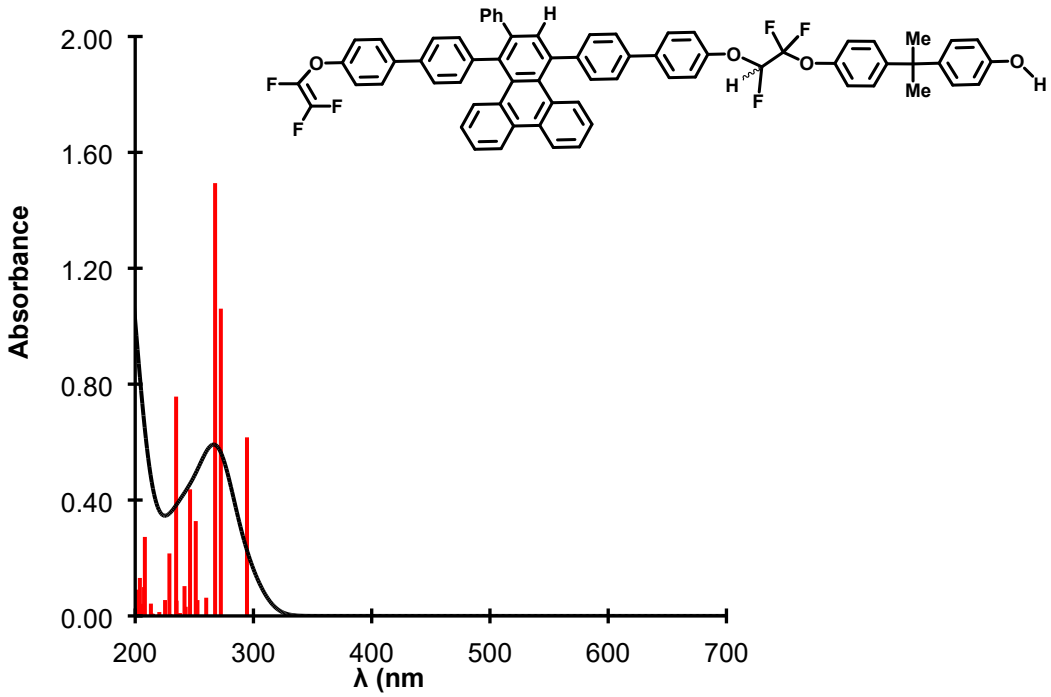
Color	Name	Angle	d Value	Net Intensity
Red	1	3.095	28.52633	36363.6
Blue	2	4.188	21.08317	35015.3
Lime	3	17.772	4.98683	58056.6
Magenta	4	38.85	2.31616	419.387
DarkRed	5	43.613	2.07365	2770.02
DarkOrange	6	47.516	1.912	1853.67
Green	7	50.639	1.80117	180.238

Computational studies

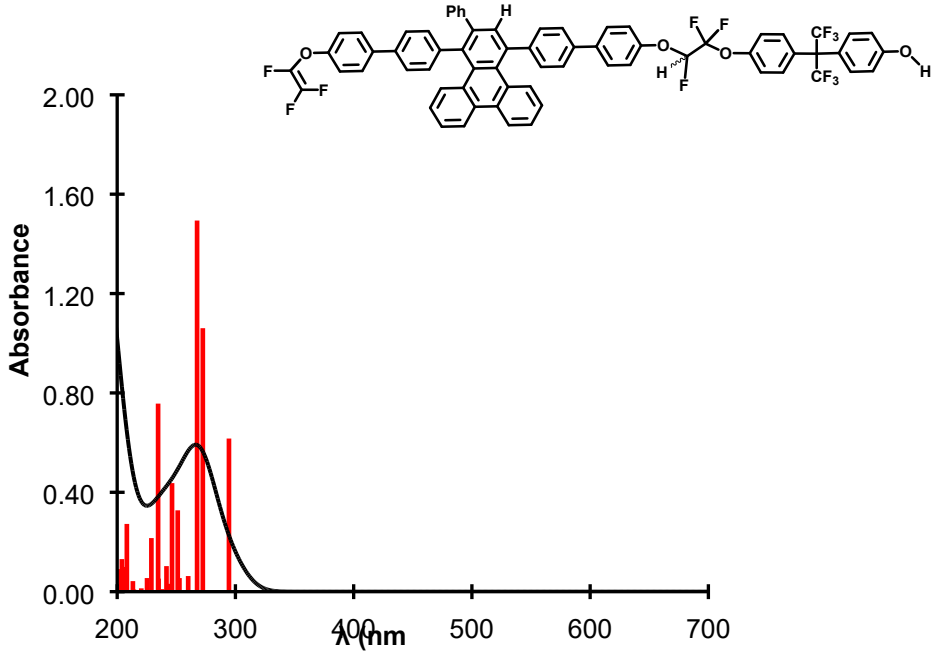
Simulated spectra

Absorption spectra of one polymer unit

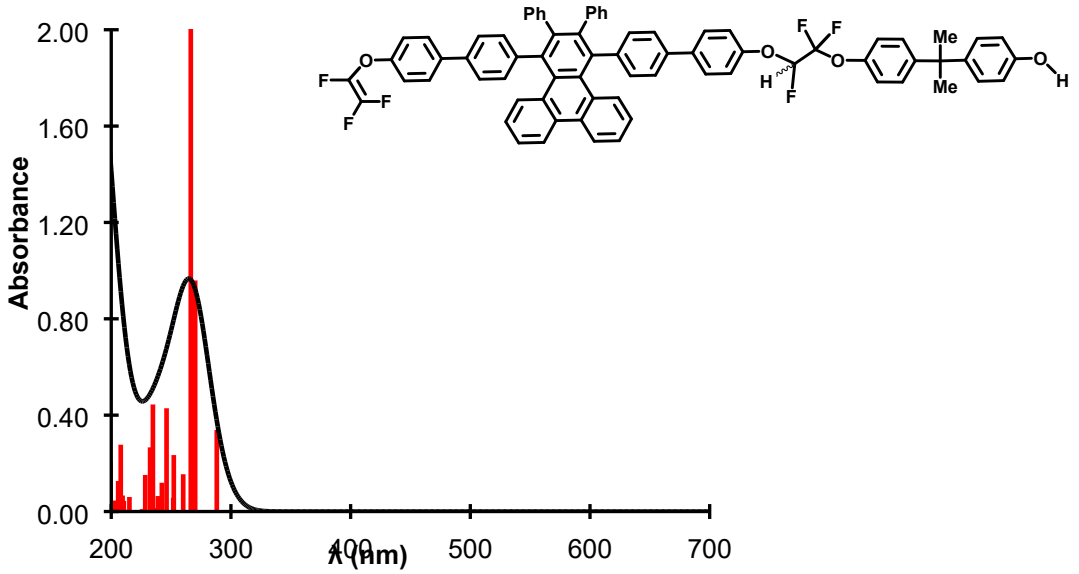
P1'



P2'



P3'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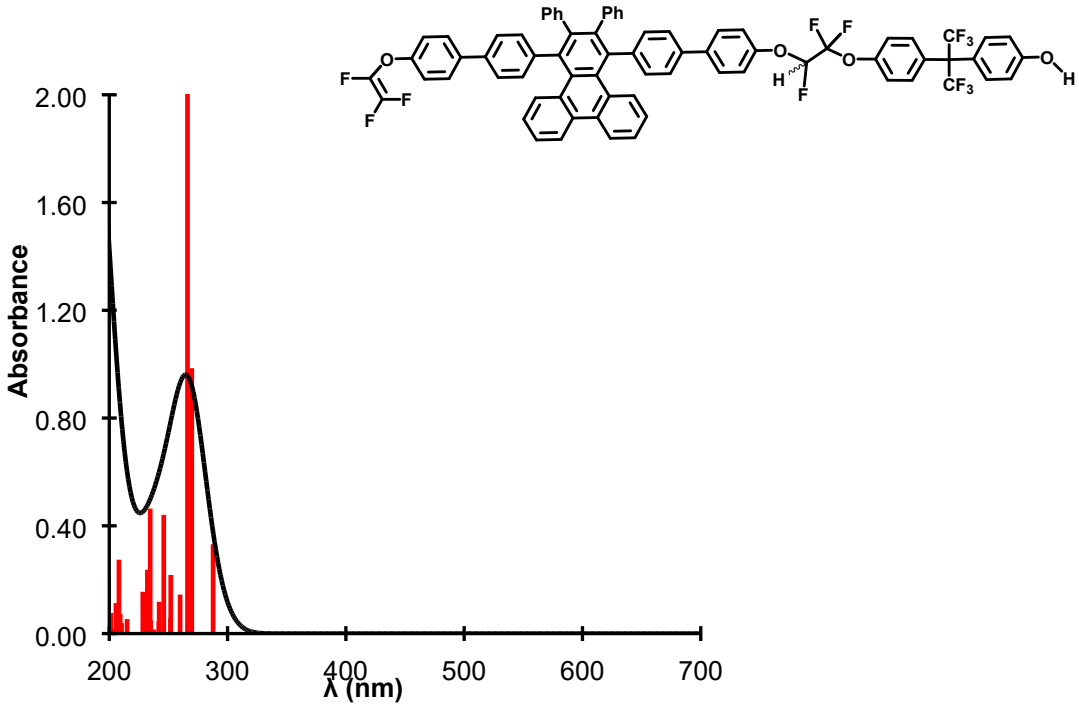
0.40
0.00
200
300
400
500
600
700
λ (nm)
Ph
Ph
F
O
F
F
F
F
O
H
F
O
Me
Me
O
H

P4'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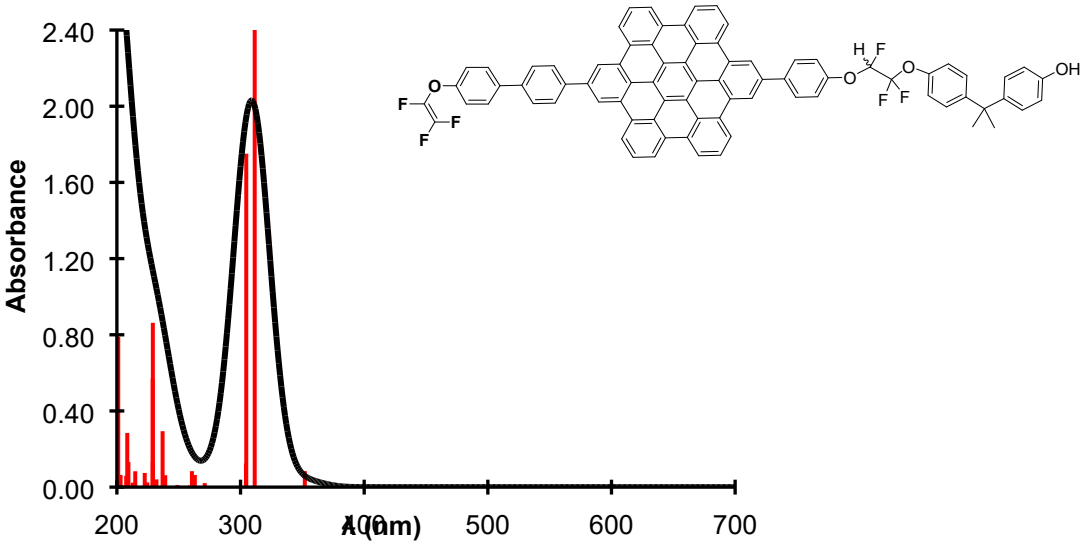
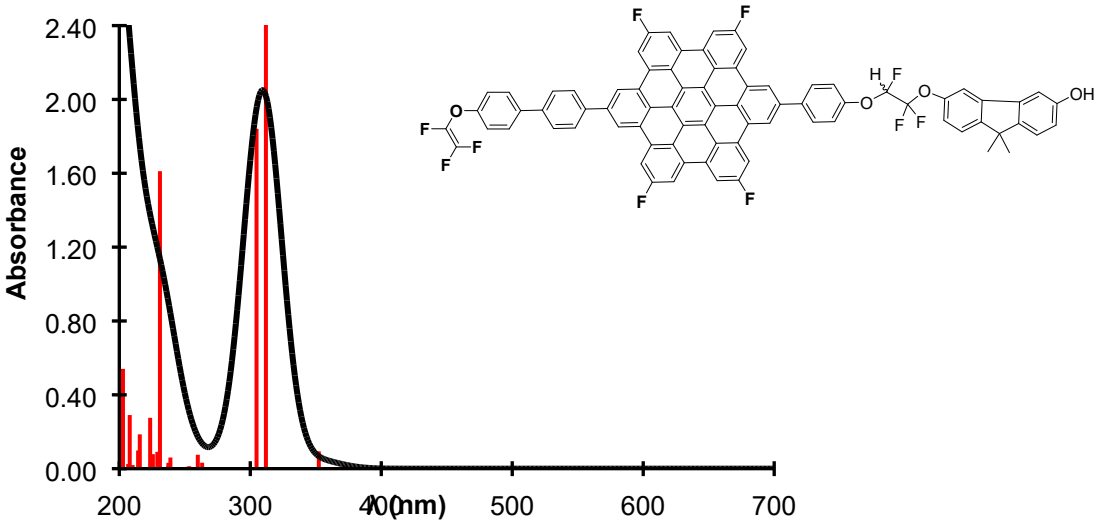
CF3
CF3
O
H

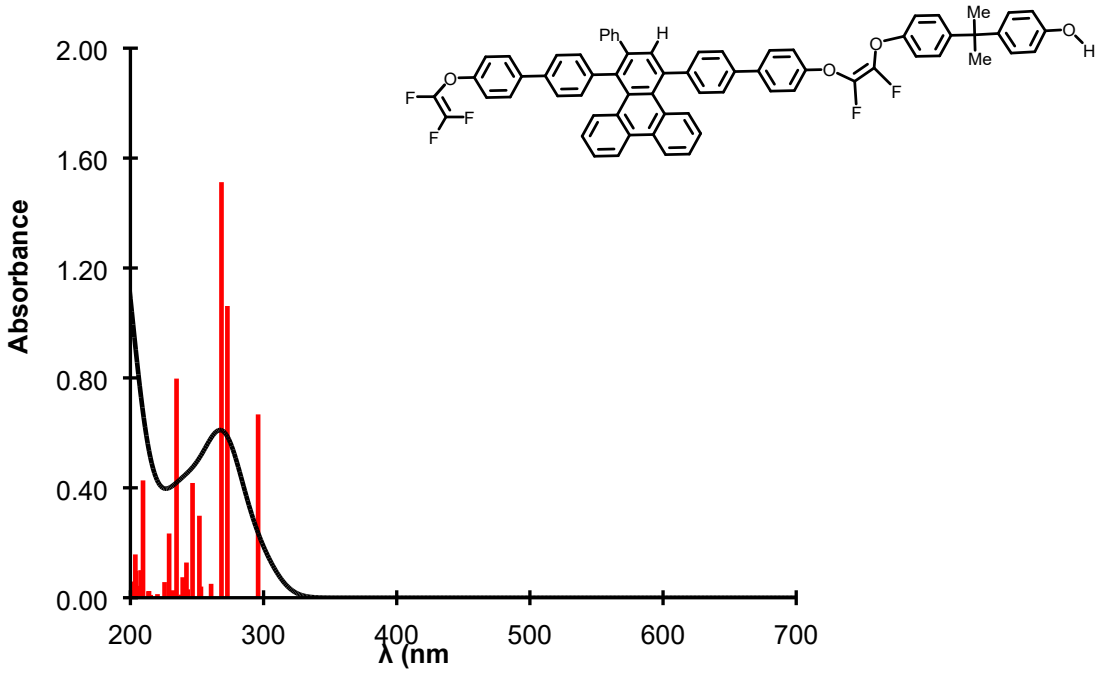
HBC-P3



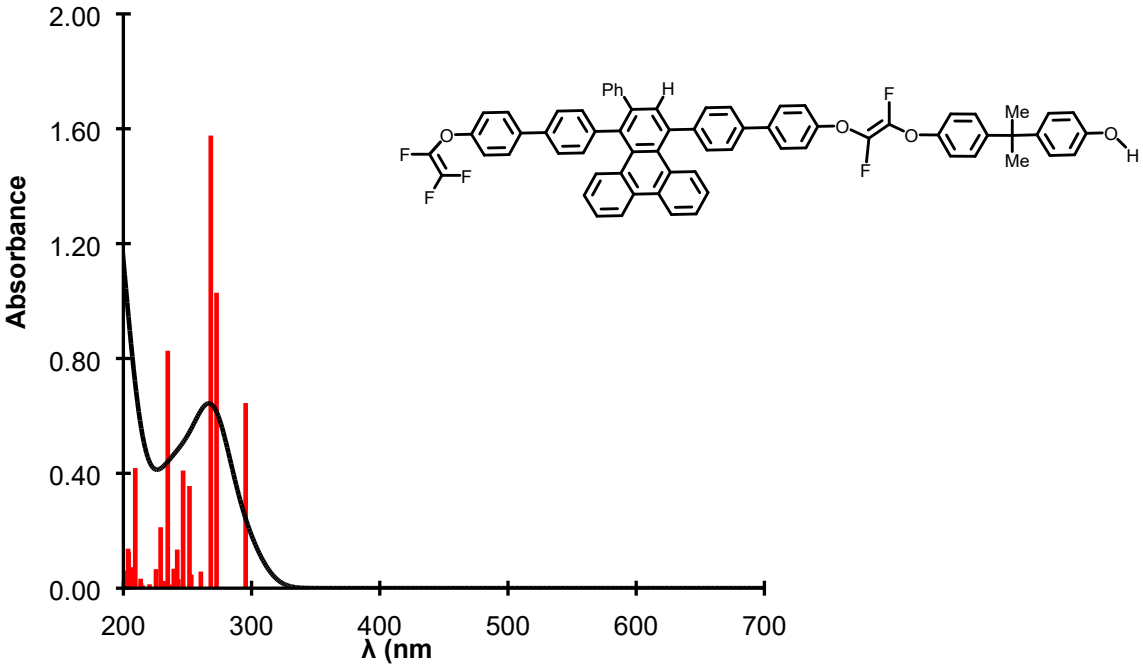
Plausible side-product of Scholl reaction



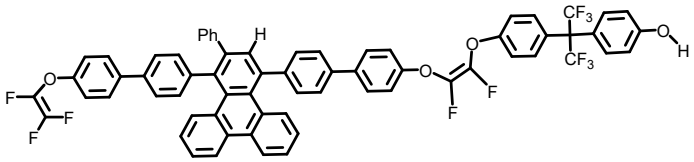
P1 (*Z*-configuration)

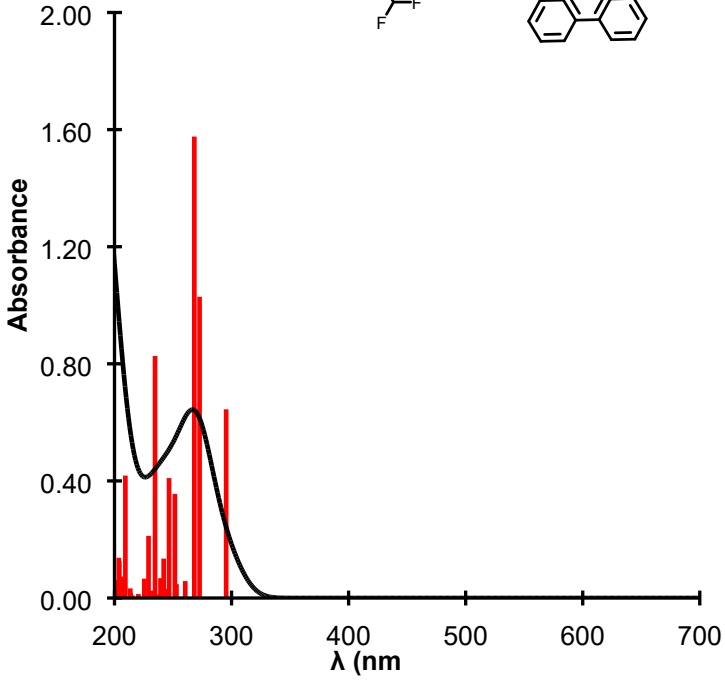


P1 (*E*-configuration)

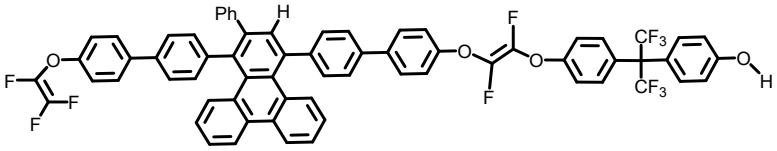


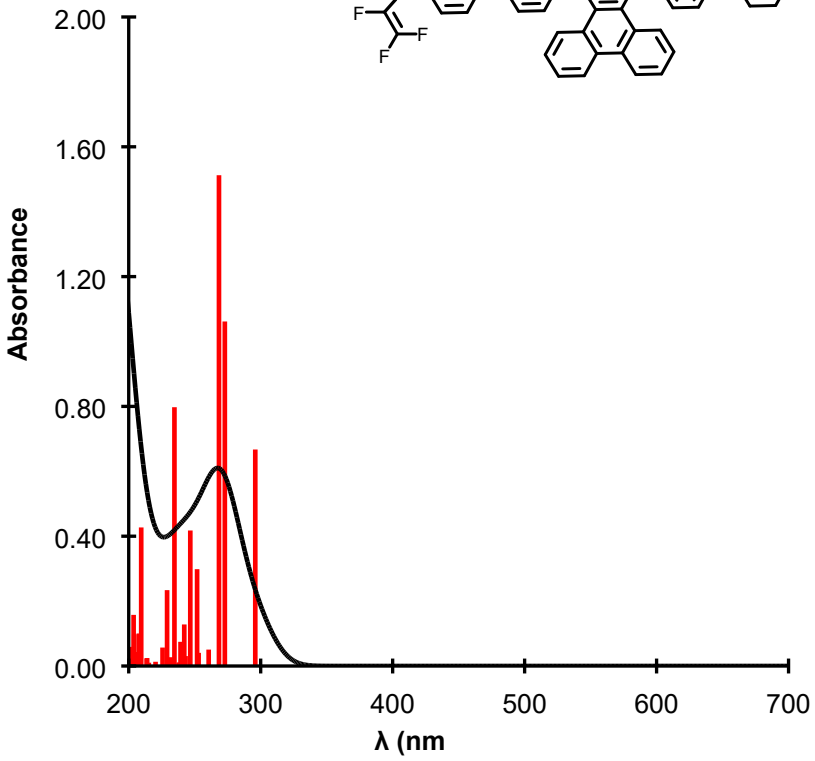
P2 (*Z*-configuration)



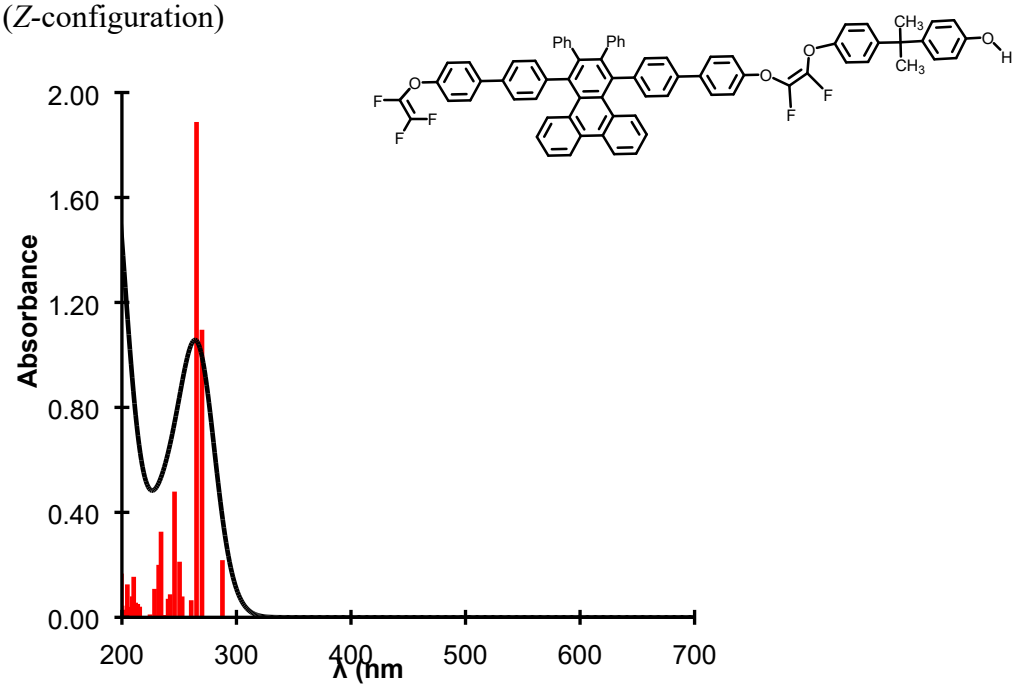


P2 (*E*-configuration)





P3 (*Z*-configuration)



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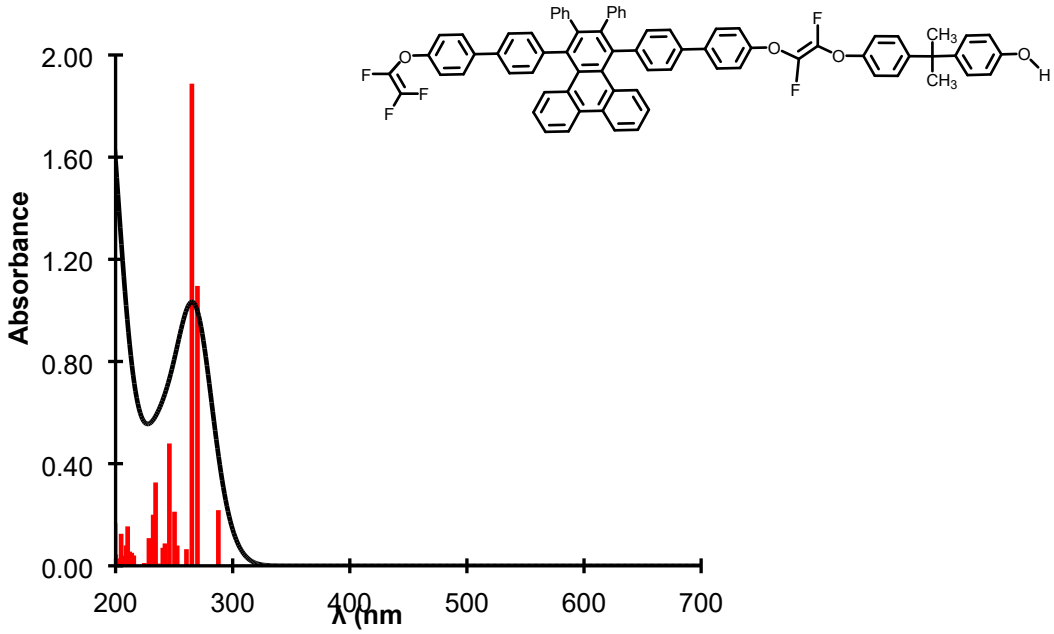
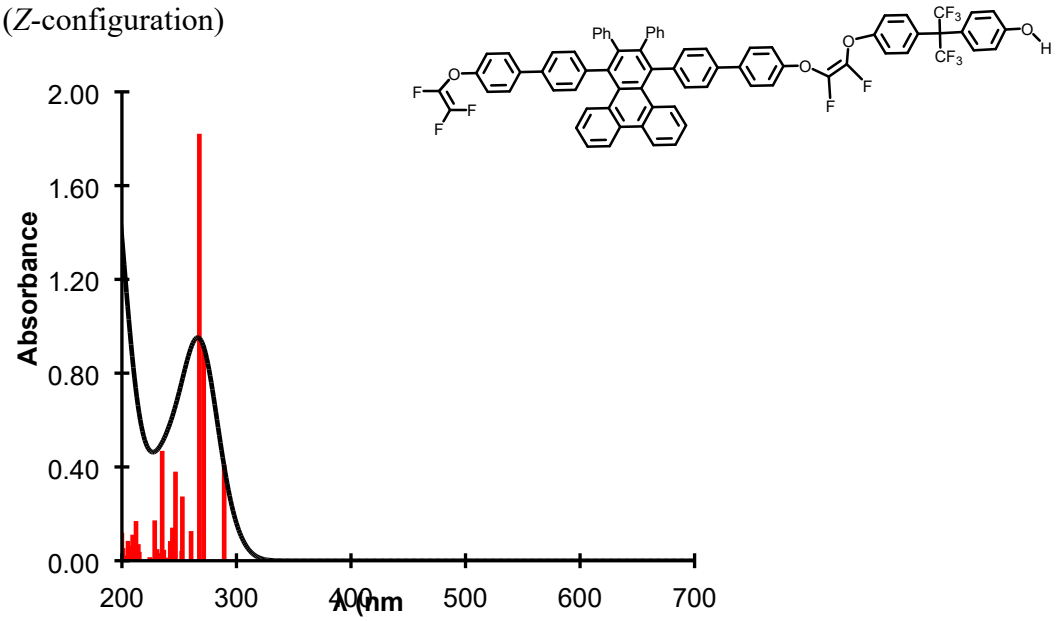


P4 (*Z*-configuration)



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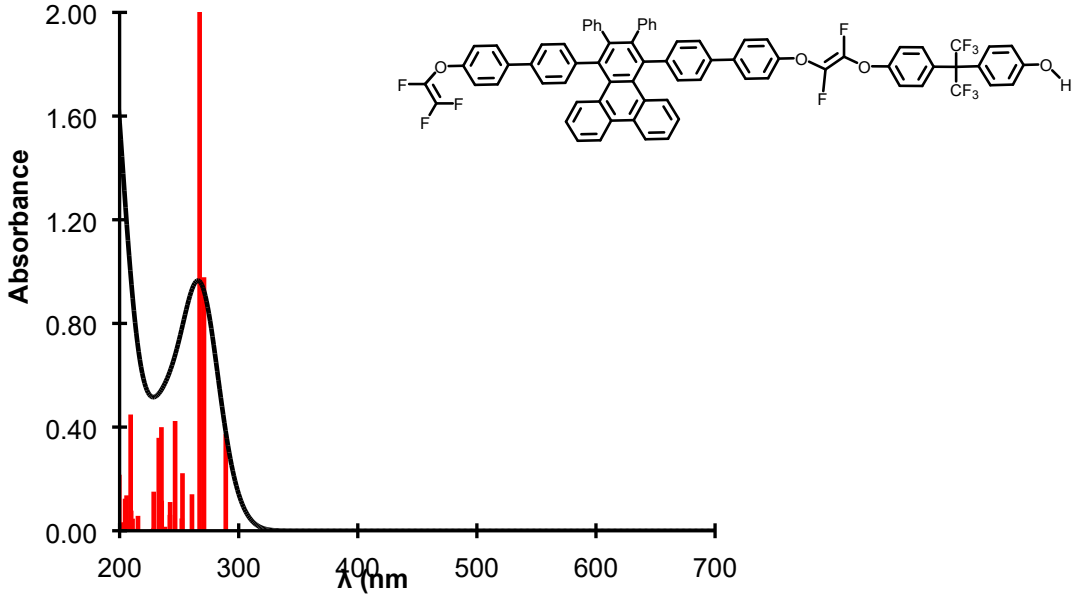
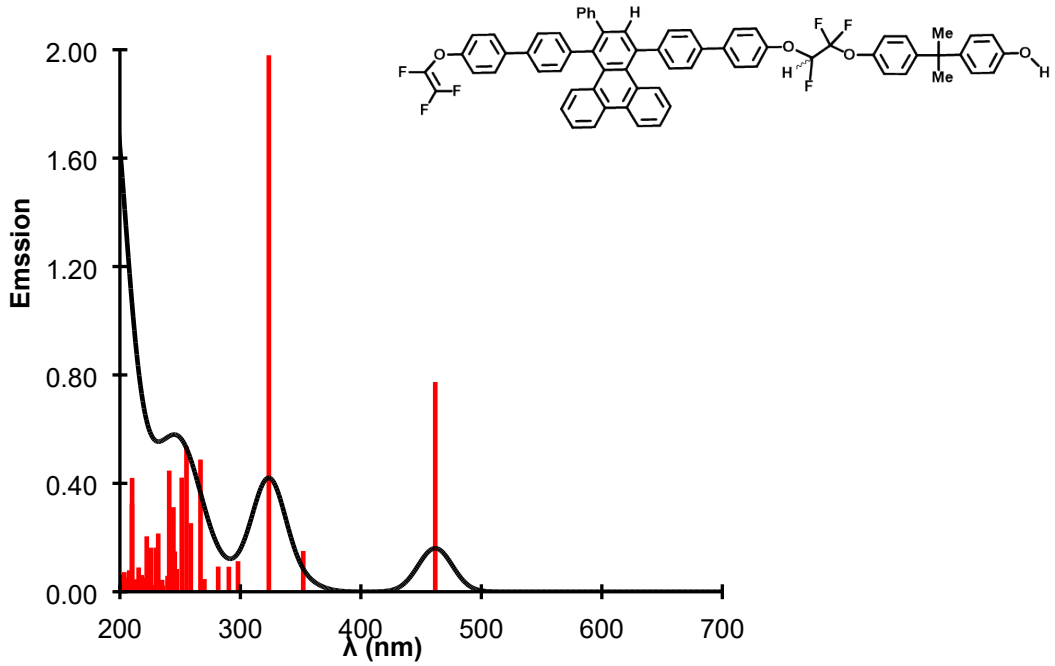
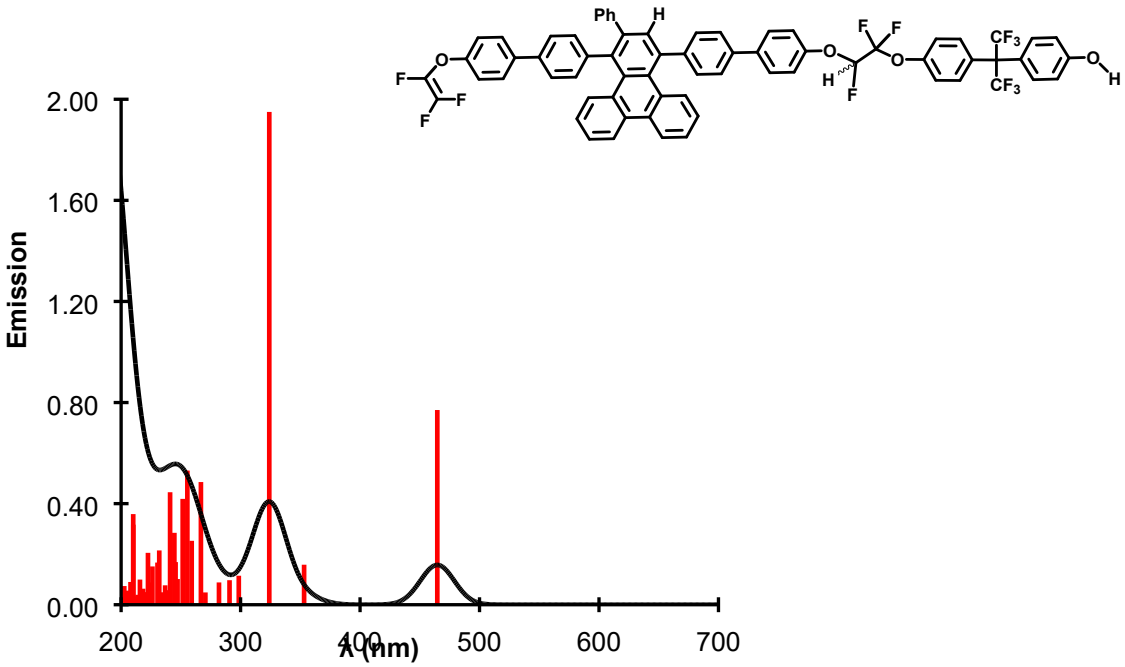


