

Electronic Supplementary Information
for

A remarkably strained cyclopyrenylene trimer that undergoes metal-free direct oxygen insertion into the biaryl C–C σ -bond

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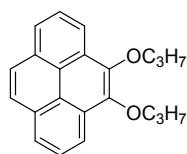
1. Instrumentation and Materials

^1H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectra were recorded with JEOL JNM-ECX500 spectrometer at ambient temperature by using tetramethylsilane as an internal standard. The high-resolution MS were measured by a JEOL JMS-700 MStation (EI magnetic sector (70 eV)) and a BRUKER Autoflex II (MALDI-spiral TOF MS). X-ray crystallographic data were recorded at 90 K with a BRUKER-APEXII X-Ray diffractometer using Mo- $K\alpha$ radiation equipped with a large area CCD detector.

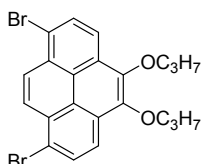
UV/Vis absorption spectra were measured with a JASCO UV/Vis/NIR spectrophotometer V-570, and fluorescence spectra were measured with a JASCO PL spectrofluorometer FP-6600. Fluorescence quantum yields were measured on a HAMAMATSU Absolute PL Quantum Yield Measurement System C9920-02G. Near infrared fluorescence measurements were performed on a Fluorolog-3 (FL3-11-NIR, Horiba Jobin Yvon), using a 450 W Xenon lamp. The emission was detected using a liquid N_2 -cooled InGaAs detector (DSS-IGA020L).

TLC, PLC and gravity column chromatography were performed on Art. 5554 (Merck KGaA) plates, Art. 13792 (Merck KGaA) plates and silica gel 60N (Kanto Chemical), respectively. All solvents and chemicals were reagent-grade quality, obtained commercially, and used without further purification. For spectral measurements, spectral-grade CH_2Cl_2 was purchased from Nacalai Tesque.

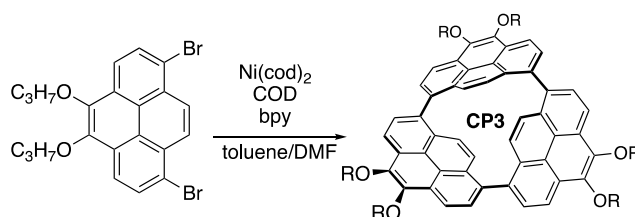
2. Experimental Section



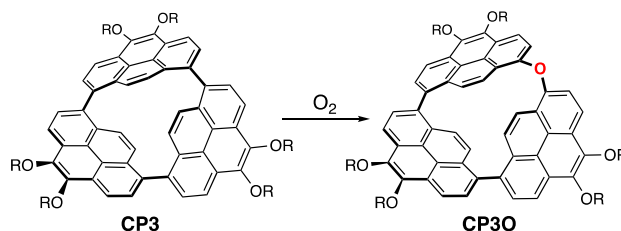
4,5-Dipropoxyppyrene (P1)^[S1]: To a solution of pyrene-4,5-dione (1.16 g, 5.00 mmol) in THF (20 mL) and H₂O (20 mL) were added tetra-*n*-butylammonium bromide (TBAB) (484 mg, 1.50 mmol) and Na₂S₂O₄ (2.61 g, 15.0 mmol). After 5 min, a solution of KOH (2.28 g, 40.0 mmol) in H₂O (20 mL) was added to the reaction mixture followed by 1-bromopropane (2.27 mL, 25.0 mmol). The red colored reaction mixture was stirred at 100°C for 12 h. The reaction mixture was cooled and extracted with AcOEt. The layers were separated and the aqueous phase was extracted with AcOEt. The combined organic extracts were washed with water followed by brine and dried over Na₂SO₄. The solvent was removed under reduced pressure. The crude products were subjected to silica gel column chromatography (*R*_f = 0.35 with CH₂Cl₂/hexanes = 1:5) to give 4,5-dipropoxyppyrene (**P1**) (1.52 g, 94%) as a colorless oil. ¹H NMR (500 MHz, CDCl₃): δ = 8.50 (d, *J* = 7.5 Hz, 2H), 8.14 (d, *J* = 7.5 Hz, 2H), 8.06 (s, 2H), 8.02 (t, *J* = 7.5 Hz, 2H), 4.31 (t, *J* = 7.0 Hz, 4H), 2.01 (m, 4H) and 1.18 (t, *J* = 7.5 Hz, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ = 144.03, 131.05, 128.89, 127.30, 125.93, 124.28, 122.83, 119.40, 75.29, 23.84 and 10.84 ppm; HR-MS (EI): *m/z*: calcd for C₂₂H₂₂O₂, 318.1620 [*M*]⁺; found: 318.1626; UV-vis (CH₂Cl₂): λ_{max} (ε [M⁻¹cm⁻¹]) = 281 (31214), 332 (20658) and 346 (25308) nm; FI (CH₂Cl₂, λ_{ex} = 346 nm): λ_{max} = 381 and 401 nm, Φ_F = 0.08; FI (solid, λ_{ex} = 346 nm): λ_{max} = 420 nm, Φ_F = 0.12.



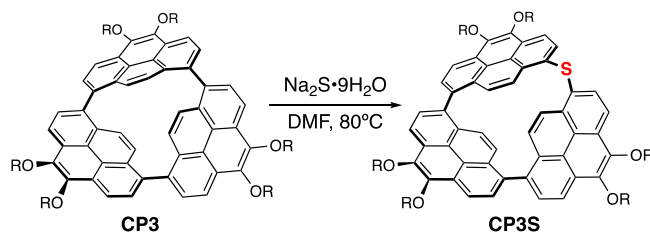
1,8-Dibromo-4,5-dipropoxyppyrene^[S1]: Bromine (0.34 mL, 6.60 mmol) was added dropwise to a solution of 4,5-dipropoxyppyrene (955 mg, 3.00 mmol) in CH₂Cl₂ (25 mL) over 5 min at room temperature. After complete addition of bromine, stirring was continued at room temperature for 5 min. The reaction mixture was poured into sodium thiosulfate solution and the layers were separated. The organic phase was washed with water followed by brine and dried over Na₂SO₄. The solvent was removed under reduced pressure. The crude products were subjected to silica gel column chromatography (*R*_f = 0.20 with CH₂Cl₂/hexanes = 1:10) to give 1,8-dibromo-4,5-dipropoxyppyrene (1.37 g, 96%) as a white solid. ¹H NMR (500 MHz, CDCl₃): δ = 8.53 (s, 2H), 8.38 (d, *J* = 8.5 Hz, 2H), 8.28 (d, *J* = 8.5 Hz, 2H), 4.29 (t, *J* = 7.0 Hz, 4H), 1.98 (m, 4H) and 1.17 (t, *J* = 7.5 Hz, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ = 143.70, 130.71, 129.39, 128.65, 127.44, 123.44, 120.81, 119.91, 75.37, 23.76 and 10.80 ppm; HR-MS (EI): *m/z*: calcd for C₂₂H₂₀Br₂O₂, 473.9830 [*M*]⁺; found: 473.9820, 475.9807, 477.9792.



1,8-Linked cyclic pyrene trimer CP3^[S2]: A mixture of 2,2'-bipyridine (300 mg, 1.92 mmol), 1,5-cyclooctadiene (0.24 mL, 1.92 mmol), Ni(cod)₂ (528 mg, 1.92 mmol) in toluene (1.76 mL) and DMF (1.76 mL) was heated at 80°C for 30 min under Ar. A solution of 1,8-dibromo-4,5-dipropoxy-pyrene (382 mg, 0.80 mmol) in toluene (7.0 mL) was added to the solution, and the whole was refluxed for 18 h under Ar. After cooling to room temperature, the reaction mixture was quenched with 10% HCl for 1 h. The solid was collected by filtration and rinsed with toluene. The filtrate was treated with water, and the organic materials were extracted with toluene. The combined organic solution was washed with brine and dried over Na₂SO₄, and evaporated to give crude products. The crude products were separated by silica gel column chromatography (*R_f* = 0.20 with CH₂Cl₂/hexanes = 1:2) and gel permeation chromatography (CHCl₃ eluent) to give **CP3** (8.9 mg, 3.5%) as a red solid. **CP3**: ¹H NMR (500 MHz, CDCl₃): δ = 8.67 (d, *J* = 8.0 Hz, 6H), 8.60 (d, *J* = 8.0 Hz, 6H), 6.99 (s, 6H), 4.39 (t, *J* = 7.0 Hz, 12H), 2.06 (m, 12H) and 1.22 (t, *J* = 7.5 Hz, 18H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ = 144.03, 134.75, 129.51, 128.33, 127.89, 125.52, 123.41, 118.94, 75.58, 23.88 and 10.88 ppm; HR-MS (Spiral MALDI): *m/z*: calcd for C₆₆H₆₀O₆, 948.4384 [*M*]⁺; found: 948.4383; UV-vis (CH₂Cl₂): λ_{max} (ε [M⁻¹ cm⁻¹]) = 298 (16906), 395 (16068) and 505 (4344) nm; FI (CH₂Cl₂, λ_{ex} = 395 nm): λ_{max} = 599 nm, Φ_F = 0.34; FI (solid, λ_{ex} = 395 nm): λ_{max} = 635 nm, Φ_F = 0.04.



CP3O: A conical flask containing **CP3** (4.6 mg, 5.0 μmol) in CH₂Cl₂ (900 mL) was left in the air under room light at r. t. for 3 days. The solvent was evaporated in vacuo to give **CP3O** in 81% NMR yield (internal reference material: HMDS). The crude products were separated by silica gel column chromatography (*R_f* = 0.18 with CH₂Cl₂/hexanes = 1:2) and were subjected to precipitation from CH₂Cl₂/MeOH to give **CP3O** (2.7 mg, 58%) as a yellow solid. **CP3O**: ¹H NMR (500 MHz, CDCl₃): δ = 8.90 (d, *J* = 10 Hz, 2H), 8.75 (d, *J* = 8.0 Hz, 2H), 8.59 (d, *J* = 8.0 Hz, 2H), 8.53 (d, *J* = 8.0 Hz, 2H), 8.43 (d, *J* = 8.5 Hz, 2H), 8.394 (d, *J* = 8.0 Hz, 2H), 8.386 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 10 Hz, 2H), 5.87 (s, 2H), 4.49 (m, 4H), 4.27 (m, 8H), 2.14 (m, 4H), 1.98 (m, 8H), 1.29 (t, *J* = 7.5 Hz, 6H) and 1.16 (t, *J* = 7.5 Hz, 12H) ppm; HR-MS (Spiral MALDI): *m/z*: calcd for C₆₆H₆₀O₇, 964.4334 [*M*]⁺; found: 964.4347; UV-vis (CH₂Cl₂): λ_{max} (ε [M⁻¹ cm⁻¹]) = 295 (55282) and 363 (38979) nm; FI (CH₂Cl₂, λ_{ex} = 363 nm): λ_{max} = 481 nm, Φ_F = 0.54; FI (solid, λ_{ex} = 363 nm): λ_{max} = 492 nm, Φ_F = 0.23.



CP3S: A Schlenk tube containing **CP3** (8.0 mg, 8.4 μmol) and $\text{Na}_2\text{S}\cdot 9\text{H}_2\text{O}$ (20 mg, 84 μmol) was evacuated and then refilled with Ar. Dry DMF (5 mL) was added and mixture was heated at 80°C for 72 h in an oil bath with stirring. After cooling to room temperature, the organic materials were extracted with Et_2O . The combined organic solution was washed with brine, dried over Na_2SO_4 , and evaporated to give crude products. The crude products were separated by PLC ($R_f = 0.58$ with $\text{CH}_2\text{Cl}_2/\text{hexanes} = 1:1$) to give **CP3S** in 67% conversion yield. **CP3S:** $^1\text{H NMR}$ (500 MHz, CDCl_3): $\delta = 9.15$ (d, $J = 9.5$ Hz, 2H), 8.77 (d, $J = 8.0$ Hz, 2H), 8.68 (d, $J = 8.5$ Hz, 2H), 8.58 (d, $J = 8.0$ Hz, 4H), 8.42 (d, $J = 8.0$ Hz, 2H), 8.41 (d, $J = 8.5$ Hz, 2H), 7.02 (d, $J = 10$ Hz, 2H), 5.87 (s, 2H), 4.51 (m, 4H), 4.29 (m, 8H), 2.15 (m, 4H), 1.98 (m, 8H), 1.30 (t, $J = 7.5$ Hz, 6H) and 1.15 (m, 12H) ppm; HR-MS (Spiral MALDI): m/z : calcd for $\text{C}_{66}\text{H}_{60}\text{O}_7$, 980.4105 [M] $^+$; found: 980.4113; UV-vis (CH_2Cl_2): λ_{max} (ϵ [$\text{M}^{-1} \text{cm}^{-1}$]) = 296 (44414) and 372 (34992) nm; FI (CH_2Cl_2 , $\lambda_{\text{ex}} = 372$ nm): $\lambda_{\text{max}} = 482$ nm, $\Phi_{\text{F}} = 0.44$; FI (solid, $\lambda_{\text{ex}} = 372$ nm): $\lambda_{\text{max}} = 525$ nm, $\Phi_{\text{F}} = 0.15$.

