

Supplementary Information

A Highly Efficient Supramolecular Photoswitch for Singlet Oxygen Generation in Water

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Materials.

All manipulations were carried out under an argon atmosphere by using standard Schlenk techniques, unless otherwise stated. THF was distilled under argon atmosphere from sodium-benzophenone. All other starting materials were obtained commercially as analytical-grade and used without further purification. Other property tests were all performed at room temperature without special statement.

Measurements.

NMR Spectroscopy. ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker AV400 spectrometer at 25 °C.

Mass spectroscopy. Mass spectra were measured in the MALDI mode.

UV-vis Spectroscopy. The optical transmittance and absorbance were measured in two quartz cells (light path, 10 mm and 1mm) on a Shimadzu UV-2401PC spectrophotometer equipped with a Thermo HAAKE-SC100 temperature controller.

Fluorescence Spectroscopy. Steady-state fluorescence spectra were recorded in a conventional quartz cell (light path, 10 mm) on a Varian Cary Eclipse equipped with a Varian Cary single-cell Peltier accessory to control the temperature. The slit width was 5 and 5 nm for excitation and emission, respectively.

TEM Measurement. TEM images were acquired using a Tecnai 20 transmission electron microscope operating at an accelerating voltage of 200 kV. The sample for TEM measurements was prepared by dropping a sample solution (20 μM) onto a copper grid. The grid was then airdried.

AFM Measurement. AFM were performed using a multi-mode IIIa AFM (Veeco Metrology, USA) under ambient conditions, the sample was prepared by dropping the solution (2 μM) onto newly clipped mica.

DLS Measurement. Solution samples (20 μM) were examined on a laser light scattering spectrometer (BI-200SM) equipped with a digital correlator (TurboCorr) at 636 nm at a scattering angle of 90°. The hydrodynamic diameter (D_h) was determined by DLS experiments at 25 °C.

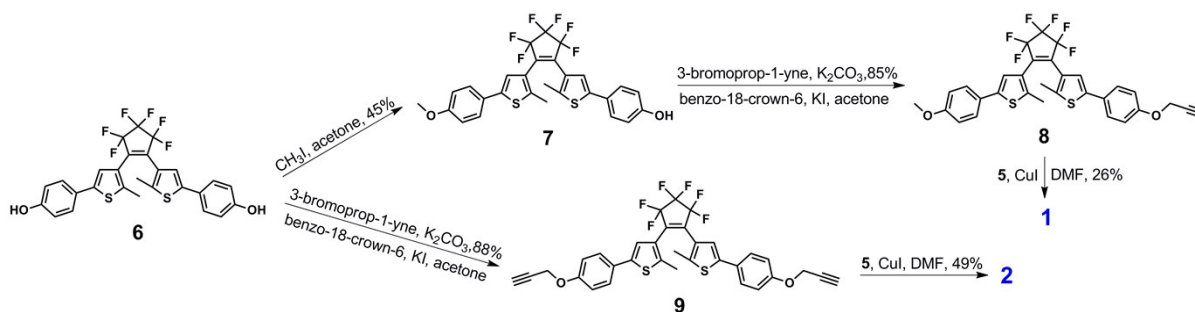
Light Irradiation Experiments. The UV light irradiation experiment was carried out using a ZF-7A lamp (254 nm, 8 W), and the visible light irradiation experiment ($\lambda > 420\text{nm}$) was carried out using a CEL-

HXF300 14V 50W xenon lamp with cutoff filter.

Liquid Chromatography Measurement. The efficiency of photoisomerization was performed on a liquid mass spectrometry apparatus (Agilent 1100).

NIR Emission Spectroscopy. The measurements were performed on a PTI QM/TM/NIR system (Photon Technology International, Birmingham, NJ, USA) equipped with a quartz cell (1cm × 1cm). The slit width was 16 and 24 nm for excitation and emission, respectively.

DFT Calculation. The geometry optimization of four structures (**3=OF-1**, **3=CF-1**, **3=OF-2** and **3=C F-2**) was performed using the semi-empirical method AM1.¹ Geometries of species listed in Figure S26. were optimized with DFT method using the B3LYP hybrid function²⁻³ and 6-31G(d) basis set.⁴⁻⁶ The energy of the T₁ state was obtained by a single-point energy calculation using B3LYP/6-31G(d) method and unrestricted wave function. Then the subtraction of the S₀ energy from the T₁ energy provided the S₀-T₁ energy gap. The S₀-S₁ energy gap was calculated using time-dependent DFT method with B3LYP function and 6-31G(d) basis set. All calculations were carried out with Gaussian 09.⁷



Scheme S1. Synthetic pathway of **1** and **2**.