Emission spectra of one polymer unit

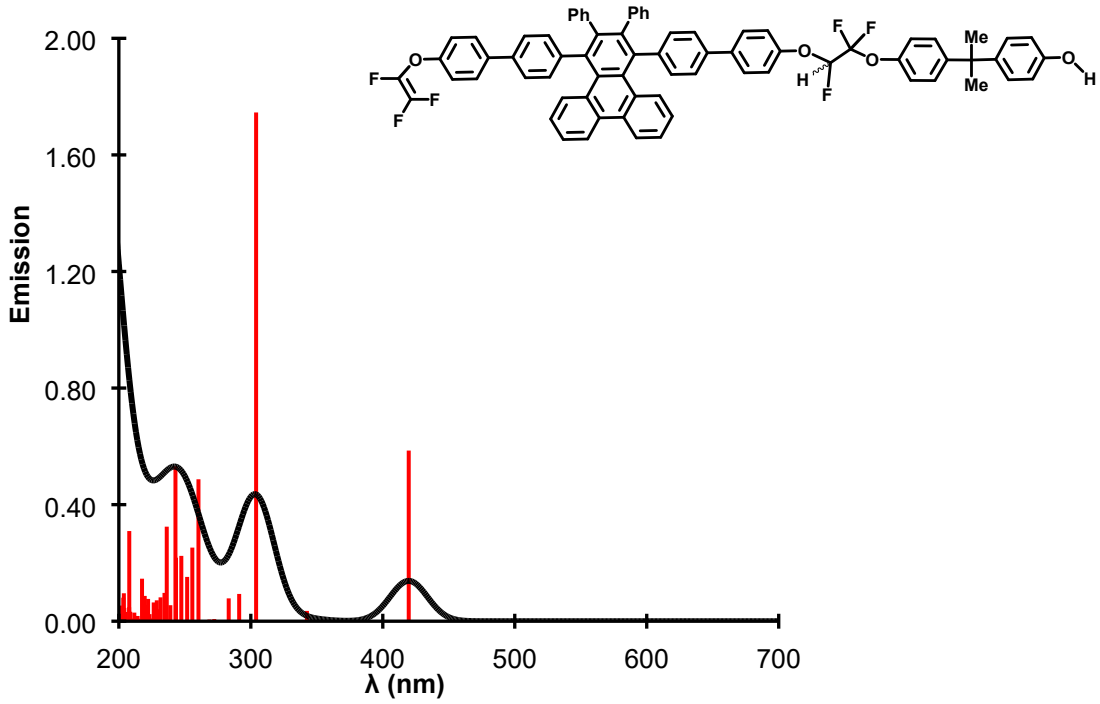
P1'



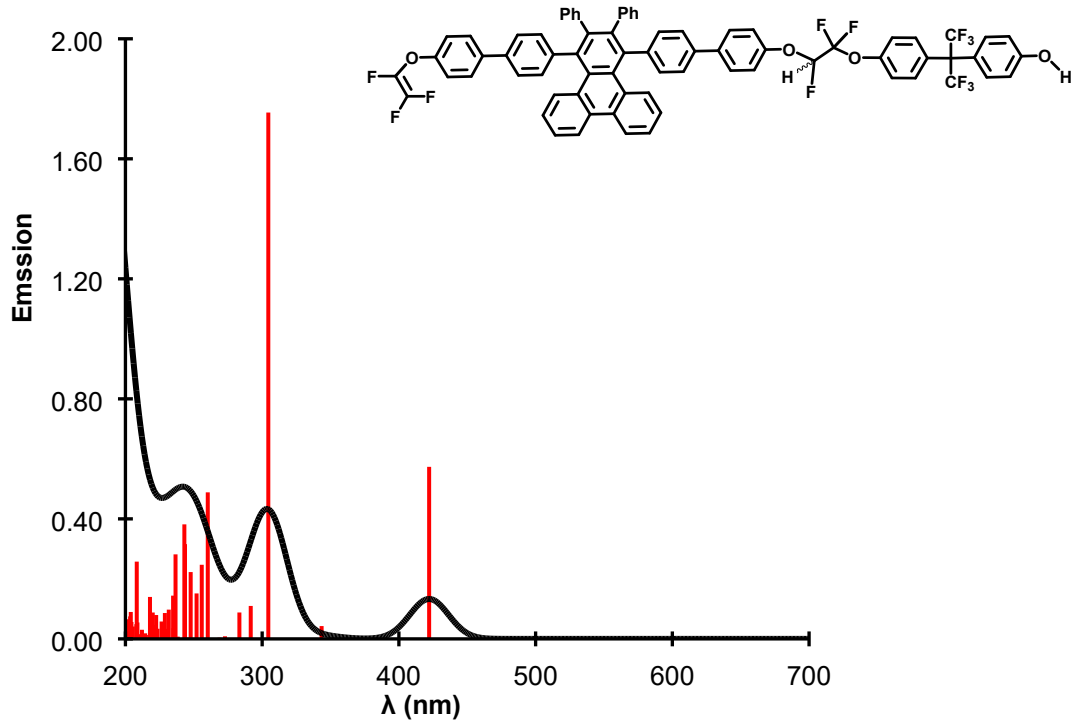
P2'



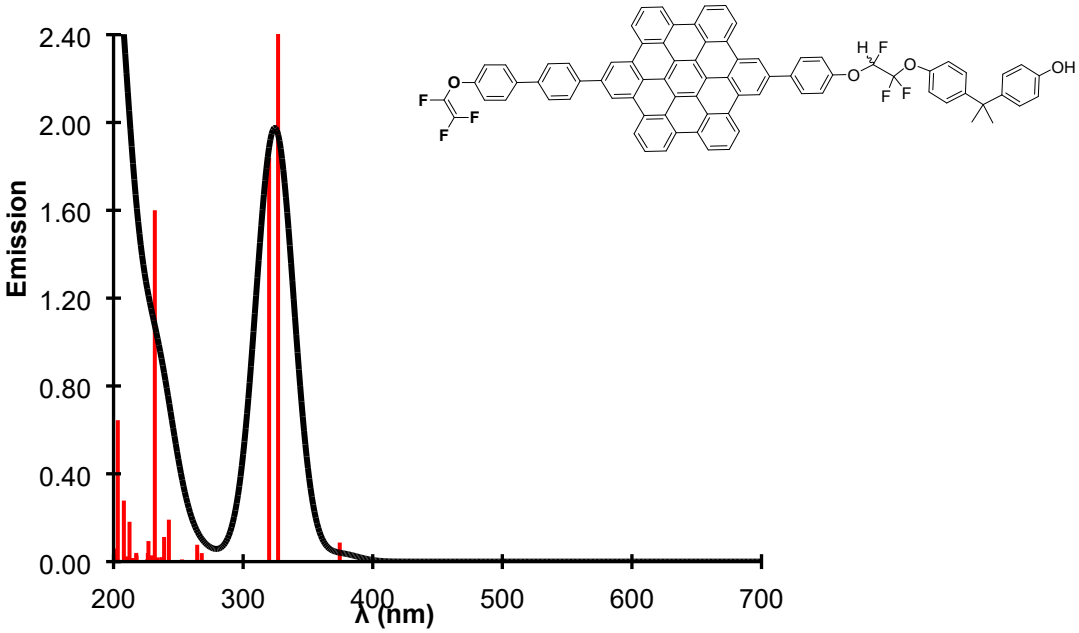
P3'


Ph
Ph
F
O
F
F
F
O
H
F
F
O
Me
Me
O
H
2.00
1.60
1.20
0.80
0.40
0.00
Emission
200
300
400
500
600
700
λ (nm)

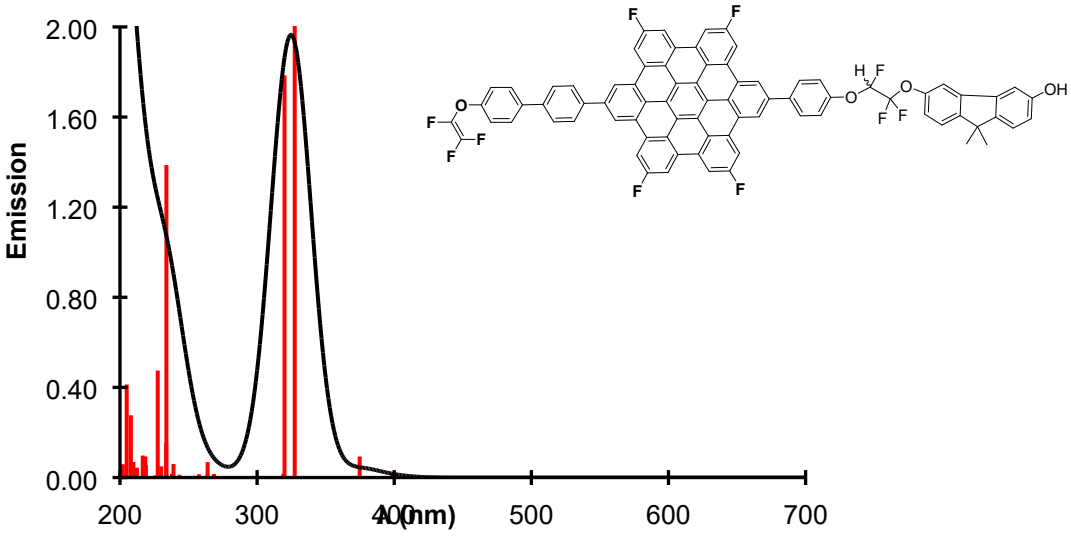
P4'


Ph
Ph
F
O
F
F
F
O
H
F
F
O
CF3
CF3
O
H
2.00
1.60
1.20
0.80
0.40
0.00
Emssion
200
300
400
500
600
700
λ (nm)

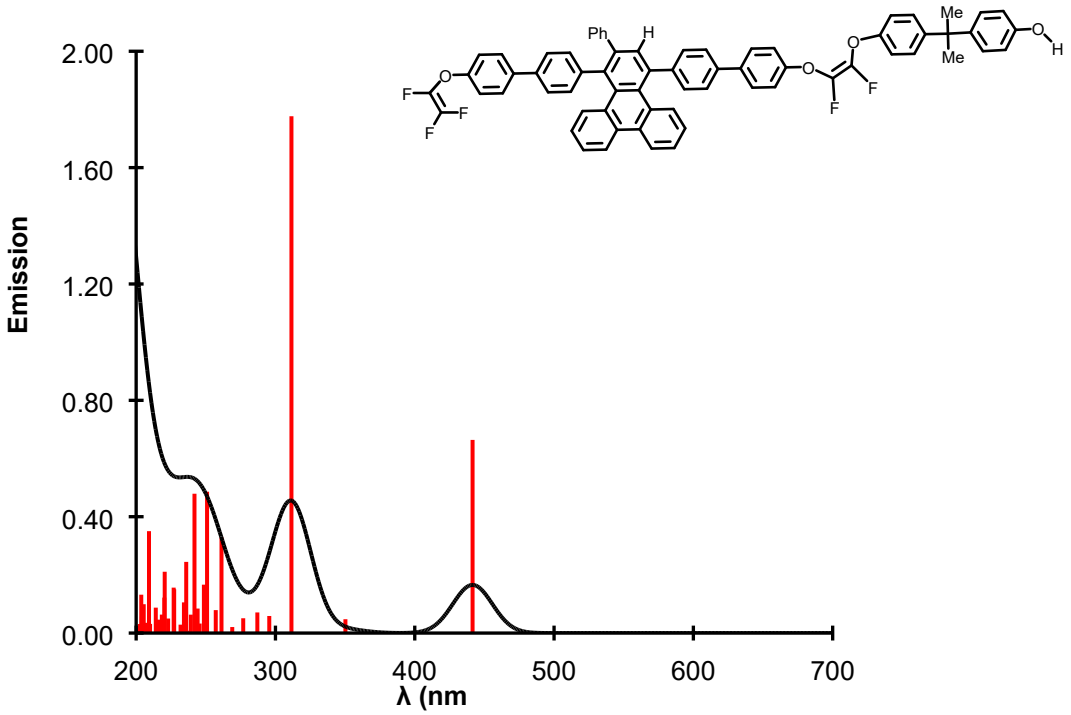
HBC-P3



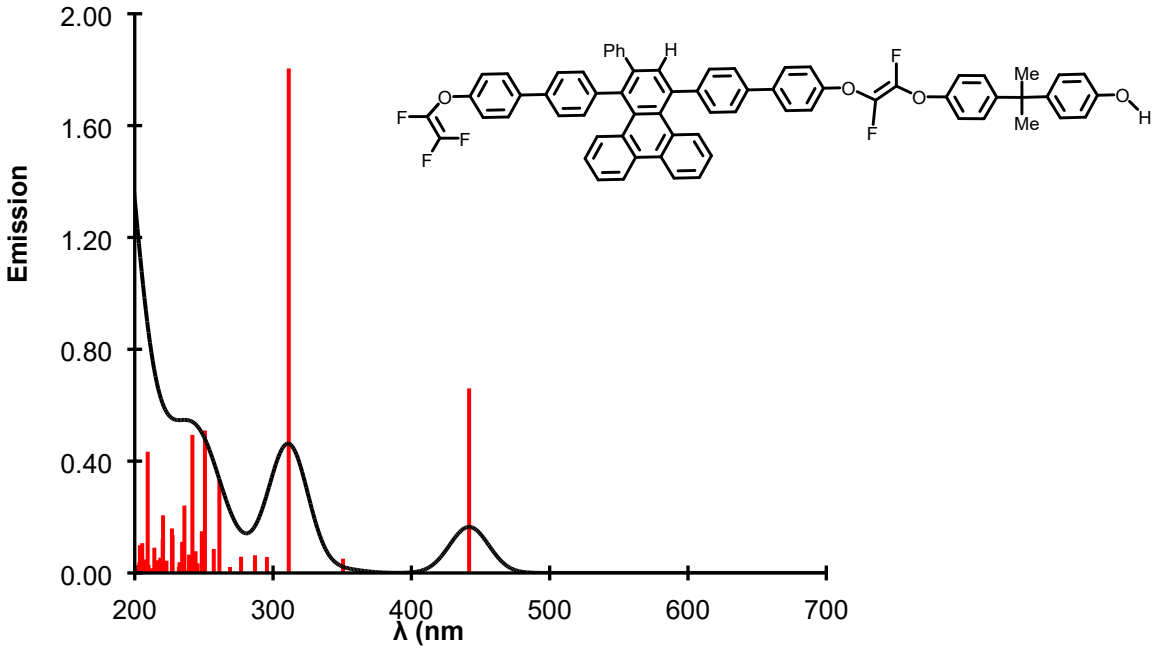
Plausible side-product of Scholl reaction



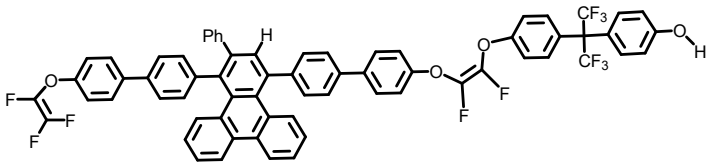
P1 (*Z*-configuration)

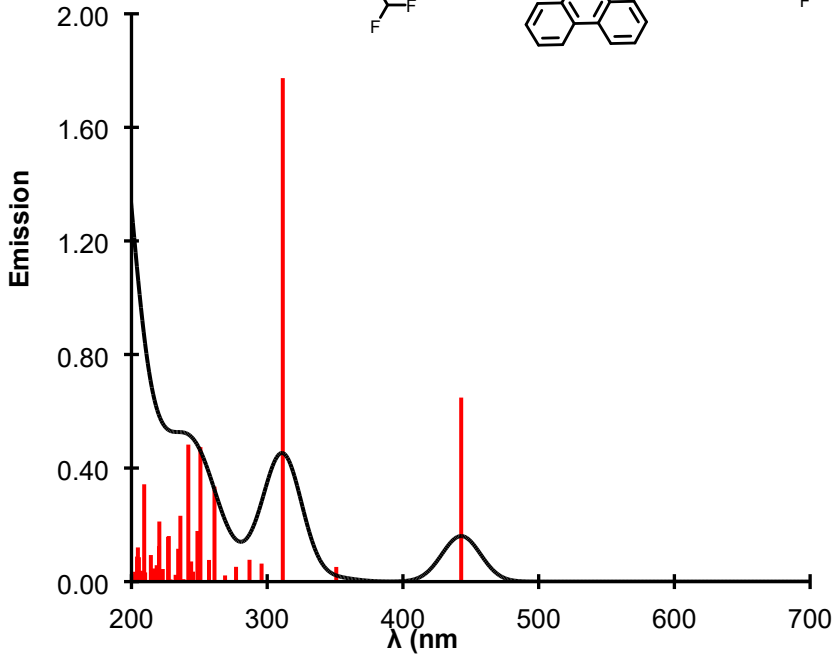


P1 (*E*-configuration)

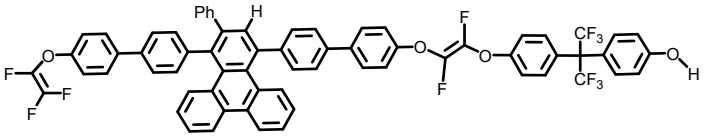


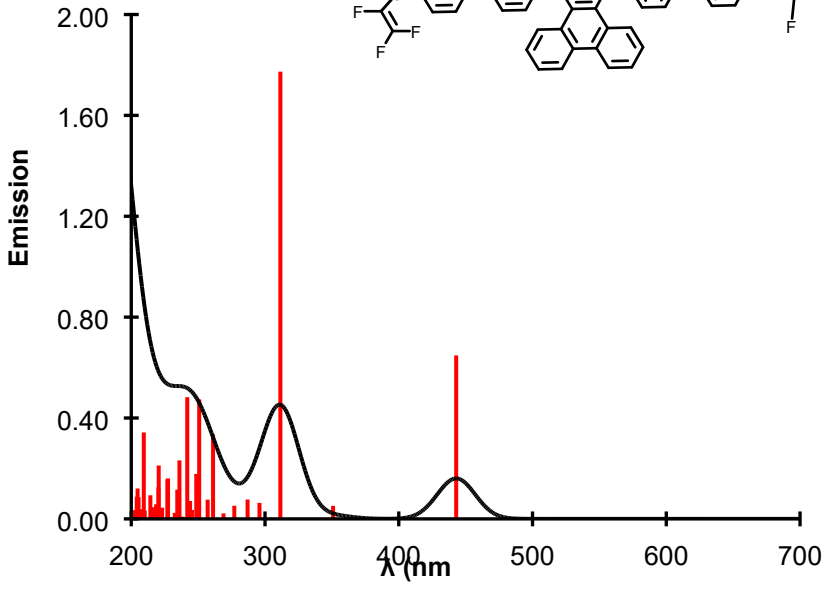
P2 (*Z*-configuration)



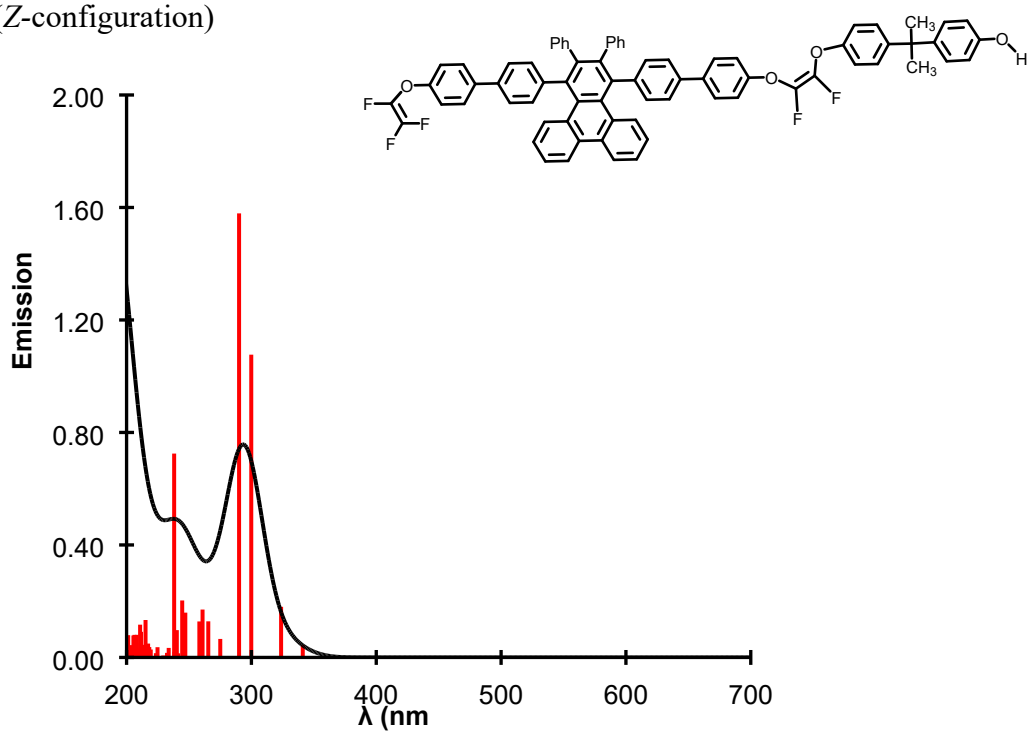


P2 (*E*-configuration)

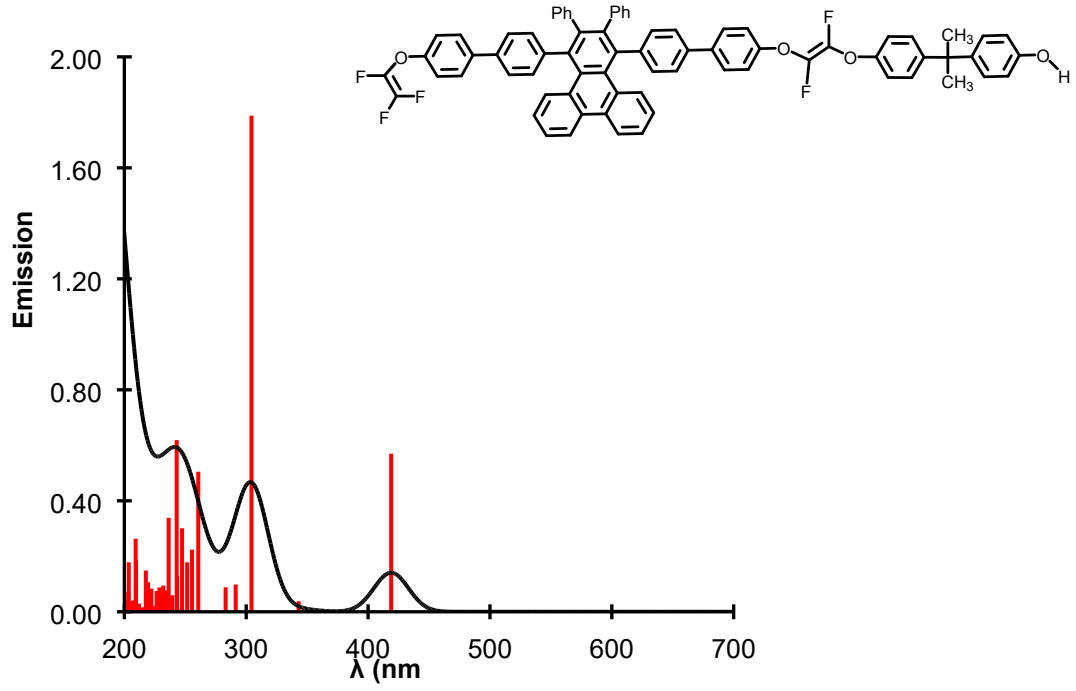




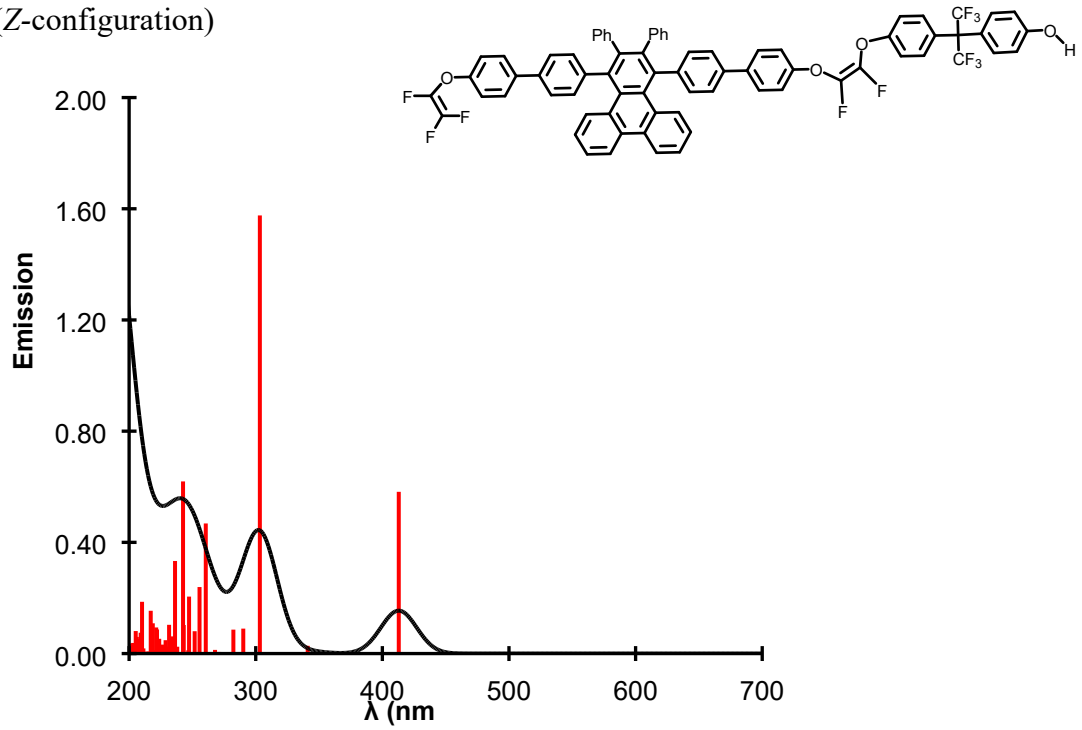
P3 (*Z*-configuration)



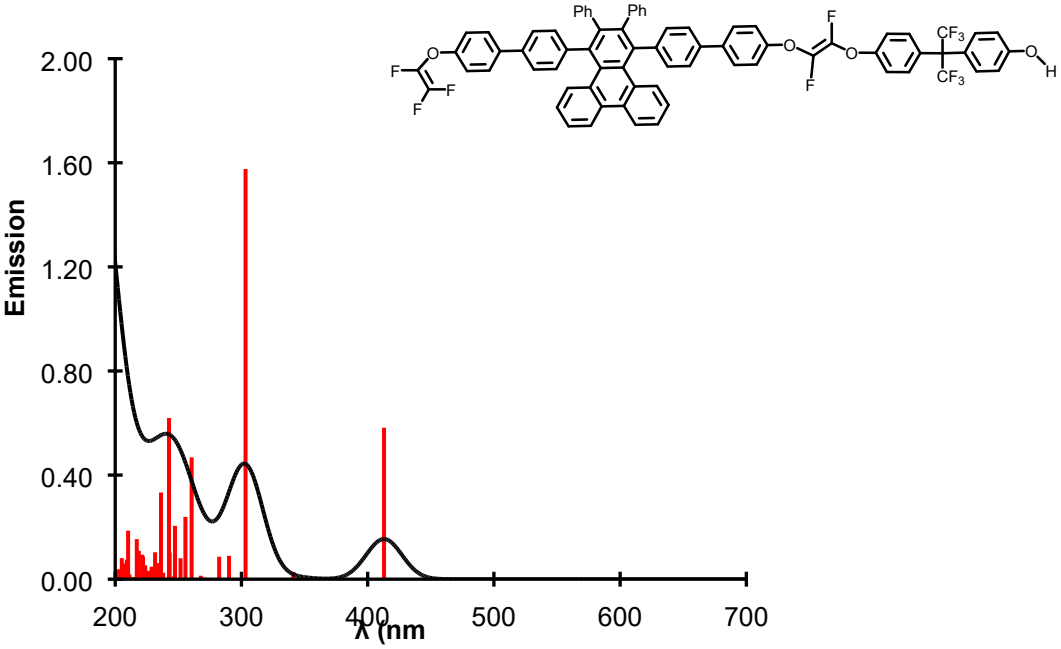
P3 (*E*-configuration)



P4 (*Z*-configuration)



P4 (*E*-configuration)



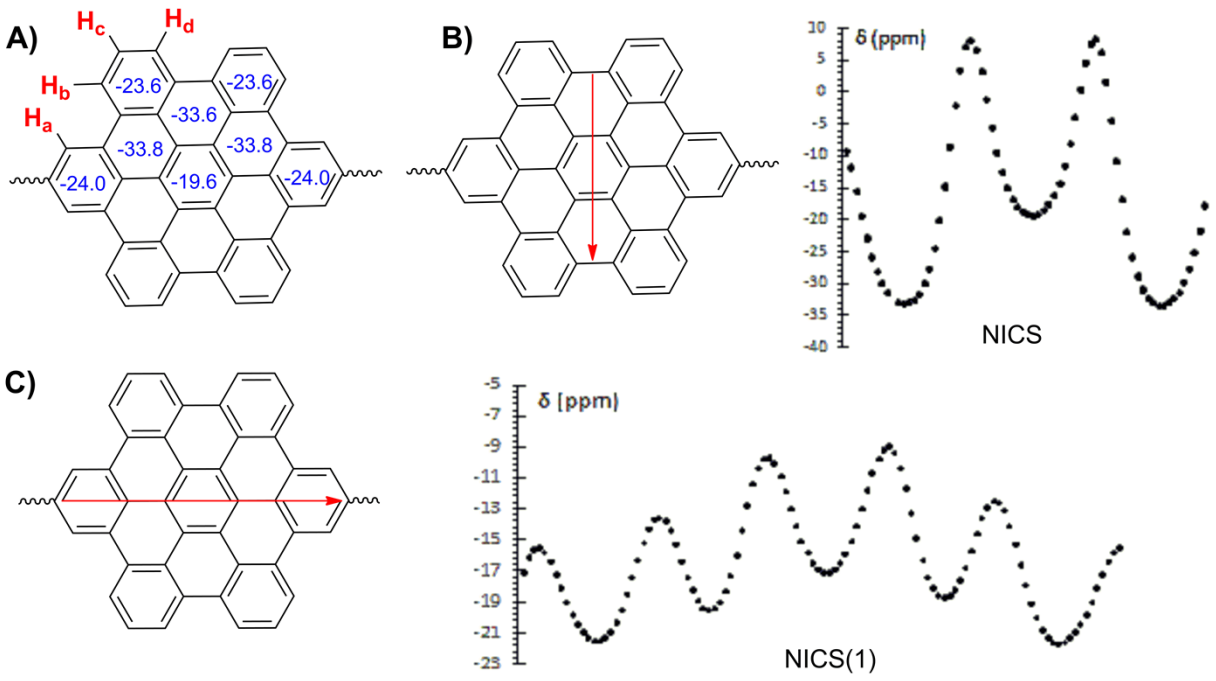


Figure S14. Computed NICS for HBC-P3 (A). NICS-XY-Scans for HBC ring value in vertical path (B) and in horizontal path (C). For the horizontal scan NICS(1) is used to avoid the overlap atom with the carbon center. All reported NICS values are calculated using GIAO method at SMD(dichloromethane)-ωB97XD/6-311++G(d,p)//SMD(DCM)-ωB97XD/BS1 level theory.

Table S5. Computed absorption and emission peaks in one and two repeating units.

Polymer	λ_{abs} (nm)		λ_{em} (nm)	
	one repeating unit	two repeating units	one repeating unit	two repeating units
P1	186, 267	192, 267	441	441
P2	186, 268	192, 267	441	442
P3	187, 264	200, 266	443	420
P4	187, 266	199, 267	437	432

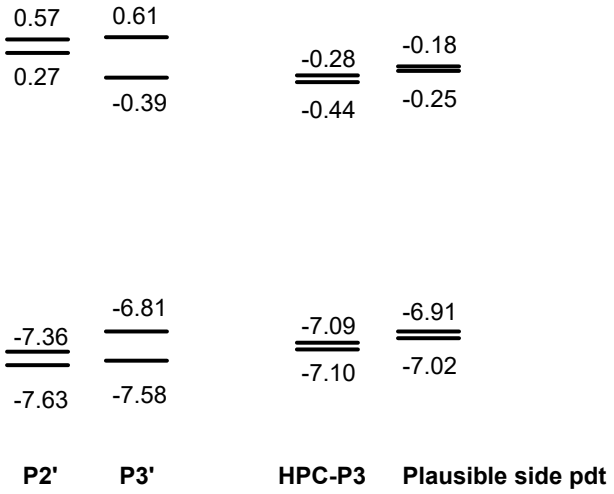


Figure S15. Comparison of computed energy diagram (eV) of frontier molecular orbitals of P2', P3', and HBC-P3.