3. NMR Spectra

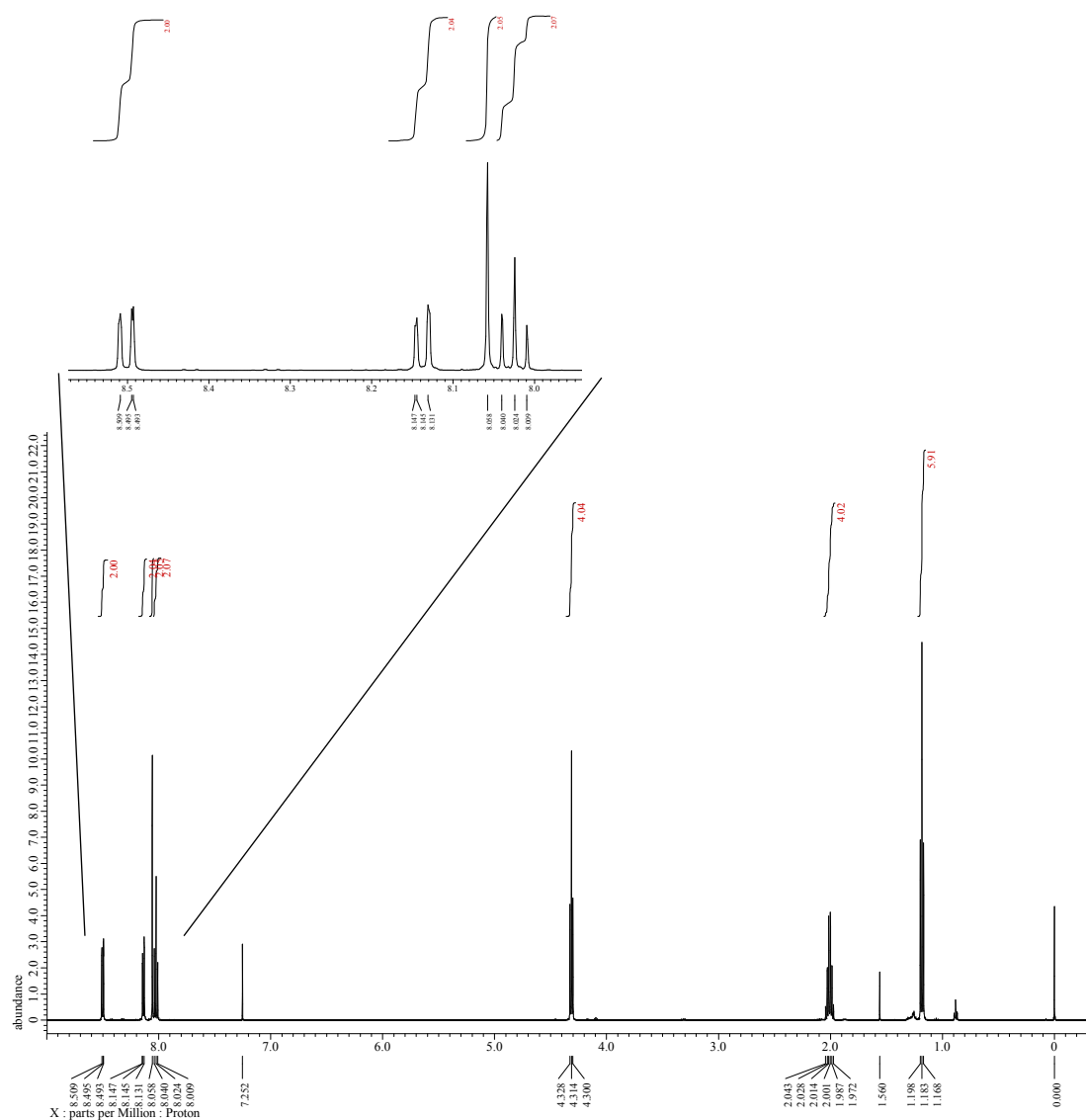


Figure S1. ¹H NMR spectrum of 4,5-dipropoxyppyrene (P1) in CDCl₃ at room temperature.

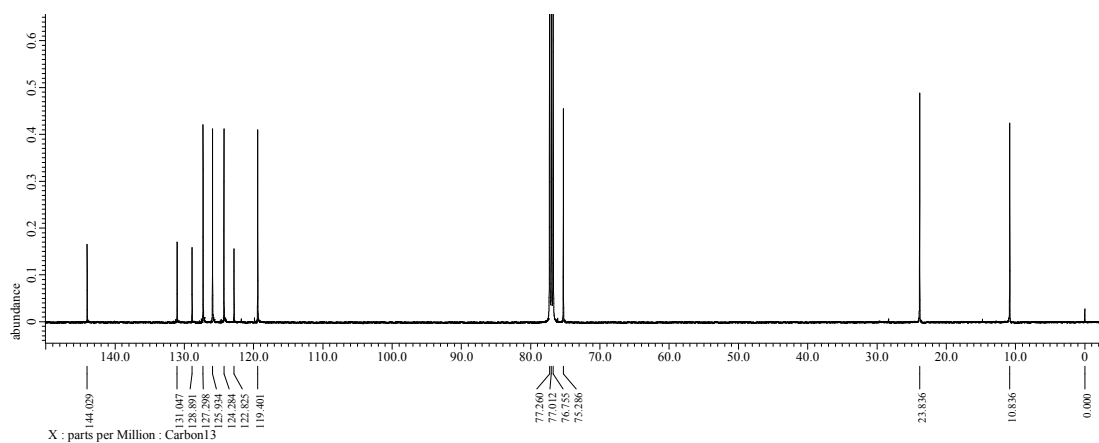


Figure S2. ¹³C NMR spectrum of 4,5-dipropoxyppyrene P1 in CDCl₃ at room temperature.

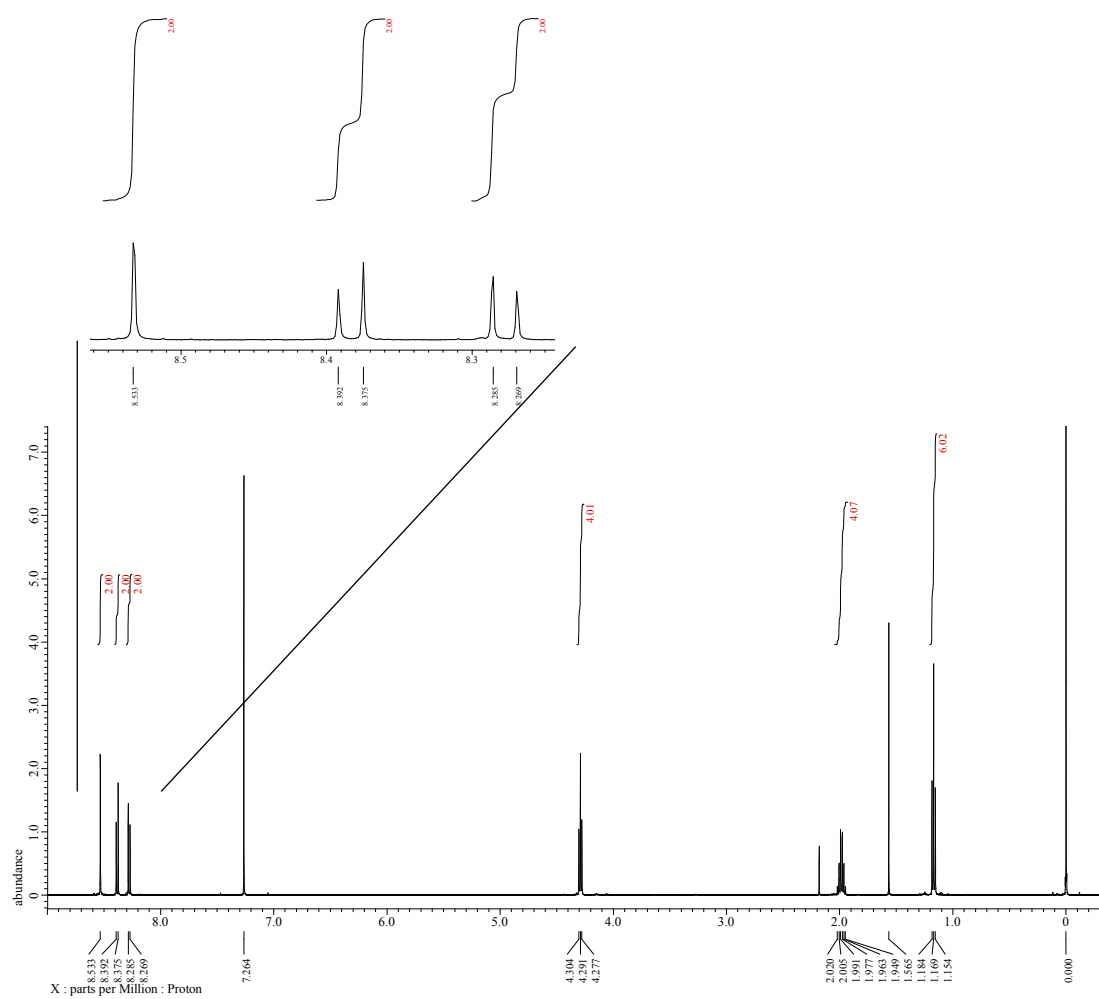


Figure S3. ^1H NMR spectrum of 1,8-dibromo-4,5-dipropoxyppyrene in CDCl_3 at room temperature.

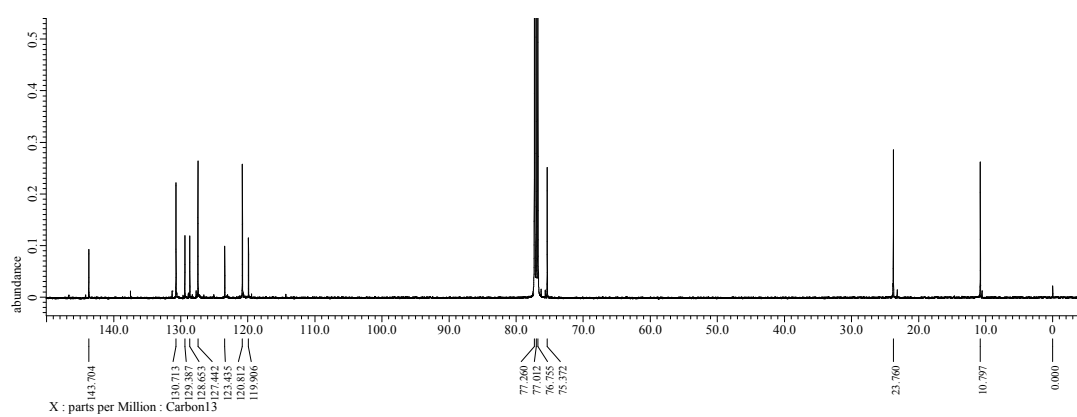


Figure S4. ^{13}C NMR spectrum of 1,8-dibromo-4,5-dipropoxyppyrene in CDCl_3 at room temperature.

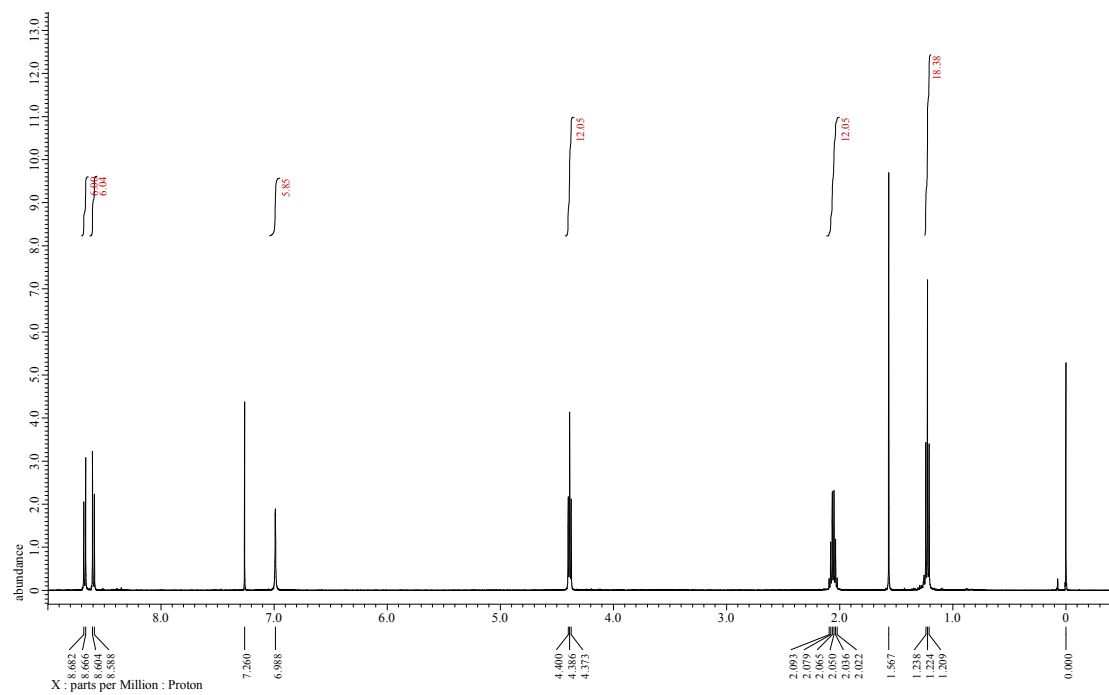


Figure S5. ^1H NMR spectrum of CP3 in CDCl_3 at room temperature.