Synthesis of **7**.

Into a 100 mL, two-necked, round-bottom flask equipped with a magnetic stirrer was placed a mixture of **6** (0.55 g, 1.00 mmol) and 50mL of acetone, then potassium carbonate (0.14 g, 1.00 mmol) was added in portions within several minutes. Afterwards, CH_3I (0.42 g, 1.00 mmol) in 15mL of acetone was added dropwise via a dropping funnel. The reaction was stirred for 24 h at 41 °C under argon atmosphere. The resulting mixture was allowed to cool to room temperature and quenched with saturated aqueous NH_4Cl . After that, the residue was extracted by ethyl acetate, and then dried over

anhydrous Na₂SO₄. After removing solvent under a reduced pressure, the residue was purified on a silica gel column using ethyl acetate / petroleum ether (1:4) as the eluent to obtain **7** as a pale green solid. Yield: 0.25 g, 45%. Compound **7**: ¹H NMR (400 MHz, CDCl₃): δ ppm = 7.48-7.41 (m, 4H), 7.15 (s, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 2H), 3.84 (s, 3H), 1.95 (s, 6H). ¹³C NMR (100 MHz, CDCl₃): δ ppm = 159.5, 155.4, 142.1, 142.0, 140.3, 140.3, 127.2, 126.9, 126.5, 126.3, 125.8, 121.4, 121.4, 115.9, 114.4, 55.4, 14.4. HRMS (FTMALDI): *m/z* = 566.08; calculated exact mass: 566.08.

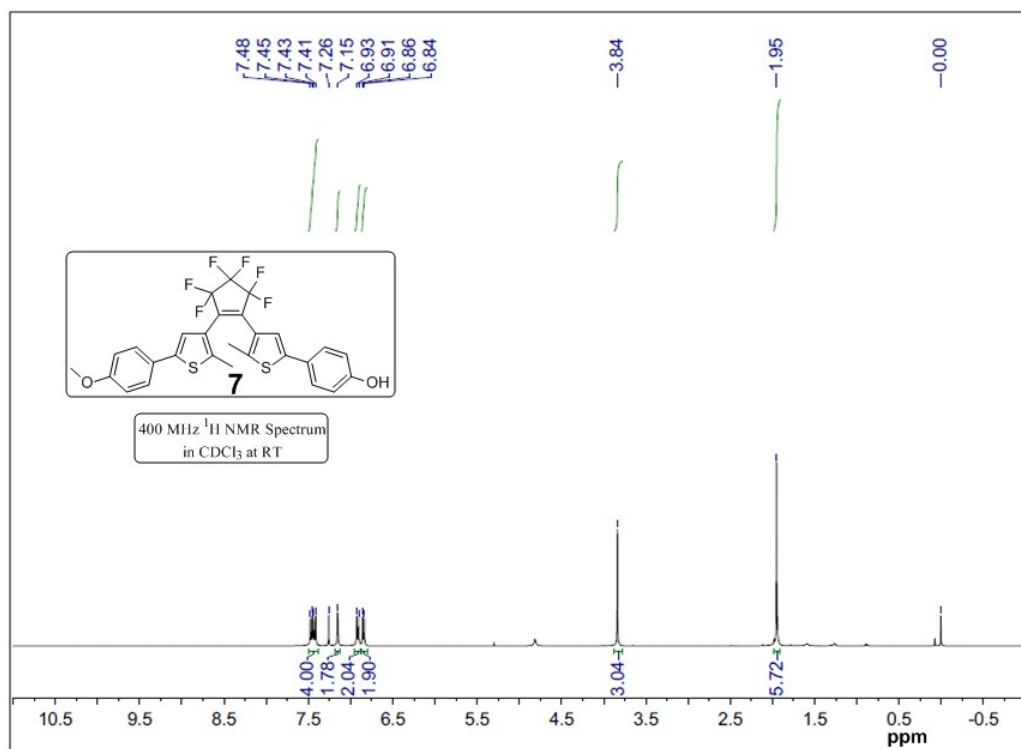


Figure S1. ¹H NMR spectrum (400 MHz, CDCl₃) of **7**.