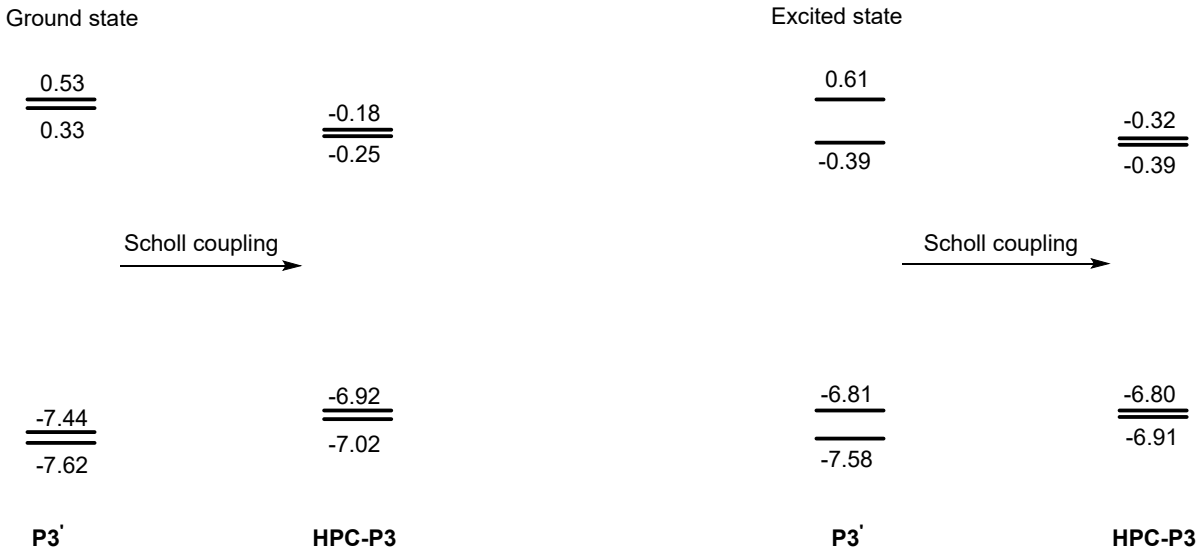
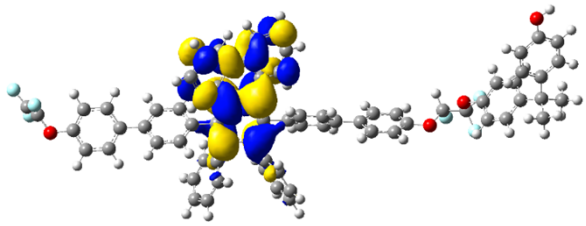
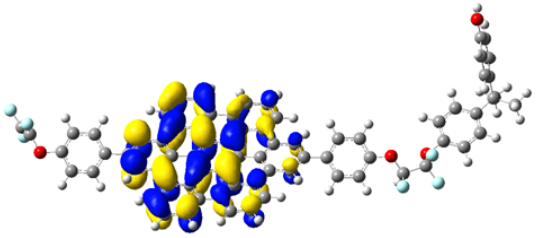
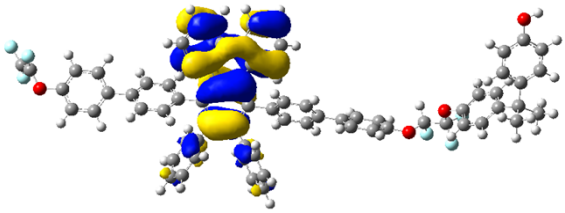
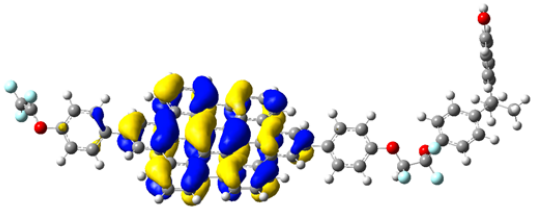
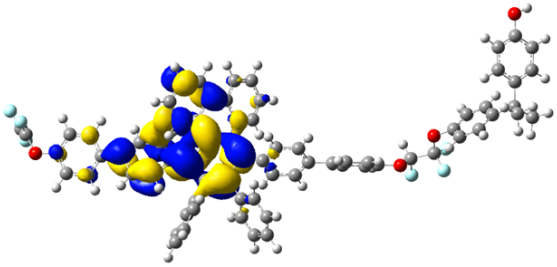
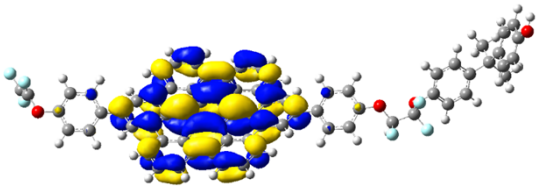
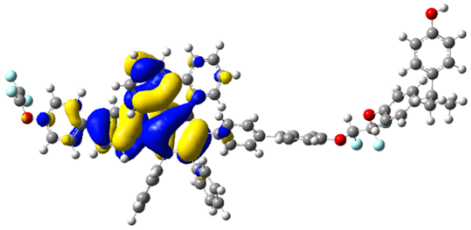
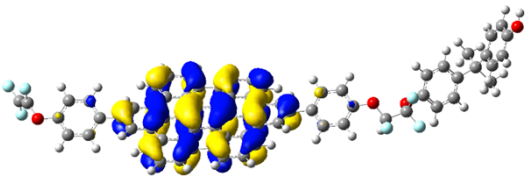


Figure S16. Computed energy diagram (eV) of frontier molecular orbitals before and after Scholl reaction.

Table S6. The visualization of HOTO (highest occupied transition orbital) and LUTO (lowest unoccupied transition orbital) responding to lowest energy excitation of P3' and HBC-P3.

Computed λ_{abs} = 267, Polymer **P3'**	*Computed* λ_{abs} = 309, *Polymer* **HBC-P3**
 LUTO	 LUTO
 HOTO	 HOTO
Computed λ_{em} = 420, Polymer **P3'**	*Computed* λ_{em} = 374, *Polymer* **HBC-P3**
 LUTO	 LUTO
 HOTO	 HOTO

Coordinates

Ground state geometries

```
P1'     el energy= -3479.66355889
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C    -4.848008 -1.407676 -0.061401
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C    -4.885847  1.023337  0.127393
C    -3.537808  1.073429 -0.310377
C    -2.787805 -0.132073 -0.331440
C    -3.020517  2.355634 -0.829384
C    -3.711506  3.556118 -0.558717
C    -4.878901  3.522565  0.326879
C    -5.479729  2.281451  0.636421
C    -1.939442  2.400397 -1.735450
C    -1.518528  3.588116 -2.306438
C    -2.184670  4.780528 -2.006668
C    -3.274400  4.754376 -1.155442
C    -5.394439  4.703138  0.895850
C    -6.470840  4.677334  1.763535
C    -7.040616  3.448861  2.109547
C    -6.544625  2.278707  1.562468
C    -7.056575 -0.309338  0.266190
C    -7.664321 -1.058272  1.279721
C    -9.048949 -1.142298  1.369712
C    -9.872203 -0.490037  0.441732
C    -9.260350  0.248588 -0.579471
C    -7.875093  0.339062 -0.664192
C   -11.351663 -0.579129  0.539845
C   -11.979126 -1.773877  0.921634
C   -13.362482 -1.859817  1.020358
C   -14.135600 -0.740644  0.730625
C   -13.547789  0.460771  0.351502
C   -12.159419  0.528777  0.258165
C    -1.300145 -0.185880 -0.395146
C    -0.643134 -1.040883 -1.286690
C     0.746712 -1.114910 -1.310966
C     1.524748 -0.341043 -0.440764
C     0.862394  0.503652  0.461782
C    -0.524658  0.578661  0.485945
C     3.008252 -0.411419 -0.472366
C     3.759448 -0.353521  0.711079
C     5.146474 -0.419483  0.685714
C     5.807355 -0.540010 -0.534838
C     5.089943 -0.586169 -1.728048
C     3.698357 -0.528942 -1.684060
O     7.183156 -0.580418 -0.473459
C     7.860644 -1.179226 -1.501236
F     8.014231 -0.315756 -2.562488
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C   -16.306661  0.128150  0.594252
C   -17.033704  0.239356 -0.507959
F   -16.385897  1.048853  1.558272
F   -16.985568 -0.625750 -1.495311
F   -17.888889  1.212581 -0.728954
H    -1.438607  1.485907 -2.027296
H    -0.685079  3.583021 -3.004866
H    -1.870095  5.717874 -2.459298
H    -3.815139  5.678243 -0.974240
H    -4.922269  5.656994  0.680898
H    -6.845961  5.602620  2.194305
H    -7.858367  3.401717  2.824828
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H    -7.046698 -1.567039  2.016179
H    -9.495990 -1.706897  2.185144
H    -9.872969  0.743089 -1.330394
H    -7.421084  0.915378 -1.467380
H   -11.380290 -2.658162  1.127011
H   -13.850264 -2.787420  1.307201
H   -14.148094  1.340566  0.136418
H   -11.701206  1.475710 -0.017831
H    -1.225183 -1.646141 -1.978667
H     1.230442 -1.796164 -2.007813
H     1.439645  1.125719  1.142529
H    -1.014612  1.247148  1.190290
H     3.252794 -0.280982  1.670697
H     5.727315 -0.391432  1.603621
H     5.598244 -0.635631 -2.686137
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C    -5.484097 -2.756382 -0.124004
C    -5.075346 -3.764096  0.757208
H    -4.318511 -3.544055  1.507829
C    -5.639852 -5.037537  0.692623
H    -5.316159 -5.806406  1.390697
C    -6.616649 -5.322126 -0.260183
H    -7.058334 -6.314722 -0.311527
C    -7.023038 -4.326482 -1.149562
H    -7.779847 -4.540834 -1.900855
C    -6.460976 -3.054358 -1.082561
H    -6.783165 -2.283198 -1.778256
H    -2.885465 -2.264386 -0.225640
O     9.909602 -0.433959 -0.577158
C    11.201809 -0.604402 -0.070439
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H    14.423020 -0.535529 -1.080033
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C    15.232015 -0.945672  1.476990
C    12.674168 -0.885961  1.801667
H    12.794193 -1.025710  2.871795
C    11.378424 -0.785588  1.291887
H    10.513562 -0.839561  1.947036
C    15.772724 -2.296572  0.969494
C    15.310244 -0.958894  3.015689
C    16.062233  0.243579  0.972163
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H    18.963399  1.065702 -0.636610
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O    18.220809  3.614679 -0.235688
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C    15.611075  1.550180  1.216861
H    14.661631  1.701456  1.727959
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H    15.808016 -2.340530 -0.125727
H    16.780708 -2.492011  1.356535
H    14.792558 -1.829897  3.437237
H    14.878921 -0.052549  3.457707
H    16.361053 -1.014082  3.324735
F     9.136211 -2.455773  0.004066
H     7.357111 -2.080879 -1.870674

123
P2'     el energy= -4074.93560593
C     4.672070  0.874505  0.110731
C     6.044328  1.140983  0.172201
C     6.940640  0.070372  0.284823
C     6.441863 -1.262784  0.257095
C     5.093104 -1.494462 -0.113874
C     4.176953 -0.411793 -0.045147
C     4.740498 -2.819362 -0.663046
C     5.612672 -3.913895 -0.479206
C     6.807670 -3.741034  0.351990
```

```
C     7.237752 -2.436570  0.683933
C     3.631718 -2.988930 -1.519407
C     3.359966 -4.202947 -2.124600
C     4.207911 -5.294081 -1.910658
C     5.324974 -5.139637 -1.109832
C     7.517861 -4.851274  0.848275
C     8.622361 -4.695924  1.665943
C     9.025328 -3.409416  2.034842
C     8.337404 -2.307383  1.558611
C     8.403770  0.365494  0.331793
C     8.958909  1.171808  1.331422
C    10.318510  1.461388  1.338790
C    11.166915  0.963678  0.340460
C    10.606882  0.162361 -0.663027
C     9.247892 -0.133197 -0.665780
C    12.617665  1.282489  0.344335
C    13.073866  2.555216  0.717219
C    14.429397  2.860600  0.721300
C    15.346821  1.885591  0.344754
C    14.931243  0.611640 -0.025186
C    13.568227  0.323215 -0.023812
C     2.696128 -0.575443 -0.033602
C     1.873627  0.209350 -0.849212
C     0.488748  0.075973 -0.804686
C    -0.119336 -0.842616  0.060098
C     0.707391 -1.616401  0.887546
C     2.089590 -1.483498  0.843889
C    -1.596394 -0.995843  0.098347
C    -2.268167 -1.229939  1.307540
C    -3.648913 -1.375734  1.346017
C    -4.381967 -1.293292  0.164400
C    -3.742897 -1.074393 -1.053821
C    -2.358144 -0.920921 -1.073252
O    -5.743933 -1.468071  0.285486
C    -6.555067 -0.910720 -0.665802
F    -6.637284 -1.721079 -1.775491
C    -7.962116 -0.808136 -0.062188
F    -7.912805 -0.017844  1.037468
O    16.680899  2.277884  0.364776
C    17.611225  1.384112  0.014728
C    18.244035  1.410446 -1.149165
F    17.926416  0.475503  0.941182
F    17.964276  2.268349 -2.103822
F    19.223865  0.596058 -1.471682
H     2.988807 -2.147751 -1.746500
H     2.500104 -4.294121 -2.783963
H     4.011093 -6.249267 -2.391683
H     6.004103 -5.979122 -0.997405
H     7.179924 -5.857061  0.617660
H     9.149075 -5.569992  2.041550
H     9.863000 -3.266913  2.713425
H     8.643052 -1.328510  1.903360
H     8.322210  1.565329  2.120308
H    10.729001  2.068848  2.142542
H    11.235899 -0.217483 -1.465387
H     8.833257 -0.752580 -1.458135
H    12.359011  3.328546  0.988595
H    14.782960  3.849529  1.000026
H    15.646928 -0.156415 -0.305470
H    13.247304 -0.679960 -0.294793
H     2.321810  0.923223 -1.537251
H    -0.126459  0.706658 -1.442949
H     0.265271 -2.346430  1.562199
H     2.709543 -2.100547  1.490330
H    -1.707942 -1.273856  2.238644
H    -4.170516 -1.541071  2.284820
H    -4.302343 -1.051113 -1.984109
H    -1.864256 -0.771313 -2.030611
C     6.475907  2.569125  0.129027
C     5.991841  3.476669  1.078161
H     5.327902  3.124353  1.865446
C     6.366107  4.819289  1.033625
H     5.987419  5.509444  1.784340
C     7.224306  5.273484  0.033505
H     7.517991  6.320128 -0.001899
C     7.702978  4.377798 -0.923574
H     8.367466  4.724421 -1.711938
C     7.331342  3.036817 -0.876647
H     7.709228  2.344238 -1.625028
H     3.972983  1.707436  0.147196
H    -6.210102  0.077769 -0.991316
O    -8.794045 -0.295902 -1.002022
C   -10.143176 -0.189402 -0.666332
C   -10.608944  0.967248 -0.055244
H    -9.919463  1.765334  0.202100
C   -11.968454  1.087090  0.208726
H   -12.331388  1.996249  0.678001
C   -12.863604  0.065323 -0.129813
C   -14.345802  0.245487  0.250998
C   -12.363320 -1.094375 -0.728924
H   -13.011557 -1.922193 -0.990202
C   -11.005315 -1.220862 -1.007293
H   -10.617651 -2.116103 -1.483905
C   -14.443505 -0.118759  1.757444
C   -15.284141 -0.708158 -0.537913
C   -14.835168  1.673092 -0.046215
C   -15.690767  2.384733  0.798076
H   -16.026623  1.970093  1.741727
C   -16.144151  3.655376  0.455703
H   -16.802829  4.193636  1.135239
C   -15.762677  4.233849 -0.755791
O   -16.170685  5.463377 -1.142437
C   -14.922961  3.526018 -1.620102
H   -14.630343  3.974774 -2.565510
C   -14.470596  2.264203 -1.264133
H   -13.815344  1.736319 -1.951224
H   -16.748203  5.843559 -0.467592
F   -13.824132 -1.272031  2.025013
F   -13.870191  0.821628  2.516105
F   -15.710219 -0.255378  2.181175
F   -15.145259 -1.996427 -0.182894
F   -15.046302 -0.631888 -1.852222
F   -16.569456 -0.397759 -0.350627
F    -8.383919 -2.018938  0.365636

133
P3'     el energy= -3710.63900589
C     3.219783 -1.587993 -0.133136
C     4.601108 -1.375396 -0.327969
C     5.133243 -0.087910 -0.205373
C     4.290676  0.993008  0.171329
C     2.994755  0.707610  0.664049
C     2.422641 -0.563866  0.387956
C     2.343289  1.722272  1.522153
C     2.829448  3.048313  1.537950
C     3.910089  3.426103  0.623391
C     4.661959  2.413762 -0.012640
C     1.348105  1.374130  2.459972
C     0.815437  2.301364  3.337984
C     1.278715  3.619973  3.326311
C     2.283093  3.976498  2.445086
C     4.195733  4.777676  0.349773
C     5.196681  5.139993 -0.532946
C     5.921380  4.142972 -1.191949
C     5.647790  2.810058 -0.941328
C     6.609389  0.088635 -0.363949
C     7.273833 -0.226545 -1.554488
C     8.651441 -0.079161 -1.661384
C     9.413907  0.378195 -0.577748
C     8.747247  0.686900  0.614524
C     7.366974  0.546464  0.718363
C    10.887112  0.528553 -0.692141
C    11.652548 -0.401674 -1.410266
C    13.030818 -0.265171 -1.522289
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C    13.659338  0.812025 -0.906842
C    12.931952  1.755808 -0.190794
C    11.550946  1.603033 -0.088826
C     0.953989 -0.809972  0.523084
C     0.438715 -1.814808  1.349534
C    -0.929829 -2.047186  1.419113
C    -1.829544 -1.287419  0.658616
C    -1.310913 -0.282409 -0.167166
C     0.058764 -0.047025 -0.232628
C    -3.291032 -1.546301  0.719672
C    -4.079598 -1.493085 -0.439282
C    -5.446298 -1.735549 -0.389931
C    -6.046293 -2.042713  0.829180
C    -5.287749 -2.116062  1.995184
C    -3.919636 -1.859173  1.929914
O    -7.401473 -2.290301  0.789414
C    -8.132676 -2.075674  1.926222
F    -8.055626 -3.162317  2.769764
C    -9.601399 -1.922935  1.509992
F   -10.020208 -3.024675  0.845610
F   -10.366940 -1.852731  2.628432
O    15.040632  0.867239 -1.059318
C    15.701310  1.885613 -0.499735
C    16.440259  1.761331  0.593109
F    15.631220  3.052920 -1.144684
F    16.534907  0.644776  1.278558
F    17.167600  2.730769  1.101628
H     1.004536  0.351156  2.531388
H     0.054508  1.990171  4.049718
H     0.877663  4.353894  4.021269
H     2.674669  4.988298  2.485393
H     3.600882  5.560426  0.810454
H     5.393456  6.190762 -0.731986
H     6.684653  4.405753 -1.920504
H     6.190818  2.065460 -1.507319
H     6.704018 -0.573137 -2.412900
H     9.138807 -0.305282 -2.607384
H     9.314977  1.020193  1.480713
H     6.870612  0.786747  1.656145
H    11.168488 -1.258399 -1.873288
H    13.625787 -0.990752 -2.070187
H    13.418788  2.606132  0.278819
H    10.981941  2.353981  0.454425
H     1.116268 -2.422373  1.944144
H    -1.301859 -2.847162  2.055726
H    -1.986186  0.335528 -0.755249
H     0.439028  0.742390 -0.877403
H    -3.616402 -1.272480 -1.398356
H    -6.057559 -1.693641 -1.287341
H    -5.743304 -2.381385  2.944451
H    -3.336982 -1.897964  2.847431
C     2.621554 -2.916569 -0.474939
C     2.899532 -4.051576  0.293137
H     3.559965 -3.967799  1.153516
C     2.338416 -5.283691 -0.035325
H     2.562230 -6.157089  0.573189
C     1.492976 -5.396522 -1.138883
H     1.054162 -6.358146 -1.395315
C     1.213085 -4.269874 -1.911567
H     0.555093 -4.348307 -2.774186
C     1.774327 -3.038064 -1.580838
H     1.549708 -2.159230 -2.181671
C     5.483204 -2.530911 -0.683203
C     5.404665 -3.135818 -1.941598
H     4.692157 -2.760083 -2.672768
C     6.230679 -4.210496 -2.263310
H     6.159952 -4.668632 -3.247339
C     7.143991 -4.696648 -1.327864
H     7.788536 -5.536160 -1.578498
C     7.225728 -4.101226 -0.069543
H     7.934255 -4.474238  0.666721
C     6.400121 -3.024952  0.249667
H     6.470375 -2.557996  1.229893
H    -7.804103 -1.191015  2.484077
O    -9.720432 -0.805849  0.757248
C   -10.985692 -0.524144  0.232298
C   -11.879054  0.244838  0.970445
H   -11.608020  0.587710  1.964853
C   -13.107037  0.570416  0.407524
H   -13.800958  1.183738  0.978661
C   -13.463303  0.139174 -0.878930
C   -14.853278  0.497376 -1.426591
C   -12.538775 -0.627725 -1.592349
H   -12.767638 -0.978080 -2.594285
C   -11.299625 -0.962446 -1.044062
H   -10.580839 -1.554416 -1.603640
C   -15.889781 -0.305316 -0.616509
C   -15.017834  0.109499 -2.908648
C   -15.063887  2.013801 -1.307678
C   -16.172856  2.587710 -0.685618
H   -16.934298  1.962086 -0.228016
C   -16.342739  3.973143 -0.627066
H   -17.218072  4.392471 -0.132445
C   -15.392388  4.817188 -1.198469
O   -15.496603  6.170542 -1.174766
C   -14.271928  4.263076 -1.826446
H   -13.529522  4.924066 -2.267027
C   -14.119319  2.884660 -1.873432
H   -13.234342  2.473294 -2.356360
H   -16.300697  6.424573 -0.704414
H   -15.668215 -1.376410 -0.698261
H   -15.876412 -0.040890  0.447697
H   -16.904967 -0.144112 -1.000548
H   -14.946625 -0.976487 -3.049990
H   -14.267110  0.591154 -3.546821
H   -16.007502  0.426953 -3.258685

133
P4'      el energy= -4305.91104013
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C     5.864712 -0.969170 -0.329321
C     6.732816  0.127023 -0.339551
C     6.209663  1.445616 -0.248775
C     4.848783  1.616619  0.102619
C     3.960047  0.517375 -0.049108
C     4.446363  2.910239  0.699056
C     5.293269  4.034505  0.581031
C     6.515915  3.930765 -0.219754
C     6.992798  2.654093 -0.590340
C     3.313231  3.024752  1.532445
C     2.995685  4.207187  2.176751
C     3.820243  5.325781  2.028243
C     4.959726  5.227387  1.251083
C     7.210074  5.080360 -0.644064
C     8.349174  4.990174 -1.422809
C     8.805235  3.731445 -1.824217
C     8.130894  2.592152 -1.422457
C     8.204216 -0.137634 -0.330008
C     8.840951 -0.830806 -1.365475
C    10.204376 -1.093845 -1.312529
C    10.976648 -0.680560 -0.218177
C    10.336316  0.010488  0.817989
C     8.972229  0.278708  0.761531
C    12.432020 -0.971913 -0.160384
C    12.939438 -2.195048 -0.622310
C    14.299895 -2.473560 -0.574092
C    15.170140 -1.521703 -0.053941
C    14.702968 -0.297918  0.411138
C    13.335896 -0.035246  0.354340
C     2.476639  0.703832 -0.070901
C     1.631701  0.052302  0.834547
C     0.254120  0.223661  0.772322
C    -0.326797  1.046544 -0.202532
C     0.520547  1.692277 -1.111402
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C    -3.845285  1.446718 -1.563360
C    -4.579837  1.552201 -0.384393
C    -3.944032  1.512743  0.854356
C    -2.561990  1.341084  0.899828
O    -5.940012  1.718531 -0.534551
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F    -6.837021  2.346189  1.441893
C    -8.160790  1.134362 -0.079633
F    -8.109921  0.141185 -0.999500
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F    17.712990 -0.033830 -0.534373
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H    14.692714 -3.424206 -0.924078
H    15.383029  0.450118  0.809787
H    12.975277  0.930553  0.700591
H     2.057356 -0.592893  1.598946
H    -0.380255 -0.306453  1.479518
H     0.099779  2.350574 -1.868652
H     2.540330  2.042204 -1.756367
H    -1.904484  1.184564 -2.425417
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H    -4.501986  1.641124  1.776972
H    -2.069619  1.327628  1.869487
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C     6.761407 -4.456813 -1.543864
H     6.647893 -5.058762 -2.442742
C     7.404334 -4.984006 -0.423953
H     7.793784 -5.999344 -0.444703
C     7.544618 -4.202724  0.722568
H     8.043797 -4.605718  1.600999
C     7.046030 -2.901660  0.747566
H     7.161507 -2.291984  1.641323
H    -6.416197  0.432772  1.001857
O    -9.000023  0.822258  0.938120
C   -10.335097  0.587802  0.611783
C   -10.751468 -0.711170  0.352354
H   -10.032832 -1.525147  0.355780
C   -12.097471 -0.949182  0.101778
H   -12.420267 -1.967979 -0.088826
C   -13.029113  0.096162  0.104166
C   -14.493637 -0.239529 -0.238486
C   -12.577761  1.396000  0.350078
H   -13.254544  2.241968  0.342548
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H   -10.887118  2.652448  0.821009
C   -14.552871 -0.352832 -1.786301
C   -15.480323  0.876129  0.201378
C   -14.956077 -1.524787  0.468692
C   -15.774911 -2.483072 -0.133375
H   -16.099360 -2.382711 -1.162923
C   -16.205162 -3.604132  0.570691
H   -16.833893 -4.342369  0.075982
C   -15.838574 -3.777457  1.906101
O   -16.226124 -4.843687  2.641280
C   -15.036484 -2.816814  2.528276
H   -14.755727 -2.949880  3.569550
C   -14.605742 -1.709039  1.813662
H   -13.978631 -0.978913  2.317532
H   -16.774282 -5.431082  2.104846
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F   -15.356154  2.002904 -0.519627
F   -15.289033  1.203689  1.484228
F   -16.751056  0.483674  0.079832
F    -8.574486  2.237796 -0.742641
C     3.546731 -1.922015 -0.497548
C     2.809109 -2.027738 -1.680763
H     2.906442 -1.256659 -2.442223
C     1.949839 -3.105395 -1.886246
H     1.382290 -3.173546 -2.811678
C     1.817489 -4.090917 -0.908620
H     1.145582 -4.931406 -1.067135
C     2.551210 -3.993307  0.273596
H     2.454018 -4.757476  1.041595
C     3.411971 -2.916757  0.475982
H     3.984934 -2.845069  1.397963

121
P1-E     el energy= -3379.18909547
C    -2.484063 -0.602261 -0.573948
C    -3.838481 -0.936139 -0.466451
C    -4.732995  0.009821  0.050801
C    -4.258768  1.310865  0.381461
C    -2.958074  1.702848 -0.025735
C    -2.025125  0.691472 -0.375794
C    -2.680178  3.145536 -0.175702
C    -3.544532  4.094526  0.411127
C    -4.644489  3.626966  1.259461
C    -5.021925  2.265846  1.218019
C    -1.664811  3.613677 -1.036672
C    -1.472918  4.964383 -1.266529
C    -2.312349  5.901982 -0.656824
C    -3.341284  5.464660  0.157530
C    -5.310651  4.504452  2.136435
C    -6.322749  4.063466  2.969333
C    -6.671488  2.709989  2.964322
C    -6.024117  1.832873  2.112079
C    -6.177723 -0.353811  0.151892
C    -6.606710 -1.445630  0.914439
C    -7.953232 -1.785048  0.976940
C    -8.914982 -1.050092  0.270616
C    -8.481393  0.036856 -0.499583
C    -7.134701  0.379870 -0.556723
C   -10.353110 -1.415616  0.336604
C   -10.755047 -2.759076  0.354015
C   -12.098776 -3.106658  0.420247
C   -13.059148 -2.101844  0.465989
C   -12.697145 -0.759746  0.452674
C   -11.345271 -0.429559  0.386306
C    -0.552475  0.905794 -0.448265
C     0.196246  0.436895 -1.533197
C     1.578455  0.597937 -1.568737
C     2.257910  1.228211 -0.518704
C     1.505566  1.686886  0.572305
C     0.126066  1.526544  0.608421
C     3.732599  1.403783 -0.558319
C     4.508023  1.266185  0.602323
C     5.887397  1.430405  0.570045
C     6.508311  1.732693 -0.637333
C     5.771039  1.878608 -1.806849
C     4.389034  1.711625 -1.755756
O     7.889587  1.866699 -0.585729
```

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C     8.540864  2.204534 -1.703524
F     8.483524  3.498933 -2.026752
C     9.242621  1.342685 -2.430826
F     9.976126  1.750701 -3.469101
O   -14.379669 -2.536223  0.516961
C   -15.343081 -1.622054  0.667936
C   -16.168360 -1.265424 -0.305548
F   -15.481096 -1.117359  1.896330
F   -16.071085 -1.713242 -1.536645
F   -17.180527 -0.442469 -0.144464
H    -1.034699  2.909212 -1.565014
H    -0.683996  5.287947 -1.941314
H    -2.179356  6.965202 -0.842211
H    -4.020028  6.199904  0.579256
H    -5.006492  5.545137  2.193019
H    -6.816601  4.760028  3.642642
H    -7.433085  2.333914  3.643329
H    -6.282130  0.783928  2.170502
H    -5.880142 -2.026947  1.477236
H    -8.262665 -2.622193  1.599076
H    -9.201948  0.609791 -1.079483
H    -6.819720  1.224867 -1.165147
H   -10.008679 -3.547985  0.295750
H   -12.411725 -4.147110  0.425591
H   -13.445428  0.026945  0.498646
H   -11.063024  0.620718  0.395749
H    -0.308730 -0.050280 -2.364778
H     2.136377  0.212412 -2.419469
H     2.003069  2.191387  1.397821
H    -0.435595  1.895388  1.463740
H     4.031230  1.007147  1.544811
H     6.489374  1.314554  1.467182
H     6.253190  2.124003 -2.749267
H     3.813793  1.847226 -2.668619
C    -4.250642 -2.304706 -0.896041
C    -3.646583 -3.429461 -0.322409
H    -2.901860 -3.296119  0.460114
C    -4.002674 -4.714201 -0.731232
H    -3.529699 -5.577400 -0.268180
C    -4.963257 -4.890639 -1.725791
H    -5.243008 -5.892145 -2.044792
C    -5.562622 -3.774674 -2.311282
H    -6.308174 -3.902320 -3.092991
C    -5.209135 -2.492274 -1.900044
H    -5.681583 -1.627307 -2.359579
H    -1.773456 -1.375350 -0.858374
O     9.227227  0.023382 -2.225747
C    10.361191 -0.575233 -1.683658
C    11.429173  0.149116 -1.162868
H    11.425330  1.236159 -1.162749
C    12.508189 -0.544669 -0.625066
H    13.335609  0.025482 -0.207388
C    12.551627 -1.944574 -0.597082
C    13.796280 -2.644826 -0.031084
C    11.458878 -2.636591 -1.125850
H    11.438636 -3.722409 -1.123252
C    10.366226 -1.962122 -1.669418
H     9.518173 -2.505652 -2.077404
C    14.956513 -2.398583 -1.014824
C    13.605171 -4.169015  0.090781
C    14.091290 -2.091124  1.370590
C    15.333109 -1.579235  1.747583
H    16.149706 -1.529353  1.032462
C    15.569625 -1.115133  3.043895
H    16.548894 -0.718193  3.308802
C    14.553465 -1.157987  3.996473
O    14.718439 -0.723192  5.272062
C    13.299563 -1.665154  3.639522
H    12.506649 -1.692089  4.383041
C    13.082497 -2.119379  2.346379
H    12.096120 -2.499000  2.084628
H    15.618148 -0.391468  5.385470
H    14.679269 -2.772686 -2.007936
H    15.194213 -1.332485 -1.113332
H    15.864666 -2.928078 -0.699853
H    13.460809 -4.635423 -0.892192
H    12.748823 -4.428004  0.725203
H    14.501402 -4.612471  0.541292

121
P2-E     el energy= -3974.46220067
C    -3.727329 -0.601312 -0.603505
C    -5.076571 -0.949930 -0.477783
C    -5.979309 -0.004148  0.025364
C    -5.519656  1.310453  0.321360
C    -4.227971  1.709694 -0.106473
C    -3.284068  0.702586 -0.439142
C    -3.971632  3.151806 -0.295240
C    -4.843968  4.103295  0.275442
C    -5.929248  3.642063  1.145854
C    -6.288062  2.275291  1.141650
C    -2.970944  3.611806 -1.177489
C    -2.800519  4.958714 -1.443720
C    -3.647639  5.899786 -0.850214
C    -4.662591  5.469172 -0.014975
C    -6.599274  4.531816  2.007380
C    -7.597194  4.097710  2.860764
C    -7.926989  2.739862  2.892550
C    -7.275570  1.850858  2.055843
C    -7.418471 -0.382996  0.147836
C    -7.827651 -1.463800  0.936646
C    -9.169905 -1.815498  1.020978
C   -10.146934 -1.104065  0.311592
C    -9.733081 -0.029000 -0.485667
C    -8.390745  0.326048 -0.565109
C   -11.580788 -1.480709  0.402365
C   -11.971036 -2.826861  0.449262
C   -13.310976 -3.184179  0.537463
C   -14.279193 -2.186606  0.576011
C   -13.928692 -0.842044  0.534675
C   -12.580537 -0.502059  0.446281
C    -1.815241  0.936184 -0.526528
C    -1.065335  0.450102 -1.603030
C     0.313589  0.634394 -1.652810
C     0.988457  1.306007 -0.625733
C     0.235291  1.780769  0.457843
C    -1.140712  1.596909  0.508292
C     2.458860  1.511655 -0.680997
C     3.243897  1.425690  0.478128
C     4.617912  1.627679  0.433472
C     5.223280  1.914540 -0.785223
C     4.477462  2.003980 -1.954817
C     3.100728  1.801682 -1.890783
O     6.601483  2.088957 -0.745528
C     7.223782  2.509338 -1.850628
F     7.046256  3.796763 -2.151837
C     8.019734  1.734951 -2.579075
F     8.726921  2.227882 -3.596912
O   -15.595354 -2.630763  0.649644
C   -16.564947 -1.721473  0.790004
C   -17.400921 -1.391202 -0.183646
F   -16.696931 -1.192816  2.008964
F   -17.310174 -1.863314 -1.406126
F   -18.418053 -0.572809 -0.030922
H    -2.335714  2.902932 -1.693672
H    -2.022613  5.275893 -2.134128
H    -3.531650  6.959668 -1.064011
H    -5.347758  6.205487  0.394290
H    -6.309178  5.577684  2.035387
H    -8.094380  4.803893  3.521496
H    -8.676815  2.370269  3.588007
H    -7.518322  0.800253  2.142661
H    -7.089026 -2.026325  1.502809
H    -9.463960 -2.643265  1.662847
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H   -10.465978  0.524792 -1.068679
H    -8.091300  1.161703 -1.193920
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H   -13.615187 -4.226874  0.565292
H   -14.682987 -0.060797  0.575485
H   -12.307075  0.550507  0.433409
H    -1.567062 -0.067891 -2.417767
H     0.872378  0.235666 -2.496869
H     0.728912  2.317131  1.265382
H    -1.703106  1.979407  1.357069
H     2.779089  1.180458  1.430209
H     5.226994  1.555986  1.330405
H     4.948157  2.232224 -2.907372
H     2.517600  1.894999 -2.803882
C    -5.474997 -2.332245 -0.874800
C    -4.852893 -3.437589 -0.283157
H    -4.103777 -3.279449  0.490492
C    -5.196513 -4.734629 -0.662771
H    -4.709480 -5.582401 -0.185980
C    -6.162607 -4.943048 -1.645752
H    -6.432528 -5.954177 -1.941986
C    -6.780176 -3.846619 -2.248935
H    -7.530287 -3.999125 -3.021765
C    -6.439100 -2.551922 -1.866844
H    -6.925778 -1.702205 -2.339819
H    -3.008871 -1.371678 -0.875431
O     8.142270  0.415737 -2.388387
C     9.267005 -0.056482 -1.730963
C    10.226565  0.775062 -1.165378
H    10.145956  1.856679 -1.227063
C    11.302814  0.200393 -0.498056
H    12.040631  0.858458 -0.049383
C    11.440957 -1.186964 -0.389638
C    12.689865 -1.739136  0.322226
C    10.473707 -1.997567 -0.992628
H    10.541893 -3.078626 -0.962452
C     9.385789 -1.438152 -1.653110
H     8.628374 -2.069097 -2.109310
C    13.843713 -1.657995 -0.713232
C    12.525136 -3.223296  0.746815
C    12.993542 -0.955230  1.610792
C    14.285334 -0.621663  2.024576
H    15.152996 -0.873810  1.425522
C    14.504311  0.048550  3.224956
H    15.519905  0.307186  3.520446
C    13.428049  0.381757  4.048715
O    13.577336  1.032308  5.224399
C    12.131502  0.035804  3.658350
H    11.294674  0.290888  4.302892
C    11.925203 -0.623404  2.455816
H    10.908079 -0.876638  2.170813
H    14.513702  1.209763  5.383471
F    13.480146 -2.166326 -1.894453
F    14.208041 -0.388548 -0.925857
F    14.942540 -2.328051 -0.329274
F    12.493748 -4.069370 -0.296620
F    11.390933 -3.400115  1.433973
F    13.528490 -3.624029  1.532269