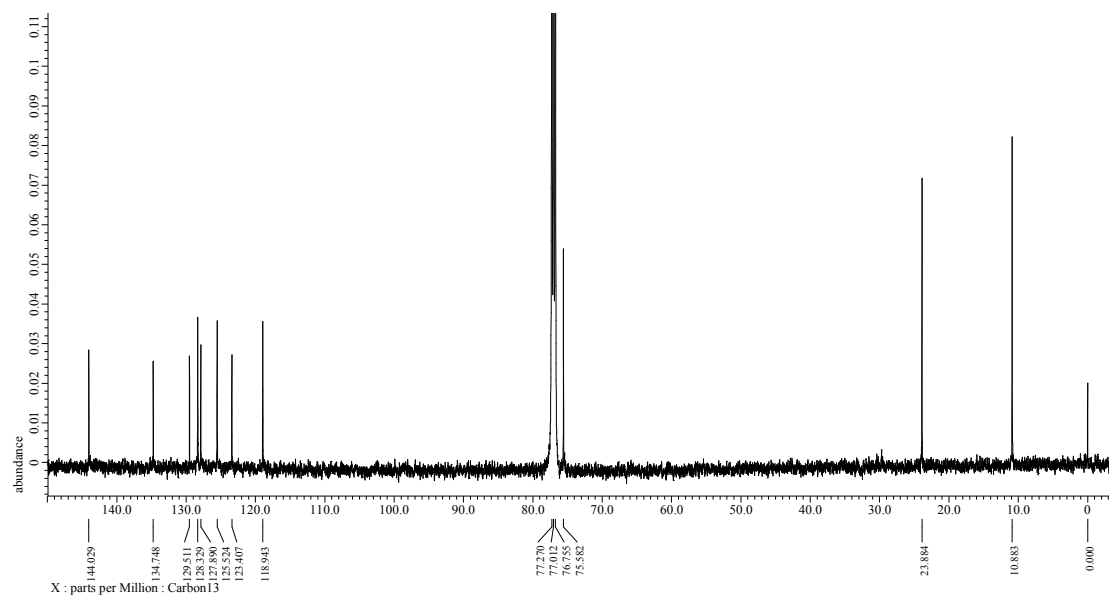


Figure S6. ^{13}C NMR spectrum of CP3 in CDCl_3 at room temperature.

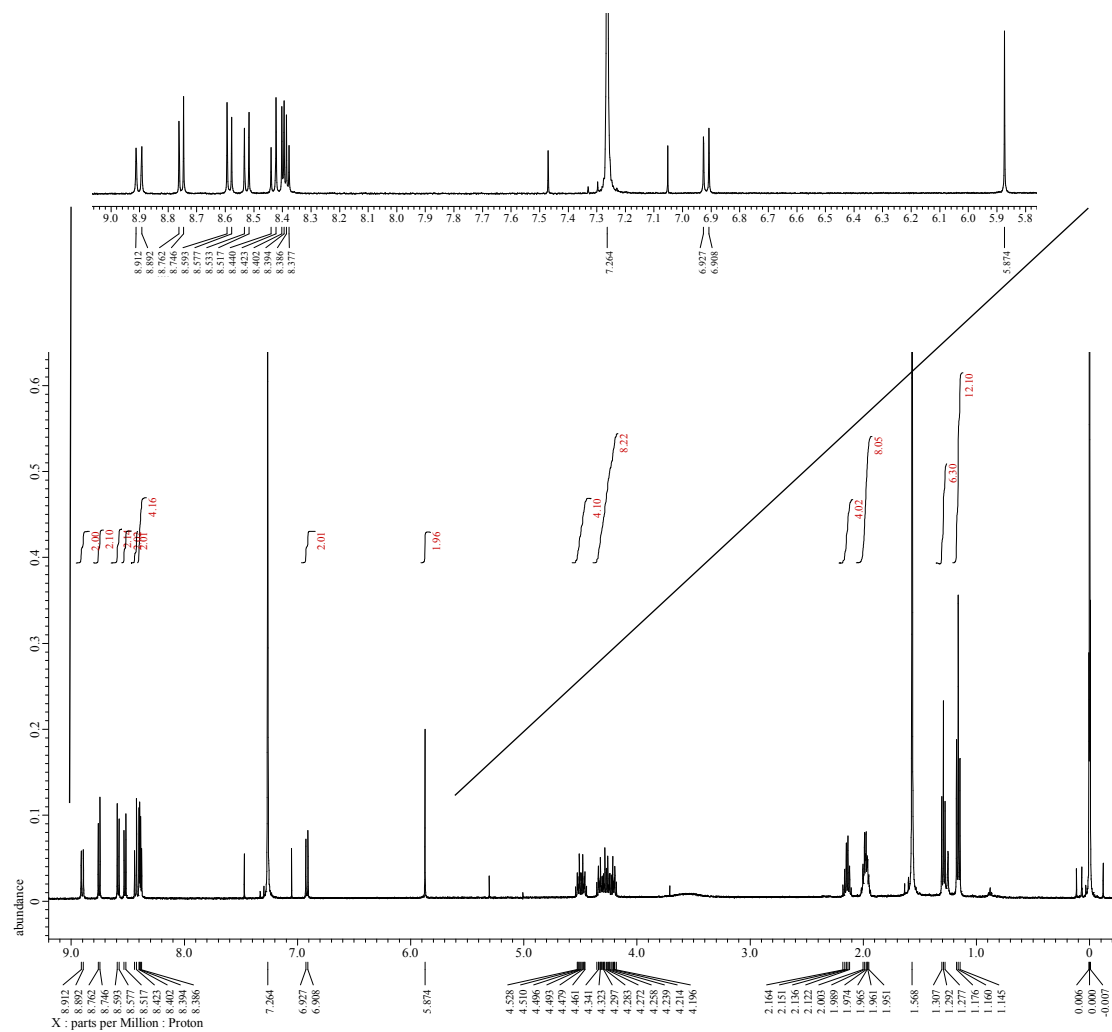


Figure S7. ^1H NMR spectrum of CP3O in CDCl_3 at room temperature.

4. HR-MS

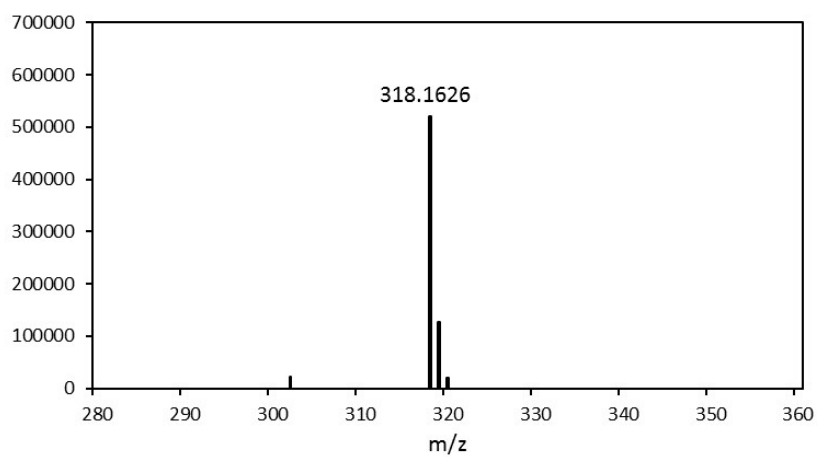


Figure S8. HR-EI mass spectrum of P1.

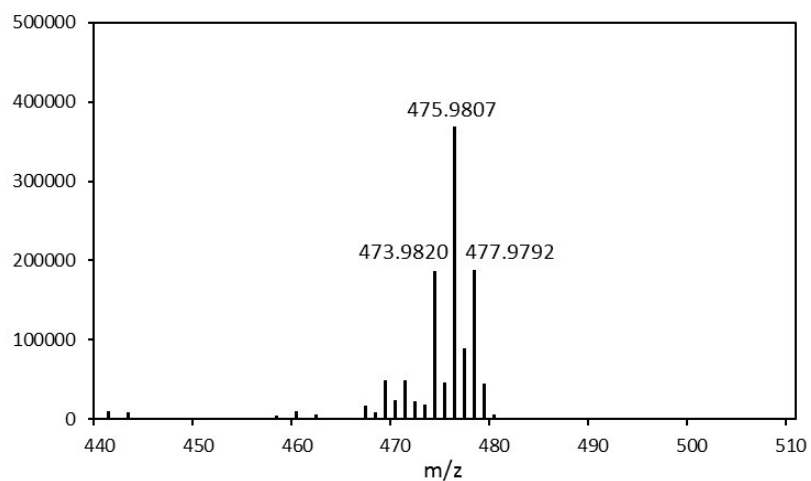


Figure S9. HR-EI mass spectrum of 1,8-dibromo-4,5-dipropoxyppyrene.

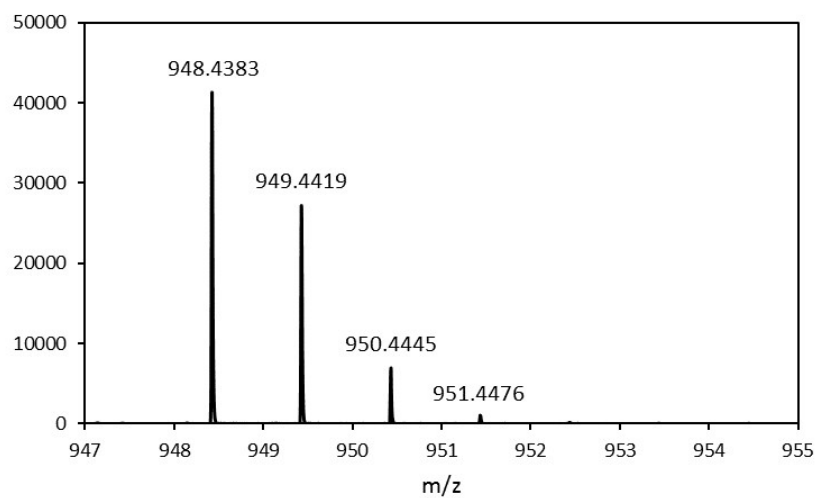


Figure S10. HR-Spiral-MALDI-TOF mass spectrum of CP3.

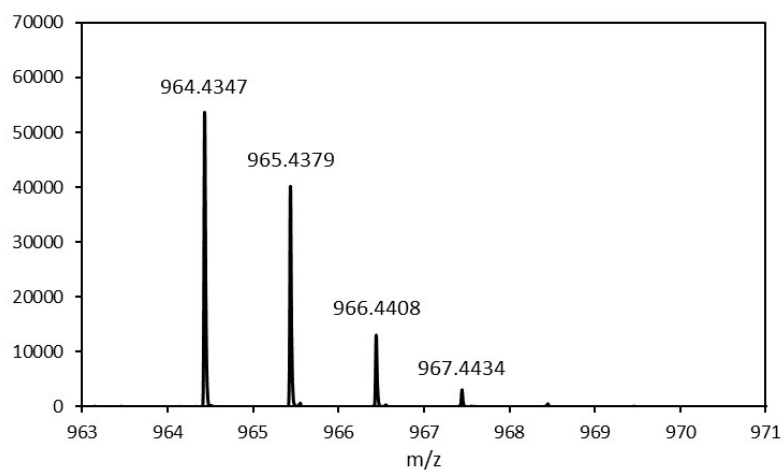


Figure S11. HR-Spiral-MALDI-TOF mass spectrum of **CP3O**.

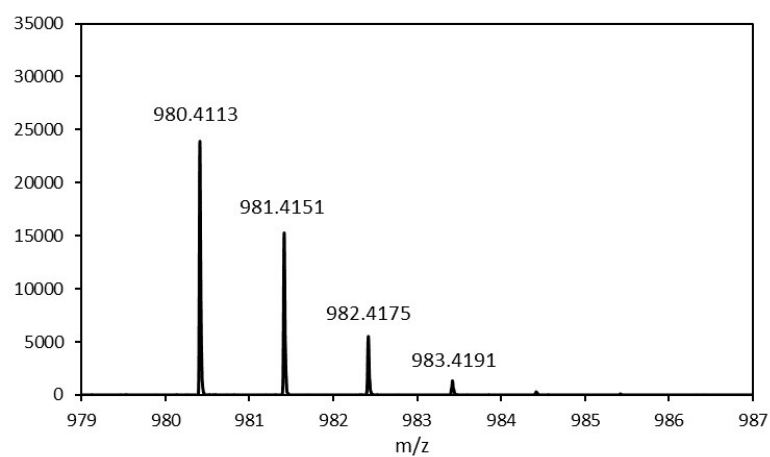


Figure S12. HR-Spiral-MALDI-TOF mass spectrum of **CP3S**.