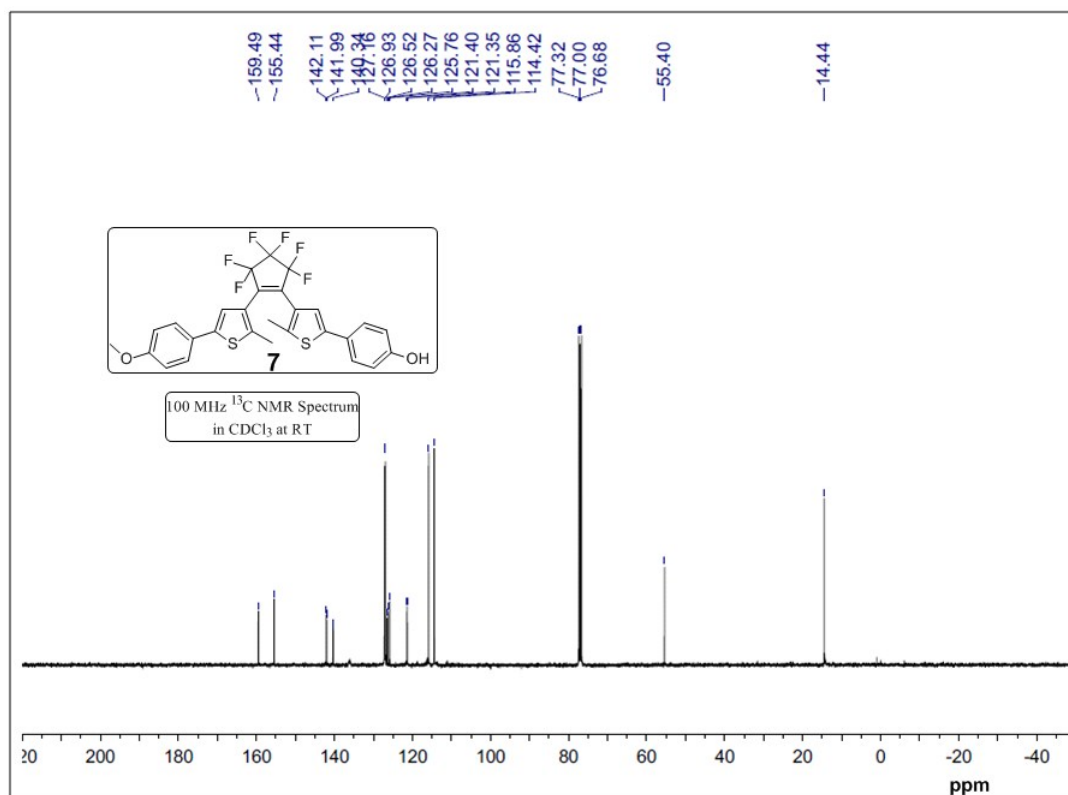


Figure S2 . ^{13}C NMR spectrum (100 MHz, CDCl_3) of **7**.

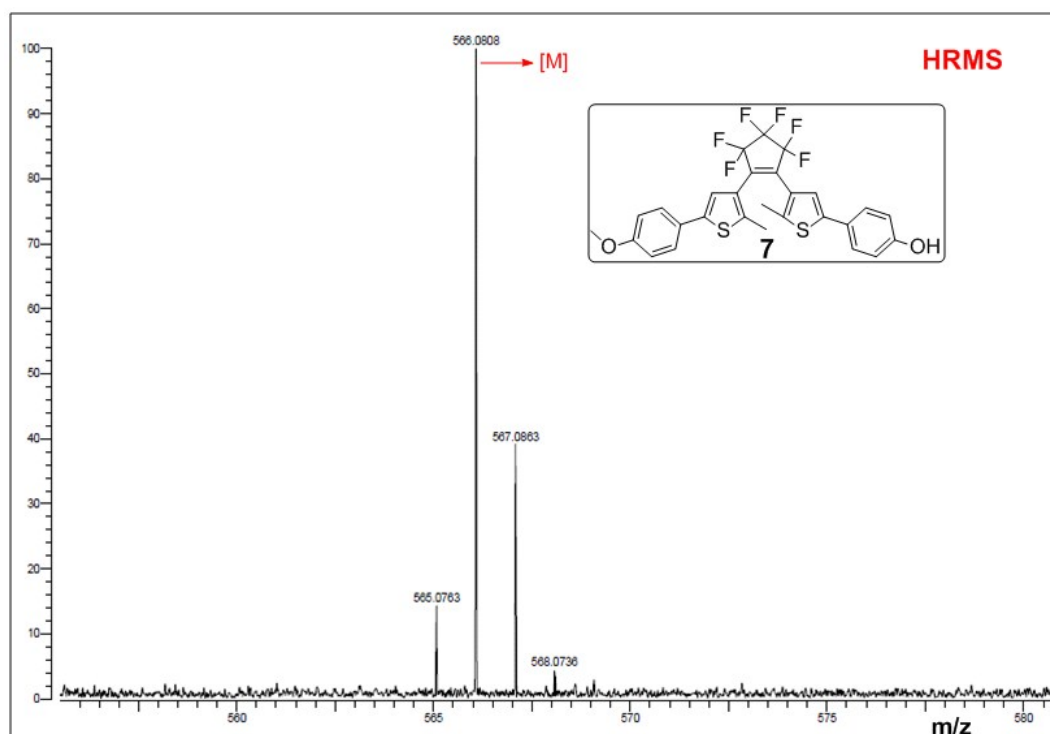


Figure S3 . HR-MS of **7**.