131
P3-E     el energy= -3610.16437164
C    -3.037685  1.258147 -0.231481
C    -4.448353  1.289248 -0.218521
C    -5.173799  0.113684 -0.435645
C    -4.487968 -1.119168 -0.611452
C    -3.106560 -1.180633 -0.308070
C    -2.366364  0.031504 -0.244937
C    -2.528885 -2.504194  0.016938
C    -3.232340 -3.682221 -0.319372
C    -4.483190 -3.579867 -1.075981
C    -5.125023 -2.326423 -1.182972
C    -1.364989 -2.634770  0.804411
C    -0.882149 -3.870544  1.196567
C    -1.564092 -5.034125  0.830261
C    -2.730683 -4.931189  0.095100
C    -5.044262 -4.702206 -1.715843
C    -6.208857 -4.605450 -2.455090
C    -6.827500 -3.360213 -2.597455
C    -6.286159 -2.246229 -1.981146
C    -6.665706  0.175601 -0.358404
C    -7.424735  0.971719 -1.223594
C    -8.808374  1.029665 -1.107914
C    -9.480028  0.300610 -0.116873
C    -8.717584 -0.490852  0.751184
C    -7.332957 -0.552795  0.631059
C   -10.958375  0.367677  0.010168
C   -11.644510  1.575625 -0.181491
C   -13.027334  1.643453 -0.063128
C   -13.739810  0.492154  0.254685
C   -13.093391 -0.723599  0.446430
C   -11.706436 -0.772904  0.324129
C    -0.872532  0.044585 -0.307110
C    -0.091693  0.613761  0.705105
C     1.294290  0.638056  0.606332
C     1.946583  0.100541 -0.511941
C     1.162353 -0.463235 -1.525973
C    -0.225039 -0.491116 -1.424400
C     3.427845  0.128768 -0.618199
C     4.058653  0.389378 -1.843252
C     5.443993  0.416963 -1.947115
C     6.216240  0.177697 -0.815192
C     5.624509 -0.080838  0.416120
C     4.234300 -0.104193  0.501802
O     7.591551  0.206035 -1.009054
C     8.387950  0.085636  0.058957
F     8.484140  1.175135  0.823304
C     9.083774 -1.009261  0.344710
F     8.986639 -2.095540 -0.424191
O   -15.116946  0.651855  0.367595
C   -15.862090 -0.425670  0.632890
C   -16.405785 -0.661552  1.818029
F   -16.091583 -1.244669 -0.396502
F   -16.202155  0.097556  2.870564
F   -17.215187 -1.666542  2.067634
H    -0.841260 -1.753396  1.148138
H     0.014917 -3.925821  1.808678
H    -1.201324 -6.010418  1.142791
H    -3.280366 -5.838533 -0.134941
H    -4.543126 -5.663648 -1.661853
H    -6.618318 -5.486212 -2.944020
H    -7.720168 -3.254175 -3.209316
H    -6.760495 -1.289716 -2.153581
H    -6.928847  1.537609 -2.008135
H    -9.375616  1.636085 -1.810923
H    -9.208730 -1.048698  1.545712
H    -6.760147 -1.169589  1.320210
H   -11.089630  2.483466 -0.406809
H   -13.558858  2.580909 -0.201734
H   -13.648624 -1.627498  0.682331
H   -11.204456 -1.728560  0.456222
H    -0.573904  1.039837  1.581278
H     1.876421  1.100308  1.400749
H     1.641583 -0.903395 -2.397934
H    -0.814108 -0.941742 -2.220291
H     3.459538  0.594451 -2.727459
H     5.933712  0.625991 -2.894327
H     6.225349 -0.275505  1.300482
H     3.774244 -0.327514  1.461630
C    -2.270878  2.543325 -0.217791
C    -2.235659  3.350907  0.923268
H    -2.772049  3.039319  1.816929
C    -1.521705  4.547192  0.922261
H    -1.501728  5.163452  1.818383
C    -0.835263  4.952382 -0.222301
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H    -0.277428  5.886083 -0.223424
C    -0.867574  4.153775 -1.365015
H    -0.335397  4.461775 -2.262314
C    -1.580740  2.956681 -1.361571
H    -1.599975  2.332671 -2.252702
C    -5.155316  2.587665  0.013644
C    -5.146638  3.595665 -0.955540
H    -4.619704  3.432598 -1.893177
C    -5.806666  4.801411 -0.728829
H    -5.793193  5.575105 -1.493365
C    -6.481522  5.015495  0.472943
H    -6.996553  5.956926  0.650544
C    -6.492281  4.016313  1.445647
H    -7.015255  4.174634  2.386221
C    -5.832691  2.810360  1.216563
H    -5.847284  2.029890  1.974571
O     9.875121 -1.135846  1.413462
C    11.251978 -1.178118  1.208382
C    11.850228 -0.831192  0.000670
H    11.253811 -0.517619 -0.852462
C    13.236630 -0.880191 -0.096717
H    13.700992 -0.594541 -1.038477
C    14.043474 -1.271957  0.979553
C    15.565964 -1.341620  0.786630
C    13.406514 -1.611000  2.176094
H    13.985489 -1.916389  3.042745
C    12.017791 -1.568211  2.296819
H    11.527624 -1.831265  3.230455
C    15.861479 -2.504059 -0.180860
C    16.309632 -1.633118  2.104213
C    16.064865  0.007820  0.248843
C    16.842724  0.135274 -0.902238
H    17.107849 -0.740311 -1.488420
C    17.302979  1.379654 -1.340269
H    17.906196  1.447658 -2.244950
C    16.988768  2.531625 -0.621770
O    17.404721  3.770012 -0.991245
C    16.207275  2.427403  0.533803
H    15.957945  3.328555  1.088745
C    15.756822  1.183322  0.951780
H    15.138789  1.125430  1.846335
H    17.922245  3.707851 -1.804095
H    15.449235 -3.434382  0.228556
H    15.410856 -2.344198 -1.167849
H    16.941498 -2.647001 -0.313314
H    16.041562 -2.618632  2.506135
H    16.101119 -0.878654  2.872374
H    17.390633 -1.631292  1.919118

131
P4-E     el energy= -4205.43749347
C     4.362173 -1.209312 -0.280094
C     5.771305 -1.230338 -0.207245
C     6.499221 -0.057500 -0.431836
C     5.815574  1.165453 -0.671464
C     4.422328  1.226073 -0.428942
C     3.685796  0.011794 -0.363577
C     3.824436  2.553829 -0.164035
C     4.534484  3.726683 -0.503298
C     5.815025  3.611800 -1.206131
C     6.468911  2.360755 -1.250198
C     2.629294  2.697470  0.572587
C     2.124722  3.940206  0.911871
C     2.815023  5.097997  0.542456
C     4.010635  4.983069 -0.142634
C     6.393158  4.719529 -1.855871
C     7.587685  4.610935 -2.544010
C     8.220809  3.367359 -2.623315
C     7.662609  2.267173 -1.997107
C     7.987156 -0.110090 -0.295820
C     8.780648 -0.923641 -1.112337
C    10.158868 -0.974342 -0.942176
C    10.790169 -0.220667  0.057046
C     9.992982  0.588358  0.876314
C     8.613885  0.643644  0.701080
C    12.262824 -0.279889  0.241712
C    12.959417 -1.488791  0.099792
C    14.337314 -1.548576  0.268708
C    15.034036 -0.388193  0.588268
C    14.376913  0.828165  0.734111
C    12.995161  0.869549  0.560666
C     2.197229 -0.007660 -0.502322
C     1.362549 -0.558576  0.476489
C    -0.016225 -0.584503  0.303718
C    -0.607738 -0.065635 -0.856374
C     0.230424  0.480243 -1.836557
C     1.610315  0.508050 -1.661900
C    -2.081359 -0.094290 -1.040790
C    -2.646041 -0.355711 -2.297572
C    -4.023800 -0.379309 -2.476378
C    -4.854823 -0.144304 -1.386318
C    -4.330173  0.118210 -0.125922
C    -2.946511  0.140151  0.034372
O    -6.219102 -0.204923 -1.646625
C    -7.068971  0.150668 -0.678569
F    -7.166835  1.462297 -0.458429
C    -7.819254 -0.708841  0.001228
O    16.407018 -0.539413  0.751742
C    17.140256  0.549895  1.001602
C    17.655491  0.823613  2.191341
F    17.388612  1.339351 -0.046251
F    17.431944  0.094171  3.260704
F    18.454761  1.839466  2.429552
H     2.096825  1.821826  0.917914
H     1.203553  4.006286  1.485905
H     2.434983  6.079868  0.814386
H     4.565355  5.886901 -0.374677
H     5.881812  5.677252 -1.850932
H     8.010406  5.480191 -3.042156
H     9.138855  3.250846 -3.194350
H     8.150327  1.310030 -2.121792
H     8.316479 -1.509617 -1.901557
H    10.754298 -1.595048 -1.608380
H    10.451743  1.165797  1.676175
H     8.013452  1.274320  1.353144
H    12.416171 -2.403253 -0.126968
H    14.876735 -2.486278  0.167481
H    14.920583  1.738350  0.972822
H    12.485546  1.825535  0.655885
H     1.796144 -0.968810  1.384951
H    -0.640098 -1.033544  1.073581
H    -0.200195  0.906548 -2.740161
H     2.241453  0.944380 -2.433113
H    -2.001243 -0.563046 -3.148383
H    -4.461831 -0.589382 -3.448337
H    -4.977538  0.309154  0.725842
H    -2.538992  0.366048  1.017045
C     6.477073 -2.515445  0.093459
C     6.512661 -3.554088 -0.842285
H     6.019413 -3.426411 -1.803424
C     7.174960 -4.745149 -0.552990
H     7.196739 -5.542907 -1.292179
C     7.808022 -4.913662  0.678446
H     8.325315 -5.843393  0.904503
C     7.773799 -3.884102  1.618369
H     8.263693 -4.006872  2.581777
C     7.112176 -2.692905  1.326717
H     7.092157 -1.888537  2.059154
O    -8.677189 -0.350982  0.965147
C   -10.033831 -0.379239  0.683994
C   -10.878629 -0.118955  1.757492
H   -10.457551  0.074295  2.739958
C   -12.250828 -0.102601  1.552243
H   -12.900622  0.111252  2.395366
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C   -12.798617 -0.346265  0.285948
C   -14.331978 -0.373506  0.148024
C   -11.927566 -0.629406 -0.767612
H   -12.295901 -0.854121 -1.761627
C   -10.546875 -0.638699 -0.579977
H    -9.894687 -0.850707 -1.422468
C   -14.778789 -1.779071  0.632520
C   -14.801137 -0.197187 -1.321897
C   -14.989705  0.764684  0.947308
C   -16.170114  0.612217  1.678436
H   -16.671124 -0.346397  1.749705
C   -16.748002  1.690375  2.342840
H   -17.662975  1.543063  2.914053
C   -16.162140  2.954951  2.270756
O   -16.676859  4.039260  2.892976
C   -14.991854  3.127637  1.526512
H   -14.538386  4.113343  1.466917
C   -14.419963  2.043790  0.877154
H   -13.506497  2.201659  0.310960
H   -17.475620  3.791566  3.376734
F   -14.051049 -2.748207  0.069634
F   -14.633516 -1.896531  1.957083
F   -16.062983 -2.049019  0.346614
F   -14.512724 -1.255577 -2.098077
F   -14.225626  0.872555 -1.882258
F   -16.122828 -0.019405 -1.397403
F    -7.723712 -2.020794 -0.214249
C     3.603153 -2.498792 -0.251560
C     2.962510 -2.960099 -1.405760
H     3.013278 -2.369506 -2.318154
C     2.257524 -4.161995 -1.392491
H     1.764072 -4.507744 -2.298125
C     2.184239 -4.917439 -0.222659
H     1.632820 -5.854873 -0.210990
C     2.821294 -4.464354  0.932439
H     2.769245 -5.046895  1.849564
C     3.527261 -3.263429  0.916827
H     4.025028 -2.914103  1.818840

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P1-Z     el energy= -3379.18886409
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C     4.490805 -1.389680 -0.185300
C     5.280665 -0.252166 -0.395807
C     4.651552  1.015712 -0.549261
C     3.269995  1.147331 -0.258187
C     2.470357 -0.025572 -0.225937
C     2.760715  2.483676  0.110482
C     3.526454  3.634185 -0.176386
C     4.772259  3.489990 -0.935309
C     5.346695  2.207777 -1.087309
C     1.600083  2.636510  0.898598
C     1.178117  3.878754  1.337536
C     1.921280  5.019876  1.019837
C     3.086361  4.889414  0.285895
C     5.391585  4.601974 -1.538030
C     6.546087  4.467985 -2.287540
C     7.094156  3.196543 -2.478752
C     6.496785  2.092470 -1.896803
C     6.766354 -0.397597 -0.353420
C     7.446529 -1.248979 -1.230929
C     8.826743 -1.395684 -1.153756
C     9.571909 -0.704748 -0.188543
C     8.887029  0.141573  0.693223
C     7.507138  0.294098  0.610392
C    11.045600 -0.868755 -0.099858
C    11.645576 -2.120086 -0.302695
C    13.023505 -2.278862 -0.219059
C    13.818488 -1.176192  0.074816
C    13.258710  0.080237  0.276518
C    11.875374  0.220751  0.189292
C     0.982505 -0.021028 -0.306987
C     0.207212 -0.780772  0.575797
C    -1.180474 -0.801617  0.469556
C    -1.838016 -0.068202 -0.525766
C    -1.057142  0.679848 -1.418734
C     0.328044  0.701441 -1.312979
C    -3.319680 -0.081743 -0.631771
C    -3.954456 -0.093760 -1.882261
C    -5.340035 -0.106184 -1.985566
C    -6.108963 -0.102760 -0.826500
C    -5.513408 -0.093727  0.429880
C    -4.123061 -0.081554  0.514709
O    -7.484963 -0.095947 -1.017500
C    -8.276209 -0.235593  0.051867
F    -8.341986 -1.470081  0.553585
C    -8.995761  0.750225  0.576076
F    -8.927705  1.984027  0.071824
O    15.184614 -1.425856  0.150920
C    16.002283 -0.408133  0.438336
C    16.570463 -0.242983  1.623908
F    16.276298  0.424184 -0.569465
F    16.327222 -1.018240  2.655978
F    17.444585  0.700399  1.894357
H     1.034671  1.765411  1.205132
H     0.282120  3.956864  1.948680
H     1.605795  5.999780  1.370152
H     3.681866  5.776754  0.094396
H     4.943350  5.586625 -1.446291
H     7.001047  5.341759 -2.747933
H     7.975587  3.063598 -3.101568
H     6.916398  1.117590 -2.106212
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H     9.333100 -2.043934 -1.865832
H     9.435268  0.671014  1.469639
H     6.995215  0.952020  1.309303
H    11.026585 -2.990268 -0.508704
H    13.488351 -3.250053 -0.365291
H    13.877243  0.947069  0.492428
H    11.442047  1.208465  0.328569
H     0.693513 -1.352049  1.363834
H    -1.757562 -1.409886  1.162735
H    -1.539618  1.268332 -2.196301
H     0.911359  1.295528 -2.012871
H    -3.358820 -0.114083 -2.791916
H    -5.832031 -0.122994 -2.954191
H    -6.111927 -0.082904  1.336946
H    -3.661173 -0.052506  1.498959
C     5.059975 -2.749403  0.048471
C     4.710738 -3.810106 -0.795120
H     4.050638 -3.626018 -1.640726
C     5.213735 -5.091375 -0.571705
H     4.939006 -5.902714 -1.242155
C     6.067492 -5.329985  0.503997
H     6.461517 -6.328603  0.678584
C     6.412649 -4.280458  1.356547
H     7.072938 -4.458580  2.202389
C     5.912333 -3.000867  1.131125
H     6.186159 -2.187264  1.798689
H     2.486992 -2.162182 -0.165063
O    -9.786547  0.611935  1.643883
C   -11.165135  0.629384  1.450538
C   -11.758499  0.629589  0.191535
H   -11.158786  0.625288 -0.714991
C   -13.146960  0.623612  0.106812
H   -13.606407  0.610203 -0.879528
C   -13.960824  0.622734  1.246874
C   -15.487313  0.659116  1.079501
C   -13.328563  0.624609  2.493038
H   -13.913004  0.621177  3.408433
C   -11.938554  0.629168  2.602143
H   -11.452688  0.626658  3.574238
C   -15.863360  2.055716  0.547663
C   -16.226606  0.454059  2.415881
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C   -15.917078 -0.464971  0.125499
C   -16.721977 -0.254334 -0.994372
H   -17.058086  0.746187 -1.252410
C   -17.119565 -1.310159 -1.818387
H   -17.746068 -1.113744 -2.687667
C   -16.712609 -2.611459 -1.530222
O   -17.061911 -3.680688 -2.290630
C   -15.903905 -2.845451 -0.412979
H   -15.583771 -3.861014 -0.193092
C   -15.517681 -1.783941  0.393199
H   -14.878506 -1.985417  1.251346
H   -17.615052 -3.387711 -3.025896
H   -15.493550  2.822085  1.239755
H   -15.423212  2.253277 -0.437272
H   -16.951683  2.173196  0.470248
H   -16.017589  1.269555  3.119923
H   -15.955700 -0.494554  2.895170
H   -17.308092  0.440240  2.234175

121
P2-Z     el energy= -3974.46401531
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C     4.486759  1.370230  0.240236
C     3.558450  0.608613  1.005629
C     2.168281  0.799934  0.802963
C     1.734633  1.997548  0.175258
C     1.253922 -0.305144  1.155396
C     1.696250 -1.341322  2.005294
C     3.031871 -1.251161  2.602428
C     3.962995 -0.322627  2.084392
C    -0.005677 -0.446446  0.534264
C    -0.823970 -1.531998  0.790474
C    -0.397779 -2.535740  1.665862
C     0.853554 -2.443463  2.247846
C     3.393529 -2.055946  3.699879
C     4.639167 -1.954168  4.291887
C     5.549698 -1.009280  3.810680
C     5.209111 -0.206336  2.736450
C     5.928742  0.993580  0.147587
C     6.946916  1.893928  0.479511
C     8.283863  1.532227  0.359334
C     8.647410  0.261505 -0.106765
C     7.625661 -0.634741 -0.446615
C     6.288359 -0.274623 -0.320029
C    10.075797 -0.123667 -0.240063
C    11.030902  0.794284 -0.700394
C    12.367734  0.437344 -0.828895
C    12.761231 -0.854636 -0.497167
C    11.842975 -1.788819 -0.031634
C    10.506751 -1.413885  0.089896
C     0.332595  2.496803  0.232928
C    -0.331167  2.932261 -0.919076
C    -1.641970  3.396385 -0.853699
C    -2.327066  3.445687  0.366433
C    -1.647547  3.040008  1.523873
C    -0.339859  2.576652  1.459021
C    -3.745450  3.882485  0.434908
C    -4.218079  4.641050  1.514307
C    -5.561011  4.997729  1.609761
C    -6.432635  4.597704  0.607868
C    -5.992461  3.873753 -0.493828
C    -4.651130  3.515040 -0.570670
O    -7.786040  4.950414  0.711935
C    -8.603308  3.907967  0.893996
F    -8.593840  3.395661  2.125961
C    -9.394094  3.387926 -0.036933
F    -9.391333  3.860236 -1.286013
O    14.113129 -1.132738 -0.668917
C    14.559177 -2.346951 -0.331827
C    14.876106 -3.278650 -1.219133
F    14.734091 -2.562661  0.974239
F    14.710142 -3.129428 -2.513647
F    15.400987 -4.442317 -0.906767
H    -0.339363  0.288183 -0.187947
H    -1.786986 -1.616497  0.293445
H    -1.035163 -3.393507  1.865009
H     1.195815 -3.257580  2.879777
H     2.673396 -2.751858  4.119283
H     4.891271 -2.582753  5.142643
H     6.517817 -0.882174  4.289325
H     5.916569  0.549444  2.422659
H     6.689912  2.883592  0.849731
H     9.055232  2.242191  0.649889
H     7.877463 -1.618947 -0.836011
H     5.511188 -0.984461 -0.594861
H    10.724542  1.798577 -0.983795
H    13.106421  1.144641 -1.195948
H    12.149742 -2.794752  0.241734
H     9.793291 -2.140654  0.471441
H     0.174663  2.885912 -1.881229
H    -2.134816  3.728916 -1.764856
H    -2.157367  3.059994  2.484577
H     0.161004  2.251875  2.368128
H    -3.530702  4.961126  2.293645
H    -5.932550  5.573656  2.452662
H    -6.692642  3.589189 -1.274723
H    -4.311496  2.919591 -1.414778
C     4.911761  3.270829 -1.400109
C     5.005786  4.653303 -1.203574
H     4.455129  5.116537 -0.386953
C     5.810341  5.435990 -2.031042
H     5.879120  6.507758 -1.858191
C     6.525989  4.846465 -3.071847
H     7.154776  5.455584 -3.717267
C     6.429154  3.470365 -3.282352
H     6.978251  3.002257 -4.096326
C     5.628443  2.689026 -2.453505
H     5.559310  1.616883 -2.622014
H     2.338788  3.709802 -0.952766
O   -10.267495  2.396249  0.190186
C    -9.851496  1.099735 -0.068013
C    -8.623587  0.793735 -0.643717
H    -7.918421  1.571188 -0.922111
C    -8.290442 -0.540364 -0.850160
H    -7.326843 -0.766928 -1.296007
C    -9.159780 -1.575028 -0.493312
C    -8.745389 -3.022591 -0.816500
C   -10.399653 -1.235747  0.059267
H   -11.123978 -1.994770  0.330755
C   -10.743754  0.093054  0.279646
H   -11.701352  0.352867  0.721708
C    -9.130931 -3.252776 -2.302432
C    -9.505787 -4.065606  0.047406
C    -7.247137 -3.256200 -0.552050
C    -6.419728 -3.994464 -1.401405
H    -6.793558 -4.422645 -2.324196
C    -5.079598 -4.208979 -1.091287
H    -4.452868 -4.780199 -1.773794
C    -4.545057 -3.701474  0.092542
O    -3.250448 -3.881321  0.446990
C    -5.363264 -2.977522  0.963079
H    -4.945174 -2.584650  1.885927
C    -6.694744 -2.762667  0.638737
H    -7.309656 -2.189824  1.326991
H    -2.780456 -4.360252 -0.248260
F   -10.384202 -2.862341 -2.552845
F    -8.331703 -2.554413 -3.116674
F    -9.050072 -4.541523 -2.671586
F   -10.807395 -4.166655 -0.271067
F    -9.439901 -3.749661  1.345433
F    -8.985655 -5.288378 -0.089485

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C    -2.764987  0.548650 -0.265611
C    -1.956445 -0.602840 -0.462057
C    -0.606125 -0.566396 -0.041633
C     0.014925  0.694120  0.159001
C     0.050535 -1.851682  0.276657
C    -0.516430 -3.062144 -0.178686
C    -1.677567 -3.014269 -1.070547
C    -2.420736 -1.817334 -1.169275
C     1.118274 -1.923632  1.194344
C     1.621931 -3.137576  1.627780
C     1.076536 -4.332181  1.150577
C     0.017297 -4.287670  0.261566
C    -2.054190 -4.131288 -1.839640
C    -3.139037 -4.084047 -2.696521
C    -3.860014 -2.893184 -2.822666
C    -3.497504 -1.782891 -2.080005
C    -4.256302  0.477679 -0.336912
C    -4.995677  1.272141 -1.220144
C    -6.383434  1.203439 -1.248256
C    -7.080185  0.344625 -0.387024
C    -6.337902 -0.444890  0.500275
C    -4.948376 -0.380200  0.523349
C    -8.563729  0.275643 -0.414640
C    -9.336251  1.432197 -0.594885
C   -10.724251  1.372619 -0.623351
C   -11.355148  0.143299 -0.465829
C   -10.621357 -1.024006 -0.288909
C    -9.230666 -0.945536 -0.263175
C     1.502761  0.859977  0.140438
C     2.217939  1.426010  1.201884
C     3.571978  1.716502  1.073600
C     4.250424  1.459686 -0.125004
C     3.541566  0.864618 -1.174920
C     2.189609  0.562070 -1.040688
C     5.687331  1.796016 -0.287254
C     6.135468  2.445340 -1.444426
C     7.484175  2.731972 -1.628479
C     8.390275  2.361607 -0.644586
C     7.975803  1.741364  0.528356
C     6.623610  1.459633  0.698107
O     9.731312  2.658837 -0.873091
C    10.630391  1.688588 -0.659603
F    11.635557  2.078266  0.119279
C    10.616961  0.474838 -1.204570
F    11.582803 -0.411388 -0.924218
O   -12.745457  0.174323 -0.494092
C   -13.408457 -0.981348 -0.385493
C   -14.044319 -1.355087  0.715340
F   -13.453428 -1.734347 -1.487319
F   -14.020533 -0.664544  1.832554
F   -14.775686 -2.443032  0.808114
H     1.539446 -1.017799  1.611871
H     2.428647 -3.154070  2.354713
H     1.462239 -5.289432  1.493534
H    -0.433797 -5.221129 -0.062039
H    -1.465152 -5.042339 -1.790862
H    -3.406542 -4.957816 -3.285989
H    -4.691776 -2.823581 -3.519722
H    -4.043429 -0.862642 -2.239655
H    -4.478346  1.938547 -1.905772
H    -6.931316  1.812970 -1.963750
H    -6.851433 -1.102838  1.198221
H    -4.392419 -0.998460  1.224900
H    -8.848131  2.398919 -0.694688
H   -11.323847  2.269427 -0.753311
H   -11.111316 -1.987461 -0.177706
H    -8.658594 -1.862808 -0.144315
H     1.704421  1.662586  2.130571
H     4.102135  2.178602  1.903862
H     4.055143  0.630427 -2.105104
H     1.653132  0.113009 -1.873812
H     5.420629  2.731975 -2.212324
H     7.840606  3.220915 -2.530767
H     8.700022  1.459643  1.288646
H     6.298519  0.944822  1.599266
C    -0.128049  3.192712  0.397020
C    -0.224591  3.871468  1.615303
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H     1.565591  6.665308  0.862839
C     1.186356  5.027331 -0.488520
H     1.735813  5.473858 -1.314324
C     0.579529  3.784227 -0.654340
H     0.661790  3.261322 -1.604849
C    -3.015318  2.964419  0.384987
C    -3.031969  4.051163 -0.494959
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C    -3.820643  5.167753 -0.226498
H    -3.824967  6.004318 -0.921772
C    -4.601200  5.212771  0.928590
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H    -5.193166  4.160512  2.716125
C    -3.799863  3.017600  1.541437
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C     8.791661 -1.537550 -0.448581
H     9.706546 -1.530515  0.136295
C     7.714391 -2.319603 -0.047815
H     7.810077 -2.906239  0.863649
C     6.518178 -2.365726 -0.775221
C     5.384459 -3.284660 -0.293710
C     6.434542 -1.588469 -1.932882
H     5.527029 -1.583470 -2.529433
C     7.499473 -0.789537 -2.349313
H     7.422318 -0.172516 -3.240195
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C    10.336316  0.010488  0.817989
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C    15.170140 -1.521703 -0.053941
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C    13.335896 -0.035246  0.354340
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C     0.520547  1.692277 -1.111402
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C    -8.160790  1.134362 -0.079633
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H    12.260070 -2.951396 -1.008502
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H     2.057356 -0.592893  1.598946
H    -0.380255 -0.306453  1.479518
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H     2.454018 -4.757476  1.041595
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246
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C    14.506134 -0.821784  1.232060
C    15.226789 -0.591987  0.030660
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C    14.196031 -0.533214  3.696794
C    13.428486 -1.781772  3.704675
C    13.003442 -2.341943  2.478927
C    15.457144  1.143394  2.488725
C    15.612531  1.886245  3.645517
C    15.065071  1.427739  4.847810
C    14.355005  0.240801  4.862256
C    13.133462 -2.447222  4.910058
C    12.442428 -3.645119  4.923780
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C	8.888801	-3.851838	-0.326221
C	9.080111	-2.647182	0.363105
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C	7.542355	-4.471093	-0.424517
C	7.129939	-5.119204	-1.598382
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C    -5.732454 -4.876449 -1.225573
H    -4.906196 -4.775864 -1.926631
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246
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266
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C	3.727857	8.401203	-1.463248
H	3.988598	8.890682	-2.394195
C	2.386498	8.073685	-1.271925
H	1.673992	8.300264	-2.055984
C	2.002167	7.468235	-0.080609
O	0.711287	7.080580	0.233753
C	2.942874	7.185325	0.905358
H	2.621991	6.716637	1.831118
C	4.276146	7.501447	0.692305
H	4.997414	7.265693	1.468846
H	-1.598392	5.906283	0.316435
F	7.914321	8.877221	-2.237626
F	6.218522	7.732458	-2.903078
F	6.045756	9.865339	-2.622526
F	7.548923	10.394560	-0.072787
F	6.275466	9.586589	1.470771
F	5.424768	10.703507	-0.159832
F	9.662502	2.973132	-0.752722
H	10.726500	1.163232	0.795956
C	-14.004167	1.304973	-2.417239
C	-13.474848	0.398202	-3.340949
H	-12.531755	-0.098681	-3.123744
C	-14.145447	0.127855	-4.531720
H	-13.722788	-0.582113	-5.239185
C	-15.353700	0.764445	-4.815253
H	-15.877566	0.553813	-5.744919
C	-15.886698	1.672101	-3.900609
H	-16.828025	2.173905	-4.113630
C	-15.215514	1.939853	-2.709074

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H   -15.635952  2.644069 -1.994121
C    19.768622 -3.075403 -1.772188
C    19.117585 -4.309647 -1.863695
H    19.401890 -5.116587 -1.191802
C    18.111307 -4.511175 -2.805909
H    17.612078 -5.475889 -2.863197
C    17.745402 -3.480513 -3.671555
H    16.959889 -3.637437 -4.407325
C    18.392330 -2.247953 -3.588987
H    18.114347 -1.438493 -4.260338
C    19.397369 -2.047641 -2.644743
H    19.896762 -1.083299 -2.578054
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Excited state geometries