5. UV-vis Absorption and Fluorescence Spectra

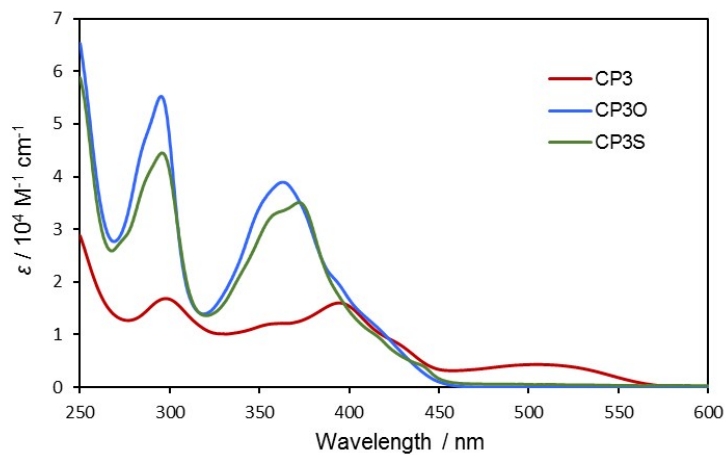


Figure S13. UV-vis absorption spectra of CP3, CP3O and CP3S in CH₂Cl₂.

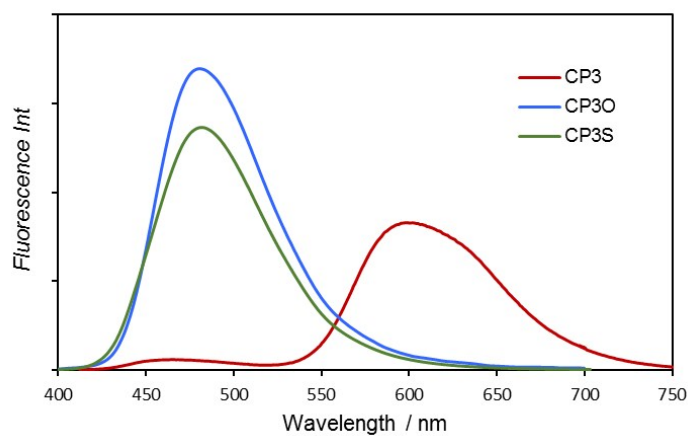


Figure S14. Fluorescence spectra of CP3, CP3O and CP3S in CH₂Cl₂.

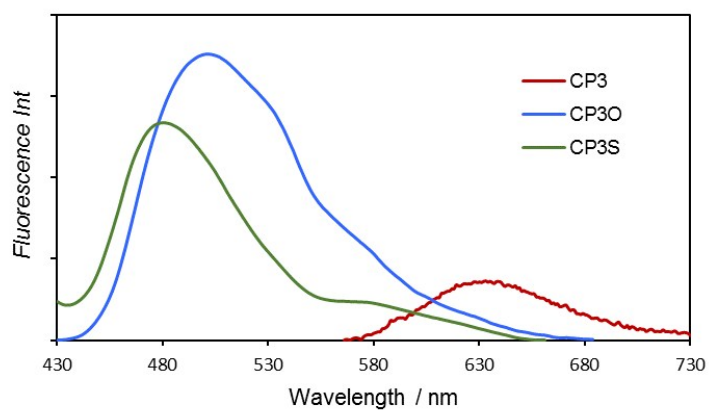


Figure S15. Fluorescence spectra of CP3, CP3O and CP3S in the solid state.

6. Fluorescence Spectral Change of CP3 to CP3O upon Oxidation

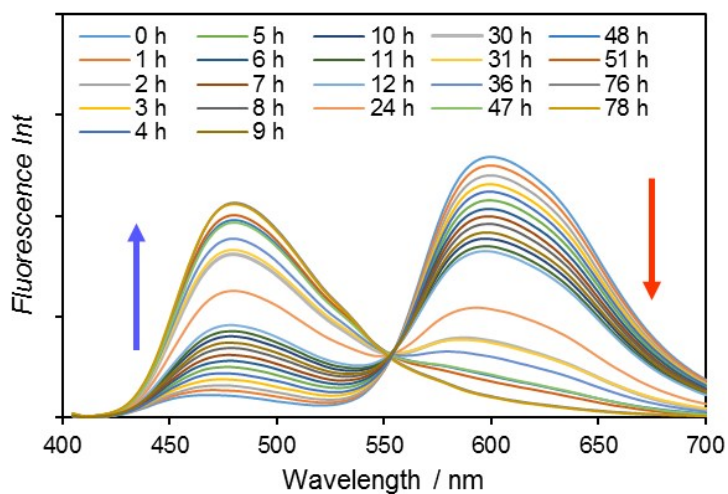


Figure S16. Fluorescence spectral change of CP3 in CH₂Cl₂ under room light at room temperature.

Measurements of singlet oxygen quantum yield (Φ_{Δ}): Measurements were performed on a Fluorolog-3 (Model: FL3-11-NIR, Horiba Jobin Yvon), using a 450 W Xenon lamp. The emission at 1274 nm was detected using a liquid nitrogen-cooled InGaAs detector (DSS-IGA020L). Singlet oxygen quantum yields Φ_{Δ} were determined in dichloromethane solutions, using tetraphenylporphyrin (TPP) in dichloromethane as reference solution (Φ_{Δ} [TPP] = 0.60) and were estimated from ¹O₂ luminescence at 1274 nm.

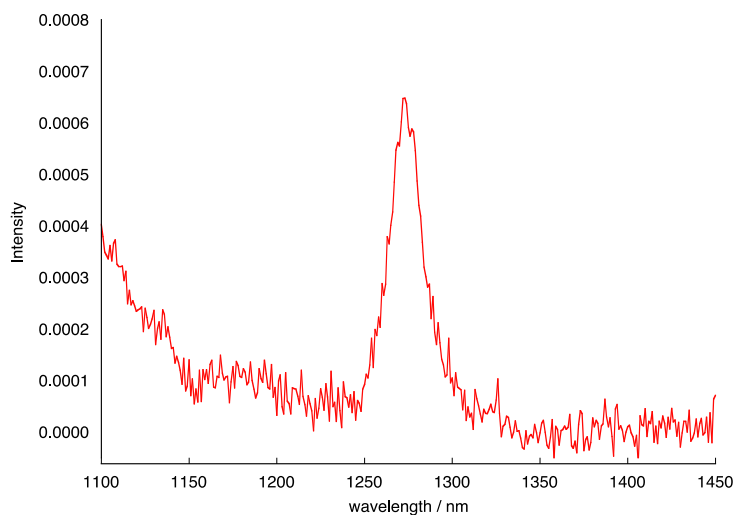


Figure S17. Emission spectrum of ¹O₂ generated by CP3 excited at 515 nm in O₂-saturated CH₂Cl₂. [CP3] = 9.3 × 10⁻⁶ M.

7. DFT Calculations

7.1. Computational Details

We focused on the model structures in which all the propyl groups were replaced by methyl groups. All the local minima and transition states were optimized (without any restrictions) at the dispersion corrected^[S3] B3LYP-D3/6-31G(d) level^[S4,S5] and the Gibbs free energy corrections at 1atm and 298.15 K were evaluated at the same level of theory. Then, the single point calculations were carried out at B3LYP-D3/6-311G(d,p) level^[S6] to refine the electronic energies. In all calculations, the solvation effect was included by the SMD continuum model^[S7] with the dielectric constant for dichloromethane. The transition states were confirmed by the intrinsic reaction coordinate (IRC) calculations.^[S8]

To find the initial guess structures of the local minima and transition states along the reaction coordinate starting from **CP3** and a singlet oxygen molecule, we used an automated reaction path search method, called the multi-component artificial force induced reaction (MC-AFIR) method.^[S9] The MC-AFIR calculations were performed via the global reaction route mapping (GRRM) program^[S10] using the energies and energy derivatives computed by the Gaussian09 program.^[S11] All the geometry optimization, frequency calculations, IRC calculations, and TD-DFT calculations were carried out using the Gaussian09 program. Mayer's bond orders^[S12] were computed with the Multiwfn software.^[S13]

7.2. Calculation results

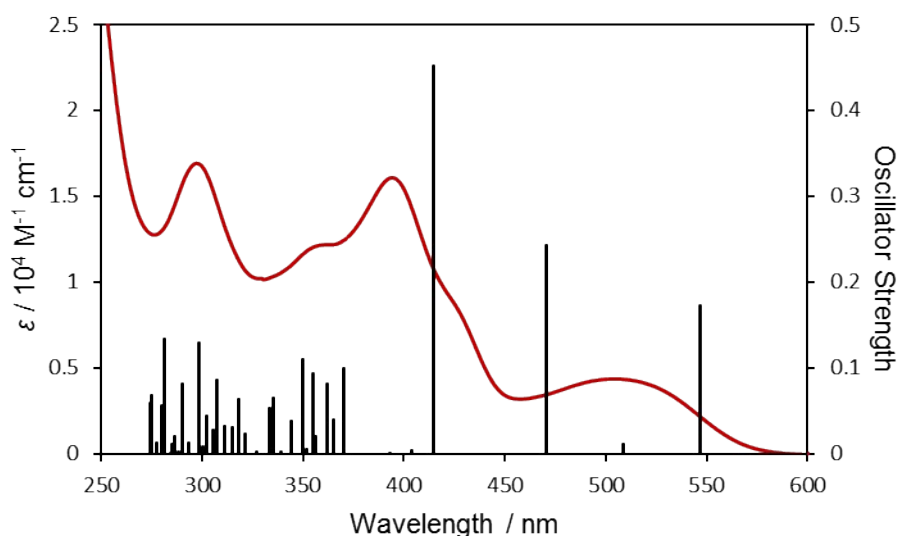


Figure S18. The excitation energies and the oscillator strengths of **CP3** calculated by the TD-DFT method (in black) and the experimental UV-vis absorption spectra (in red).

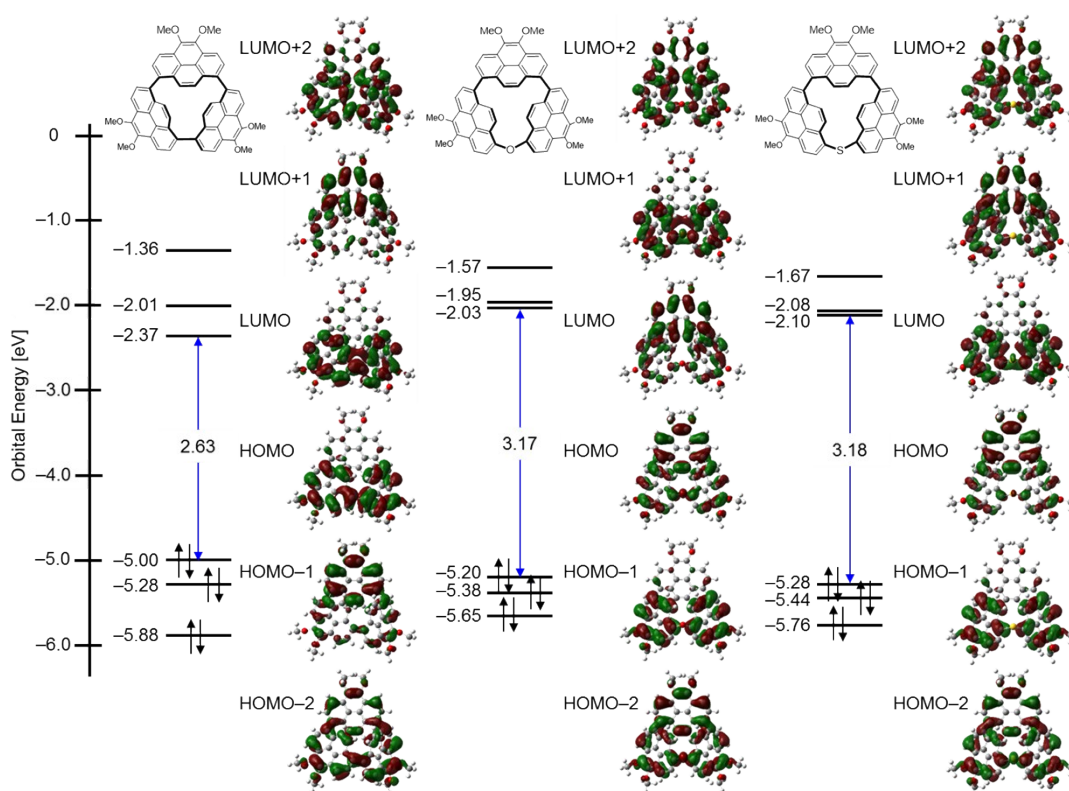


Figure S19. MO diagrams of CP3, CP3O and CP3S based on calculations at the B3LYP-D3 /6-311G(d,p)//B3LYP-D3/6-31G(d) level including the SMD solvation model. The propyl groups were replaced by methyl groups.