Synthesis of **8**.

In a 100 mL two-necked, round-bottom flask equipped with a magnetic stirrer was placed a mixture of **7** (0.57 g, 1.00 mmol), 3-bromoprop-1-yne (0.24 g, 2.00 mmol), KI (0.01 g, 0.06 mmol), benzo-18-crown-

6 (0.02 g, 0.06 mmol) and potassium carbonate (0.55 g, 4.00 mmol), then 60mL of acetone was added. The reaction mixture was refluxed for 24 h under an argon atmosphere. The resulting mixture was cooled to ambient temperature and filtered. After that, the solvent was removed under vacuum, and the residue was extracted by ethyl acetate, dried over anhydrous Na₂SO₄. After removing solvent under a reduced pressure, the residue was purified on a silica gel column using petroleum ether/ethyl acetate (5:1) as the eluent to obtain compound **8** as a light-green solid. Yield: 0.51 g, 85%. Compound **8**: ¹H NMR (400 MHz, CDCl₃): δ ppm = 7.49-7.45 (m, 4H), 7.17 (d, *J* = 4 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 12.0 Hz, 2H), 4.73 (d, *J* = 4.0 Hz, 2H), 3.84 (s, 3H), 2.54 (t, *J* = 4.0 Hz, 1H), 1.96 (d, *J* = 4.0 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃): δ ppm = 159.51, 157.36, 142.14, 141.85, 140.52, 140.27, 127.11, 126.90, 126.88, 126.20, 125.80, 125.74, 121.59, 121.29, 115.42, 114.39, 78.28, 75.74, 55.88, 55.34, 14.43. HRMS (FTMALDI): *m/z* = 604.10; calculated exact mass: 604.10.

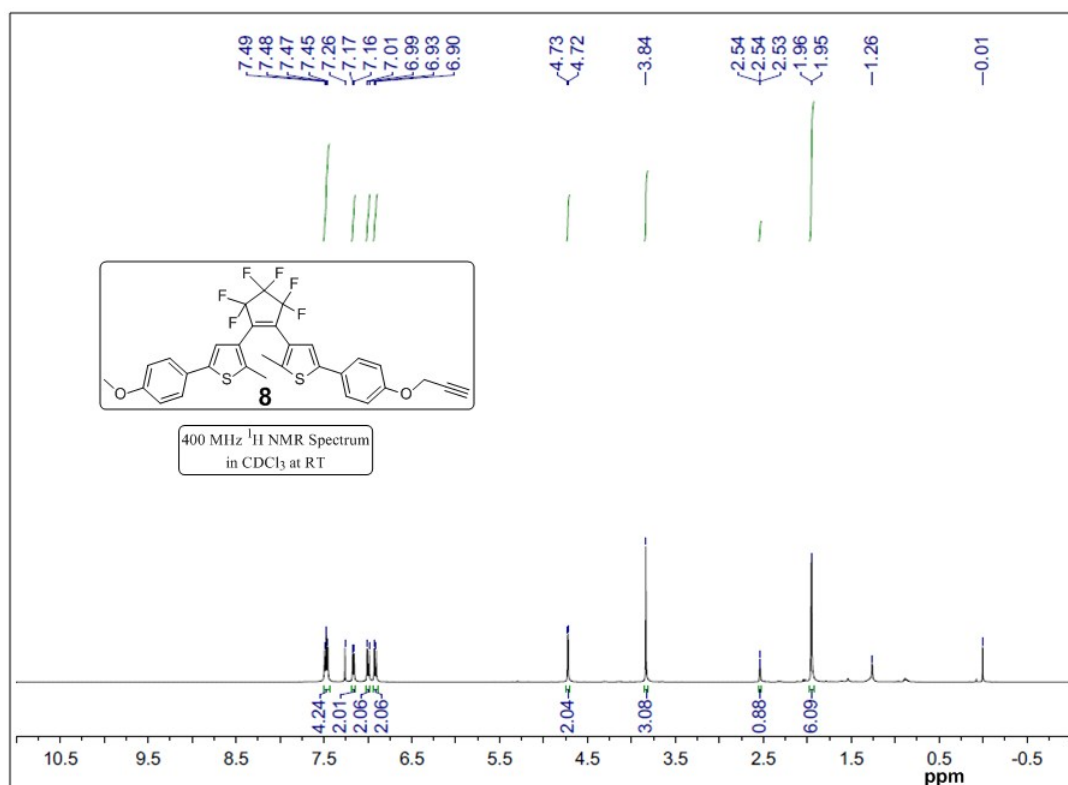


Figure S4 . ¹H NMR spectrum (400 MHz, CDCl₃) of **8**.