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123
P1'-ES     el energy= -3479.63577212
C    -3.590625 -1.534512 -1.386348
C    -4.929677 -1.503781 -1.084945
C    -5.536769 -0.272124 -0.589109
C    -4.798919  0.909101 -0.609127
C    -3.509978  0.908538 -1.239917
C    -2.777047 -0.370086 -1.300875
C    -3.093488  2.068880 -1.935535
C    -3.763430  3.324384 -1.716659
C    -4.759264  3.403374 -0.651535
C    -5.261174  2.209278 -0.080802
C    -2.055423  2.021948 -2.923528
C    -1.716006  3.138180 -3.655359
C    -2.382731  4.354824 -3.438239
C    -3.390660  4.433319 -2.484617
C    -5.187953  4.640688 -0.126672
C    -6.064283  4.704523  0.941490
C    -6.513679  3.522640  1.541828
C    -6.109332  2.297490  1.038583
C    -6.958769 -0.311176 -0.160495
C    -7.385089 -1.174236  0.857141
C    -8.719957 -1.218079  1.243140
C    -9.679140 -0.413628  0.613367
C    -9.253570  0.439464 -0.414536
C    -7.917721  0.491505 -0.792531
C   -11.106791 -0.467692  1.017631
C   -11.712254 -1.683654  1.367087
C   -13.048613 -1.739497  1.743460
C   -13.797040 -0.567594  1.769327
C   -13.228699  0.656322  1.435137
C   -11.887653  0.693468  1.059617
C    -1.365392 -0.441159 -1.142188
C    -0.615368 -1.622013 -1.451881
C     0.752851 -1.659180 -1.328336
C     1.491602 -0.547890 -0.849334
C     0.763720  0.606247 -0.501257
C    -0.606362  0.672367 -0.651503
C     2.955486 -0.607005 -0.717069
C     3.631955  0.136859  0.269062
C     5.010775  0.073188  0.401798
C     5.751213 -0.736212 -0.459014
C     5.116446 -1.469837 -1.460021
C     3.731178 -1.406668 -1.572946
O     7.113818 -0.736015 -0.264941
C     7.829009 -1.820677 -0.698439
F     8.115976 -1.717745 -2.040169
C     9.158011 -1.844659  0.065331
F     9.870340 -2.924854 -0.344275
O   -15.128481 -0.714603  2.143251
C   -15.893049  0.379770  2.211005
C   -16.817021  0.679418  1.309679
F   -15.720499  1.146862  3.290263
F   -17.019763 -0.026761  0.220738
F   -17.638066  1.700704  1.410990
H    -1.576390  1.074747 -3.144433
H    -0.942815  3.068586 -4.417064
H    -2.122543  5.233967 -4.022804
H    -3.905122  5.380806 -2.351654
H    -4.800922  5.567708 -0.539648
H    -6.374489  5.671281  1.331025
H    -7.166745  3.560227  2.410440
H    -6.441858  1.391041  1.532306
H    -6.660089 -1.808124  1.362557
H    -9.016714 -1.875448  2.057697
H    -9.980650  1.053029 -0.942394
H    -7.612254  1.153805 -1.599284
H   -11.137907 -2.606112  1.324840
H   -13.521561 -2.682415  2.004006
H   -13.807623  1.575297  1.468014
H   -11.440308  1.654539  0.816765
H    -1.122409 -2.507268 -1.823875
H     1.274416 -2.580115 -1.579625
H     1.287200  1.484629 -0.130267
H    -1.121822  1.578198 -0.350641
H     3.068670  0.748339  0.969378
H     5.525169  0.631633  1.179207
H     5.687446 -2.063927 -2.167229
H     3.253838 -1.964321 -2.374730
C    -5.715296 -2.757897 -1.235627
C    -5.254121 -3.952050 -0.664234
H    -4.340921 -3.942053 -0.072352
C    -5.962224 -5.141872 -0.825360
H    -5.590858 -6.055459 -0.366203
C    -7.144771 -5.158629 -1.563139
H    -7.700150 -6.085510 -1.687204
C    -7.612065 -3.976937 -2.140430
H    -8.530322 -3.979978 -2.723571
C    -6.906478 -2.788591 -1.976846
H    -7.278508 -1.875268 -2.434404
H    -3.146343 -2.492295 -1.644175
O     9.837515 -0.696296 -0.135999
C    11.087641 -0.581141  0.480783
C    12.228047 -0.941137 -0.229007
H    12.135520 -1.345368 -1.233078
C    13.471481 -0.762943  0.364368
H    14.364889 -1.031166 -0.195749
C    13.599035 -0.236868  1.658738
C    15.000474 -0.108005  2.275075
C    12.431997  0.117764  2.339664
H    12.481664  0.535583  3.340665
C    11.174046 -0.049763  1.757689
H    10.270381  0.235534  2.288624
C    15.520439 -1.533838  2.542727
C    14.983674  0.641761  3.620933
C    15.902909  0.673003  1.308670
C    17.135403  0.199999  0.857694
H    17.497323 -0.777635  1.164091
C    17.940420  0.957233  0.003182
H    18.897202  0.561570 -0.335455
C    17.519444  2.217250 -0.417442
O    18.254966  3.002439 -1.245383
C    16.285550  2.709993  0.020134
H    15.956602  3.690705 -0.314819
C    15.498263  1.942553  0.866807
H    14.535660  2.338410  1.186738
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H    19.072949  2.546095 -1.479704
H    14.819612 -2.060990  3.201496
H    15.616514 -2.118352  1.619841
H    16.497201 -1.512861  3.042413
H    14.407380  0.095057  4.378235
H    14.561782  1.649607  3.526582
H    16.010582  0.742753  3.992442
F     8.896181 -2.053942  1.379945
H     7.298121 -2.766873 -0.537279

123
P2'-ES     el energy= -4074.90740993
C    -4.789626  0.424626  1.783014
C    -6.105043  0.722189  1.528320
C    -6.876449 -0.110138  0.610377
C    -6.333121 -1.309482  0.155749
C    -5.084341 -1.753932  0.705090
C    -4.163435 -0.728966  1.231151
C    -4.880090 -3.142345  0.892158
C    -5.728509 -4.095647  0.226071
C    -6.686438 -3.603047 -0.759960
C    -6.973189 -2.218184 -0.817630
C    -3.885573 -3.640740  1.796538
C    -3.749597 -4.990493  2.034104
C    -4.586820 -5.910139  1.382042
C    -5.559048 -5.458001  0.497921
C    -7.286432 -4.461768 -1.704763
C    -8.121989 -3.973253 -2.692769
C    -8.355523 -2.596271 -2.785546
C    -7.782220 -1.736640 -1.863517
C    -8.257394  0.317220  0.266819
C    -8.502522  1.559723 -0.331707
C    -9.798031  1.962145 -0.635837
C   -10.896013  1.144491 -0.336202
C   -10.650283 -0.092681  0.275798
C    -9.354784 -0.499770  0.569377
C   -12.280388  1.577175 -0.654058
C   -12.671585  2.915515 -0.501968
C   -13.965331  3.325046 -0.800735
C   -14.887195  2.387818 -1.254624
C   -14.534128  1.053435 -1.419774
C   -13.232684  0.660641 -1.115518
C    -2.754054 -0.824867  1.070643
C    -1.840022  0.023962  1.775997
C    -0.479586 -0.111951  1.640045
C     0.094254 -1.070001  0.765939
C    -0.792565 -1.880789  0.031177
C    -2.160530 -1.779721  0.179751
C     1.553275 -1.203510  0.635758
C     2.146455 -1.655936 -0.559170
C     3.522571 -1.776137 -0.681576
C     4.343190 -1.451107  0.397810
C     3.789892 -1.017394  1.601197
C     2.408626 -0.889374  1.705331
O     5.695988 -1.610957  0.198473
C     6.556852 -0.879289  0.972879
F     6.750713 -1.483448  2.193659
C     7.909731 -0.849986  0.249607
F     7.745359 -0.278281 -0.967789
O   -16.161316  2.878777 -1.519149
C   -17.076272  2.037241 -2.010529
C   -18.085499  1.561257 -1.295869
F   -16.959374  1.739136 -3.306833
F   -18.241994  1.805415 -0.014661
F   -19.044351  0.809574 -1.788863
H    -3.275416 -2.937440  2.352121
H    -3.004124 -5.340656  2.744332
H    -4.486634 -6.975312  1.576232
H    -6.207509 -6.189043  0.023491
H    -7.067491 -5.525440 -1.685584
H    -8.566704 -4.656039 -3.412914
H    -8.973202 -2.195527 -3.585703
H    -7.948102 -0.669939 -1.966104
H    -7.667483  2.212319 -0.575896
H    -9.955154  2.918871 -1.129491
H   -11.484612 -0.735884  0.547451
H    -9.188951 -1.459704  1.053025
H   -11.961255  3.647416 -0.124610
H   -14.271714  4.359873 -0.674297
H   -15.249378  0.321521 -1.785106
H   -12.953447 -0.379790 -1.264778
H    -2.215459  0.778040  2.461141
H     0.168756  0.556642  2.201990
H    -0.400790 -2.630017 -0.652899
H    -2.800447 -2.415268 -0.422972
H     1.525736 -1.885958 -1.421362
H     3.975704 -2.105889 -1.612583
H     4.416114 -0.807397  2.462844
H     1.992300 -0.575061  2.658862
C    -6.695811  1.925050  2.174472
C    -6.046474  3.164125  2.087486
H    -5.129050  3.245705  1.507826
C    -6.574374  4.293007  2.712283
H    -6.059343  5.247146  2.624407
C    -7.760848  4.201113  3.438050
H    -8.176096  5.081590  3.923109
C    -8.413582  2.971383  3.536727
H    -9.336577  2.887375  4.106157
C    -7.888183  1.845386  2.909931
H    -8.403693  0.892167  2.996625
H    -4.213426  1.124409  2.382603
H     6.203143  0.143166  1.150589
O     8.783222 -0.148596  1.012522
C    10.097966 -0.056419  0.557882
C    10.458093  0.976838 -0.297201
H     9.710344  1.679824 -0.651155
C    11.789101  1.101029 -0.677720
H    12.069180  1.915863 -1.338026
C    12.760913  0.206590 -0.213058
C    14.206430  0.381805 -0.718245
C    12.365004 -0.835848  0.629871
H    13.074125 -1.567732  0.997538
C    11.036183 -0.964746  1.024506
H    10.730262 -1.766118  1.690224
C    14.241920 -0.255946 -2.133441
C    15.242019 -0.357745  0.171907
C    14.625533  1.862136 -0.724240
C    15.398645  2.440476 -1.733912
H    15.715981  1.870790 -2.599941
C    15.792312  3.773816 -1.662494
H    16.386466  4.203876 -2.467090
C    15.434322  4.553183 -0.561338
O    15.786781  5.852075 -0.434793
C    14.678655  3.982865  0.466621
H    14.405106  4.588444  1.326389
C    14.284516  2.656144  0.379739
H    13.693797  2.237531  1.189429
H    16.309932  6.126071 -1.199523
F    13.678815 -1.467587 -2.140008
F    13.571964  0.495267 -3.014087
F    15.488804 -0.409319 -2.607339
F    15.156535 -1.695313  0.079746
F    15.077384 -0.037885  1.460530
F    16.494340 -0.032249 -0.158694
F     8.352516 -2.105510  0.017318

133
P3'-ES     el energy= -3710.61114351
C     3.267136 -1.877610 -0.699958
C     4.631249 -1.787023 -0.913405
C     5.282844 -0.510501 -0.805009
C     4.393291  0.670547 -0.789237
C     3.073895  0.534001 -0.250334
C     2.486445 -0.724679 -0.278703
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C     2.419860  1.767956  0.228501
C     2.837866  3.015333 -0.291867
C     3.922455  3.055972 -1.268684
C     4.734333  1.877349 -1.447414
C     1.462290  1.749487  1.259120
C     0.882034  2.917618  1.725088
C     1.258525  4.148625  1.176315
C     2.232547  4.192767  0.195213
C     4.238560  4.213847 -1.987154
C     5.321994  4.262703 -2.856691
C     6.124724  3.125467 -3.037142
C     5.846163  1.963875 -2.352049
C     6.681521 -0.311544 -0.585718
C     7.722926 -1.162044 -1.082882
C     9.051468 -0.881443 -0.864764
C     9.472141  0.248727 -0.121508
C     8.462525  1.100342  0.368609
C     7.127781  0.851319  0.130211
C    10.897069  0.524907  0.111693
C    11.841909 -0.517984  0.171287
C    13.186413 -0.263014  0.398802
C    13.612625  1.050501  0.572712
C    12.712772  2.109825  0.511949
C    11.367588  1.838217  0.285742
C     1.036399 -0.926455 -0.008818
C     0.589168 -1.766240  1.018639
C    -0.769264 -1.956471  1.243950
C    -1.729093 -1.322614  0.442985
C    -1.279837 -0.489146 -0.589896
C     0.078787 -0.294182 -0.810906
C    -3.180394 -1.530172  0.680264
C    -4.078148 -1.640877 -0.392128
C    -5.437242 -1.827815 -0.175227
C    -5.919927 -1.913875  1.128683
C    -5.051440 -1.824863  2.213949
C    -3.692551 -1.625216  1.979172
O    -7.276863 -2.116858  1.258479
C    -7.889392 -1.690341  2.405762
F    -7.759724 -2.627608  3.407166
C    -9.386458 -1.546266  2.103058
F    -9.892011 -2.718838  1.656509
F   -10.042919 -1.277434  3.260279
O    14.972111  1.214791  0.806319
C    15.440590  2.453872  0.989489
C    15.787321  2.932490  2.175369
F    15.605159  3.185227 -0.115405
F    15.633858  2.265430  3.296352
F    16.331883  4.114164  2.359516
H     1.181953  0.805947  1.713788
H     0.146939  2.873281  2.525146
H     0.811438  5.071537  1.538101
H     2.552674  5.161036 -0.177917
H     3.619392  5.100232 -1.883591
H     5.534576  5.177371 -3.404868
H     6.957967  3.150965 -3.735646
H     6.436875  1.078590 -2.555008
H     7.476229 -2.006018 -1.713882
H     9.795890 -1.531038 -1.319449
H     8.728428  1.963717  0.974321
H     6.387948  1.519750  0.560042
H    11.519268 -1.550771  0.067402
H    13.909042 -1.072398  0.458100
H    13.043184  3.138391  0.628489
H    10.678613  2.675788  0.213138
H     1.313107 -2.273827  1.651327
H    -1.087244 -2.625401  2.040880
H    -2.000916  0.028189 -1.219411
H     0.404798  0.361916 -1.614915
H    -3.708625 -1.593356 -1.413865
H    -6.132963 -1.910584 -1.005863
H    -5.415624 -1.919659  3.232429
H    -3.023681 -1.534297  2.832005
C     2.563509 -3.184893 -0.877935
C     2.729776 -4.239070  0.026700
H     3.389924 -4.111090  0.881169
C     2.051626 -5.442957 -0.152710
H     2.190777 -6.251024  0.562158
C     1.195744 -5.609974 -1.240857
H     0.665336 -6.549192 -1.380746
C     1.022670 -4.564830 -2.147922
H     0.357009 -4.684923 -2.999862
C     1.700353 -3.361186 -1.965566
H     1.557946 -2.545591 -2.671730
C     5.397543 -3.047068 -1.159025
C     5.448876 -3.602467 -2.440110
H     4.931808 -3.107134 -3.259194
C     6.158056 -4.780910 -2.670663
H     6.190758 -5.203595 -3.672383
C     6.821262 -5.415245 -1.620893
H     7.375183 -6.333849 -1.800760
C     6.766983 -4.869367 -0.337811
H     7.277649 -5.361521  0.486944
C     6.057141 -3.693275 -0.108348
H     6.018241 -3.265117  0.891108
H    -7.484967 -0.741762  2.777288
O    -9.547247 -0.552839  1.199673
C   -10.843368 -0.325538  0.726237
C   -11.687267  0.539684  1.414386
H   -11.354029  1.005818  2.337099
C   -12.948381  0.801331  0.892449
H   -13.604782  1.487541  1.423598
C   -13.385362  0.213681 -0.303954
C   -14.808402  0.506912 -0.803121
C   -12.508276 -0.645766 -0.970336
H   -12.800498 -1.118976 -1.902939
C   -11.237931 -0.919771 -0.461639
H   -10.556720 -1.585772 -0.983826
C   -15.786957 -0.200951  0.154169
C   -15.058957 -0.046150 -2.219256
C   -15.025365  2.026487 -0.842626
C   -16.096073  2.664176 -0.215665
H   -16.818803  2.092568  0.360034
C   -16.275620  4.046768 -0.301856
H   -17.119674  4.517249  0.200770
C   -15.374567  4.823563 -1.027428
O   -15.492119  6.170635 -1.148751
C   -14.292572  4.205131 -1.662860
H   -13.587974  4.813915 -2.224216
C   -14.129266  2.830494 -1.564662
H   -13.273973  2.369709 -2.056402
H   -16.268162  6.472537 -0.659927
H   -15.561840 -1.274093  0.179977
H   -15.710484  0.182161  1.178884
H   -16.824937 -0.085313 -0.182576
H   -14.992406 -1.141325 -2.240429
H   -14.348929  0.357609 -2.951170
H   -16.068833  0.232438 -2.543742

133
P4'-ES     el energy= -4305.88255665
C     4.563372  1.173749  1.137069
C     5.918844  1.451916  1.139541
C     6.860390  0.385033  0.937580
C     6.321069 -0.985280  1.073480
C     4.950502 -1.223131  0.733898
C     4.063252 -0.159324  0.836774
C     4.586356 -2.607446  0.371315
C     5.386310 -3.674258  0.844322
C     6.565921 -3.380937  1.653389
C     7.057022 -2.025545  1.690604
C     3.526284 -2.893480 -0.508415
C     3.217605 -4.195636 -0.865995
C     3.978297 -5.255554 -0.359976
C     5.054412 -4.992649  0.468400
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C     7.269350 -4.377524  2.337838
C     8.438080 -4.098892  3.036969
C     8.934494 -2.786302  3.073358
C     8.269585 -1.774410  2.417326
C     8.212491  0.541546  0.499643
C     9.057576  1.657671  0.807417
C    10.364908  1.713240  0.383148
C    10.949239  0.686856 -0.398895
C    10.134694 -0.420384 -0.706711
C     8.833509 -0.507262 -0.260253
C    12.345380  0.768818 -0.852523
C    12.968466  2.012326 -1.074012
C    14.284543  2.094704 -1.504844
C    15.005706  0.924973 -1.725670
C    14.428570 -0.323047 -1.514212
C    13.107771 -0.389666 -1.083341
C     2.589027 -0.348790  0.761877
C     1.815819  0.303341 -0.206497
C     0.438907  0.120430 -0.260805
C    -0.215420 -0.712881  0.656928
C     0.558670 -1.355089  1.632673
C     1.936265 -1.175563  1.683838
C    -1.686079 -0.909645  0.595758
C    -2.450154 -1.019844  1.767239
C    -3.825933 -1.203410  1.713896
C    -4.460683 -1.284904  0.476624
C    -3.728137 -1.193062 -0.704493
C    -2.350338 -0.998635 -0.632943
O    -5.824304 -1.486265  0.508268
C    -6.566615 -1.055282 -0.557906
F    -6.544103 -1.980396 -1.577609
C    -8.020249 -0.932546 -0.081816
F    -8.076592 -0.045047  0.940998
O    16.311946  1.099351 -2.165185
C    17.066281  0.013384 -2.365410
C    17.371073 -0.448381 -3.569381
F    17.563249 -0.562483 -1.268209
F    16.899251  0.067162 -4.681443
F    18.184065 -1.458202 -3.784289
H     2.946418 -2.081583 -0.932662
H     2.394237 -4.386629 -1.550032
H     3.746468 -6.280819 -0.638550
H     5.669299 -5.822623  0.803788
H     6.893596 -5.396719  2.342978
H     8.955866 -4.896486  3.564170
H     9.835703 -2.559487  3.638350
H     8.633117 -0.758053  2.511308
H     8.696647  2.447401  1.453472
H    10.972959  2.557148  0.701057
H    10.521752 -1.220969 -1.332734
H     8.237759 -1.366515 -0.552883
H    12.408895  2.933751 -0.935296
H    14.757033  3.056363 -1.685623
H    14.991355 -1.239131 -1.671665
H    12.677348 -1.369909 -0.895159
H     2.298453  0.957161 -0.928812
H    -0.137727  0.649927 -1.016232
H     0.082696 -2.020217  2.350139
H     2.518178 -1.690396  2.445051
H    -1.967111 -0.934632  2.737903
H    -4.419535 -1.271267  2.621502
H    -4.208614 -1.300003 -1.672138
H    -1.782960 -0.948280 -1.559441
C     6.355655  2.876475  1.261550
C     6.471012  3.474611  2.519041
H     6.241952  2.894784  3.410668
C     6.878802  4.803346  2.633537
H     6.965246  5.258177  3.617846
C     7.174341  5.545735  1.490785
H     7.494479  6.581347  1.580101
C     7.052390  4.956183  0.231916
H     7.276479  5.530716 -0.664161
C     6.642908  3.629918  0.118499
H     6.552978  3.168022 -0.862504
H    -6.215184 -0.098038 -0.960150
O    -8.780734 -0.528704 -1.129142
C   -10.159295 -0.470950 -0.928906
C   -10.734047  0.680009 -0.406006
H   -10.110707  1.518687 -0.111942
C   -12.116917  0.741656 -0.278337
H   -12.564238  1.645699  0.123011
C   -12.928386 -0.331022 -0.667124
C   -14.447460 -0.209557 -0.437955
C   -12.320185 -1.482252 -1.175931
H   -12.901484 -2.347761 -1.470208
C   -10.937067 -1.551709 -1.316404
H   -10.463912 -2.441265 -1.721197
C   -14.674297 -0.522815  1.066086
C   -15.261072 -1.235024 -1.273132
C   -14.969194  1.180790 -0.838883
C   -15.946384  1.872500 -0.119222
H   -16.365834  1.469615  0.795590
C   -16.418811  3.107255 -0.554255
H   -17.173891  3.630858  0.029150
C   -15.933156  3.667995 -1.736381
O   -16.352949  4.863787 -2.207096
C   -14.971591  2.977445 -2.479153
H   -14.598421  3.411362 -3.402865
C   -14.502248  1.751519 -2.031191
H   -13.751521  1.236210 -2.623601
H   -17.018806  5.233822 -1.612819
F   -14.030878 -1.633042  1.438522
F   -14.221889  0.472727  1.836006
F   -15.968214 -0.707792  1.373255
F   -15.092409 -2.502617 -0.860886
F   -14.907495 -1.187175 -2.562411
F   -16.571922 -0.986344 -1.213648
F    -8.453997 -2.109960  0.419592
C     3.571120  2.251327  1.436744
C     2.864724  2.214603  2.644906
H     3.052417  1.406065  3.348568
C     1.927081  3.198367  2.951272
H     1.389580  3.155434  3.896028
C     1.678070  4.232835  2.049620
H     0.944772  5.000479  2.286287
C     2.373502  4.275869  0.841752
H     2.183994  5.076567  0.130196
C     3.312488  3.292012  0.538364
H     3.846478  3.326268 -0.408124

121
P1-E-ES     el energy= -3379.16128821
C    -2.725882  1.178856 -1.851705
C    -4.022755  0.737953 -1.760140
C    -4.681250  0.675635 -0.458666
C    -4.058348  1.244480  0.649552
C    -2.850270  1.993866  0.454254
C    -2.015805  1.656590 -0.714430
C    -2.617781  3.130480  1.265393
C    -3.370260  3.320513  2.477812
C    -4.245970  2.242461  2.927681
C    -4.574426  1.196173  2.033165
C    -1.693907  4.156229  0.878155
C    -1.539687  5.298767  1.631674
C    -2.286700  5.476300  2.807539
C    -3.186543  4.497452  3.212021
C    -4.720896  2.178548  4.254360
C    -5.476438  1.107889  4.696926
C    -5.751327  0.046139  3.827064
C    -5.299048  0.091964  2.518893
C    -6.040263  0.079955 -0.384410
C    -6.277761 -1.237038 -0.798410
C    -7.554039 -1.784795 -0.738433
C    -8.641967 -1.029906 -0.279561
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C    -8.405796  0.293158  0.119641
C    -7.128231  0.836839  0.070451
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C   -10.458973 -2.485554 -1.224107
C   -11.733715 -3.036264 -1.175764
C   -12.574747 -2.711395 -0.116821
C   -12.158637 -1.853182  0.894614
C   -10.877031 -1.310738  0.830171
C    -0.594850  1.672194 -0.657772
C     0.223186  1.594978 -1.831565
C     1.594672  1.646447 -1.759149
C     2.275909  1.738118 -0.518941
C     1.485720  1.775654  0.646107
C     0.107305  1.757639  0.589763
C     3.745270  1.784445 -0.454169
C     4.443733  1.268302  0.654419
C     5.828529  1.312978  0.720609
C     6.545381  1.877241 -0.330793
C     5.893029  2.399200 -1.443084
C     4.503908  2.346015 -1.495570
O     7.925205  1.867363 -0.189091
C     8.670880  2.466560 -1.123914
F     8.723667  3.797806 -1.041482
C     9.363054  1.802133 -2.042302
F    10.192173  2.435501 -2.875319
O   -13.836579 -3.295401 -0.152495
C   -14.676720 -3.055898  0.859257
C   -15.716964 -2.240614  0.764056
F   -14.449523 -3.742365  1.981770
F   -15.979578 -1.527255 -0.307269
F   -16.603345 -2.065565  1.718577
H    -1.157364  4.059857 -0.059011
H    -0.851513  6.073359  1.301156
H    -2.173400  6.383058  3.396788
H    -3.768350  4.667274  4.113678
H    -4.463229  2.963726  4.959356
H    -5.825229  1.079129  5.726529
H    -6.305643 -0.821767  4.176188
H    -5.494566 -0.750846  1.865014
H    -5.450173 -1.845013 -1.156578
H    -7.702274 -2.820587 -1.036669
H    -9.235622  0.913949  0.450877
H    -6.970457  1.868386  0.376858
H    -9.814273 -2.723473 -2.066882
H   -12.088227 -3.704434 -1.955873
H   -12.809488 -1.606362  1.729071
H   -10.547346 -0.655898  1.633464
H    -0.237465  1.523632 -2.812334
H     2.166774  1.585160 -2.682143
H     1.962663  1.848982  1.620743
H    -0.453247  1.766900  1.518335
H     3.899988  0.796446  1.468742
H     6.363612  0.902414  1.572569
H     6.447937  2.849075 -2.262104
H     4.004775  2.782338 -2.356949
C    -4.707330  0.293172 -3.003654
C    -4.091275 -0.631861 -3.857889
H    -3.127615 -1.054560 -3.580377
C    -4.708914 -1.033018 -5.041515
H    -4.217613 -1.758988 -5.685718
C    -5.953862 -0.513701 -5.392789
H    -6.438776 -0.828363 -6.314101
C    -6.574973  0.411851 -4.552813
H    -7.543605  0.828245 -4.820507
C    -5.959680  0.809473 -3.369646
H    -6.451616  1.533646 -2.725034
H    -2.227674  1.106440 -2.814912
O     9.249456  0.486533 -2.240582
C    10.268173 -0.344293 -1.782284
C    11.344376  0.113625 -1.028246
H    11.442756  1.163913 -0.766088
C    12.297298 -0.804046 -0.598564
H    13.129494 -0.444236  0.003269
C    12.208224 -2.167629 -0.906899
C    13.317629 -3.116826 -0.429340
C    11.114470 -2.588657 -1.667970
H    10.993961 -3.635347 -1.931467
C    10.145879 -1.687053 -2.107630
H     9.294277 -2.020767 -2.694569
C    14.595775 -2.776169 -1.219892
C    12.980550 -4.595105 -0.703258
C    13.505075 -2.948294  1.085751
C    14.741858 -2.701916  1.682286
H    15.635041 -2.589137  1.073963
C    14.876173 -2.590734  3.068421
H    15.854925 -2.396329  3.505548
C    13.759351 -2.727144  3.890609
O    13.821736 -2.630106  5.243453
C    12.508619 -2.971209  3.313558
H    11.637832 -3.071399  3.956888
C    12.394360 -3.077059  1.934624
H    11.410322 -3.256120  1.504308
H    14.735257 -2.472930  5.513858
H    14.396139 -2.867267 -2.294567
H    14.938056 -1.751966 -1.028346
H    15.413100 -3.465578 -0.972773
H    12.899120 -4.795412 -1.779317
H    12.042837 -4.899718 -0.222893
H    13.781460 -5.230075 -0.305514

121
P2-E-ES     el energy= -3974.43402530
C    -4.003401  0.881448 -2.044444
C    -5.286398  0.422950 -1.874632
C    -5.965669  0.613217 -0.595874
C    -5.386201  1.432685  0.369055
C    -4.202913  2.169763  0.027765
C    -3.332922  1.617169 -1.027611
C    -4.028529  3.464202  0.572237
C    -4.811938  3.885222  1.704819
C    -5.658412  2.897583  2.369367
C    -5.926647  1.666826  1.723990
C    -3.132527  4.414894 -0.018608
C    -3.031883  5.699082  0.468894
C    -3.807407  6.099992  1.568607
C    -4.681939  5.199861  2.166049
C    -6.162454  3.106631  3.670124
C    -6.884568  2.127393  4.328248
C    -7.095759  0.888600  3.712081
C    -6.616384  0.665441  2.432022
C    -7.297889 -0.016744 -0.405643
C    -7.464918 -1.402533 -0.523366
C    -8.714711 -1.987379 -0.354391
C    -9.844934 -1.206144 -0.078813
C    -9.679212  0.182285  0.023329
C    -8.428258  0.765748 -0.135069
C   -11.180616 -1.830739  0.096230
C   -11.579315 -2.917163 -0.696210
C   -12.828407 -3.504149 -0.535542
C   -13.697438 -3.001093  0.426741
C   -13.333767 -1.929370  1.234180
C   -12.077823 -1.352649  1.058509
C    -1.914885  1.694816 -0.950755
C    -1.063975  1.391102 -2.062265
C     0.303206  1.503861 -1.974224
C     0.945971  1.887634 -0.770522
C     0.124183  2.152992  0.341431
C    -1.251146  2.076260  0.261521
C     2.411426  1.997467 -0.686714
C     3.092384  1.746420  0.519739
C     4.472660  1.855609  0.606204
C     5.200403  2.217714 -0.523203
C     4.566033  2.471865 -1.734600
C     3.181244  2.358505 -1.805804
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O     6.577349  2.285044 -0.355699
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C     8.114209  2.149372 -2.122965
F     8.930717  2.757119 -2.984582
O   -14.930683 -3.638210  0.511987
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C   -16.879196 -2.508884  1.158428
F   -15.552017 -3.620477  2.690175
F   -17.164129 -2.073418 -0.047675
F   -17.788298 -2.172647  2.046042
H    -2.575524  4.138076 -0.906640
H    -2.363604  6.408107 -0.014328
H    -3.736172  7.116538  1.947810
H    -5.285142  5.541953  3.002206
H    -5.956367  4.038624  4.188493
H    -7.256292  2.311569  5.333492
H    -7.622005  0.095179  4.237335
H    -6.762612 -0.308404  1.977701
H    -6.603144 -2.031599 -0.734223
H    -8.808493 -3.069264 -0.420202
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H    -8.324690  1.845761 -0.059422
H   -10.912983 -3.299144 -1.466115
H   -13.141875 -4.339226 -1.156004
H   -14.004703 -1.542862  1.996611
H   -11.787914 -0.526663  1.703829
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H     0.903842  1.261838 -2.848101
H     0.572999  2.453706  1.285418
H    -1.840054  2.271133  1.151438
H     2.538893  1.435372  1.402067
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H     2.693619  2.586895 -2.750207
C    -5.934281 -0.299487 -3.001841
C    -5.272599 -1.360326 -3.635648
H    -4.299752 -1.679040 -3.266503
C    -5.856165 -2.024703 -4.713254
H    -5.329526 -2.851365 -5.185120
C    -7.112110 -1.637554 -5.177758
H    -7.570394 -2.156956 -6.016289
C    -7.778661 -0.579404 -4.557996
H    -8.756311 -0.264908 -4.916563
C    -7.197480  0.081216 -3.479867
H    -7.724554  0.906494 -3.007642
H    -3.484755  0.622845 -2.964161
O     8.134823  0.812021 -2.167450
C     9.195032  0.146257 -1.572474
C    10.127299  0.773807 -0.754634
H    10.073814  1.839990 -0.552016
C    11.137499  0.009624 -0.180376
H    11.855944  0.505808  0.465037
C    11.234212 -1.366610 -0.409563
C    12.418948 -2.125544  0.216250
C    10.293173 -1.965478 -1.253431
H    10.331933 -3.023091 -1.486046
C     9.271878 -1.216812 -1.827006
H     8.535847 -1.685028 -2.474207
C    13.639233 -1.841848 -0.701253
C    12.189091 -3.660364  0.253033
C    12.660112 -1.692246  1.672496
C    13.932405 -1.530146  2.226156
H    14.828603 -1.667196  1.631756
C    14.094728 -1.186769  3.565251
H    15.096769 -1.055206  3.969965
C    12.979005 -1.019498  4.386892
O    13.073367 -0.689167  5.694531
C    11.700062 -1.197858  3.852357
H    10.832002 -1.072296  4.493842
C    11.550685 -1.529866  2.513984
H    10.546511 -1.658269  2.120034
H    14.002733 -0.604328  5.944596
F    13.337199 -2.023585 -1.990262
F    14.054197 -0.577173 -0.568062
F    14.690674 -2.635203 -0.438864
F    12.205024 -4.223881 -0.966719
F    11.008146 -3.952900  0.809124
F    13.128017 -4.281627  0.971740