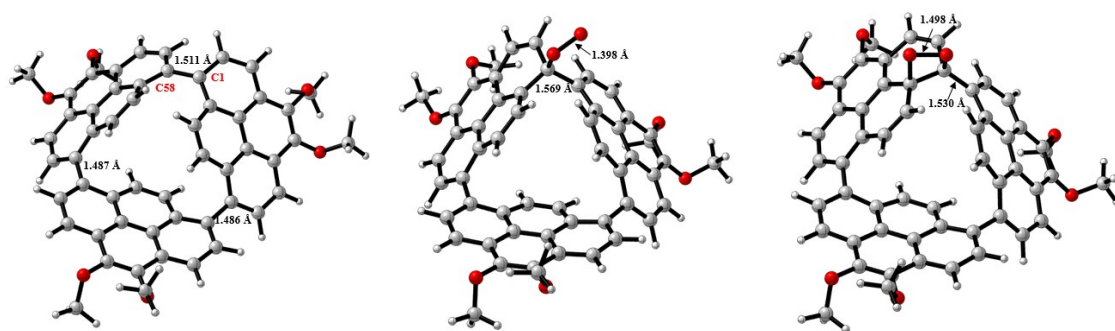


Figure S21. Structures of CP3, INT1, and INT2 optimized at B3LYP-D3/6-31G(d) level with the SMD solvation model. The propyl groups were replaced by methyl groups.

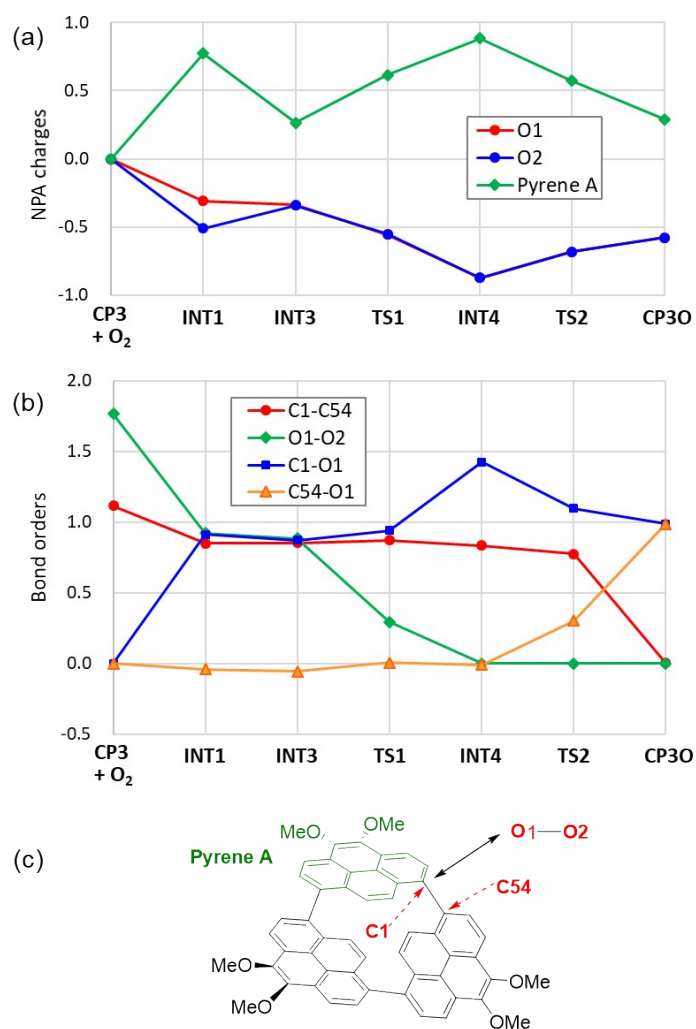


Figure S22. NPA charges (a) and Mayer's bond orders (b) on and between the reactive atoms and moiety at the critical structures along the reaction. The names of the reactive atoms (O1, O2, C1, and C54) and the moiety (Pyrene A) were defined in (c). All the values were calculated at the B3LYP-D3/6-311G(d,p)/B3LYP-D3/6-31G(d) level including the SMD solvation model. The propyl groups were replaced by methyl groups.

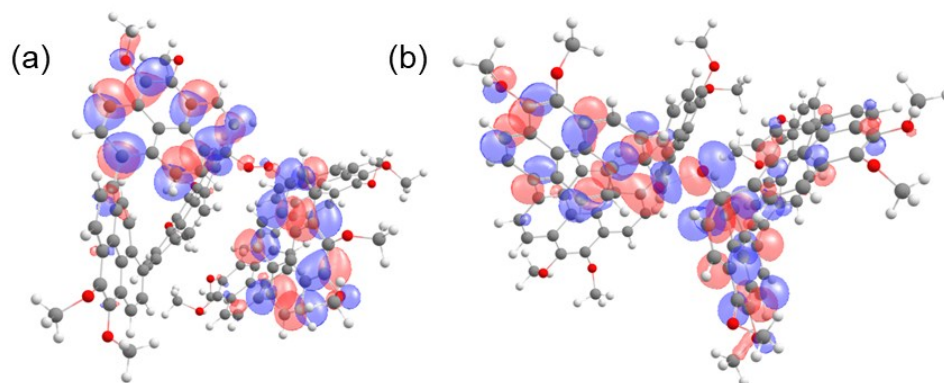


Figure S23. HOMOs of **INT3** (a) and **TS1** (b) calculated at the B3LYP-D3/6-311G(d,p)//B3LYP-D3/6-31G(d) level including the SMD solvation model for dichloromethane. The propyl groups were replaced by methyl groups.

8. X-ray Crystal Structures

Table S1. Crystal data and structure refinement for CP3.

Empirical formula	C ₆₆ H ₆₀ O ₆	
Formula weight	949.14	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	$a = 8.9771(10)$ Å	$\alpha = 116.5169(19)^\circ$
	$b = 17.626(2)$ Å	$\beta = 93.784(2)^\circ$
	$c = 17.763(2)$ Å	$\gamma = 102.495(2)^\circ$
Volume	2412.5(5) Å ³	
<i>Z</i>	2	
Density (calculated)	1.307 g/cm ³	
Absorption coefficient	0.082 mm ⁻¹	
<i>F</i> (000)	1008	
Crystal size	0.10 x 0.10 x 0.02 mm ³	
Theta range for data collection	1.304 to 25.999°	
Index ranges	$-10 \leq h \leq 11$, $-21 \leq k \leq 14$, $-19 \leq l \leq 21$	
Reflections collected	14199	
Independent reflections	9398 [<i>R</i> (int) = 0.0365]	
Completeness to theta = 25.242°	99.4%	
Max. and min. transmission	0.998 and 0.972	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	9398 / 0 / 655	
Goodness-of-fit on <i>F</i> ²	1.061	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0738, <i>wR</i> ₂ = 0.1592	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1256, <i>wR</i> ₂ = 0.2024	
Largest diff. peak and hole	1.100 and -1.029 e.Å ⁻³	

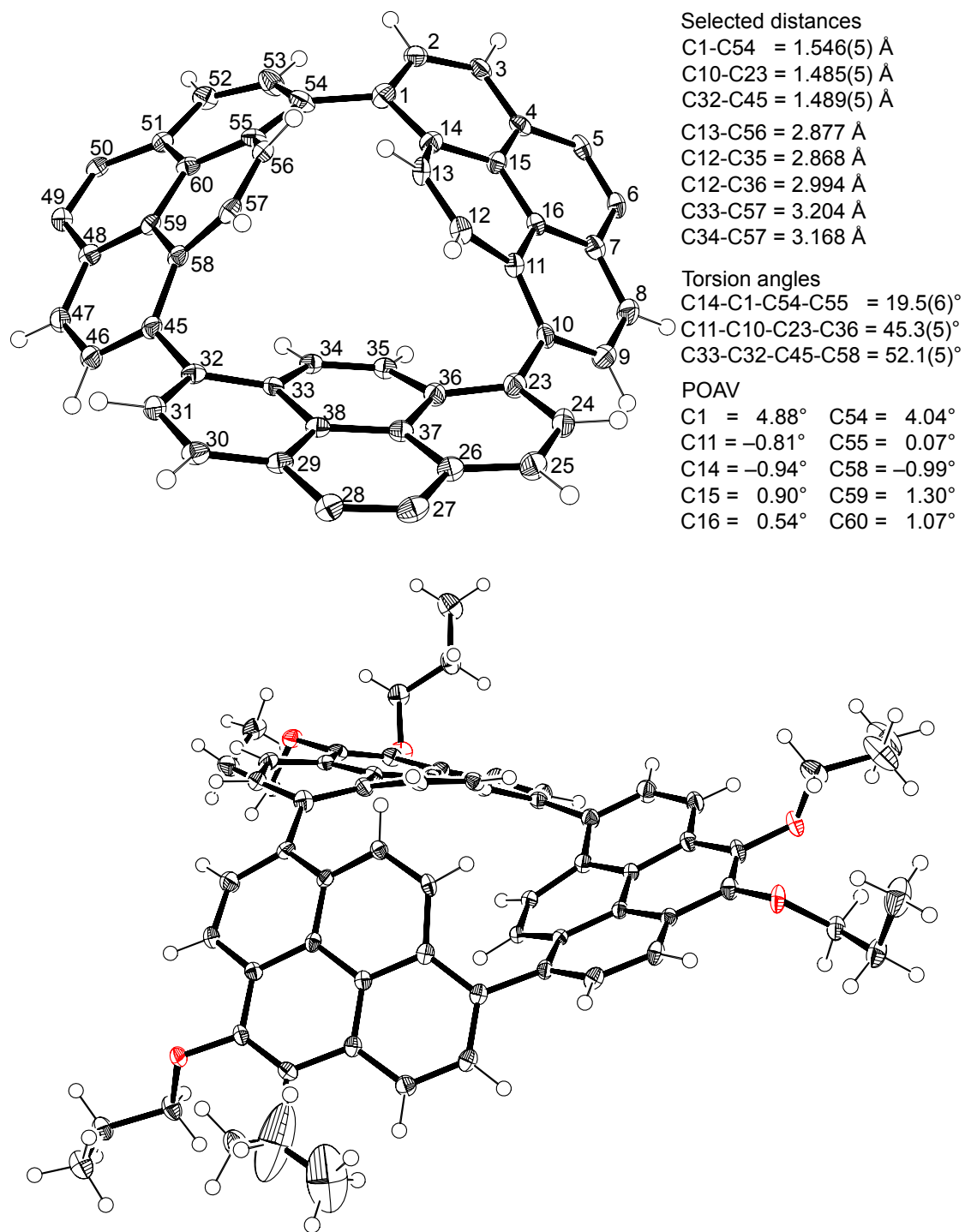


Figure S24. X-ray structure of CP3. The thermal ellipsoids are scaled to the 50% probability.

Table S2. Crystal data and structure refinement for **CP3O**.

Empirical formula	C ₆₆ H ₆₀ O ₇ ·(methanol) _{0.51} ·(dichloromethane) _{0.39}	
Formula weight	1012.83	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 17.7176(19) Å	<i>α</i> = 109.8071(19) °
	<i>b</i> = 18.088(2) Å	<i>β</i> = 114.3435(19) °
	<i>c</i> = 18.855(2) Å	<i>γ</i> = 91.189(2) °
Volume	5088.2(10) Å ³	
<i>Z</i>	4	
Density (calculated)	1.322 g/cm ³	
Absorption coefficient	0.124 mm ⁻¹	
<i>F</i> (000)	2143	
Crystal size	0.30 x 0.20 x 0.05 mm ³	
Theta range for data collection	1.392 to 24.462 °	
Index ranges	-19 ≤ <i>h</i> ≤ 20, -20 ≤ <i>k</i> ≤ 21, -21 ≤ <i>l</i> ≤ 12	
Reflections collected	26337	
Independent reflections	16673 [<i>R</i> (int) = 0.0408]	
Completeness to theta = 23.5 °	98.9%	
Max. and min. transmission	0.994 and 0.906	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	16673 / 35 / 1514	
Goodness-of-fit on <i>F</i> ²	1.025	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0829, <i>wR</i> ₂ = 0.2091	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1777, <i>wR</i> ₂ = 0.2715	
Largest diff. peak and hole	0.533 and -0.359 e.Å ⁻³	

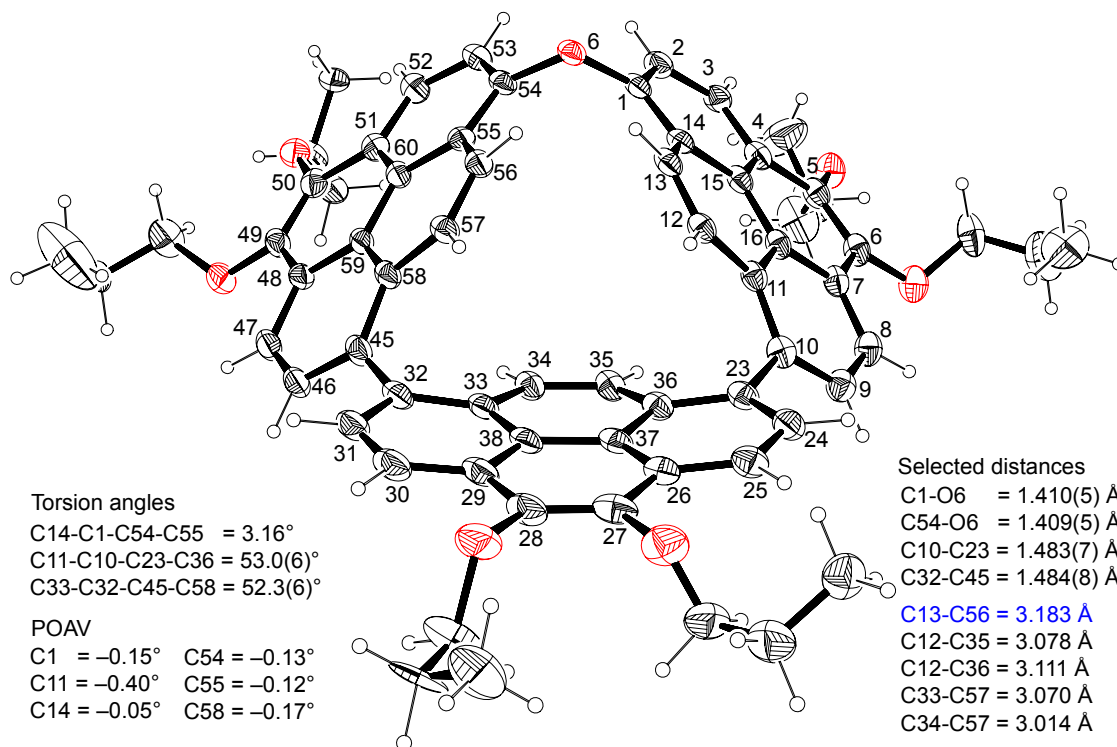


Figure S25. X-ray structure of CP30. The thermal ellipsoids are scaled to the 25% probability. The crystallographic asymmetric unit of CP30 contains two identical molecules of slightly different structures.