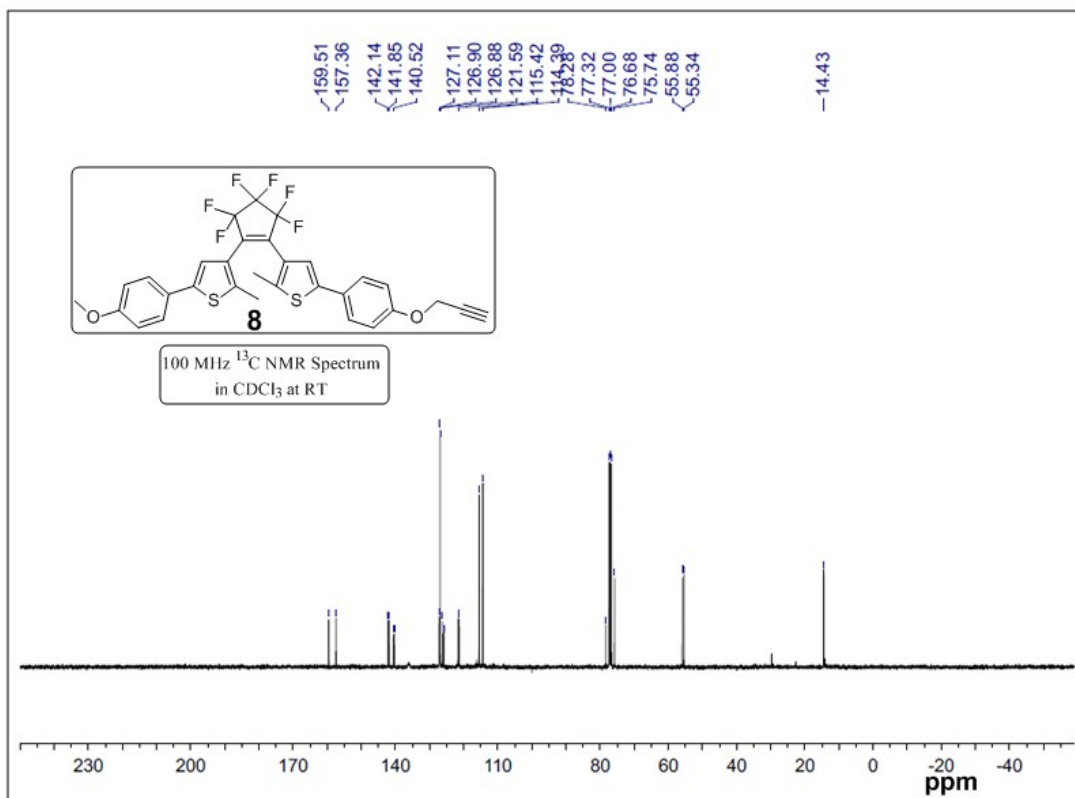


Figure S5 . ^{13}C NMR spectrum (100 MHz, CDCl_3) of **8**.