131
P3-E-ES     el energy= -3610.13664372
C    -3.093616  1.830460 -0.566688
C    -4.471799  1.941468 -0.496825
C    -5.288597  0.778011 -0.702029
C    -4.605421 -0.398429 -1.282240
C    -3.210922 -0.586235 -1.015572
C    -2.445624  0.538726 -0.737870
C    -2.691511 -1.963268 -1.132107
C    -3.376810 -2.889029 -1.953543
C    -4.593335 -2.468834 -2.643574
C    -5.230857 -1.241288 -2.232201
C    -1.593244 -2.410231 -0.375187
C    -1.137236 -3.714898 -0.467839
C    -1.784524 -4.619357 -1.316941
C    -2.895798 -4.212753 -2.033434
C    -5.193160 -3.243954 -3.641462
C    -6.394603 -2.872206 -4.233936
C    -7.031560 -1.685636 -3.837888
C    -6.472649 -0.890155 -2.862728
C    -6.648939  0.634950 -0.282930
C    -7.611722  1.695286 -0.233929
C    -8.917820  1.469327  0.134379
C    -9.385146  0.184768  0.504504
C    -8.453582 -0.870423  0.459017
C    -7.149335 -0.666318  0.061181
C   -10.784117 -0.038263  0.898560
C   -11.538502  0.975910  1.519214
C   -12.857994  0.767585  1.894056
C   -13.449243 -0.469078  1.653080
C   -12.739584 -1.495391  1.038034
C   -11.417048 -1.272189  0.669368
C    -0.957914  0.495452 -0.720863
C    -0.223838  0.864371  0.413219
C     1.165848  0.829155  0.405448
C     1.870976  0.435027 -0.739999
C     1.134945  0.074241 -1.876428
C    -0.254723  0.103921 -1.866391
C     3.355545  0.402090 -0.751505
C     4.076297  0.795822 -1.888514
C     5.465126  0.762916 -1.907020
C     6.150714  0.328949 -0.777221
C     5.469145 -0.063625  0.369359
C     4.076593 -0.024556  0.369933
O     7.535609  0.309480 -0.885949
C     8.255045 -0.010064  0.195476
F     8.361276  0.952621  1.113280
C     8.870078 -1.176116  0.358694
F     8.762236 -2.135870 -0.562186
O   -14.768311 -0.595188  2.071002
C   -15.423081 -1.723693  1.778047
C   -15.716095 -2.649739  2.679429
F   -15.834625 -1.847546  0.514185
F   -15.322806 -2.589420  3.931223
F   -16.442045 -3.715881  2.427264
H    -1.100628 -1.729062  0.309499
H    -0.287299 -4.033451  0.130890
H    -1.437156 -5.647025 -1.392866
H    -3.419538 -4.945186 -2.640427
H    -4.709451 -4.154226 -3.984049
H    -6.828857 -3.494767 -5.012454
H    -7.958510 -1.378284 -4.316553
H    -6.944406  0.054410 -2.619512
H    -7.339438  2.688528 -0.566928
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H    -9.616244  2.302226  0.093018
H    -8.752066 -1.869783  0.767614
H    -6.461972 -1.506690  0.076122
H   -11.080443  1.936818  1.739654
H   -13.433069  1.549000  2.383328
H   -13.201467 -2.458241  0.836577
H   -10.880931 -2.071402  0.164015
H    -0.746715  1.178912  1.313089
H     1.710611  1.133742  1.296636
H     1.653918 -0.250950 -2.775674
H    -0.806010 -0.186238 -2.758025
H     3.545955  1.152456 -2.768454
H     6.024130  1.073232 -2.785594
H     6.002039 -0.407772  1.251803
H     3.546085 -0.352697  1.260854
C    -2.230427  3.045010 -0.445244
C    -2.089777  3.735000  0.763650
H    -2.623924  3.386292  1.644076
C    -1.264506  4.854244  0.851544
H    -1.164675  5.376039  1.800804
C    -0.566708  5.300817 -0.270032
H     0.078755  6.173587 -0.201524
C    -0.699581  4.619930 -1.479888
H    -0.159474  4.959860 -2.360843
C    -1.523695  3.500018 -1.565036
H    -1.619640  2.967609 -2.509159
C    -5.061106  3.261076 -0.113949
C    -5.226613  4.264999 -1.071476
H    -4.927830  4.077666 -2.100688
C    -5.770549  5.498355 -0.714066
H    -5.894002  6.272479 -1.468178
C    -6.153574  5.738423  0.605003
H    -6.578852  6.699894  0.883790
C    -5.984115  4.741872  1.566982
H    -6.275979  4.923743  2.598970
C    -5.439350  3.511020  1.209341
H    -5.310837  2.732211  1.958172
O     9.582593 -1.500904  1.440994
C    10.966071 -1.594517  1.314513
C    11.659209 -1.153623  0.191034
H    11.138193 -0.716878 -0.657135
C    13.045199 -1.269016  0.172974
H    13.584112 -0.910980 -0.701981
C    13.759278 -1.817568  1.246164
C    15.285840 -1.952182  1.139252
C    13.028568 -2.248238  2.356654
H    13.532610 -2.677540  3.217519
C    11.638738 -2.142000  2.396904
H    11.076025 -2.476373  3.264467
C    15.584541 -3.036412  0.085609
C    15.927303 -2.401828  2.466127
C    15.885469 -0.589504  0.761644
C    16.755060 -0.405573 -0.313705
H    17.024625 -1.240389 -0.954708
C    17.303857  0.845792 -0.604741
H    17.978686  0.959143 -1.452460
C    16.987039  1.947757  0.187165
O    17.484534  3.189846 -0.042848
C    16.116676  1.786434  1.270335
H    15.866992  2.648933  1.883476
C    15.580048  0.536106  1.543024
H    14.894508  0.434169  2.382757
H    18.053232  3.170189 -0.822968
H    15.095806 -3.974094  0.377049
H    15.211394 -2.758872 -0.907664
H    16.661733 -3.231514  0.008452
H    15.590934 -3.405948  2.754605
H    15.700533 -1.712105  3.288195
H    17.017260 -2.436257  2.349446

131
P4-E-ES     el energy= -4205.42838610
C     4.345648 -1.440898 -0.160043
C     5.771094 -1.464896 -0.069163
C     6.512436 -0.286391 -0.326847
C     5.822164  0.925345 -0.643538
C     4.407785  1.013691 -0.299374
C     3.660603 -0.206784 -0.274297
C     3.879180  2.307767  0.014195
C     4.585033  3.487498 -0.417783
C     5.782047  3.341879 -1.213595
C     6.407255  2.047642 -1.317405
C     2.709001  2.484716  0.804679
C     2.229631  3.737897  1.122228
C     2.907740  4.888197  0.674158
C     4.064564  4.754577 -0.070050
C     6.376872  4.434082 -1.885477
C     7.521279  4.285123 -2.645940
C     8.110065  3.013376 -2.786295
C     7.558795  1.925074 -2.144419
C     7.991078 -0.283585 -0.202684
C     8.804369 -1.203557 -0.881433
C    10.186622 -1.165501 -0.752943
C    10.811792 -0.216961  0.069026
C     9.999290  0.697603  0.753226
C     8.617231  0.669136  0.614461
C    12.289339 -0.182701  0.207604
C    13.038212 -1.368424  0.241185
C    14.421481 -1.342543  0.369300
C    15.071971 -0.117312  0.468667
C    14.363057  1.078092  0.432263
C    12.976570  1.033230  0.304794
C     2.186799 -0.174337 -0.445785
C     1.309084 -0.809133  0.446018
C    -0.066122 -0.747925  0.259838
C    -0.619400 -0.059405 -0.828902
C     0.256966  0.572555 -1.721779
C     1.632016  0.521249 -1.530201
C    -2.089093 -0.002713 -1.029449
C    -2.645603 -0.078535 -2.314785
C    -4.020752 -0.030030 -2.507693
C    -4.858153  0.092566 -1.403989
C    -4.341534  0.176409 -0.115870
C    -2.960481  0.126113  0.058715
O    -6.219947  0.114280 -1.681843
C    -7.072614  0.302635 -0.670135
F    -7.162016  1.556536 -0.224980
C    -7.830168 -0.656476 -0.150782
O    16.454673 -0.180851  0.601343
C    17.129614  0.961379  0.765802
C    17.632263  1.347876  1.929261
F    17.332388  1.685386 -0.338037
F    17.452920  0.685131  3.049130
F    18.372384  2.421890  2.089897
H     2.196526  1.614241  1.197063
H     1.338251  3.833437  1.737586
H     2.538072  5.877906  0.930423
H     4.590971  5.654666 -0.372224
H     5.918316  5.416619 -1.830002
H     7.948549  5.145296 -3.155441
H     8.986137  2.882260 -3.416654
H     7.998578  0.946858 -2.299086
H     8.351073 -1.941420 -1.537688
H    10.790263 -1.871059 -1.319805
H    10.450832  1.428907  1.420278
H     8.008669  1.388523  1.157709
H    12.532492 -2.329676  0.188113
H    15.000957 -2.260898  0.406553
H    14.870273  2.037128  0.490067
H    12.427420  1.970586  0.255641
H     1.706430 -1.349984  1.300480
H    -0.719452 -1.260347  0.962999
H    -0.140870  1.129851 -2.567346
H     2.290644  1.029788 -2.230641
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H    -1.996595 -0.198728 -3.179062
H    -4.452163 -0.099737 -3.502506
H    -4.992860  0.285157  0.747141
H    -2.559211  0.211406  1.065842
C     6.471280 -2.728675  0.291431
C     6.431923 -3.848874 -0.549432
H     5.877506 -3.797713 -1.483595
C     7.099916 -5.020690 -0.203574
H     7.063007 -5.878275 -0.871731
C     7.813871 -5.094559  0.992710
H     8.334568 -6.010346  1.263355
C     7.856645 -3.986863  1.839085
H     8.409100 -4.034595  2.774908
C     7.192680 -2.813267  1.489635
H     7.233387 -1.949747  2.150027
O    -8.685989 -0.464694  0.861068
C   -10.042177 -0.429955  0.580508
C   -10.881588 -0.272540  1.678107
H   -10.456843 -0.197236  2.674973
C   -12.252833 -0.203106  1.478729
H   -12.897821 -0.069117  2.341726
C   -12.805358 -0.291893  0.194143
C   -14.338925 -0.262374  0.058074
C   -11.940490 -0.475679 -0.886031
H   -12.313441 -0.579075 -1.898186
C   -10.560325 -0.537801 -0.703287
H    -9.912984 -0.672855 -1.565042
C   -14.826036 -1.693859  0.410889
C   -14.802317  0.063286 -1.387529
C   -14.962903  0.814997  0.962051
C   -16.152871  0.632035  1.670398
H   -16.687239 -0.310744  1.643268
C   -16.696820  1.657846  2.438239
H   -17.620084  1.486549  2.989046
C   -16.066230  2.901581  2.495761
O   -16.545197  3.934891  3.224310
C   -14.887130  3.107079  1.774187
H   -14.399466  4.077272  1.814420
C   -14.349654  2.074418  1.020360
H   -13.428965  2.257088  0.473527
H   -17.354351  3.668314  3.679810
F   -14.122915 -2.626323 -0.238598
F   -14.689122 -1.937025  1.719163
F   -16.116060 -1.901601  0.100533
F   -14.540097 -0.924553 -2.259916
F   -14.199165  1.165984 -1.845653
F   -16.118940  0.281501 -1.444118
F    -7.743499 -1.911513 -0.591453
C     3.583559 -2.719685 -0.132236
C     2.859086 -3.129773 -1.259121
H     2.858337 -2.505647 -2.150019
C     2.143233 -4.324490 -1.247118
H     1.589571 -4.629214 -2.132429
C     2.134528 -5.124665 -0.104855
H     1.572380 -6.055684 -0.093663
C     2.850504 -4.723885  1.023454
H     2.847712 -5.339975  1.919878
C     3.572007 -3.533046  1.008505
H     4.129496 -3.226482  1.890469

121
P1-Z-ES     el energy= -3379.16095350
C     3.120503 -0.934539  1.403705
C     4.471624 -1.085644  1.211729
C     5.221672 -0.070756  0.478031
C     4.601299  1.133278  0.152031
C     3.284922  1.392390  0.660517
C     2.429424  0.231446  0.969377
C     2.943105  2.718684  1.018153
C     3.743415  3.822531  0.556087
C     4.800575  3.554243 -0.414940
C     5.214715  2.219394 -0.639301
C     1.850021  3.001080  1.901837
C     1.579187  4.287191  2.313205
C     2.373128  5.354567  1.862990
C     3.436583  5.113519  1.001387
C     5.375683  4.583608 -1.189441
C     6.309936  4.309044 -2.171770
C     6.672652  2.982498 -2.433210
C     6.125034  1.957591 -1.679969
C     6.654303 -0.331198  0.182488
C     7.047948 -1.455055 -0.555266
C     8.390640 -1.702616 -0.816903
C     9.388986 -0.844891 -0.335904
C     8.994922  0.271405  0.415267
C     7.652304  0.524503  0.667778
C    10.823357 -1.114770 -0.609255
C    11.325845 -2.424193 -0.596212
C    12.666959 -2.682316 -0.851851
C    13.523808 -1.620766 -1.121839
C    13.059808 -0.310513 -1.148699
C    11.712329 -0.070212 -0.889152
C     1.030619  0.233615  0.711811
C     0.152020 -0.774901  1.225068
C    -1.201977 -0.737347  0.991552
C    -1.796503  0.276153  0.198630
C    -0.939844  1.252071 -0.345833
C     0.416868  1.248512 -0.094077
C    -3.246935  0.298946 -0.049370
C    -3.774083  0.819757 -1.246569
C    -5.140165  0.836942 -1.487255
C    -6.010200  0.334974 -0.523548
C    -5.528873 -0.187620  0.672609
C    -4.156295 -0.200910  0.898392
O    -7.359711  0.401188 -0.838053
C    -8.237531 -0.160497  0.001574
F    -8.273579 -1.493893 -0.020117
C    -9.063426  0.530516  0.779402
F    -9.026727  1.864186  0.793790
O    14.850868 -1.965770 -1.354880
C    15.722242 -0.989492 -1.627446
C    16.618903 -0.549089 -0.756953
F    15.687812 -0.506992 -2.872189
F    16.690286 -0.973445  0.484133
F    17.540269  0.344295 -1.040463
H     1.268783  2.178993  2.304286
H     0.760389  4.470814  3.005068
H     2.167075  6.368990  2.195771
H     4.047321  5.954540  0.685248
H     5.059023  5.612197 -1.043857
H     6.733182  5.120478 -2.759171
H     7.370750  2.750399 -3.233910
H     6.392361  0.933000 -1.913580
H     6.292717 -2.135452 -0.941979
H     8.664542 -2.566591 -1.418742
H     9.749033  0.938422  0.827927
H     7.370547  1.391201  1.261351
H    10.664449 -3.255179 -0.362240
H    13.059296 -3.695384 -0.831426
H    13.724155  0.519112 -1.374859
H    11.347437  0.953466 -0.929561
H     0.546065 -1.579520  1.838738
H    -1.824512 -1.527724  1.404954
H    -1.351586  2.050212 -0.959466
H     1.036461  2.012243 -0.552011
H    -3.105093  1.191412 -2.018503
H    -5.541469  1.229144 -2.417705
H    -6.206122 -0.571493  1.430834
H    -3.794216 -0.586488  1.848173
C     5.124102 -2.317922  1.729860
C     4.587551 -3.578014  1.431756
H     3.717834 -3.646550  0.781221
C     5.168183 -4.740002  1.937537
H     4.740853 -5.708444  1.686700
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C     6.295712 -4.661295  2.753298
H     6.752003 -5.566952  3.146387
C     6.836554 -3.411902  3.060858
H     7.712599 -3.339149  3.701577
C     6.258664 -2.252197  2.552967
H     6.686760 -1.284451  2.802229
H     2.572561 -1.757479  1.855093
O    -9.940866 -0.025089  1.619459
C   -11.293482  0.041931  1.293763
C   -11.753007  0.429224  0.038661
H   -11.061217  0.712140 -0.750639
C   -13.123334  0.436052 -0.198752
H   -13.477309  0.724931 -1.186406
C   -14.049607  0.070911  0.786827
C   -15.550336  0.136468  0.464871
C   -13.550002 -0.312396  2.034210
H   -14.224480 -0.609747  2.831845
C   -12.179928 -0.327980  2.294216
H   -11.797265 -0.630432  3.265382
C   -15.932950  1.622000  0.319089
C   -16.416522 -0.458863  1.591419
C   -15.822549 -0.666505 -0.815838
C   -16.493479 -0.144517 -1.922064
H   -16.834202  0.887232 -1.924593
C   -16.747521 -0.919632 -3.056586
H   -17.270997 -0.482935 -3.906404
C   -16.328870 -2.248093 -3.101243
O   -16.542590 -3.055934 -4.171200
C   -15.652157 -2.791298 -2.003976
H   -15.321239 -3.826215 -2.044176
C   -15.407036 -2.005608 -0.886947
H   -14.867577 -2.443889 -0.048846
H   -17.005447 -2.564258 -4.861408
H   -15.678184  2.157542  1.241777
H   -15.399206  2.106533 -0.507398
H   -17.010894  1.740565  0.150857
H   -16.317491  0.116584  2.520702
H   -16.157554 -1.503351  1.802800
H   -17.471263 -0.429941  1.292279

121
P2-Z-ES     el energy= -3974.43686012
C     2.395015  2.097651 -1.281374
C     3.732825  1.786783 -1.289575
C     4.306992  1.005599 -0.197891
C     3.463502  0.426991  0.746912
C     2.045061  0.495793  0.538666
C     1.521153  1.611301 -0.271261
C     1.242620 -0.594108  0.951462
C     1.761337 -1.567027  1.878808
C     3.067917 -1.321608  2.484065
C     3.908404 -0.319305  1.942502
C    -0.074581 -0.803557  0.422001
C    -0.826764 -1.896677  0.789679
C    -0.311218 -2.835084  1.697047
C     0.966433 -2.667186  2.219323
C     3.489911 -2.010509  3.640516
C     4.688395 -1.709093  4.261681
C     5.489179 -0.677037  3.759689
C     5.096546  0.007824  2.621841
C     5.776972  0.788464 -0.185119
C     6.669605  1.867079 -0.144478
C     8.043745  1.656075 -0.141731
C     8.574545  0.360309 -0.198913
C     7.679688 -0.717320 -0.256461
C     6.306424 -0.507186 -0.246271
C    10.042008  0.133803 -0.201748
C    10.906378  0.999558 -0.887890
C    12.280058  0.790222 -0.891806
C    12.803664 -0.299973 -0.205101
C    11.977666 -1.175691  0.490293
C    10.602964 -0.951111  0.482547
C     0.273688  2.229374  0.022697
C    -0.408689  3.074248 -0.911094
C    -1.663653  3.569398 -0.646037
C    -2.323293  3.313107  0.582082
C    -1.630563  2.552325  1.541615
C    -0.387670  2.014760  1.276575
C    -3.693748  3.789944  0.831085
C    -4.129765  4.118654  2.127397
C    -5.443930  4.503180  2.370848
C    -6.334045  4.563613  1.307195
C    -5.934462  4.275321  0.007122
C    -4.619288  3.891475 -0.224039
O    -7.668524  4.924372  1.548933
C    -8.497424  3.875328  1.596387
F    -8.469264  3.187292  2.739881
C    -9.307245  3.498637  0.614260
F    -9.327905  4.149482 -0.551571
O    14.185630 -0.441215 -0.267311
C    14.744746 -1.492885  0.339756
C    15.205651 -2.549623 -0.313387
F    14.876780 -1.401225  1.665626
F    15.089646 -2.702485 -1.612843
F    15.837351 -3.549505  0.259553
H    -0.457587 -0.125095 -0.331398
H    -1.815829 -2.044534  0.363676
H    -0.906730 -3.698326  1.983875
H     1.349803 -3.422211  2.899772
H     2.852516 -2.771100  4.081427
H     4.986753 -2.251623  5.155671
H     6.410581 -0.399287  4.265889
H     5.712204  0.825182  2.263536
H     6.283555  2.882736 -0.097533
H     8.712505  2.511669 -0.075953
H     8.061253 -1.733157 -0.333511
H     5.631310 -1.358297 -0.298541
H    10.500645  1.839172 -1.447483
H    12.949204  1.454024 -1.432444
H    12.385018 -2.018812  1.041303
H     9.961048 -1.626836  1.043066
H     0.041917  3.298731 -1.873509
H    -2.150048  4.189530 -1.395950
H    -2.094316  2.341304  2.502559
H     0.112205  1.440716  2.049708
H    -3.431820  4.084212  2.960047
H    -5.780755  4.748738  3.374136
H    -6.652808  4.332392 -0.806205
H    -4.320321  3.629396 -1.235710
C     4.570972  2.305268 -2.403732
C     4.532724  3.665230 -2.741716
H     3.918991  4.343928 -2.152675
C     5.288316  4.159305 -3.803781
H     5.251113  5.219776 -4.043275
C     6.094323  3.300164 -4.548975
H     6.687029  3.684388 -5.376017
C     6.136974  1.943161 -4.225286
H     6.757694  1.263024 -4.804425
C     5.385467  1.450756 -3.162534
H     5.424225  0.391228 -2.922144
H     2.021593  2.776455 -2.043733
O   -10.179328  2.484571  0.705874
C    -9.762689  1.230448  0.286528
C    -8.493655  0.975397 -0.221198
H    -7.753092  1.764404 -0.317958
C    -8.168590 -0.323154 -0.598584
H    -7.172582 -0.511537 -0.987663
C    -9.086064 -1.371174 -0.479669
C    -8.671792 -2.765520 -0.985120
C   -10.362673 -1.079761  0.013072
H   -11.122292 -1.847384  0.104410
C   -10.699655  0.211278  0.403015
H   -11.687634  0.432851  0.796207
C    -8.888880 -2.741477 -2.522344
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C    -9.552300 -3.897908 -0.390139
C    -7.220970 -3.103953 -0.598834
C    -6.331820 -3.762693 -1.451548
H    -6.614756 -4.036029 -2.461570
C    -5.046689 -4.094940 -1.032307
H    -4.369551 -4.600309 -1.718584
C    -4.633096 -3.790543  0.264493
O    -3.397966 -4.096433  0.729766
C    -5.514818 -3.146176  1.135346
H    -5.191011 -2.911076  2.145584
C    -6.789886 -2.811662  0.702875
H    -7.456448 -2.306871  1.396259
H    -2.878379 -4.518146  0.032624
F   -10.090068 -2.251194 -2.842467
F    -7.975905 -1.969055 -3.121734
F    -8.810910 -3.959464 -3.082956
F   -10.812207 -3.886535 -0.857368
F    -9.623321 -3.796720  0.941763
F    -9.054799 -5.105796 -0.668788

131
P3-Z-ES     el energy= -3610.17131791
C    -0.769048  2.083857  0.312918
C    -2.190878  1.991904  0.239101
C    -2.784307  0.757985 -0.128069
C    -1.958462 -0.388375 -0.333428
C    -0.592255 -0.363552  0.169876
C     0.036844  0.919977  0.244567
C     0.002738 -1.601031  0.565906
C    -0.583668 -2.841715  0.129597
C    -1.666654 -2.802913 -0.825413
C    -2.351563 -1.558531 -1.067973
C     1.092426 -1.666355  1.476720
C     1.560949 -2.871686  1.955977
C     0.981618 -4.083357  1.530827
C    -0.066627 -4.057393  0.630271
C    -2.090437 -3.950636 -1.533185
C    -3.115771 -3.895050 -2.457697
C    -3.750625 -2.668935 -2.737456
C    -3.366305 -1.529503 -2.064480
C    -4.257586  0.632372 -0.234170
C    -5.029317  1.506368 -1.014793
C    -6.407521  1.360367 -1.098491
C    -7.072666  0.347321 -0.392475
C    -6.303445 -0.519190  0.396280
C    -4.922958 -0.383576  0.468591
C    -8.546617  0.196247 -0.479181
C    -9.386020  1.318203 -0.546610
C   -10.766320  1.179984 -0.626174
C   -11.322633 -0.094664 -0.636318
C   -10.521207 -1.229173 -0.578413
C    -9.139575 -1.071924 -0.497517
C     1.510349  1.043647  0.106370
C     2.309614  1.735298  1.029170
C     3.669114  1.916242  0.802555
C     4.276200  1.427441 -0.361572
C     3.486731  0.706769 -1.267917
C     2.132334  0.503885 -1.029501
C     5.716665  1.658615 -0.631547
C     6.142549  2.078714 -1.898202
C     7.491417  2.283013 -2.169885
C     8.421481  2.058453 -1.164263
C     8.031806  1.659455  0.109162
C     6.679047  1.459502  0.366562
O     9.760421  2.273557 -1.480623
C    10.647170  1.340418 -1.109004
F    11.657849  1.834904 -0.399184
C    10.613086  0.055687 -1.452294
F    11.564227 -0.791195 -1.035230
O   -12.710431 -0.143631 -0.707847
C   -13.305572 -1.340543 -0.682442
C   -13.936192 -1.817012  0.381047
F   -13.288024 -2.026835 -1.828040
F   -13.973146 -1.194958  1.537356
F   -14.600882 -2.950601  0.394563
H     1.538213 -0.748835  1.844867
H     2.372616 -2.881047  2.678178
H     1.348799 -5.031252  1.916186
H    -0.518152 -4.998677  0.330093
H    -1.583799 -4.897871 -1.375485
H    -3.410385 -4.795375 -2.991536
H    -4.527099 -2.614862 -3.496304
H    -3.831873 -0.584354 -2.318868
H    -4.541866  2.292805 -1.584368
H    -6.973166  2.031827 -1.740866
H    -6.791508 -1.297681  0.978774
H    -4.349008 -1.065566  1.091621
H    -8.958578  2.317598 -0.514005
H   -11.417437  2.048883 -0.666161
H   -10.951604 -2.226390 -0.603949
H    -8.514551 -1.961514 -0.472948
H     1.858658  2.148380  1.927529
H     4.261743  2.473229  1.525588
H     3.941887  0.293242 -2.165695
H     1.537115 -0.054787 -1.748574
H     5.409003  2.254001 -2.681873
H     7.828830  2.597343 -3.153554
H     8.774356  1.487181  0.884310
H     6.371698  1.118986  1.352756
C    -0.130014  3.420165  0.468413
C    -0.281432  4.152943  1.651910
H    -0.874716  3.740575  2.464772
C     0.324960  5.398424  1.795035
H     0.204193  5.952276  2.723276
C     1.082441  5.933310  0.752849
H     1.554159  6.906968  0.864252
C     1.231540  5.213891 -0.432672
H     1.818552  5.624305 -1.251217
C     0.632705  3.964295 -0.572504
H     0.758265  3.401769 -1.494880
C    -3.037082  3.179847  0.541080
C    -2.985775  4.336344 -0.249199
H    -2.312184  4.371758 -1.102240
C    -3.790777  5.434848  0.041822
H    -3.738635  6.321429 -0.586430
C    -4.662859  5.397595  1.129998
H    -5.291441  6.255576  1.357674
C    -4.723094  4.252562  1.924055
H    -5.398017  4.213147  2.776338
C    -3.918128  3.154215  1.630658
H    -3.971626  2.262347  2.251520
O     9.672081 -0.473050 -2.243183
C     8.634558 -1.189250 -1.645755
C     8.745370 -1.772704 -0.387064
H     9.662894 -1.698138  0.188959
C     7.650633 -2.454836  0.131771
H     7.736218 -2.894400  1.123457
C     6.450266 -2.583321 -0.578622
C     5.296784 -3.387812  0.040381
C     6.381178 -1.995460 -1.844067
H     5.471455 -2.059451 -2.433835
C     7.463721 -1.298945 -2.380551
H     7.398022 -0.827320 -3.357103
C     5.696443 -4.875299  0.010253
C     3.986695 -3.242718 -0.756659
C     5.056394 -2.879571  1.468631
C     5.120872 -3.693334  2.598916
H     5.357549 -4.749836  2.506703
C     4.887525 -3.184513  3.880311
H     4.948423 -3.843442  4.745572
C     4.581476 -1.835303  4.050848
O     4.348859 -1.278580  5.266771
C     4.509467 -1.001969  2.928690
H     4.263283  0.049375  3.058481
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C     4.744854 -1.525843  1.666258
H     4.684587 -0.860605  0.808378
H     4.440670 -1.951317  5.953274
H     5.880753 -5.183915 -1.026080
H     6.611282 -5.069406  0.583213
H     4.895042 -5.508885  0.411800
H     4.092439 -3.642366 -1.773336
H     3.656019 -2.199506 -0.826311
H     3.191499 -3.809435 -0.258990

133
P4-Z-ES     el energy= -4305.88255665
C     4.563372  1.173749  1.137069
C     5.918844  1.451916  1.139541
C     6.860390  0.385033  0.937580
C     6.321069 -0.985280  1.073480
C     4.950502 -1.223131  0.733898
C     4.063252 -0.159324  0.836774
C     4.586356 -2.607446  0.371315
C     5.386310 -3.674258  0.844322
C     6.565921 -3.380937  1.653389
C     7.057022 -2.025545  1.690604
C     3.526284 -2.893480 -0.508415
C     3.217605 -4.195636 -0.865995
C     3.978297 -5.255554 -0.359976
C     5.054412 -4.992649  0.468400
C     7.269350 -4.377524  2.337838
C     8.438080 -4.098892  3.036969
C     8.934494 -2.786302  3.073358
C     8.269585 -1.774410  2.417326
C     8.212491  0.541546  0.499643
C     9.057576  1.657671  0.807417
C    10.364908  1.713240  0.383148
C    10.949239  0.686856 -0.398895
C    10.134694 -0.420384 -0.706711
C     8.833509 -0.507262 -0.260253
C    12.345380  0.768818 -0.852523
C    12.968466  2.012326 -1.074012
C    14.284543  2.094704 -1.504844
C    15.005706  0.924973 -1.725670
C    14.428570 -0.323047 -1.514212
C    13.107771 -0.389666 -1.083341
C     2.589027 -0.348790  0.761877
C     1.815819  0.303341 -0.206497
C     0.438907  0.120430 -0.260805
C    -0.215420 -0.712881  0.656928
C     0.558670 -1.355089  1.632673
C     1.936265 -1.175563  1.683838
C    -1.686079 -0.909645  0.595758
C    -2.450154 -1.019844  1.767239
C    -3.825933 -1.203410  1.713896
C    -4.460683 -1.284904  0.476624
C    -3.728137 -1.193062 -0.704493
C    -2.350338 -0.998635 -0.632943
O    -5.824304 -1.486265  0.508268
C    -6.566615 -1.055282 -0.557906
F    -6.544103 -1.980396 -1.577609
C    -8.020249 -0.932546 -0.081816
F    -8.076592 -0.045047  0.940998
O    16.311946  1.099351 -2.165185
C    17.066281  0.013384 -2.365410
C    17.371073 -0.448381 -3.569381
F    17.563249 -0.562483 -1.268209
F    16.899251  0.067162 -4.681443
F    18.184065 -1.458202 -3.784289
H     2.946418 -2.081583 -0.932662
H     2.394237 -4.386629 -1.550032
H     3.746468 -6.280819 -0.638550
H     5.669299 -5.822623  0.803788
H     6.893596 -5.396719  2.342978
H     8.955866 -4.896486  3.564170
H     9.835703 -2.559487  3.638350
H     8.633117 -0.758053  2.511308
H     8.696647  2.447401  1.453472
H    10.972959  2.557148  0.701057
H    10.521752 -1.220969 -1.332734
H     8.237759 -1.366515 -0.552883
H    12.408895  2.933751 -0.935296
H    14.757033  3.056363 -1.685623
H    14.991355 -1.239131 -1.671665
H    12.677348 -1.369909 -0.895159
H     2.298453  0.957161 -0.928812
H    -0.137727  0.649927 -1.016232
H     0.082696 -2.020217  2.350139
H     2.518178 -1.690396  2.445051
H    -1.967111 -0.934632  2.737903
H    -4.419535 -1.271267  2.621502
H    -4.208614 -1.300003 -1.672138
H    -1.782960 -0.948280 -1.559441
C     6.355655  2.876475  1.261550
C     6.471012  3.474611  2.519041
H     6.241952  2.894784  3.410668
C     6.878802  4.803346  2.633537
H     6.965246  5.258177  3.617846
C     7.174341  5.545735  1.490785
H     7.494479  6.581347  1.580101
C     7.052390  4.956183  0.231916
H     7.276479  5.530716 -0.664161
C     6.642908  3.629918  0.118499
H     6.552978  3.168022 -0.862504
H    -6.215184 -0.098038 -0.960150
O    -8.780734 -0.528704 -1.129142
C   -10.159295 -0.470950 -0.928906
C   -10.734047  0.680009 -0.406006
H   -10.110707  1.518687 -0.111942
C   -12.116917  0.741656 -0.278337
H   -12.564238  1.645699  0.123011
C   -12.928386 -0.331022 -0.667124
C   -14.447460 -0.209557 -0.437955
C   -12.320185 -1.482252 -1.175931
H   -12.901484 -2.347761 -1.470208
C   -10.937067 -1.551709 -1.316404
H   -10.463912 -2.441265 -1.721197
C   -14.674297 -0.522815  1.066086
C   -15.261072 -1.235024 -1.273132
C   -14.969194  1.180790 -0.838883
C   -15.946384  1.872500 -0.119222
H   -16.365834  1.469615  0.795590
C   -16.418811  3.107255 -0.554255
H   -17.173891  3.630858  0.029150
C   -15.933156  3.667995 -1.736381
O   -16.352949  4.863787 -2.207096
C   -14.971591  2.977445 -2.479153
H   -14.598421  3.411362 -3.402865
C   -14.502248  1.751519 -2.031191
H   -13.751521  1.236210 -2.623601
H   -17.018806  5.233822 -1.612819
F   -14.030878 -1.633042  1.438522
F   -14.221889  0.472727  1.836006
F   -15.968214 -0.707792  1.373255
F   -15.092409 -2.502617 -0.860886
F   -14.907495 -1.187175 -2.562411
F   -16.571922 -0.986344 -1.213648
F    -8.453997 -2.109960  0.419592
C     3.571120  2.251327  1.436744
C     2.864724  2.214603  2.644906
H     3.052417  1.406065  3.348568
C     1.927081  3.198367  2.951272
H     1.389580  3.155434  3.896028
C     1.678070  4.232835  2.049620
H     0.944772  5.000479  2.286287
C     2.373502  4.275869  0.841752
H     2.183994  5.076567  0.130196
C     3.312488  3.292012  0.538364
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H     3.846478  3.326268 -0.408124

123
P1'-ES     el energy= -3479.63577212
C    -3.590625 -1.534512 -1.386348
C    -4.929677 -1.503781 -1.084945
C    -5.536769 -0.272124 -0.589109
C    -4.798919  0.909101 -0.609127
C    -3.509978  0.908538 -1.239917
C    -2.777047 -0.370086 -1.300875
C    -3.093488  2.068880 -1.935535
C    -3.763430  3.324384 -1.716659
C    -4.759264  3.403374 -0.651535
C    -5.261174  2.209278 -0.080802
C    -2.055423  2.021948 -2.923528
C    -1.716006  3.138180 -3.655359
C    -2.382731  4.354824 -3.438239
C    -3.390660  4.433319 -2.484617
C    -5.187953  4.640688 -0.126672
C    -6.064283  4.704523  0.941490
C    -6.513679  3.522640  1.541828
C    -6.109332  2.297490  1.038583
C    -6.958769 -0.311176 -0.160495
C    -7.385089 -1.174236  0.857141
C    -8.719957 -1.218079  1.243140
C    -9.679140 -0.413628  0.613367
C    -9.253570  0.439464 -0.414536
C    -7.917721  0.491505 -0.792531
C   -11.106791 -0.467692  1.017631
C   -11.712254 -1.683654  1.367087
C   -13.048613 -1.739497  1.743460
C   -13.797040 -0.567594  1.769327
C   -13.228699  0.656322  1.435137
C   -11.887653  0.693468  1.059617
C    -1.365392 -0.441159 -1.142188
C    -0.615368 -1.622013 -1.451881
C     0.752851 -1.659180 -1.328336
C     1.491602 -0.547890 -0.849334
C     0.763720  0.606247 -0.501257
C    -0.606362  0.672367 -0.651503
C     2.955486 -0.607005 -0.717069
C     3.631955  0.136859  0.269062
C     5.010775  0.073188  0.401798
C     5.751213 -0.736212 -0.459014
C     5.116446 -1.469837 -1.460021
C     3.731178 -1.406668 -1.572946
O     7.113818 -0.736015 -0.264941
C     7.829009 -1.820677 -0.698439
F     8.115976 -1.717745 -2.040169
C     9.158011 -1.844659  0.065331
F     9.870340 -2.924854 -0.344275
O   -15.128481 -0.714603  2.143251
C   -15.893049  0.379770  2.211005
C   -16.817021  0.679418  1.309679
F   -15.720499  1.146862  3.290263
F   -17.019763 -0.026761  0.220738
F   -17.638066  1.700704  1.410990
H    -1.576390  1.074747 -3.144433
H    -0.942815  3.068586 -4.417064
H    -2.122543  5.233967 -4.022804
H    -3.905122  5.380806 -2.351654
H    -4.800922  5.567708 -0.539648
H    -6.374489  5.671281  1.331025
H    -7.166745  3.560227  2.410440
H    -6.441858  1.391041  1.532306
H    -6.660089 -1.808124  1.362557
H    -9.016714 -1.875448  2.057697
H    -9.980650  1.053029 -0.942394
H    -7.612254  1.153805 -1.599284
H   -11.137907 -2.606112  1.324840
H   -13.521561 -2.682415  2.004006
H   -13.807623  1.575297  1.468014
H   -11.440308  1.654539  0.816765
H    -1.122409 -2.507268 -1.823875
H     1.274416 -2.580115 -1.579625
H     1.287200  1.484629 -0.130267
H    -1.121822  1.578198 -0.350641
H     3.068670  0.748339  0.969378
H     5.525169  0.631633  1.179207
H     5.687446 -2.063927 -2.167229
H     3.253838 -1.964321 -2.374730
C    -5.715296 -2.757897 -1.235627
C    -5.254121 -3.952050 -0.664234
H    -4.340921 -3.942053 -0.072352
C    -5.962224 -5.141872 -0.825360
H    -5.590858 -6.055459 -0.366203
C    -7.144771 -5.158629 -1.563139
H    -7.700150 -6.085510 -1.687204
C    -7.612065 -3.976937 -2.140430
H    -8.530322 -3.979978 -2.723571
C    -6.906478 -2.788591 -1.976846
H    -7.278508 -1.875268 -2.434404
H    -3.146343 -2.492295 -1.644175
O     9.837515 -0.696296 -0.135999
C    11.087641 -0.581141  0.480783
C    12.228047 -0.941137 -0.229007
H    12.135520 -1.345368 -1.233078
C    13.471481 -0.762943  0.364368
H    14.364889 -1.031166 -0.195749
C    13.599035 -0.236868  1.658738
C    15.000474 -0.108005  2.275075
C    12.431997  0.117764  2.339664
H    12.481664  0.535583  3.340665
C    11.174046 -0.049763  1.757689
H    10.270381  0.235534  2.288624
C    15.520439 -1.533838  2.542727
C    14.983674  0.641761  3.620933
C    15.902909  0.673003  1.308670
C    17.135403  0.199999  0.857694
H    17.497323 -0.777635  1.164091
C    17.940420  0.957233  0.003182
H    18.897202  0.561570 -0.335455
C    17.519444  2.217250 -0.417442
O    18.254966  3.002439 -1.245383
C    16.285550  2.709993  0.020134
H    15.956602  3.690705 -0.314819
C    15.498263  1.942553  0.866807
H    14.535660  2.338410  1.186738
H    19.072949  2.546095 -1.479704
H    14.819612 -2.060990  3.201496
H    15.616514 -2.118352  1.619841
H    16.497201 -1.512861  3.042413
H    14.407380  0.095057  4.378235
H    14.561782  1.649607  3.526582
H    16.010582  0.742753  3.992442
F     8.896181 -2.053942  1.379945
H     7.298121 -2.766873 -0.537279