9. Cartesian Coordinates

The cartesian coordinates (in Å) optimized at the B3LYP-D3/6-31G(d) level including the SMD solvation models are shown.

CP3

C	2.32905965	-0.56980056	0.00000000
C	3.61353365	-1.15321356	0.16083500
H	4.40367365	-0.56727156	0.61848100
C	3.94226865	-2.41964856	-0.29806900
H	4.95186565	-2.79719256	-0.17793100
C	2.99933265	-3.18105056	-1.01203700
C	3.34828865	-4.37491456	-1.73208400
C	2.40899365	-5.05524156	-2.47315300
C	1.04161865	-4.60699056	-2.51838400
C	0.06682865	-5.23847756	-3.31601900
H	0.36016565	-6.08767356	-3.92369000
C	-1.23782535	-4.75458956	-3.37534400
H	-1.94788135	-5.21929556	-4.05442900
C	-1.65275035	-3.66098056	-2.59727000
C	-0.70678035	-3.08028156	-1.71007700
C	-1.05632335	-2.10829356	-0.72248800
H	-2.09584735	-1.97034856	-0.45114000
C	-0.10987235	-1.34668156	-0.11678800
H	-0.43674435	-0.66733056	0.64297500
C	1.29270965	-1.49475156	-0.37191900
C	1.65119865	-2.72698156	-1.01842700
C	0.66211565	-3.47543956	-1.73837200
C	-3.03151335	-3.10961256	-2.65316200
C	-4.14659835	-3.95535056	-2.53270200
H	-3.99039435	-5.03087456	-2.52378200
C	-5.43169435	-3.45344856	-2.35012200
H	-6.27264935	-4.13018856	-2.24499700
C	-5.64703635	-2.07102256	-2.20683600
C	-6.93671035	-1.53150656	-1.86044500
C	-7.10038635	-0.18705556	-1.62557200
C	-5.98362235	0.72058244	-1.70248700
C	-6.10983835	2.08362244	-1.38312200
H	-7.07943135	2.46537444	-1.08284700
C	-4.99968735	2.92392844	-1.40176500
H	-5.11046135	3.96244044	-1.10102800

C	-3.72934135	2.45915444	-1.77077900
C	-3.59250435	1.10492844	-2.18858600
C	-2.37853135	0.57749144	-2.75204000
H	-1.56682735	1.25625644	-2.98425400
C	-2.22234535	-0.75163156	-2.99461700
H	-1.28742235	-1.11084356	-3.40949700
C	-3.25504735	-1.70259156	-2.68712800
C	-4.54256535	-1.18105356	-2.36012000
C	-4.70784935	0.21719444	-2.09791900
C	-2.53723535	3.34868544	-1.77353100
C	-2.49539035	4.49316644	-2.58376500
H	-3.39915135	4.80255844	-3.10237000
C	-1.31200335	5.19782844	-2.78996900
H	-1.30088135	6.07391744	-3.42899000
C	-0.09702235	4.72171244	-2.26491000
C	1.16704765	5.32618144	-2.59660000
C	2.34558965	4.73955144	-2.20221300
C	2.34294165	3.52529744	-1.43097800
C	3.52010065	2.81675844	-1.14847300
H	4.47467865	3.22149144	-1.46665100
C	3.45757565	1.54910844	-0.59316200
H	4.38180565	0.98586144	-0.57913900
C	2.25724965	0.93199744	-0.15082300
C	1.08926565	1.75961944	-0.21314600
C	-0.16139535	1.49649044	0.44564000
H	-0.14932035	0.88962044	1.34138000
C	-1.33747335	2.02122144	-0.00185900
H	-2.27397035	1.74461544	0.47289100
C	-1.36000535	2.97311344	-1.07543500
C	-0.11441235	3.57547344	-1.41556200
C	1.11047665	2.96814044	-0.99040800
O	4.65411865	-4.80083456	-1.65115300
O	2.73788365	-6.15705256	-3.22685300
O	-7.98651435	-2.41608856	-1.78276800
O	-8.31389735	0.34237044	-1.25446100
O	1.13874465	6.45596044	-3.37885800
O	3.57123265	5.27246444	-2.52699000
C	-9.33808535	0.28909844	-2.26310700
H	-10.20479935	0.80229044	-1.83971800
H	-9.01099635	0.81062644	-3.17118600

H	-9.60295435	-0.74405956	-2.50866300
C	-8.53234535	-2.60306756	-0.46484200
H	-8.98690235	-1.68207956	-0.08672500
H	-9.29519535	-3.37929156	-0.56188700
H	-7.75322735	-2.94045556	0.22984200
C	1.64707065	7.64653844	-2.75201300
H	1.49120465	8.45499744	-3.47024000
H	1.09224665	7.86297144	-1.83053800
H	2.71358565	7.55400644	-2.52433300
C	3.89670865	5.24340844	-3.92818500
H	3.21826865	5.87646344	-4.50868900
H	4.91763965	5.62435544	-4.00859400
H	3.85763465	4.21607644	-4.31096000
C	5.40921065	-4.67309456	-2.86872300
H	5.41712765	-3.63040556	-3.20989700
H	6.42808765	-4.98522856	-2.62705100
H	5.00279465	-5.31421856	-3.65746700
C	3.11989465	-7.32151556	-2.47380200
H	3.28012565	-8.11551256	-3.20714100
H	4.04127665	-7.14652156	-1.90971600
H	2.31723265	-7.61512356	-1.78590200

O₂ (Singlet, ¹Δ_g)

O	1.91579008	0.42735042	0.02507907
O	1.91579008	0.42735042	-1.19071093

INT1

C	2.69919867	-0.78347577	0.03533445
C	1.45699567	-0.46656177	-0.52965655
H	0.61313167	-1.12491377	-0.35957155
C	1.24770867	0.66784523	-1.30949955
H	0.26008067	0.88511723	-1.70163055
C	2.31609467	1.51142523	-1.63671155
C	2.15689067	2.63861623	-2.52260855
C	3.23888767	3.38364823	-2.92014455
C	4.57097967	3.02315923	-2.50247955
C	5.71172867	3.64805623	-3.03391455
H	5.58499367	4.46847723	-3.73168255
C	6.98382367	3.14249423	-2.76642455
H	7.84197067	3.54433123	-3.29909355

C	7.17090867	2.06716923	-1.88958655
C	6.04864567	1.56680723	-1.17609955
C	6.16209567	0.63799223	-0.08706055
H	7.13923867	0.47393023	0.35681045
C	5.07250167	-0.00905877	0.41128845
H	5.16319467	-0.62065177	1.29545345
C	3.77680467	0.11251623	-0.20162755
C	3.60549267	1.20925123	-1.10876155
C	4.73634667	1.95808123	-1.56632055
C	8.43995267	1.28776023	-1.87512555
C	9.67629267	1.81612723	-1.48433155
H	9.73255767	2.85879823	-1.18317955
C	10.82522267	1.02583623	-1.43880055
H	11.77026467	1.45579623	-1.12535455
C	10.76937967	-0.34462277	-1.74580155
C	11.91799967	-1.20921777	-1.62269555
C	11.81774267	-2.56130277	-1.85575355
C	10.55272567	-3.16387677	-2.19549955
C	10.39544167	-4.55517677	-2.33436055
H	11.26159467	-5.19622177	-2.21308355
C	9.13460967	-5.11338977	-2.54071555
H	9.02132567	-6.19416077	-2.54539555
C	7.99544967	-4.30744677	-2.67193555
C	8.15454967	-2.89485877	-2.69012355
C	7.07780767	-2.00356277	-3.01750055
H	6.15805167	-2.41181477	-3.42027955
C	7.18679467	-0.66327677	-2.83142055
H	6.35277267	-0.02546877	-3.09448755
C	8.37763767	-0.07378977	-2.28197755
C	9.52623267	-0.90885077	-2.15693855
C	9.41668467	-2.31908677	-2.36917955
C	6.61645867	-4.85541777	-2.66376955
C	6.13697867	-5.74755477	-3.62343755
H	6.81883667	-6.14086477	-4.37179055
C	4.78232467	-6.09235177	-3.68044055
H	4.43780067	-6.78038777	-4.44414255
C	3.84633267	-5.51421277	-2.80471155
C	2.43274167	-5.80343177	-2.88663455
C	1.54123867	-5.20977377	-1.98057855
C	1.99862167	-4.31307277	-0.99187555

C	1.13032267	-3.82699377	0.04897345
H	0.15426067	-4.29021877	0.15353445
C	1.53859967	-2.86351477	0.90879445
H	0.92454967	-2.52824877	1.73753845
C	2.85929367	-2.15834577	0.77451445
C	3.85429267	-3.06887677	0.05180445
C	5.23335567	-3.02522877	0.31120345
H	5.59684767	-2.49956377	1.18135945
C	6.13571367	-3.65223377	-0.52330855
H	7.19457967	-3.58682777	-0.30251555
C	5.70476867	-4.36889177	-1.66911155
C	4.31005767	-4.61937677	-1.79974555
C	3.39096467	-3.97199677	-0.92691455
O	0.87875267	2.92752023	-2.94140555
O	3.11954867	4.44013023	-3.79195255
O	13.10868767	-0.61695977	-1.27906155
O	12.89416067	-3.40494277	-1.71768055
O	2.09792667	-6.64510977	-3.87429955
O	0.19736667	-5.50141677	-2.03450955
C	13.94993967	-3.21080377	-2.67564055
H	14.68314167	-3.99653377	-2.47878255
H	13.56546867	-3.31590077	-3.69767455
H	14.41905567	-2.22881077	-2.55950655
C	13.64099667	-1.00081477	0.00198345
H	13.91424267	-2.06024377	0.02015445
H	14.53117267	-0.38590677	0.15378945
H	12.91356367	-0.79509277	0.79670245
C	0.89532167	-7.44234477	-3.86176755
H	1.08211567	-8.22758277	-4.59720255
H	0.72917167	-7.88292477	-2.87662155
H	0.02585467	-6.85473177	-4.16235255
C	-0.58273833	-4.52054377	-2.74300255
H	-0.27272033	-4.45909477	-3.79364555
H	-1.62042933	-4.85599777	-2.68326055
H	-0.48767833	-3.53134177	-2.27955855
C	0.63997267	2.73666223	-4.34664155
H	0.86980067	1.70458323	-4.63939055
H	-0.42409733	2.93113523	-4.50107155
H	1.23436467	3.42906523	-4.95111755
C	2.38403467	5.56850223	-3.28767455

H	2.44282467	6.33679823	-4.06240055
H	1.33696367	5.31154423	-3.09947255
H	2.84135367	5.94398323	-2.36396955
O	2.62654367	-1.03684677	2.78581445
O	3.37799667	-2.00429577	2.11259045

INT2

C	1.24633184	1.36752135	0.01631538
C	0.10705984	1.86029235	-0.64817262
H	-0.80625316	1.27856735	-0.64255062
C	0.08907284	3.06301635	-1.34189062
H	-0.82673816	3.40888535	-1.80808762
C	1.26550984	3.80491635	-1.50129162
C	1.30434884	5.00270035	-2.30186062
C	2.49519384	5.62960435	-2.57375862
C	3.73876584	5.06539135	-2.11305562
C	4.98170784	5.55593235	-2.54725362
H	5.00816684	6.42834335	-3.19066562
C	6.15210584	4.85329235	-2.26623562
H	7.08349884	5.15532935	-2.73821162
C	6.14060284	3.70723035	-1.46050362
C	4.92787484	3.34093035	-0.81834562
C	4.85056084	2.36279535	0.22919738
H	5.76843584	2.04856035	0.71678938
C	3.65498684	1.84889135	0.63340838
H	3.60484984	1.19751535	1.49207138
C	2.43322484	2.15136735	-0.06084962
C	2.46224984	3.31314235	-0.90386662
C	3.70560984	3.93388135	-1.24402862
C	7.28533184	2.75705135	-1.46936462
C	8.57712084	3.10900135	-1.05692762
H	8.75655984	4.11796735	-0.69498062
C	9.62442684	2.18961235	-1.07385062
H	10.61482084	2.48383235	-0.74411062
C	9.40711084	0.85982235	-1.47436662
C	10.45084584	-0.13417465	-1.42894962
C	10.19549384	-1.44592765	-1.75219962
C	8.86700484	-1.87534365	-2.11137762
C	8.54790084	-3.22810765	-2.32608362
H	9.33496384	-3.97107365	-2.25863062