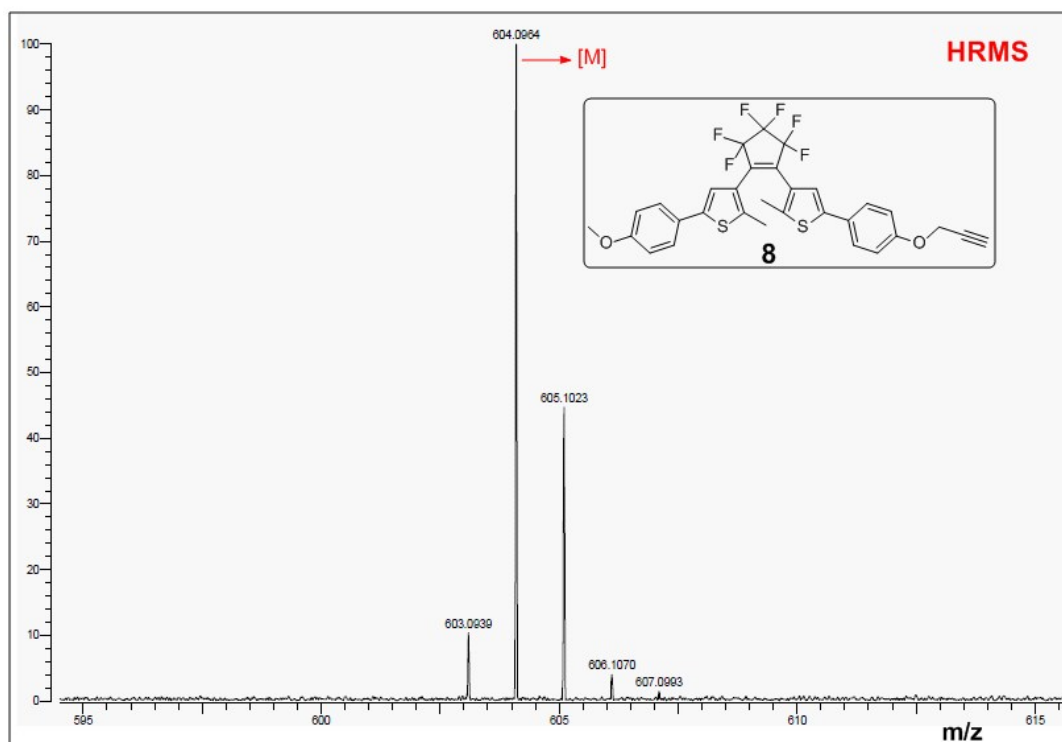


Figure S6 . HR-MS of **8**.

Synthesis of **1**.

6-Deoxy-6-azide-permethyl- β -cyclodextrin **5** was prepared according to the literature procedures. **5**

(0.10 mmol, 0.15 g) and **8** (0.1 mmol, 0.06 g) were dissolved in 15 mL of DMF, to which CuI (0.20 mmol, 0.04 g) was added under nitrogen atmosphere. The solution was stirred at 70°C for 24 h, After cooling to room temperature, the mixture was filtered to remove any insoluble copper salt, and the filtrate was evaporated under a reduced pressure to remove excess DMF. The residue was purified by silica gel column by using chloroform/ methanol (v/v = 25:1) to obtain compound **OF-1** as a light-green solid. Yield: 0.05 g, 26%. Compound **OF-1**: ^1H NMR (400 MHz, CDCl_3): δ ppm = δ 7.75 (s, 1H), 7.46 (d, J = 8 Hz, 4H), 7.16 (s, 2H), 6.98 (d, J = 8 Hz, 2H), 6.91 (d, J = 8 Hz, 2H), 5.28 (d, J = 4 Hz, 1H), 5.20 (s, 2H), 5.13 (s, 8H), 3.83 (br, 9H), 3.65 (br, 34H), 3.50 (br, 36H), 3.38 (br, 18H), 3.31 (s, 6H), 1.93 (s, 6H). ^{19}F NMR (400 MHz, CDCl_3) δ ppm = 109.76 (s, 4F), 131.82 (s, 2F). ^{13}C NMR (100 MHz, CDCl_3): δ ppm = 159.42, 158.02, 143.16, 142.07, 141.73, 140.45, 140.19, 126.89, 126.84, 126.74, 126.11, 125.75, 125.66, 125.03, 121.39, 121.17, 115.08, 114.31, 99.18, 98.90, 98.86, 98.80, 98.70, 98.21, 82.83, 81.99, 81.95, 81.87, 81.82, 81.71, 81.59, 81.07, 80.24, 80.15, 79.83, 79.20, 71.45, 71.34, 71.28, 71.22, 70.86, 70.76, 70.70, 70.65, 70.24, 62.00, 61.69, 61.40, 61.35, 61.26, 59.11, 59.04, 58.97, 58.94, 58.91, 58.89, 58.59, 58.52, 58.46, 58.40, 58.36, 55.32, 51.36, 29.62, 14.43. HRMS (FTMALDI): m/z = 2066.78 [$\text{M} + \text{Na}^+$], 2082.75 [$\text{M} + \text{K}^+$]; calculated exact mass: 2043.79.