123
P2'-ES     el energy= -4074.90740993
C    -4.789626  0.424626  1.783014
C    -6.105043  0.722189  1.528320
C    -6.876449 -0.110138  0.610377
C    -6.333121 -1.309482  0.155749
C    -5.084341 -1.753932  0.705090
C    -4.163435 -0.728966  1.231151
C    -4.880090 -3.142345  0.892158
C    -5.728509 -4.095647  0.226071
C    -6.686438 -3.603047 -0.759960
C    -6.973189 -2.218184 -0.817630
C    -3.885573 -3.640740  1.796538
C    -3.749597 -4.990493  2.034104
C    -4.586820 -5.910139  1.382042
C    -5.559048 -5.458001  0.497921
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C    -7.286432 -4.461768 -1.704763
C    -8.121989 -3.973253 -2.692769
C    -8.355523 -2.596271 -2.785546
C    -7.782220 -1.736640 -1.863517
C    -8.257394  0.317220  0.266819
C    -8.502522  1.559723 -0.331707
C    -9.798031  1.962145 -0.635837
C   -10.896013  1.144491 -0.336202
C   -10.650283 -0.092681  0.275798
C    -9.354784 -0.499770  0.569377
C   -12.280388  1.577175 -0.654058
C   -12.671585  2.915515 -0.501968
C   -13.965331  3.325046 -0.800735
C   -14.887195  2.387818 -1.254624
C   -14.534128  1.053435 -1.419774
C   -13.232684  0.660641 -1.115518
C    -2.754054 -0.824867  1.070643
C    -1.840022  0.023962  1.775997
C    -0.479586 -0.111951  1.640045
C     0.094254 -1.070001  0.765939
C    -0.792565 -1.880789  0.031177
C    -2.160530 -1.779721  0.179751
C     1.553275 -1.203510  0.635758
C     2.146455 -1.655936 -0.559170
C     3.522571 -1.776137 -0.681576
C     4.343190 -1.451107  0.397810
C     3.789892 -1.017394  1.601197
C     2.408626 -0.889374  1.705331
O     5.695988 -1.610957  0.198473
C     6.556852 -0.879289  0.972879
F     6.750713 -1.483448  2.193659
C     7.909731 -0.849986  0.249607
F     7.745359 -0.278281 -0.967789
O   -16.161316  2.878777 -1.519149
C   -17.076272  2.037241 -2.010529
C   -18.085499  1.561257 -1.295869
F   -16.959374  1.739136 -3.306833
F   -18.241994  1.805415 -0.014661
F   -19.044351  0.809574 -1.788863
H    -3.275416 -2.937440  2.352121
H    -3.004124 -5.340656  2.744332
H    -4.486634 -6.975312  1.576232
H    -6.207509 -6.189043  0.023491
H    -7.067491 -5.525440 -1.685584
H    -8.566704 -4.656039 -3.412914
H    -8.973202 -2.195527 -3.585703
H    -7.948102 -0.669939 -1.966104
H    -7.667483  2.212319 -0.575896
H    -9.955154  2.918871 -1.129491
H   -11.484612 -0.735884  0.547451
H    -9.188951 -1.459704  1.053025
H   -11.961255  3.647416 -0.124610
H   -14.271714  4.359873 -0.674297
H   -15.249378  0.321521 -1.785106
H   -12.953447 -0.379790 -1.264778
H    -2.215459  0.778040  2.461141
H     0.168756  0.556642  2.201990
H    -0.400790 -2.630017 -0.652899
H    -2.800447 -2.415268 -0.422972
H     1.525736 -1.885958 -1.421362
H     3.975704 -2.105889 -1.612583
H     4.416114 -0.807397  2.462844
H     1.992300 -0.575061  2.658862
C    -6.695811  1.925050  2.174472
C    -6.046474  3.164125  2.087486
H    -5.129050  3.245705  1.507826
C    -6.574374  4.293007  2.712283
H    -6.059343  5.247146  2.624407
C    -7.760848  4.201113  3.438050
H    -8.176096  5.081590  3.923109
C    -8.413582  2.971383  3.536727
H    -9.336577  2.887375  4.106157
C    -7.888183  1.845386  2.909931
H    -8.403693  0.892167  2.996625
H    -4.213426  1.124409  2.382603
H     6.203143  0.143166  1.150589
O     8.783222 -0.148596  1.012522
C    10.097966 -0.056419  0.557882
C    10.458093  0.976838 -0.297201
H     9.710344  1.679824 -0.651155
C    11.789101  1.101029 -0.677720
H    12.069180  1.915863 -1.338026
C    12.760913  0.206590 -0.213058
C    14.206430  0.381805 -0.718245
C    12.365004 -0.835848  0.629871
H    13.074125 -1.567732  0.997538
C    11.036183 -0.964746  1.024506
H    10.730262 -1.766118  1.690224
C    14.241920 -0.255946 -2.133441
C    15.242019 -0.357745  0.171907
C    14.625533  1.862136 -0.724240
C    15.398645  2.440476 -1.733912
H    15.715981  1.870790 -2.599941
C    15.792312  3.773816 -1.662494
H    16.386466  4.203876 -2.467090
C    15.434322  4.553183 -0.561338
O    15.786781  5.852075 -0.434793
C    14.678655  3.982865  0.466621
H    14.405106  4.588444  1.326389
C    14.284516  2.656144  0.379739
H    13.693797  2.237531  1.189429
H    16.309932  6.126071 -1.199523
F    13.678815 -1.467587 -2.140008
F    13.571964  0.495267 -3.014087
F    15.488804 -0.409319 -2.607339
F    15.156535 -1.695313  0.079746
F    15.077384 -0.037885  1.460530
F    16.494340 -0.032249 -0.158694
F     8.352516 -2.105510  0.017318

133
P3'-ES     el energy= -3710.61114351
C     3.267136 -1.877610 -0.699958
C     4.631249 -1.787023 -0.913405
C     5.282844 -0.510501 -0.805009
C     4.393291  0.670547 -0.789237
C     3.073895  0.534001 -0.250334
C     2.486445 -0.724679 -0.278703
C     2.419860  1.767956  0.228501
C     2.837866  3.015333 -0.291867
C     3.922455  3.055972 -1.268684
C     4.734333  1.877349 -1.447414
C     1.462290  1.749487  1.259120
C     0.882034  2.917618  1.725088
C     1.258525  4.148625  1.176315
C     2.232547  4.192767  0.195213
C     4.238560  4.213847 -1.987154
C     5.321994  4.262703 -2.856691
C     6.124724  3.125467 -3.037142
C     5.846163  1.963875 -2.352049
C     6.681521 -0.311544 -0.585718
C     7.722926 -1.162044 -1.082882
C     9.051468 -0.881443 -0.864764
C     9.472141  0.248727 -0.121508
C     8.462525  1.100342  0.368609
C     7.127781  0.851319  0.130211
C    10.897069  0.524907  0.111693
C    11.841909 -0.517984  0.171287
C    13.186413 -0.263014  0.398802
C    13.612625  1.050501  0.572712
C    12.712772  2.109825  0.511949
C    11.367588  1.838217  0.285742
C     1.036399 -0.926455 -0.008818
C     0.589168 -1.766240  1.018639
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C    -0.769264 -1.956471  1.243950
C    -1.729093 -1.322614  0.442985
C    -1.279837 -0.489146 -0.589896
C     0.078787 -0.294182 -0.810906
C    -3.180394 -1.530172  0.680264
C    -4.078148 -1.640877 -0.392128
C    -5.437242 -1.827815 -0.175227
C    -5.919927 -1.913875  1.128683
C    -5.051440 -1.824863  2.213949
C    -3.692551 -1.625216  1.979172
O    -7.276863 -2.116858  1.258479
C    -7.889392 -1.690341  2.405762
F    -7.759724 -2.627608  3.407166
C    -9.386458 -1.546266  2.103058
F    -9.892011 -2.718838  1.656509
F   -10.042919 -1.277434  3.260279
O    14.972111  1.214791  0.806319
C    15.440590  2.453872  0.989489
C    15.787321  2.932490  2.175369
F    15.605159  3.185227 -0.115405
F    15.633858  2.265430  3.296352
F    16.331883  4.114164  2.359516
H     1.181953  0.805947  1.713788
H     0.146939  2.873281  2.525146
H     0.811438  5.071537  1.538101
H     2.552674  5.161036 -0.177917
H     3.619392  5.100232 -1.883591
H     5.534576  5.177371 -3.404868
H     6.957967  3.150965 -3.735646
H     6.436875  1.078590 -2.555008
H     7.476229 -2.006018 -1.713882
H     9.795890 -1.531038 -1.319449
H     8.728428  1.963717  0.974321
H     6.387948  1.519750  0.560042
H    11.519268 -1.550771  0.067402
H    13.909042 -1.072398  0.458100
H    13.043184  3.138391  0.628489
H    10.678613  2.675788  0.213138
H     1.313107 -2.273827  1.651327
H    -1.087244 -2.625401  2.040880
H    -2.000916  0.028189 -1.219411
H     0.404798  0.361916 -1.614915
H    -3.708625 -1.593356 -1.413865
H    -6.132963 -1.910584 -1.005863
H    -5.415624 -1.919659  3.232429
H    -3.023681 -1.534297  2.832005
C     2.563509 -3.184893 -0.877935
C     2.729776 -4.239070  0.026700
H     3.389924 -4.111090  0.881169
C     2.051626 -5.442957 -0.152710
H     2.190777 -6.251024  0.562158
C     1.195744 -5.609974 -1.240857
H     0.665336 -6.549192 -1.380746
C     1.022670 -4.564830 -2.147922
H     0.357009 -4.684923 -2.999862
C     1.700353 -3.361186 -1.965566
H     1.557946 -2.545591 -2.671730
C     5.397543 -3.047068 -1.159025
C     5.448876 -3.602467 -2.440110
H     4.931808 -3.107134 -3.259194
C     6.158056 -4.780910 -2.670663
H     6.190758 -5.203595 -3.672383
C     6.821262 -5.415245 -1.620893
H     7.375183 -6.333849 -1.800760
C     6.766983 -4.869367 -0.337811
H     7.277649 -5.361521  0.486944
C     6.057141 -3.693275 -0.108348
H     6.018241 -3.265117  0.891108
H    -7.484967 -0.741762  2.777288
O    -9.547247 -0.552839  1.199673
C   -10.843368 -0.325538  0.726237
C   -11.687267  0.539684  1.414386
H   -11.354029  1.005818  2.337099
C   -12.948381  0.801331  0.892449
H   -13.604782  1.487541  1.423598
C   -13.385362  0.213681 -0.303954
C   -14.808402  0.506912 -0.803121
C   -12.508276 -0.645766 -0.970336
H   -12.800498 -1.118976 -1.902939
C   -11.237931 -0.919771 -0.461639
H   -10.556720 -1.585772 -0.983826
C   -15.786957 -0.200951  0.154169
C   -15.058957 -0.046150 -2.219256
C   -15.025365  2.026487 -0.842626
C   -16.096073  2.664176 -0.215665
H   -16.818803  2.092568  0.360034
C   -16.275620  4.046768 -0.301856
H   -17.119674  4.517249  0.200770
C   -15.374567  4.823563 -1.027428
O   -15.492119  6.170635 -1.148751
C   -14.292572  4.205131 -1.662860
H   -13.587974  4.813915 -2.224216
C   -14.129266  2.830494 -1.564662
H   -13.273973  2.369709 -2.056402
H   -16.268162  6.472537 -0.659927
H   -15.561840 -1.274093  0.179977
H   -15.710484  0.182161  1.178884
H   -16.824937 -0.085313 -0.182576
H   -14.992406 -1.141325 -2.240429
H   -14.348929  0.357609 -2.951170
H   -16.068833  0.232438 -2.543742

133
P4'-ES     el energy= -4305.88255665
C     4.563372  1.173749  1.137069
C     5.918844  1.451916  1.139541
C     6.860390  0.385033  0.937580
C     6.321069 -0.985280  1.073480
C     4.950502 -1.223131  0.733898
C     4.063252 -0.159324  0.836774
C     4.586356 -2.607446  0.371315
C     5.386310 -3.674258  0.844322
C     6.565921 -3.380937  1.653389
C     7.057022 -2.025545  1.690604
C     3.526284 -2.893480 -0.508415
C     3.217605 -4.195636 -0.865995
C     3.978297 -5.255554 -0.359976
C     5.054412 -4.992649  0.468400
C     7.269350 -4.377524  2.337838
C     8.438080 -4.098892  3.036969
C     8.934494 -2.786302  3.073358
C     8.269585 -1.774410  2.417326
C     8.212491  0.541546  0.499643
C     9.057576  1.657671  0.807417
C    10.364908  1.713240  0.383148
C    10.949239  0.686856 -0.398895
C    10.134694 -0.420384 -0.706711
C     8.833509 -0.507262 -0.260253
C    12.345380  0.768818 -0.852523
C    12.968466  2.012326 -1.074012
C    14.284543  2.094704 -1.504844
C    15.005706  0.924973 -1.725670
C    14.428570 -0.323047 -1.514212
C    13.107771 -0.389666 -1.083341
C     2.589027 -0.348790  0.761877
C     1.815819  0.303341 -0.206497
C     0.438907  0.120430 -0.260805
C    -0.215420 -0.712881  0.656928
C     0.558670 -1.355089  1.632673
C     1.936265 -1.175563  1.683838
C    -1.686079 -0.909645  0.595758
C    -2.450154 -1.019844  1.767239
C    -3.825933 -1.203410  1.713896
C    -4.460683 -1.284904  0.476624
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C    -3.728137 -1.193062 -0.704493
C    -2.350338 -0.998635 -0.632943
O    -5.824304 -1.486265  0.508268
C    -6.566615 -1.055282 -0.557906
F    -6.544103 -1.980396 -1.577609
C    -8.020249 -0.932546 -0.081816
F    -8.076592 -0.045047  0.940998
O    16.311946  1.099351 -2.165185
C    17.066281  0.013384 -2.365410
C    17.371073 -0.448381 -3.569381
F    17.563249 -0.562483 -1.268209
F    16.899251  0.067162 -4.681443
F    18.184065 -1.458202 -3.784289
H     2.946418 -2.081583 -0.932662
H     2.394237 -4.386629 -1.550032
H     3.746468 -6.280819 -0.638550
H     5.669299 -5.822623  0.803788
H     6.893596 -5.396719  2.342978
H     8.955866 -4.896486  3.564170
H     9.835703 -2.559487  3.638350
H     8.633117 -0.758053  2.511308
H     8.696647  2.447401  1.453472
H    10.972959  2.557148  0.701057
H    10.521752 -1.220969 -1.332734
H     8.237759 -1.366515 -0.552883
H    12.408895  2.933751 -0.935296
H    14.757033  3.056363 -1.685623
H    14.991355 -1.239131 -1.671665
H    12.677348 -1.369909 -0.895159
H     2.298453  0.957161 -0.928812
H    -0.137727  0.649927 -1.016232
H     0.082696 -2.020217  2.350139
H     2.518178 -1.690396  2.445051
H    -1.967111 -0.934632  2.737903
H    -4.419535 -1.271267  2.621502
H    -4.208614 -1.300003 -1.672138
H    -1.782960 -0.948280 -1.559441
C     6.355655  2.876475  1.261550
C     6.471012  3.474611  2.519041
H     6.241952  2.894784  3.410668
C     6.878802  4.803346  2.633537
H     6.965246  5.258177  3.617846
C     7.174341  5.545735  1.490785
H     7.494479  6.581347  1.580101
C     7.052390  4.956183  0.231916
H     7.276479  5.530716 -0.664161
C     6.642908  3.629918  0.118499
H     6.552978  3.168022 -0.862504
H    -6.215184 -0.098038 -0.960150
O    -8.780734 -0.528704 -1.129142
C   -10.159295 -0.470950 -0.928906
C   -10.734047  0.680009 -0.406006
H   -10.110707  1.518687 -0.111942
C   -12.116917  0.741656 -0.278337
H   -12.564238  1.645699  0.123011
C   -12.928386 -0.331022 -0.667124
C   -14.447460 -0.209557 -0.437955
C   -12.320185 -1.482252 -1.175931
H   -12.901484 -2.347761 -1.470208
C   -10.937067 -1.551709 -1.316404
H   -10.463912 -2.441265 -1.721197
C   -14.674297 -0.522815  1.066086
C   -15.261072 -1.235024 -1.273132
C   -14.969194  1.180790 -0.838883
C   -15.946384  1.872500 -0.119222
H   -16.365834  1.469615  0.795590
C   -16.418811  3.107255 -0.554255
H   -17.173891  3.630858  0.029150
C   -15.933156  3.667995 -1.736381
O   -16.352949  4.863787 -2.207096
C   -14.971591  2.977445 -2.479153
H   -14.598421  3.411362 -3.402865
C   -14.502248  1.751519 -2.031191
H   -13.751521  1.236210 -2.623601
H   -17.018806  5.233822 -1.612819
F   -14.030878 -1.633042  1.438522
F   -14.221889  0.472727  1.836006
F   -15.968214 -0.707792  1.373255
F   -15.092409 -2.502617 -0.860886
F   -14.907495 -1.187175 -2.562411
F   -16.571922 -0.986344 -1.213648
F    -8.453997 -2.109960  0.419592
C     3.571120  2.251327  1.436744
C     2.864724  2.214603  2.644906
H     3.052417  1.406065  3.348568
C     1.927081  3.198367  2.951272
H     1.389580  3.155434  3.896028
C     1.678070  4.232835  2.049620
H     0.944772  5.000479  2.286287
C     2.373502  4.275869  0.841752
H     2.183994  5.076567  0.130196
C     3.312488  3.292012  0.538364
H     3.846478  3.326268 -0.408124

121
P1-E-ES     el energy= -3379.16128821
C    -2.725882  1.178856 -1.851705
C    -4.022755  0.737953 -1.760140
C    -4.681250  0.675635 -0.458666
C    -4.058348  1.244480  0.649552
C    -2.850270  1.993866  0.454254
C    -2.015805  1.656590 -0.714430
C    -2.617781  3.130480  1.265393
C    -3.370260  3.320513  2.477812
C    -4.245970  2.242461  2.927681
C    -4.574426  1.196173  2.033165
C    -1.693907  4.156229  0.878155
C    -1.539687  5.298767  1.631674
C    -2.286700  5.476300  2.807539
C    -3.186543  4.497452  3.212021
C    -4.720896  2.178548  4.254360
C    -5.476438  1.107889  4.696926
C    -5.751327  0.046139  3.827064
C    -5.299048  0.091964  2.518893
C    -6.040263  0.079955 -0.384410
C    -6.277761 -1.237038 -0.798410
C    -7.554039 -1.784795 -0.738433
C    -8.641967 -1.029906 -0.279561
C    -8.405796  0.293158  0.119641
C    -7.128231  0.836839  0.070451
C   -10.006138 -1.613438 -0.223272
C   -10.458973 -2.485554 -1.224107
C   -11.733715 -3.036264 -1.175764
C   -12.574747 -2.711395 -0.116821
C   -12.158637 -1.853182  0.894614
C   -10.877031 -1.310738  0.830171
C    -0.594850  1.672194 -0.657772
C     0.223186  1.594978 -1.831565
C     1.594672  1.646447 -1.759149
C     2.275909  1.738118 -0.518941
C     1.485720  1.775654  0.646107
C     0.107305  1.757639  0.589763
C     3.745270  1.784445 -0.454169
C     4.443733  1.268302  0.654419
C     5.828529  1.312978  0.720609
C     6.545381  1.877241 -0.330793
C     5.893029  2.399200 -1.443084
C     4.503908  2.346015 -1.495570
O     7.925205  1.867363 -0.189091
C     8.670880  2.466560 -1.123914
F     8.723667  3.797806 -1.041482
C     9.363054  1.802133 -2.042302
F    10.192173  2.435501 -2.875319
O   -13.836579 -3.295401 -0.152495
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C   -14.676720 -3.055898  0.859257
C   -15.716964 -2.240614  0.764056
F   -14.449523 -3.742365  1.981770
F   -15.979578 -1.527255 -0.307269
F   -16.603345 -2.065565  1.718577
H    -1.157364  4.059857 -0.059011
H    -0.851513  6.073359  1.301156
H    -2.173400  6.383058  3.396788
H    -3.768350  4.667274  4.113678
H    -4.463229  2.963726  4.959356
H    -5.825229  1.079129  5.726529
H    -6.305643 -0.821767  4.176188
H    -5.494566 -0.750846  1.865014
H    -5.450173 -1.845013 -1.156578
H    -7.702274 -2.820587 -1.036669
H    -9.235622  0.913949  0.450877
H    -6.970457  1.868386  0.376858
H    -9.814273 -2.723473 -2.066882
H   -12.088227 -3.704434 -1.955873
H   -12.809488 -1.606362  1.729071
H   -10.547346 -0.655898  1.633464
H    -0.237465  1.523632 -2.812334
H     2.166774  1.585160 -2.682143
H     1.962663  1.848982  1.620743
H    -0.453247  1.766900  1.518335
H     3.899988  0.796446  1.468742
H     6.363612  0.902414  1.572569
H     6.447937  2.849075 -2.262104
H     4.004775  2.782338 -2.356949
C    -4.707330  0.293172 -3.003654
C    -4.091275 -0.631861 -3.857889
H    -3.127615 -1.054560 -3.580377
C    -4.708914 -1.033018 -5.041515
H    -4.217613 -1.758988 -5.685718
C    -5.953862 -0.513701 -5.392789
H    -6.438776 -0.828363 -6.314101
C    -6.574973  0.411851 -4.552813
H    -7.543605  0.828245 -4.820507
C    -5.959680  0.809473 -3.369646
H    -6.451616  1.533646 -2.725034
H    -2.227674  1.106440 -2.814912
O     9.249456  0.486533 -2.240582
C    10.268173 -0.344293 -1.782284
C    11.344376  0.113625 -1.028246
H    11.442756  1.163913 -0.766088
C    12.297298 -0.804046 -0.598564
H    13.129494 -0.444236  0.003269
C    12.208224 -2.167629 -0.906899
C    13.317629 -3.116826 -0.429340
C    11.114470 -2.588657 -1.667970
H    10.993961 -3.635347 -1.931467
C    10.145879 -1.687053 -2.107630
H     9.294277 -2.020767 -2.694569
C    14.595775 -2.776169 -1.219892
C    12.980550 -4.595105 -0.703258
C    13.505075 -2.948294  1.085751
C    14.741858 -2.701916  1.682286
H    15.635041 -2.589137  1.073963
C    14.876173 -2.590734  3.068421
H    15.854925 -2.396329  3.505548
C    13.759351 -2.727144  3.890609
O    13.821736 -2.630106  5.243453
C    12.508619 -2.971209  3.313558
H    11.637832 -3.071399  3.956888
C    12.394360 -3.077059  1.934624
H    11.410322 -3.256120  1.504308
H    14.735257 -2.472930  5.513858
H    14.396139 -2.867267 -2.294567
H    14.938056 -1.751966 -1.028346
H    15.413100 -3.465578 -0.972773
H    12.899120 -4.795412 -1.779317
H    12.042837 -4.899718 -0.222893
H    13.781460 -5.230075 -0.305514

121
P2-E-ES     el energy= -3974.43402530
C    -4.003401  0.881448 -2.044444
C    -5.286398  0.422950 -1.874632
C    -5.965669  0.613217 -0.595874
C    -5.386201  1.432685  0.369055
C    -4.202913  2.169763  0.027765
C    -3.332922  1.617169 -1.027611
C    -4.028529  3.464202  0.572237
C    -4.811938  3.885222  1.704819
C    -5.658412  2.897583  2.369367
C    -5.926647  1.666826  1.723990
C    -3.132527  4.414894 -0.018608
C    -3.031883  5.699082  0.468894
C    -3.807407  6.099992  1.568607
C    -4.681939  5.199861  2.166049
C    -6.162454  3.106631  3.670124
C    -6.884568  2.127393  4.328248
C    -7.095759  0.888600  3.712081
C    -6.616384  0.665441  2.432022
C    -7.297889 -0.016744 -0.405643
C    -7.464918 -1.402533 -0.523366
C    -8.714711 -1.987379 -0.354391
C    -9.844934 -1.206144 -0.078813
C    -9.679212  0.182285  0.023329
C    -8.428258  0.765748 -0.135069
C   -11.180616 -1.830739  0.096230
C   -11.579315 -2.917163 -0.696210
C   -12.828407 -3.504149 -0.535542
C   -13.697438 -3.001093  0.426741
C   -13.333767 -1.929370  1.234180
C   -12.077823 -1.352649  1.058509
C    -1.914885  1.694816 -0.950755
C    -1.063975  1.391102 -2.062265
C     0.303206  1.503861 -1.974224
C     0.945971  1.887634 -0.770522
C     0.124183  2.152992  0.341431
C    -1.251146  2.076260  0.261521
C     2.411426  1.997467 -0.686714
C     3.092384  1.746420  0.519739
C     4.472660  1.855609  0.606204
C     5.200403  2.217714 -0.523203
C     4.566033  2.471865 -1.734600
C     3.181244  2.358505 -1.805804
O     6.577349  2.285044 -0.355699
C     7.311059  2.842358 -1.323798
F     7.232641  4.171365 -1.403452
C     8.114209  2.149372 -2.122965
F     8.930717  2.757119 -2.984582
O   -14.930683 -3.638210  0.511987
C   -15.798130 -3.221616  1.439756
C   -16.879196 -2.508884  1.158428
F   -15.552017 -3.620477  2.690175
F   -17.164129 -2.073418 -0.047675
F   -17.788298 -2.172647  2.046042
H    -2.575524  4.138076 -0.906640
H    -2.363604  6.408107 -0.014328
H    -3.736172  7.116538  1.947810
H    -5.285142  5.541953  3.002206
H    -5.956367  4.038624  4.188493
H    -7.256292  2.311569  5.333492
H    -7.622005  0.095179  4.237335
H    -6.762612 -0.308404  1.977701
H    -6.603144 -2.031599 -0.734223
H    -8.808493 -3.069264 -0.420202
H   -10.543561  0.817225  0.206548
H    -8.324690  1.845761 -0.059422
H   -10.912983 -3.299144 -1.466115
H   -13.141875 -4.339226 -1.156004
H   -14.004703 -1.542862  1.996611
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H   -11.787914 -0.526663  1.703829
H    -1.495478  1.090950 -3.012521
H     0.903842  1.261838 -2.848101
H     0.572999  2.453706  1.285418
H    -1.840054  2.271133  1.151438
H     2.538893  1.435372  1.402067
H     4.995422  1.652097  1.536818
H     5.132965  2.759658 -2.616374
H     2.693619  2.586895 -2.750207
C    -5.934281 -0.299487 -3.001841
C    -5.272599 -1.360326 -3.635648
H    -4.299752 -1.679040 -3.266503
C    -5.856165 -2.024703 -4.713254
H    -5.329526 -2.851365 -5.185120
C    -7.112110 -1.637554 -5.177758
H    -7.570394 -2.156956 -6.016289
C    -7.778661 -0.579404 -4.557996
H    -8.756311 -0.264908 -4.916563
C    -7.197480  0.081216 -3.479867
H    -7.724554  0.906494 -3.007642
H    -3.484755  0.622845 -2.964161
O     8.134823  0.812021 -2.167450
C     9.195032  0.146257 -1.572474
C    10.127299  0.773807 -0.754634
H    10.073814  1.839990 -0.552016
C    11.137499  0.009624 -0.180376
H    11.855944  0.505808  0.465037
C    11.234212 -1.366610 -0.409563
C    12.418948 -2.125544  0.216250
C    10.293173 -1.965478 -1.253431
H    10.331933 -3.023091 -1.486046
C     9.271878 -1.216812 -1.827006
H     8.535847 -1.685028 -2.474207
C    13.639233 -1.841848 -0.701253
C    12.189091 -3.660364  0.253033
C    12.660112 -1.692246  1.672496
C    13.932405 -1.530146  2.226156
H    14.828603 -1.667196  1.631756
C    14.094728 -1.186769  3.565251
H    15.096769 -1.055206  3.969965
C    12.979005 -1.019498  4.386892
O    13.073367 -0.689167  5.694531
C    11.700062 -1.197858  3.852357
H    10.832002 -1.072296  4.493842
C    11.550685 -1.529866  2.513984
H    10.546511 -1.658269  2.120034
H    14.002733 -0.604328  5.944596
F    13.337199 -2.023585 -1.990262
F    14.054197 -0.577173 -0.568062
F    14.690674 -2.635203 -0.438864
F    12.205024 -4.223881 -0.966719
F    11.008146 -3.952900  0.809124
F    13.128017 -4.281627  0.971740

131
P3-E-ES     el energy= -3610.13664372
C    -3.093616  1.830460 -0.566688
C    -4.471799  1.941468 -0.496825
C    -5.288597  0.778011 -0.702029
C    -4.605421 -0.398429 -1.282240
C    -3.210922 -0.586235 -1.015572
C    -2.445624  0.538726 -0.737870
C    -2.691511 -1.963268 -1.132107
C    -3.376810 -2.889029 -1.953543
C    -4.593335 -2.468834 -2.643574
C    -5.230857 -1.241288 -2.232201
C    -1.593244 -2.410231 -0.375187
C    -1.137236 -3.714898 -0.467839
C    -1.784524 -4.619357 -1.316941
C    -2.895798 -4.212753 -2.033434
C    -5.193160 -3.243954 -3.641462
C    -6.394603 -2.872206 -4.233936
C    -7.031560 -1.685636 -3.837888
C    -6.472649 -0.890155 -2.862728
C    -6.648939  0.634950 -0.282930
C    -7.611722  1.695286 -0.233929
C    -8.917820  1.469327  0.134379
C    -9.385146  0.184768  0.504504
C    -8.453582 -0.870423  0.459017
C    -7.149335 -0.666318  0.061181
C   -10.784117 -0.038263  0.898560
C   -11.538502  0.975910  1.519214
C   -12.857994  0.767585  1.894056
C   -13.449243 -0.469078  1.653080
C   -12.739584 -1.495391  1.038034
C   -11.417048 -1.272189  0.669368
C    -0.957914  0.495452 -0.720863
C    -0.223838  0.864371  0.413219
C     1.165848  0.829155  0.405448
C     1.870976  0.435027 -0.739999
C     1.134945  0.074241 -1.876428
C    -0.254723  0.103921 -1.866391
C     3.355545  0.402090 -0.751505
C     4.076297  0.795822 -1.888514
C     5.465126  0.762916 -1.907020
C     6.150714  0.328949 -0.777221
C     5.469145 -0.063625  0.369359
C     4.076593 -0.024556  0.369933
O     7.535609  0.309480 -0.885949
C     8.255045 -0.010064  0.195476
F     8.361276  0.952621  1.113280
C     8.870078 -1.176116  0.358694
F     8.762236 -2.135870 -0.562186
O   -14.768311 -0.595188  2.071002
C   -15.423081 -1.723693  1.778047
C   -15.716095 -2.649739  2.679429
F   -15.834625 -1.847546  0.514185
F   -15.322806 -2.589420  3.931223
F   -16.442045 -3.715881  2.427264
H    -1.100628 -1.729062  0.309499
H    -0.287299 -4.033451  0.130890
H    -1.437156 -5.647025 -1.392866
H    -3.419538 -4.945186 -2.640427
H    -4.709451 -4.154226 -3.984049
H    -6.828857 -3.494767 -5.012454
H    -7.958510 -1.378284 -4.316553
H    -6.944406  0.054410 -2.619512
H    -7.339438  2.688528 -0.566928
H    -9.616244  2.302226  0.093018
H    -8.752066 -1.869783  0.767614
H    -6.461972 -1.506690  0.076122
H   -11.080443  1.936818  1.739654
H   -13.433069  1.549000  2.383328
H   -13.201467 -2.458241  0.836577
H   -10.880931 -2.071402  0.164015
H    -0.746715  1.178912  1.313089
H     1.710611  1.133742  1.296636
H     1.653918 -0.250950 -2.775674
H    -0.806010 -0.186238 -2.758025
H     3.545955  1.152456 -2.768454
H     6.024130  1.073232 -2.785594
H     6.002039 -0.407772  1.251803
H     3.546085 -0.352697  1.260854
C    -2.230427  3.045010 -0.445244
C    -2.089777  3.735000  0.763650
H    -2.623924  3.386292  1.644076
C    -1.264506  4.854244  0.851544
H    -1.164675  5.376039  1.800804
C    -0.566708  5.300817 -0.270032
H     0.078755  6.173587 -0.201524
C    -0.699581  4.619930 -1.479888
H    -0.159474  4.959860 -2.360843
C    -1.523695  3.500018 -1.565036
H    -1.619640  2.967609 -2.509159
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C    -5.061106  3.261076 -0.113949
C    -5.226613  4.264999 -1.071476
H    -4.927830  4.077666 -2.100688
C    -5.770549  5.498355 -0.714066
H    -5.894002  6.272479 -1.468178
C    -6.153574  5.738423  0.605003
H    -6.578852  6.699894  0.883790
C    -5.984115  4.741872  1.566982
H    -6.275979  4.923743  2.598970
C    -5.439350  3.511020  1.209341
H    -5.310837  2.732211  1.958172
O     9.582593 -1.500904  1.440994
C    10.966071 -1.594517  1.314513
C    11.659209 -1.153623  0.191034
H    11.138193 -0.716878 -0.657135
C    13.045199 -1.269016  0.172974
H    13.584112 -0.910980 -0.701981
C    13.759278 -1.817568  1.246164
C    15.285840 -1.952182  1.139252
C    13.028568 -2.248238  2.356654
H    13.532610 -2.677540  3.217519
C    11.638738 -2.142000  2.396904
H    11.076025 -2.476373  3.264467
C    15.584541 -3.036412  0.085609
C    15.927303 -2.401828  2.466127
C    15.885469 -0.589504  0.761644
C    16.755060 -0.405573 -0.313705
H    17.024625 -1.240389 -0.954708
C    17.303857  0.845792 -0.604741
H    17.978686  0.959143 -1.452460
C    16.987039  1.947757  0.187165
O    17.484534  3.189846 -0.042848
C    16.116676  1.786434  1.270335
H    15.866992  2.648933  1.883476
C    15.580048  0.536106  1.543024
H    14.894508  0.434169  2.382757
H    18.053232  3.170189 -0.822968
H    15.095806 -3.974094  0.377049
H    15.211394 -2.758872 -0.907664
H    16.661733 -3.231514  0.008452
H    15.590934 -3.405948  2.754605
H    15.700533 -1.712105  3.288195
H    17.017260 -2.436257  2.349446