C	7.22681684	-3.62248365	-2.52761562
H	6.98878084	-4.68184765	-2.57874562
C	6.18338084	-2.68698165	-2.59518062
C	6.51083184	-1.30556565	-2.55941162
C	5.54522684	-0.27522865	-2.81754762
H	4.58222884	-0.55190565	-3.23184162
C	5.80688784	1.02859635	-2.54071562
H	5.05023884	1.77278035	-2.75297462
C	7.05745284	1.44061035	-1.95988762
C	8.10411784	0.47221335	-1.90695962
C	7.83372184	-0.89834865	-2.21686662
C	4.75821584	-3.11378765	-2.55338362
C	4.23481484	-4.05363565	-3.48140462
H	4.90167884	-4.48013465	-4.22564562
C	2.90219484	-4.39987365	-3.47319062
H	2.51054784	-5.10532865	-4.19763762
C	2.00147784	-3.80354465	-2.54784062
C	0.60676184	-4.08613965	-2.57212362
C	-0.25994016	-3.41670165	-1.71537762
C	0.23688384	-2.47322165	-0.77722662
C	-0.69084916	-1.66677265	0.01742838
H	-1.72628716	-1.98752165	0.06197338
C	-0.30416016	-0.53134965	0.61234438
H	-1.01429416	0.07060435	1.17251538
C	1.12973884	-0.02442065	0.64032438
C	2.08958684	-1.25265065	0.34829638
C	3.57039184	-1.10755165	0.35433238
H	3.98871984	-0.60700265	1.21235738
C	4.38890484	-1.75350965	-0.48561962
H	5.45712784	-1.68943865	-0.31782162
C	3.90614984	-2.58682365	-1.57153962
C	2.50537384	-2.88290365	-1.57923162
C	1.61009484	-2.25000365	-0.66960062
O	0.10339684	5.47433435	-2.77670062
O	2.57134284	6.75003235	-3.36314262
O	11.70484384	0.29335835	-1.06149462
O	11.16851984	-2.41476065	-1.68520162
O	0.14986684	-4.97154365	-3.51183762
O	-1.61561016	-3.64544865	-1.75199662
C	12.23886284	-2.27424665	-2.63595162

H	12.87751284	-3.15056965	-2.50188262
H	11.84446484	-2.26144865	-3.65957362
H	12.81730284	-1.36305265	-2.45454662
C	12.18685284	-0.22758065	0.19011438
H	12.33000284	-1.31157565	0.14319838
H	13.14523084	0.26449935	0.37199638
H	11.49029184	0.01603935	1.00177138
C	-0.47921816	-6.16165965	-2.99875962
H	-0.71453416	-6.77381265	-3.87211862
H	0.21242084	-6.70564765	-2.34420262
H	-1.39608616	-5.92532665	-2.45153662
C	-2.27937816	-3.15159165	-2.92983262
H	-1.91417816	-3.65411365	-3.83128362
H	-3.34120816	-3.36758165	-2.79106262
H	-2.13452516	-2.06854265	-3.02743162
C	-0.05307116	5.41458835	-4.20604862
H	0.08025284	4.38655835	-4.56469062
H	-1.07455416	5.74342635	-4.41118162
H	0.65753984	6.07425735	-4.71385562
C	1.92619184	7.92221935	-2.83367062
H	2.14562584	8.72869835	-3.53707662
H	0.84374284	7.78289535	-2.75496362
H	2.33685184	8.17321335	-1.84802562
O	1.81379284	-1.60352465	1.79711338
O	1.52169884	-0.15697965	2.05437838

INT3

C	-0.66239311	0.31339031	0.00000000
C	-1.42666911	0.09128531	-1.15417200
H	-1.69562111	-0.92218869	-1.42469200
C	-1.86708811	1.12229831	-1.97971000
H	-2.48523311	0.90080431	-2.84275500
C	-1.48504911	2.44634931	-1.73111500
C	-1.86285411	3.52956531	-2.60645500
C	-1.37446311	4.79615031	-2.40826200
C	-0.47099711	5.07781131	-1.32271300
C	0.14012489	6.33448931	-1.16965200
H	-0.09734311	7.12148431	-1.87697500
C	1.10939589	6.53930231	-0.18788900
H	1.65477089	7.47921531	-0.16210500

C	1.44848189	5.53024931	0.72270000
C	0.71291789	4.31433731	0.69307600
C	0.82337589	3.31102031	1.71141000
H	1.31703589	3.56193431	2.64418600
C	0.30028089	2.06842531	1.54388100
H	0.31054889	1.38107431	2.36930400
C	-0.33309511	1.66030131	0.31959100
C	-0.67602811	2.71595731	-0.58883700
C	-0.16651411	4.04036631	-0.39209400
C	2.64708189	5.61944931	1.59816500
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C	-5.30154611	4.44872231	3.40517400
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TS1

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H	-0.24799326	8.62202730	-1.30215100
C	2.31470874	7.25588730	-0.68232600
H	1.98426974	7.08899530	-1.71315600
H	2.88862074	8.18416930	-0.62538200

H	2.93850274	6.41710130	-0.35400400
C	-7.42016526	-3.49250670	0.45774600
H	-8.49797926	-3.34136070	0.35993000
H	-6.97031826	-3.57566270	-0.53953300
H	-7.22482426	-4.40827670	1.02460500
C	-6.41596826	-3.77318970	3.79334100
H	-7.25883826	-3.20555370	3.38663000
H	-6.78093626	-4.68625970	4.26990600
H	-5.88483326	-3.16130270	4.53303600
C	-0.33342826	-2.99860470	8.76442600
H	-1.06503326	-3.27673470	7.99544900
H	-0.16110826	-3.84801970	9.42964400
H	-0.71178426	-2.14829570	9.34197800
C	1.73294574	-0.35731070	9.89239100
H	1.44957074	0.01302130	10.88007400
H	1.90691274	-1.43569770	9.93278600
H	2.64342874	0.15286230	9.55561500

INT4

C	2.02991437	-0.58404558	0.00000000
C	0.79618437	-0.22668258	-0.56681500
H	-0.06065763	-0.87786758	-0.42780500
C	0.60999337	0.93156142	-1.31827600
H	-0.37078263	1.17637842	-1.71262200
C	1.69592337	1.76398142	-1.62107000
C	1.56762437	2.90990742	-2.48712400
C	2.67015537	3.63168742	-2.87265600
C	3.99222137	3.22831942	-2.46248700
C	5.15062237	3.82346342	-2.99073600
H	5.04850537	4.65567942	-3.67855000
C	6.40551137	3.27182642	-2.73460800
H	7.27457237	3.65040442	-3.26683500
C	6.56118737	2.18058242	-1.87030200
C	5.42765937	1.70937142	-1.15540000
C	5.51390437	0.76595042	-0.07437100
H	6.48682937	0.56919442	0.36618800
C	4.40476437	0.14638842	0.41599500
H	4.44868537	-0.48527958	1.29155800
C	3.11614337	0.31087942	-0.20298700
C	2.97557837	1.42544442	-1.09270000

C	4.12741437	2.14795642	-1.53907400
C	7.80610737	1.36231542	-1.87751500
C	9.06074337	1.85181842	-1.49420400
H	9.14707737	2.88704142	-1.17498000
C	10.19057137	1.03354142	-1.48140300
H	11.15035637	1.43396342	-1.17362400
C	10.09720237	-0.32792458	-1.81696100
C	11.22758437	-1.22056758	-1.73123600
C	11.09304537	-2.56436358	-1.99221000
C	9.80903237	-3.13018458	-2.32349400
C	9.61870037	-4.51462958	-2.48756700
H	10.47228237	-5.17691458	-2.39511600
C	8.34236537	-5.04018458	-2.67988900
H	8.20404137	-6.11783358	-2.70080600
C	7.21898737	-4.20657358	-2.77274900
C	7.40886937	-2.79732358	-2.77055700
C	6.34801537	-1.87428658	-3.06147600
H	5.41160437	-2.25277158	-3.45495800
C	6.49105237	-0.54095058	-2.84878700
H	5.66722137	0.12091542	-3.08286100
C	7.70401337	0.01017042	-2.30781600
C	8.83464237	-0.85408858	-2.21931800
C	8.68959337	-2.25672858	-2.46031000
C	5.83369837	-4.73590658	-2.73365100
C	5.33512837	-5.65130558	-3.66670400
H	6.00046837	-6.05449958	-4.42427900
C	3.98516837	-6.00809958	-3.67630900
H	3.62394637	-6.71132758	-4.41835500
C	3.07110137	-5.42443858	-2.77939500
C	1.65994537	-5.73657658	-2.80297900
C	0.78677037	-5.11913458	-1.89048100
C	1.26438637	-4.18493358	-0.94760600
C	0.40232437	-3.64682358	0.07874900
H	-0.57749963	-4.09760358	0.20250700
C	0.80970937	-2.61623958	0.85822000
H	0.15033937	-2.20702558	1.61923800
C	2.18131237	-1.94741658	0.80832600
C	3.12741537	-2.87481258	-0.01265000
C	4.51342937	-2.85146258	0.23013300
H	4.86906537	-2.33233758	1.10678200

C	5.39928337	-3.48448558	-0.60935900
H	6.46260737	-3.41579658	-0.41113400
C	4.94671637	-4.23323658	-1.73181000
C	3.55202737	-4.49857558	-1.81510200
C	2.65181937	-3.82707658	-0.93948700
O	0.29806137	3.24006642	-2.90290700
O	2.57895637	4.70440542	-3.72946000
O	12.43655837	-0.66323358	-1.39360100
O	12.15138037	-3.43545058	-1.88954200
O	1.31165437	-6.62715858	-3.73487800
O	-0.55361063	-5.43223358	-1.89359500
C	13.19970037	-3.24214158	-2.85576000
H	13.91574537	-4.05024658	-2.68839700
H	12.80039337	-3.31144458	-3.87515600
H	13.69428837	-2.27520458	-2.72067600
C	12.97748937	-1.08534658	-0.12818300
H	13.22105237	-2.15212458	-0.13342900
H	13.88686537	-0.49842358	0.02049200
H	12.26835037	-0.87408758	0.68144900
C	0.09595837	-7.40611058	-3.69208300
H	0.27151937	-8.21676258	-4.40174600
H	-0.07232863	-7.81014858	-2.69246500
H	-0.76386563	-6.81495858	-4.01168100
C	-1.36975463	-4.48996058	-2.61412100
H	-1.09532663	-4.46595658	-3.67617700
H	-2.40013463	-4.83612558	-2.50717400
H	-1.27378763	-3.48206658	-2.19342500
C	0.05710137	3.08135942	-4.31146500
H	0.26370637	2.05000342	-4.62361600
H	-1.00212563	3.30266942	-4.46353200
H	0.66791037	3.77121242	-4.90232900
C	1.87994337	5.84563142	-3.20422800
H	1.95843337	6.62472042	-3.96646700
H	0.82617137	5.61714342	-3.01579400
H	2.35141437	6.19270942	-2.27637300
O	2.63355037	-1.82538658	2.07459000

TS2

C	1.93019928	0.07122507	0.00000000
C	0.60090128	0.47215207	-0.27271200

H	-0.22727972	-0.15185493	0.03225500
C	0.31680528	1.60607607	-1.01605300
H	-0.71677072	1.85080507	-1.23751400
C	1.33878128	2.40101307	-1.56209800
C	1.06232028	3.51631007	-2.42149300
C	2.08251528	4.24905407	-2.98457900
C	3.45585928	3.89892607	-2.74294000
C	4.51867228	4.57234507	-3.37436600
H	4.29280328	5.39854407	-4.03950900
C	5.83182028	4.13001307	-3.22452400
H	6.62205128	4.59129107	-3.81161700
C	6.14776628	3.05272307	-2.38753100
C	5.10838228	2.47514007	-1.60101700
C	5.35731028	1.54008307	-0.54753300
H	6.37568128	1.39597707	-0.20227600
C	4.34454328	0.84040907	0.03973600
H	4.54448628	0.21460907	0.89177200
C	2.98900428	0.95401007	-0.39660400
C	2.69045328	2.05582807	-1.26265300
C	3.74967928	2.81981807	-1.85292400
C	7.47763428	2.39269107	-2.41323000
C	8.67659428	3.06052207	-2.12475800
H	8.64950228	4.12892507	-1.92684700
C	9.88804928	2.37684307	-2.03173000
H	10.79989928	2.91338807	-1.79290100
C	9.93868928	0.97815007	-2.17484400
C	11.14944828	0.22386207	-1.96828800
C	11.15041728	-1.15120493	-2.03323700
C	9.93414328	-1.88373893	-2.28101500
C	9.88196528	-3.28977893	-2.25718300
H	10.79408528	-3.84565293	-2.06991600
C	8.66846528	-3.96234893	-2.39939800
H	8.63977428	-5.04382593	-2.29616300
C	7.47265628	-3.26544493	-2.61614700
C	7.52069428	-1.85485393	-2.77669000
C	6.37911828	-1.09114493	-3.19598200
H	5.49436528	-1.60981693	-3.54547500
C	6.38687828	0.26583207	-3.16413000
H	5.50796628	0.80878207	-3.48880200
C	7.52845328	0.99915207	-2.69251200