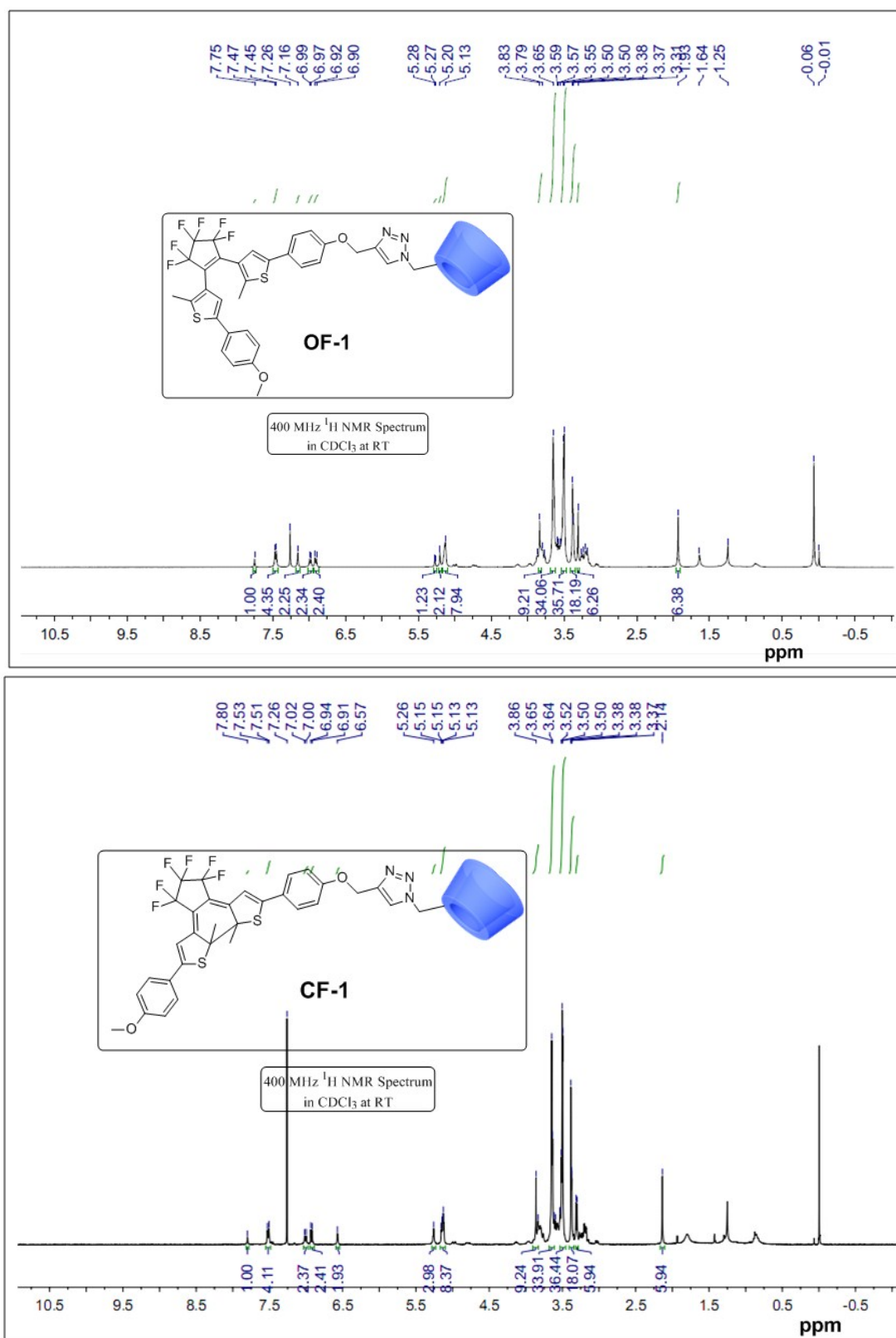


Figure S7. ^1H NMR spectrum (400 MHz, CDCl_3) of **OF-1** and **CF-1**.