131
P4-E-ES     el energy= -4205.42838610
C     4.345648 -1.440898 -0.160043
C     5.771094 -1.464896 -0.069163
C     6.512436 -0.286391 -0.326847
C     5.822164  0.925345 -0.643538
C     4.407785  1.013691 -0.299374
C     3.660603 -0.206784 -0.274297
C     3.879180  2.307767  0.014195
C     4.585033  3.487498 -0.417783
C     5.782047  3.341879 -1.213595
C     6.407255  2.047642 -1.317405
C     2.709001  2.484716  0.804679
C     2.229631  3.737897  1.122228
C     2.907740  4.888197  0.674158
C     4.064564  4.754577 -0.070050
C     6.376872  4.434082 -1.885477
C     7.521279  4.285123 -2.645940
C     8.110065  3.013376 -2.786295
C     7.558795  1.925074 -2.144419
C     7.991078 -0.283585 -0.202684
C     8.804369 -1.203557 -0.881433
C    10.186622 -1.165501 -0.752943
C    10.811792 -0.216961  0.069026
C     9.999290  0.697603  0.753226
C     8.617231  0.669136  0.614461
C    12.289339 -0.182701  0.207604
C    13.038212 -1.368424  0.241185
C    14.421481 -1.342543  0.369300
C    15.071971 -0.117312  0.468667
C    14.363057  1.078092  0.432263
C    12.976570  1.033230  0.304794
C     2.186799 -0.174337 -0.445785
C     1.309084 -0.809133  0.446018
C    -0.066122 -0.747925  0.259838
C    -0.619400 -0.059405 -0.828902
C     0.256966  0.572555 -1.721779
C     1.632016  0.521249 -1.530201
C    -2.089093 -0.002713 -1.029449
C    -2.645603 -0.078535 -2.314785
C    -4.020752 -0.030030 -2.507693
C    -4.858153  0.092566 -1.403989
C    -4.341534  0.176409 -0.115870
C    -2.960481  0.126113  0.058715
O    -6.219947  0.114280 -1.681843
C    -7.072614  0.302635 -0.670135
F    -7.162016  1.556536 -0.224980
C    -7.830168 -0.656476 -0.150782
O    16.454673 -0.180851  0.601343
C    17.129614  0.961379  0.765802
C    17.632263  1.347876  1.929261
F    17.332388  1.685386 -0.338037
F    17.452920  0.685131  3.049130
F    18.372384  2.421890  2.089897
H     2.196526  1.614241  1.197063
H     1.338251  3.833437  1.737586
H     2.538072  5.877906  0.930423
H     4.590971  5.654666 -0.372224
H     5.918316  5.416619 -1.830002
H     7.948549  5.145296 -3.155441
H     8.986137  2.882260 -3.416654
H     7.998578  0.946858 -2.299086
H     8.351073 -1.941420 -1.537688
H    10.790263 -1.871059 -1.319805
H    10.450832  1.428907  1.420278
H     8.008669  1.388523  1.157709
H    12.532492 -2.329676  0.188113
H    15.000957 -2.260898  0.406553
H    14.870273  2.037128  0.490067
H    12.427420  1.970586  0.255641
H     1.706430 -1.349984  1.300480
H    -0.719452 -1.260347  0.962999
H    -0.140870  1.129851 -2.567346
H     2.290644  1.029788 -2.230641
H    -1.996595 -0.198728 -3.179062
H    -4.452163 -0.099737 -3.502506
H    -4.992860  0.285157  0.747141
H    -2.559211  0.211406  1.065842
C     6.471280 -2.728675  0.291431
C     6.431923 -3.848874 -0.549432
H     5.877506 -3.797713 -1.483595
C     7.099916 -5.020690 -0.203574
H     7.063007 -5.878275 -0.871731
C     7.813871 -5.094559  0.992710
H     8.334568 -6.010346  1.263355
C     7.856645 -3.986863  1.839085
H     8.409100 -4.034595  2.774908
C     7.192680 -2.813267  1.489635
H     7.233387 -1.949747  2.150027
O    -8.685989 -0.464694  0.861068
C   -10.042177 -0.429955  0.580508
C   -10.881588 -0.272540  1.678107
H   -10.456843 -0.197236  2.674973
C   -12.252833 -0.203106  1.478729
H   -12.897821 -0.069117  2.341726
C   -12.805358 -0.291893  0.194143
C   -14.338925 -0.262374  0.058074
C   -11.940490 -0.475679 -0.886031
H   -12.313441 -0.579075 -1.898186
C   -10.560325 -0.537801 -0.703287
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H    -9.912984 -0.672855 -1.565042
C   -14.826036 -1.693859  0.410889
C   -14.802317  0.063286 -1.387529
C   -14.962903  0.814997  0.962051
C   -16.152871  0.632035  1.670398
H   -16.687239 -0.310744  1.643268
C   -16.696820  1.657846  2.438239
H   -17.620084  1.486549  2.989046
C   -16.066230  2.901581  2.495761
O   -16.545197  3.934891  3.224310
C   -14.887130  3.107079  1.774187
H   -14.399466  4.077272  1.814420
C   -14.349654  2.074418  1.020360
H   -13.428965  2.257088  0.473527
H   -17.354351  3.668314  3.679810
F   -14.122915 -2.626323 -0.238598
F   -14.689122 -1.937025  1.719163
F   -16.116060 -1.901601  0.100533
F   -14.540097 -0.924553 -2.259916
F   -14.199165  1.165984 -1.845653
F   -16.118940  0.281501 -1.444118
F    -7.743499 -1.911513 -0.591453
C     3.583559 -2.719685 -0.132236
C     2.859086 -3.129773 -1.259121
H     2.858337 -2.505647 -2.150019
C     2.143233 -4.324490 -1.247118
H     1.589571 -4.629214 -2.132429
C     2.134528 -5.124665 -0.104855
H     1.572380 -6.055684 -0.093663
C     2.850504 -4.723885  1.023454
H     2.847712 -5.339975  1.919878
C     3.572007 -3.533046  1.008505
H     4.129496 -3.226482  1.890469

121
P1-Z-ES     el energy= -3379.16095350
C     3.120503 -0.934539  1.403705
C     4.471624 -1.085644  1.211729
C     5.221672 -0.070756  0.478031
C     4.601299  1.133278  0.152031
C     3.284922  1.392390  0.660517
C     2.429424  0.231446  0.969377
C     2.943105  2.718684  1.018153
C     3.743415  3.822531  0.556087
C     4.800575  3.554243 -0.414940
C     5.214715  2.219394 -0.639301
C     1.850021  3.001080  1.901837
C     1.579187  4.287191  2.313205
C     2.373128  5.354567  1.862990
C     3.436583  5.113519  1.001387
C     5.375683  4.583608 -1.189441
C     6.309936  4.309044 -2.171770
C     6.672652  2.982498 -2.433210
C     6.125034  1.957591 -1.679969
C     6.654303 -0.331198  0.182488
C     7.047948 -1.455055 -0.555266
C     8.390640 -1.702616 -0.816903
C     9.388986 -0.844891 -0.335904
C     8.994922  0.271405  0.415267
C     7.652304  0.524503  0.667778
C    10.823357 -1.114770 -0.609255
C    11.325845 -2.424193 -0.596212
C    12.666959 -2.682316 -0.851851
C    13.523808 -1.620766 -1.121839
C    13.059808 -0.310513 -1.148699
C    11.712329 -0.070212 -0.889152
C     1.030619  0.233615  0.711811
C     0.152020 -0.774901  1.225068
C    -1.201977 -0.737347  0.991552
C    -1.796503  0.276153  0.198630
C    -0.939844  1.252071 -0.345833
C     0.416868  1.248512 -0.094077
C    -3.246935  0.298946 -0.049370
C    -3.774083  0.819757 -1.246569
C    -5.140165  0.836942 -1.487255
C    -6.010200  0.334974 -0.523548
C    -5.528873 -0.187620  0.672609
C    -4.156295 -0.200910  0.898392
O    -7.359711  0.401188 -0.838053
C    -8.237531 -0.160497  0.001574
F    -8.273579 -1.493893 -0.020117
C    -9.063426  0.530516  0.779402
F    -9.026727  1.864186  0.793790
O    14.850868 -1.965770 -1.354880
C    15.722242 -0.989492 -1.627446
C    16.618903 -0.549089 -0.756953
F    15.687812 -0.506992 -2.872189
F    16.690286 -0.973445  0.484133
F    17.540269  0.344295 -1.040463
H     1.268783  2.178993  2.304286
H     0.760389  4.470814  3.005068
H     2.167075  6.368990  2.195771
H     4.047321  5.954540  0.685248
H     5.059023  5.612197 -1.043857
H     6.733182  5.120478 -2.759171
H     7.370750  2.750399 -3.233910
H     6.392361  0.933000 -1.913580
H     6.292717 -2.135452 -0.941979
H     8.664542 -2.566591 -1.418742
H     9.749033  0.938422  0.827927
H     7.370547  1.391201  1.261351
H    10.664449 -3.255179 -0.362240
H    13.059296 -3.695384 -0.831426
H    13.724155  0.519112 -1.374859
H    11.347437  0.953466 -0.929561
H     0.546065 -1.579520  1.838738
H    -1.824512 -1.527724  1.404954
H    -1.351586  2.050212 -0.959466
H     1.036461  2.012243 -0.552011
H    -3.105093  1.191412 -2.018503
H    -5.541469  1.229144 -2.417705
H    -6.206122 -0.571493  1.430834
H    -3.794216 -0.586488  1.848173
C     5.124102 -2.317922  1.729860
C     4.587551 -3.578014  1.431756
H     3.717834 -3.646550  0.781221
C     5.168183 -4.740002  1.937537
H     4.740853 -5.708444  1.686700
C     6.295712 -4.661295  2.753298
H     6.752003 -5.566952  3.146387
C     6.836554 -3.411902  3.060858
H     7.712599 -3.339149  3.701577
C     6.258664 -2.252197  2.552967
H     6.686760 -1.284451  2.802229
H     2.572561 -1.757479  1.855093
O    -9.940866 -0.025089  1.619459
C   -11.293482  0.041931  1.293763
C   -11.753007  0.429224  0.038661
H   -11.061217  0.712140 -0.750639
C   -13.123334  0.436052 -0.198752
H   -13.477309  0.724931 -1.186406
C   -14.049607  0.070911  0.786827
C   -15.550336  0.136468  0.464871
C   -13.550002 -0.312396  2.034210
H   -14.224480 -0.609747  2.831845
C   -12.179928 -0.327980  2.294216
H   -11.797265 -0.630432  3.265382
C   -15.932950  1.622000  0.319089
C   -16.416522 -0.458863  1.591419
C   -15.822549 -0.666505 -0.815838
C   -16.493479 -0.144517 -1.922064
H   -16.834202  0.887232 -1.924593
C   -16.747521 -0.919632 -3.056586
H   -17.270997 -0.482935 -3.906404
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C   -16.328870 -2.248093 -3.101243
O   -16.542590 -3.055934 -4.171200
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H   -15.321239 -3.826215 -2.044176
C   -15.407036 -2.005608 -0.886947
H   -14.867577 -2.443889 -0.048846
H   -17.005447 -2.564258 -4.861408
H   -15.678184  2.157542  1.241777
H   -15.399206  2.106533 -0.507398
H   -17.010894  1.740565  0.150857
H   -16.317491  0.116584  2.520702
H   -16.157554 -1.503351  1.802800
H   -17.471263 -0.429941  1.292279

121
P2-Z-ES     el energy= -3974.43686012
C     2.395015  2.097651 -1.281374
C     3.732825  1.786783 -1.289575
C     4.306992  1.005599 -0.197891
C     3.463502  0.426991  0.746912
C     2.045061  0.495793  0.538666
C     1.521153  1.611301 -0.271261
C     1.242620 -0.594108  0.951462
C     1.761337 -1.567027  1.878808
C     3.067917 -1.321608  2.484065
C     3.908404 -0.319305  1.942502
C    -0.074581 -0.803557  0.422001
C    -0.826764 -1.896677  0.789679
C    -0.311218 -2.835084  1.697047
C     0.966433 -2.667186  2.219323
C     3.489911 -2.010509  3.640516
C     4.688395 -1.709093  4.261681
C     5.489179 -0.677037  3.759689
C     5.096546  0.007824  2.621841
C     5.776972  0.788464 -0.185119
C     6.669605  1.867079 -0.144478
C     8.043745  1.656075 -0.141731
C     8.574545  0.360309 -0.198913
C     7.679688 -0.717320 -0.256461
C     6.306424 -0.507186 -0.246271
C    10.042008  0.133803 -0.201748
C    10.906378  0.999558 -0.887890
C    12.280058  0.790222 -0.891806
C    12.803664 -0.299973 -0.205101
C    11.977666 -1.175691  0.490293
C    10.602964 -0.951111  0.482547
C     0.273688  2.229374  0.022697
C    -0.408689  3.074248 -0.911094
C    -1.663653  3.569398 -0.646037
C    -2.323293  3.313107  0.582082
C    -1.630563  2.552325  1.541615
C    -0.387670  2.014760  1.276575
C    -3.693748  3.789944  0.831085
C    -4.129765  4.118654  2.127397
C    -5.443930  4.503180  2.370848
C    -6.334045  4.563613  1.307195
C    -5.934462  4.275321  0.007122
C    -4.619288  3.891475 -0.224039
O    -7.668524  4.924372  1.548933
C    -8.497424  3.875328  1.596387
F    -8.469264  3.187292  2.739881
C    -9.307245  3.498637  0.614260
F    -9.327905  4.149482 -0.551571
O    14.185630 -0.441215 -0.267311
C    14.744746 -1.492885  0.339756
C    15.205651 -2.549623 -0.313387
F    14.876780 -1.401225  1.665626
F    15.089646 -2.702485 -1.612843
F    15.837351 -3.549505  0.259553
H    -0.457587 -0.125095 -0.331398
H    -1.815829 -2.044534  0.363676
H    -0.906730 -3.698326  1.983875
H     1.349803 -3.422211  2.899772
H     2.852516 -2.771100  4.081427
H     4.986753 -2.251623  5.155671
H     6.410581 -0.399287  4.265889
H     5.712204  0.825182  2.263536
H     6.283555  2.882736 -0.097533
H     8.712505  2.511669 -0.075953
H     8.061253 -1.733157 -0.333511
H     5.631310 -1.358297 -0.298541
H    10.500645  1.839172 -1.447483
H    12.949204  1.454024 -1.432444
H    12.385018 -2.018812  1.041303
H     9.961048 -1.626836  1.043066
H     0.041917  3.298731 -1.873509
H    -2.150048  4.189530 -1.395950
H    -2.094316  2.341304  2.502559
H     0.112205  1.440716  2.049708
H    -3.431820  4.084212  2.960047
H    -5.780755  4.748738  3.374136
H    -6.652808  4.332392 -0.806205
H    -4.320321  3.629396 -1.235710
C     4.570972  2.305268 -2.403732
C     4.532724  3.665230 -2.741716
H     3.918991  4.343928 -2.152675
C     5.288316  4.159305 -3.803781
H     5.251113  5.219776 -4.043275
C     6.094323  3.300164 -4.548975
H     6.687029  3.684388 -5.376017
C     6.136974  1.943161 -4.225286
H     6.757694  1.263024 -4.804425
C     5.385467  1.450756 -3.162534
H     5.424225  0.391228 -2.922144
H     2.021593  2.776455 -2.043733
O   -10.179328  2.484571  0.705874
C    -9.762689  1.230448  0.286528
C    -8.493655  0.975397 -0.221198
H    -7.753092  1.764404 -0.317958
C    -8.168590 -0.323154 -0.598584
H    -7.172582 -0.511537 -0.987663
C    -9.086064 -1.371174 -0.479669
C    -8.671792 -2.765520 -0.985120
C   -10.362673 -1.079761  0.013072
H   -11.122292 -1.847384  0.104410
C   -10.699655  0.211278  0.403015
H   -11.687634  0.432851  0.796207
C    -8.888880 -2.741477 -2.522344
C    -9.552300 -3.897908 -0.390139
C    -7.220970 -3.103953 -0.598834
C    -6.331820 -3.762693 -1.451548
H    -6.614756 -4.036029 -2.461570
C    -5.046689 -4.094940 -1.032307
H    -4.369551 -4.600309 -1.718584
C    -4.633096 -3.790543  0.264493
O    -3.397966 -4.096433  0.729766
C    -5.514818 -3.146176  1.135346
H    -5.191011 -2.911076  2.145584
C    -6.789886 -2.811662  0.702875
H    -7.456448 -2.306871  1.396259
H    -2.878379 -4.518146  0.032624
F   -10.090068 -2.251194 -2.842467
F    -7.975905 -1.969055 -3.121734
F    -8.810910 -3.959464 -3.082956
F   -10.812207 -3.886535 -0.857368
F    -9.623321 -3.796720  0.941763
F    -9.054799 -5.105796 -0.668788

131
P3-Z-ES     el energy= -3610.17131791
C    -0.769048  2.083857  0.312918
C    -2.190878  1.991904  0.239101
C    -2.784307  0.757985 -0.128069
C    -1.958462 -0.388375 -0.333428
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C    -0.592255 -0.363552  0.169876
C     0.036844  0.919977  0.244567
C     0.002738 -1.601031  0.565906
C    -0.583668 -2.841715  0.129597
C    -1.666654 -2.802913 -0.825413
C    -2.351563 -1.558531 -1.067973
C     1.092426 -1.666355  1.476720
C     1.560949 -2.871686  1.955977
C     0.981618 -4.083357  1.530827
C    -0.066627 -4.057393  0.630271
C    -2.090437 -3.950636 -1.533185
C    -3.115771 -3.895050 -2.457697
C    -3.750625 -2.668935 -2.737456
C    -3.366305 -1.529503 -2.064480
C    -4.257586  0.632372 -0.234170
C    -5.029317  1.506368 -1.014793
C    -6.407521  1.360367 -1.098491
C    -7.072666  0.347321 -0.392475
C    -6.303445 -0.519190  0.396280
C    -4.922958 -0.383576  0.468591
C    -8.546617  0.196247 -0.479181
C    -9.386020  1.318203 -0.546610
C   -10.766320  1.179984 -0.626174
C   -11.322633 -0.094664 -0.636318
C   -10.521207 -1.229173 -0.578413
C    -9.139575 -1.071924 -0.497517
C     1.510349  1.043647  0.106370
C     2.309614  1.735298  1.029170
C     3.669114  1.916242  0.802555
C     4.276200  1.427441 -0.361572
C     3.486731  0.706769 -1.267917
C     2.132334  0.503885 -1.029501
C     5.716665  1.658615 -0.631547
C     6.142549  2.078714 -1.898202
C     7.491417  2.283013 -2.169885
C     8.421481  2.058453 -1.164263
C     8.031806  1.659455  0.109162
C     6.679047  1.459502  0.366562
O     9.760421  2.273557 -1.480623
C    10.647170  1.340418 -1.109004
F    11.657849  1.834904 -0.399184
C    10.613086  0.055687 -1.452294
F    11.564227 -0.791195 -1.035230
O   -12.710431 -0.143631 -0.707847
C   -13.305572 -1.340543 -0.682442
C   -13.936192 -1.817012  0.381047
F   -13.288024 -2.026835 -1.828040
F   -13.973146 -1.194958  1.537356
F   -14.600882 -2.950601  0.394563
H     1.538213 -0.748835  1.844867
H     2.372616 -2.881047  2.678178
H     1.348799 -5.031252  1.916186
H    -0.518152 -4.998677  0.330093
H    -1.583799 -4.897871 -1.375485
H    -3.410385 -4.795375 -2.991536
H    -4.527099 -2.614862 -3.496304
H    -3.831873 -0.584354 -2.318868
H    -4.541866  2.292805 -1.584368
H    -6.973166  2.031827 -1.740866
H    -6.791508 -1.297681  0.978774
H    -4.349008 -1.065566  1.091621
H    -8.958578  2.317598 -0.514005
H   -11.417437  2.048883 -0.666161
H   -10.951604 -2.226390 -0.603949
H    -8.514551 -1.961514 -0.472948
H     1.858658  2.148380  1.927529
H     4.261743  2.473229  1.525588
H     3.941887  0.293242 -2.165695
H     1.537115 -0.054787 -1.748574
H     5.409003  2.254001 -2.681873
H     7.828830  2.597343 -3.153554
H     8.774356  1.487181  0.884310
H     6.371698  1.118986  1.352756
C    -0.130014  3.420165  0.468413
C    -0.281432  4.152943  1.651910
H    -0.874716  3.740575  2.464772
C     0.324960  5.398424  1.795035
H     0.204193  5.952276  2.723276
C     1.082441  5.933310  0.752849
H     1.554159  6.906968  0.864252
C     1.231540  5.213891 -0.432672
H     1.818552  5.624305 -1.251217
C     0.632705  3.964295 -0.572504
H     0.758265  3.401769 -1.494880
C    -3.037082  3.179847  0.541080
C    -2.985775  4.336344 -0.249199
H    -2.312184  4.371758 -1.102240
C    -3.790777  5.434848  0.041822
H    -3.738635  6.321429 -0.586430
C    -4.662859  5.397595  1.129998
H    -5.291441  6.255576  1.357674
C    -4.723094  4.252562  1.924055
H    -5.398017  4.213147  2.776338
C    -3.918128  3.154215  1.630658
H    -3.971626  2.262347  2.251520
O     9.672081 -0.473050 -2.243183
C     8.634558 -1.189250 -1.645755
C     8.745370 -1.772704 -0.387064
H     9.662894 -1.698138  0.188959
C     7.650633 -2.454836  0.131771
H     7.736218 -2.894400  1.123457
C     6.450266 -2.583321 -0.578622
C     5.296784 -3.387812  0.040381
C     6.381178 -1.995460 -1.844067
H     5.471455 -2.059451 -2.433835
C     7.463721 -1.298945 -2.380551
H     7.398022 -0.827320 -3.357103
C     5.696443 -4.875299  0.010253
C     3.986695 -3.242718 -0.756659
C     5.056394 -2.879571  1.468631
C     5.120872 -3.693334  2.598916
H     5.357549 -4.749836  2.506703
C     4.887525 -3.184513  3.880311
H     4.948423 -3.843442  4.745572
C     4.581476 -1.835303  4.050848
O     4.348859 -1.278580  5.266771
C     4.509467 -1.001969  2.928690
H     4.263283  0.049375  3.058481
C     4.744854 -1.525843  1.666258
H     4.684587 -0.860605  0.808378
H     4.440670 -1.951317  5.953274
H     5.880753 -5.183915 -1.026080
H     6.611282 -5.069406  0.583213
H     4.895042 -5.508885  0.411800
H     4.092439 -3.642366 -1.773336
H     3.656019 -2.199506 -0.826311
H     3.191499 -3.809435 -0.258990

133
P4-Z-ES     el energy= -4305.88255665
C     4.563372  1.173749  1.137069
C     5.918844  1.451916  1.139541
C     6.860390  0.385033  0.937580
C     6.321069 -0.985280  1.073480
C     4.950502 -1.223131  0.733898
C     4.063252 -0.159324  0.836774
C     4.586356 -2.607446  0.371315
C     5.386310 -3.674258  0.844322
C     6.565921 -3.380937  1.653389
C     7.057022 -2.025545  1.690604
C     3.526284 -2.893480 -0.508415
C     3.217605 -4.195636 -0.865995
C     3.978297 -5.255554 -0.359976
C     5.054412 -4.992649  0.468400
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C     7.269350 -4.377524  2.337838
C     8.438080 -4.098892  3.036969
C     8.934494 -2.786302  3.073358
C     8.269585 -1.774410  2.417326
C     8.212491  0.541546  0.499643
C     9.057576  1.657671  0.807417
C    10.364908  1.713240  0.383148
C    10.949239  0.686856 -0.398895
C    10.134694 -0.420384 -0.706711
C     8.833509 -0.507262 -0.260253
C    12.345380  0.768818 -0.852523
C    12.968466  2.012326 -1.074012
C    14.284543  2.094704 -1.504844
C    15.005706  0.924973 -1.725670
C    14.428570 -0.323047 -1.514212
C    13.107771 -0.389666 -1.083341
C     2.589027 -0.348790  0.761877
C     1.815819  0.303341 -0.206497
C     0.438907  0.120430 -0.260805
C    -0.215420 -0.712881  0.656928
C     0.558670 -1.355089  1.632673
C     1.936265 -1.175563  1.683838
C    -1.686079 -0.909645  0.595758
C    -2.450154 -1.019844  1.767239
C    -3.825933 -1.203410  1.713896
C    -4.460683 -1.284904  0.476624
C    -3.728137 -1.193062 -0.704493
C    -2.350338 -0.998635 -0.632943
O    -5.824304 -1.486265  0.508268
C    -6.566615 -1.055282 -0.557906
F    -6.544103 -1.980396 -1.577609
C    -8.020249 -0.932546 -0.081816
F    -8.076592 -0.045047  0.940998
O    16.311946  1.099351 -2.165185
C    17.066281  0.013384 -2.365410
C    17.371073 -0.448381 -3.569381
F    17.563249 -0.562483 -1.268209
F    16.899251  0.067162 -4.681443
F    18.184065 -1.458202 -3.784289
H     2.946418 -2.081583 -0.932662
H     2.394237 -4.386629 -1.550032
H     3.746468 -6.280819 -0.638550
H     5.669299 -5.822623  0.803788
H     6.893596 -5.396719  2.342978
H     8.955866 -4.896486  3.564170
H     9.835703 -2.559487  3.638350
H     8.633117 -0.758053  2.511308
H     8.696647  2.447401  1.453472
H    10.972959  2.557148  0.701057
H    10.521752 -1.220969 -1.332734
H     8.237759 -1.366515 -0.552883
H    12.408895  2.933751 -0.935296
H    14.757033  3.056363 -1.685623
H    14.991355 -1.239131 -1.671665
H    12.677348 -1.369909 -0.895159
H     2.298453  0.957161 -0.928812
H    -0.137727  0.649927 -1.016232
H     0.082696 -2.020217  2.350139
H     2.518178 -1.690396  2.445051
H    -1.967111 -0.934632  2.737903
H    -4.419535 -1.271267  2.621502
H    -4.208614 -1.300003 -1.672138
H    -1.782960 -0.948280 -1.559441
C     6.355655  2.876475  1.261550
C     6.471012  3.474611  2.519041
H     6.241952  2.894784  3.410668
C     6.878802  4.803346  2.633537
H     6.965246  5.258177  3.617846
C     7.174341  5.545735  1.490785
H     7.494479  6.581347  1.580101
C     7.052390  4.956183  0.231916
H     7.276479  5.530716 -0.664161
C     6.642908  3.629918  0.118499
H     6.552978  3.168022 -0.862504
H    -6.215184 -0.098038 -0.960150
O    -8.780734 -0.528704 -1.129142
C   -10.159295 -0.470950 -0.928906
C   -10.734047  0.680009 -0.406006
H   -10.110707  1.518687 -0.111942
C   -12.116917  0.741656 -0.278337
H   -12.564238  1.645699  0.123011
C   -12.928386 -0.331022 -0.667124
C   -14.447460 -0.209557 -0.437955
C   -12.320185 -1.482252 -1.175931
H   -12.901484 -2.347761 -1.470208
C   -10.937067 -1.551709 -1.316404
H   -10.463912 -2.441265 -1.721197
C   -14.674297 -0.522815  1.066086
C   -15.261072 -1.235024 -1.273132
C   -14.969194  1.180790 -0.838883
C   -15.946384  1.872500 -0.119222
H   -16.365834  1.469615  0.795590
C   -16.418811  3.107255 -0.554255
H   -17.173891  3.630858  0.029150
C   -15.933156  3.667995 -1.736381
O   -16.352949  4.863787 -2.207096
C   -14.971591  2.977445 -2.479153
H   -14.598421  3.411362 -3.402865
C   -14.502248  1.751519 -2.031191
H   -13.751521  1.236210 -2.623601
H   -17.018806  5.233822 -1.612819
F   -14.030878 -1.633042  1.438522
F   -14.221889  0.472727  1.836006
F   -15.968214 -0.707792  1.373255
F   -15.092409 -2.502617 -0.860886
F   -14.907495 -1.187175 -2.562411
F   -16.571922 -0.986344 -1.213648
F    -8.453997 -2.109960  0.419592
C     3.571120  2.251327  1.436744
C     2.864724  2.214603  2.644906
H     3.052417  1.406065  3.348568
C     1.927081  3.198367  2.951272
H     1.389580  3.155434  3.896028
C     1.678070  4.232835  2.049620
H     0.944772  5.000479  2.286287
C     2.373502  4.275869  0.841752
H     2.183994  5.076567  0.130196
C     3.312488  3.292012  0.538364
H     3.846478  3.326268 -0.408124

246
P1'-2-units-ES     el energy= -
6959.37121606
C   -14.602138  1.049240 -1.289653
C   -13.351214  1.669363 -1.379017
C   -12.723871  2.107923 -0.205671
C   -13.335992  1.845690  1.052654
C   -14.437278  0.954635  1.119399
C   -15.153756  0.673611 -0.073687
C   -14.707597  0.276745  2.403367
C   -14.134881  0.770348  3.595252
C   -13.368527  2.019130  3.553295
C   -12.941365  2.528737  2.306340
C   -15.388544 -0.958226  2.454469
C   -15.548230 -1.651303  3.641119
C   -15.007095 -1.140960  4.825180
C   -14.298399  0.046368  4.791876
C   -13.076270  2.734016  4.730831
C   -12.386731  3.932330  4.696360
C   -11.998673  4.462985  3.462946
C   -12.282345  3.776442  2.295498
C   -11.382635  2.755703 -0.313480
C   -11.188342  3.917541 -1.068439
C    -9.926182  4.488141 -1.184898
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C	-8.813651	3.910211	-0.558448
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C	-10.274582	2.176748	0.313666
C	-7.463934	4.515887	-0.690473
C	-7.040067	5.074440	-1.905508
C	-5.776256	5.635835	-2.035563
C	-4.915066	5.650613	-0.940793
C	-5.313137	5.119033	0.283659
C	-6.580269	4.549746	0.393960
C	-16.520982	0.082277	-0.104734
C	-16.832951	-0.975897	-0.965235
C	-18.124553	-1.491748	-1.022414
C	-19.147597	-0.963261	-0.225310
C	-18.834140	0.105016	0.627518
C	-17.545118	0.620286	0.685232
C	-20.525064	-1.516225	-0.284146
C	-21.645032	-0.675621	-0.199081
C	-22.934474	-1.188026	-0.261194
C	-23.122926	-2.560784	-0.405698
C	-22.030945	-3.422947	-0.475610
C	-20.743993	-2.891538	-0.422286
O	-24.432108	-2.988858	-0.445855
C	-24.707982	-4.169574	-1.081295
F	-24.490560	-5.242395	-0.246630
C	-26.194259	-4.164199	-1.457957
F	-26.477046	-5.318650	-2.114108
O	-3.685527	6.238698	-1.148272
C	-2.635590	5.840423	-0.365468
C	-1.345145	6.207343	-1.113877
F	-2.632576	6.519516	0.831072
F	-1.326172	7.525336	-1.407428
F	-1.342244	5.549975	-2.303046
H	-15.771114	-1.404749	1.545249
H	-16.074048	-2.603094	3.640945
H	-15.114701	-1.684284	5.760930
H	-13.835886	0.401731	5.707664
H	-13.425829	2.362869	5.689414
H	-12.179189	4.468268	5.619512
H	-11.495088	5.425309	3.410156
H	-12.015377	4.240333	1.355385
H	-12.037046	4.388325	-1.558934
H	-9.808179	5.406293	-1.756411
H	-8.161008	2.259229	0.669787
H	-10.403283	1.267019	0.896131
H	-7.697090	5.046926	-2.771875
H	-5.440329	6.051612	-2.981605
H	-4.664484	5.166679	1.153185
H	-6.892286	4.152964	1.357291
H	-16.054009	-1.408896	-1.589437
H	-18.341134	-2.306968	-1.709549
H	-19.604436	0.528845	1.268311
H	-17.325976	1.445701	1.358798
H	-21.509068	0.399732	-0.109282
H	-23.801633	-0.534905	-0.213607
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