C	8.73997328	0.27602007	-2.49504900
C	8.73615928	-1.15312793	-2.53690600
C	6.13130928	-3.90307593	-2.62091100
C	5.73054628	-4.79887193	-3.61677500
H	6.46662328	-5.16323493	-4.32794800
C	4.39360928	-5.16980693	-3.76193500
H	4.10648928	-5.85361693	-4.55259400
C	3.39480528	-4.61343793	-2.93969700
C	1.99604428	-4.90274593	-3.13357200
C	1.04315228	-4.33590293	-2.28767800
C	1.42359228	-3.47336293	-1.23005200
C	0.47545628	-3.01539993	-0.25441200
H	-0.52361072	-3.43920393	-0.27108800
C	0.84432028	-2.13109293	0.70759700
H	0.14679228	-1.82085793	1.48010300
C	2.14815328	-1.41242693	0.67643300
C	3.18566028	-2.24126093	-0.01335500
C	4.55457428	-2.16556193	0.31337500
H	4.84272628	-1.65546193	1.22441500
C	5.51451328	-2.73472993	-0.49274100
H	6.56233728	-2.64040893	-0.22842500
C	5.16175328	-3.45378393	-1.67171800
C	3.78167328	-3.73564393	-1.88536300
C	2.79797228	-3.12521793	-1.05407600
O	-0.25987372	3.83246807	-2.63409800
O	1.83593928	5.30310707	-3.83521400
O	12.29556528	0.93993607	-1.71825200
O	12.28926128	-1.88811893	-1.80878700
O	1.72275228	-5.71380193	-4.17774300
O	-0.29593872	-4.61465993	-2.45607000
C	13.32266528	-1.73332093	-2.79752000
H	14.11506128	-2.43124393	-2.51684300
H	12.94299828	-1.99125893	-3.79392700
H	13.71563328	-0.71189193	-2.80799500
C	12.85747528	0.76205307	-0.40553100
H	13.20224128	-0.26546693	-0.25414100
H	13.70457528	1.44940207	-0.34543700
H	12.12117528	1.01982807	0.36561500
C	0.59704528	-6.61225093	-4.16472500
H	0.85088628	-7.38923093	-4.88987000

H	0.46198828	-7.05775393	-3.17564000
H	-0.32174772	-6.10825393	-4.47221200
C	-0.98083472	-3.65083393	-3.27478600
H	-0.56956572	-3.63780193	-4.29209000
H	-2.02741772	-3.96272493	-3.30535600
H	-0.90793172	-2.64558393	-2.84182300
C	-0.72329772	3.64804607	-3.98279200
H	-0.56368472	2.61182807	-4.30643000
H	-1.79450172	3.86334407	-3.96579100
H	-0.21941572	4.32959307	-4.67512300
C	1.23967528	6.45468107	-3.21426600
H	1.16572128	7.21564907	-3.99513100
H	0.24216528	6.22577007	-2.82556600
H	1.87442528	6.82632507	-2.40006300
O	2.45755728	-0.62381893	1.75183500

CP30

O	1.03276345	0.71225070	0.00000000
C	0.84380445	1.88767070	-0.74486400
C	-0.44439455	2.33450270	-1.04083300
H	-1.29833755	1.79537870	-0.64768000
C	-0.64247555	3.45602570	-1.84410100
H	-1.64873555	3.79423470	-2.06478900
C	0.44790345	4.13424570	-2.41131900
C	0.27324145	5.23752970	-3.32372200
C	1.35350745	5.83102470	-3.92947900
C	2.69146745	5.34636870	-3.69644900
C	3.80126645	5.85398570	-4.39312000
H	3.65284745	6.66021370	-5.10305100
C	5.05944645	5.27570670	-4.23998800
H	5.88357545	5.61880670	-4.86000200
C	5.28030645	4.21847270	-3.34589100
C	4.20654145	3.79330670	-2.51894700
C	4.37870745	2.86040470	-1.43851800
H	5.38469245	2.59872370	-1.12940000
C	3.31336545	2.30989170	-0.79768200
H	3.46828345	1.65071970	0.04355100
C	1.96858745	2.60772770	-1.19577200
C	1.76857745	3.69713770	-2.09933600
C	2.89108245	4.29384470	-2.75409500

C	6.57359945	3.48277570	-3.32522900
C	7.78829245	4.13614970	-3.07505300
H	7.78457145	5.21338870	-2.93087200
C	8.98671845	3.43469870	-2.96368700
H	9.91206545	3.96260270	-2.76065700
C	9.00814545	2.03258570	-3.05565300
C	10.21497145	1.27201170	-2.84656100
C	10.19809845	-0.10169230	-2.86936900
C	8.96827945	-0.82483630	-3.07806500
C	8.90849345	-2.22758330	-3.01673400
H	9.81937945	-2.78493530	-2.82782900
C	7.68965545	-2.89247430	-3.12982900
H	7.65643745	-3.97141130	-3.00310000
C	6.49162645	-2.20067330	-3.35784900
C	6.54517045	-0.79229830	-3.54593400
C	5.40296645	-0.01890330	-3.94910800
H	4.50362545	-0.53469330	-4.26375100
C	5.42225045	1.33984270	-3.94176700
H	4.53746045	1.88396970	-4.24968300
C	6.58637345	2.07583170	-3.53055300
C	7.79185745	1.33866970	-3.32921700
C	7.77060945	-0.09233530	-3.33289500
C	5.17845345	-2.90005830	-3.36555200
C	4.92537945	-3.96524830	-4.24185200
H	5.73423545	-4.33216930	-4.86829600
C	3.65571645	-4.52462530	-4.36739100
H	3.48341945	-5.33837630	-5.06321500
C	2.56584445	-3.99293730	-3.65718200
C	1.21827245	-4.46770030	-3.85268600
C	0.15774445	-3.86059230	-3.22557200
C	0.36285345	-2.74779130	-2.33114300
C	-0.70727055	-2.06284930	-1.73341800
H	-1.72033455	-2.40492130	-1.91338600
C	-0.48190555	-0.93127230	-0.95072900
H	-1.32034955	-0.39115530	-0.52564900
C	0.81584045	-0.47793230	-0.71257800
C	1.92362545	-1.20863030	-1.18719700
C	3.27849445	-0.91280730	-0.82711600
H	3.45679245	-0.23362230	-0.00784800
C	4.32533545	-1.49190230	-1.47234100

H	5.33884645	-1.23733930	-1.18356700
C	4.12302845	-2.44262730	-2.53154900
C	2.79663945	-2.92851530	-2.73571900
C	1.69411045	-2.31225330	-2.06519900
O	-1.01414355	5.66655270	-3.54441300
O	1.20916245	6.86196170	-4.82827000
O	11.37405845	1.98217670	-2.63918900
O	11.33070045	-0.84707930	-2.64094500
O	1.04323845	-5.50798630	-4.73523800
O	-1.13714655	-4.28548430	-3.40620100
C	12.35071745	-0.73488730	-3.64889900
H	13.13838945	-1.43465730	-3.35956100
H	11.95296945	-1.01699630	-4.63162600
H	12.75633545	0.28055470	-3.69547700
C	11.95043445	1.84413670	-1.32835700
H	12.27886245	0.81676770	-1.14263800
H	12.81066945	2.51737070	-1.30518200
H	11.22976945	2.14429770	-0.55764300
C	0.55625945	-6.72826230	-4.15021400
H	0.54431345	-7.46543530	-4.95665400
H	1.22891145	-7.06847930	-3.35303300
H	-0.45413755	-6.60290730	-3.74842100
C	-1.66617955	-4.09344730	-4.73032300
H	-1.13006855	-4.70049130	-5.46642900
H	-2.71232555	-4.40538230	-4.68472500
H	-1.61121355	-3.03588730	-5.01662900
C	-1.50779355	5.46140670	-4.88019600
H	-1.44967355	4.40041370	-5.15283200
H	-2.55341355	5.77809970	-4.86671900
H	-0.94928455	6.05771970	-5.60837900
C	0.71046045	8.09091070	-4.27208300
H	0.72537545	8.81849070	-5.08713400
H	-0.31178155	7.97449570	-3.89859100
H	1.36095445	8.43785270	-3.45956500

CP3S

S	-3.056133	-0.006138	3.361294
C	-3.191113	1.406436	2.226978
C	-4.469376	1.870161	1.894856
H	-5.338550	1.386385	2.329638

C	-4.649623	2.935503	1.017301
H	-5.649120	3.284194	0.782555
C	-3.546501	3.555335	0.408560
C	-3.711144	4.624836	-0.545536
C	-2.624003	5.192620	-1.163466
C	-1.292258	4.695705	-0.917841
C	-0.177366	5.184330	-1.618566
H	-0.317894	5.978062	-2.343904
C	1.079797	4.610726	-1.443752
H	1.908122	4.948796	-2.060849
C	1.294199	3.569344	-0.529927
C	0.208732	3.152649	0.289616
C	0.366960	2.228364	1.377502
H	1.368377	1.939954	1.676567
C	-0.702015	1.716125	2.045440
H	-0.543422	1.041053	2.875462
C	-2.049995	2.049584	1.685025
C	-2.231534	3.100652	0.727899
C	-1.103805	3.658881	0.045220
C	2.604513	2.861102	-0.468498
C	3.796963	3.546116	-0.193228
H	3.766599	4.624434	-0.060140
C	5.009014	2.875833	-0.042405
H	5.914283	3.431318	0.177112
C	5.068955	1.473560	-0.115466
C	6.287636	0.743639	0.137088
C	6.305531	-0.630288	0.120392
C	5.096903	-1.384878	-0.107954
C	5.063896	-2.787441	-0.024532
H	5.980085	-3.323497	0.197402
C	3.863129	-3.481166	-0.158824
H	3.853719	-4.558646	-0.016315
C	2.656226	-2.820638	-0.431003
C	2.685151	-1.414184	-0.636106
C	1.539264	-0.673319	-1.086441
H	0.663625	-1.214975	-1.424043
C	1.527923	0.685855	-1.099302
H	0.643217	1.206440	-1.446283
C	2.660333	1.453557	-0.659896
C	3.877648	0.747845	-0.416227

C	3.889616	-0.683483	-0.402427
C	1.359172	-3.553321	-0.482344
C	1.162916	-4.607694	-1.385414
H	1.996861	-4.937271	-1.999515
C	-0.083954	-5.204834	-1.554267
H	-0.210668	-6.007969	-2.271744
C	-1.207222	-4.728362	-0.858615
C	-2.530079	-5.250409	-1.099647
C	-3.627032	-4.694715	-0.488250
C	-3.481145	-3.612309	0.454245
C	-4.595353	-3.004447	1.054713
H	-5.588471	-3.372900	0.823189
C	-4.433983	-1.925836	1.919436
H	-5.311581	-1.451032	2.347210
C	-3.164032	-1.436908	2.247452
C	-2.011204	-2.068080	1.716111
C	-0.668917	-1.710232	2.075916
H	-0.521161	-1.026696	2.901309
C	0.408778	-2.210755	1.412936
H	1.405253	-1.903653	1.710015
C	0.266686	-3.147462	0.333377
C	-1.036836	-3.678712	0.093946
C	-2.174288	-3.132333	0.770055
O	-4.993220	5.061267	-0.783997
O	-2.754909	6.200043	-2.088133
O	7.424987	1.480883	0.371496
O	7.450204	-1.345048	0.384768
O	-2.643924	-6.269749	-2.013612
O	-4.901270	-5.155757	-0.722363
C	8.484457	-1.244185	-0.609519
H	9.283609	-1.912912	-0.280972
H	8.113002	-1.572682	-1.587703
H	8.866310	-0.221744	-0.685984
C	7.946220	1.399824	1.709635
H	8.267759	0.382392	1.951696
H	8.804812	2.074881	1.739588
H	7.195588	1.731888	2.436915
C	-3.096954	-7.528712	-1.484953
H	-3.072591	-8.231090	-2.321404
H	-2.422902	-7.878993	-0.694048

H	-4.115892	-7.454437	-1.093894
C	-5.415948	-4.899686	-2.041264
H	-4.835349	-5.425635	-2.805120
H	-6.444127	-5.269198	-2.039767
H	-5.414767	-3.823933	-2.253841
C	-5.502920	4.783959	-2.100528
H	-5.483571	3.706392	-2.302761
H	-6.537126	5.136219	-2.102857
H	-4.930859	5.312204	-2.869230
C	-3.233579	7.455869	-1.574787
H	-3.216913	8.150058	-2.418228
H	-4.253211	7.367406	-1.188556
H	-2.570486	7.826149	-0.783757

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