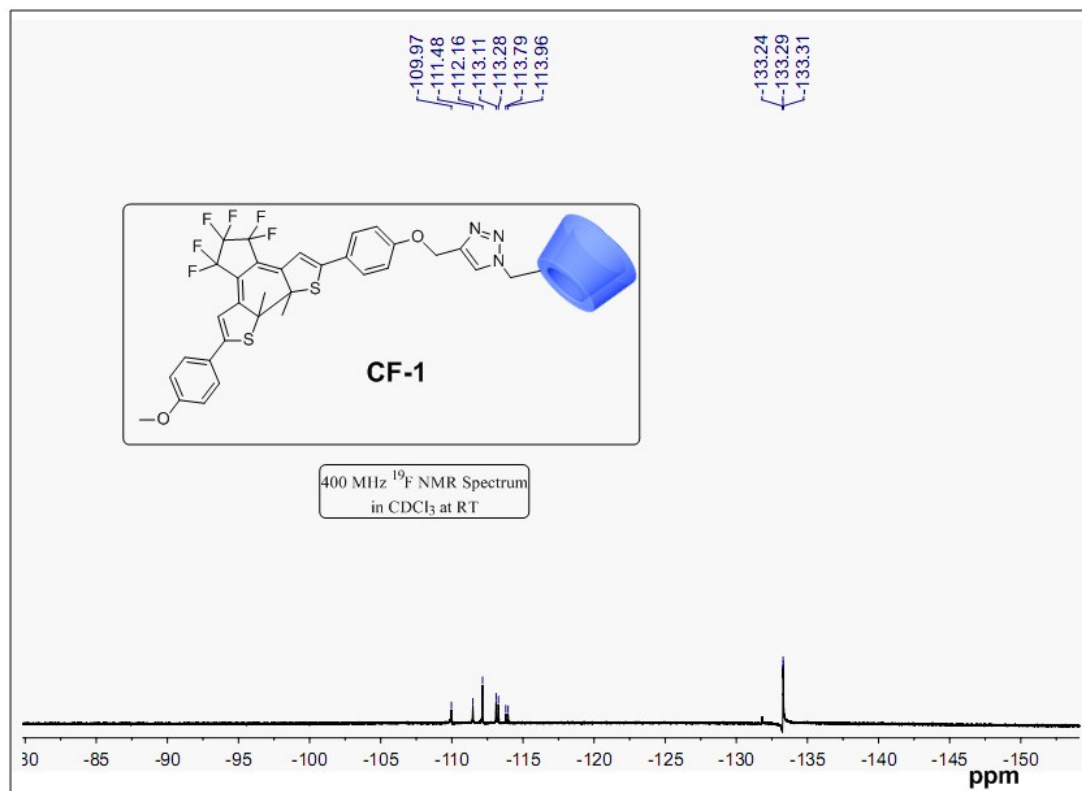
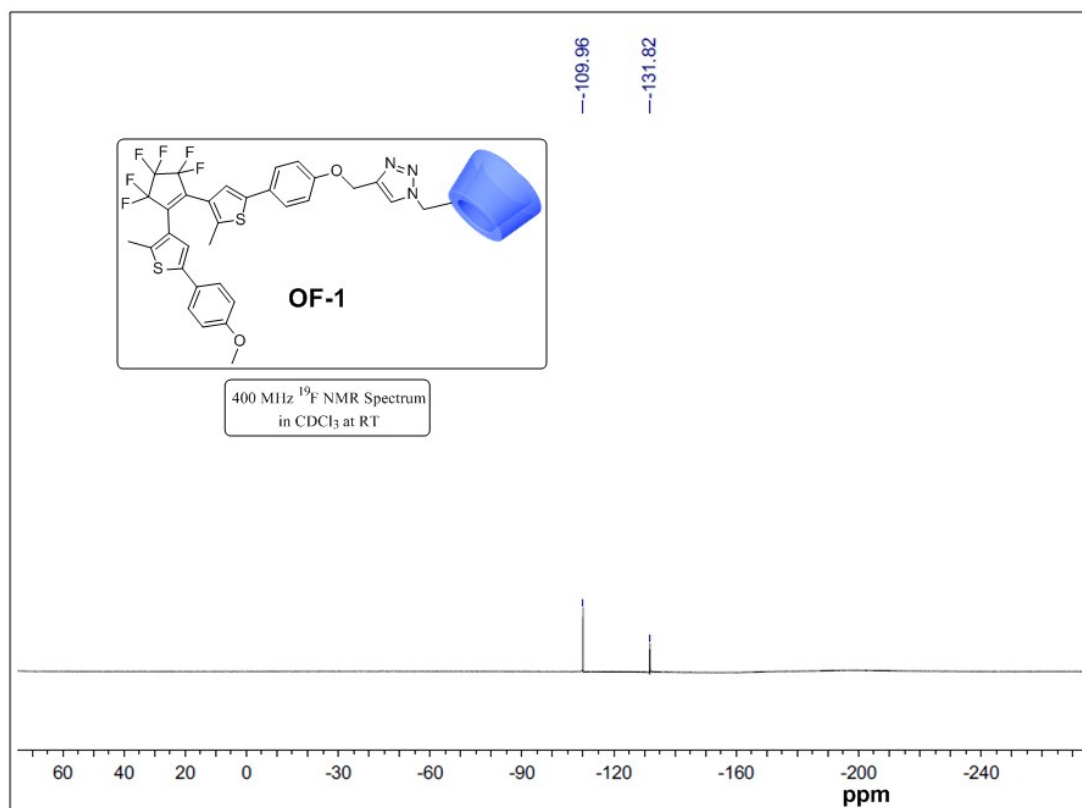


Figure S8. ^{19}F NMR spectrum (400 MHz, CDCl_3) of **OF-1** and **CF-1**.

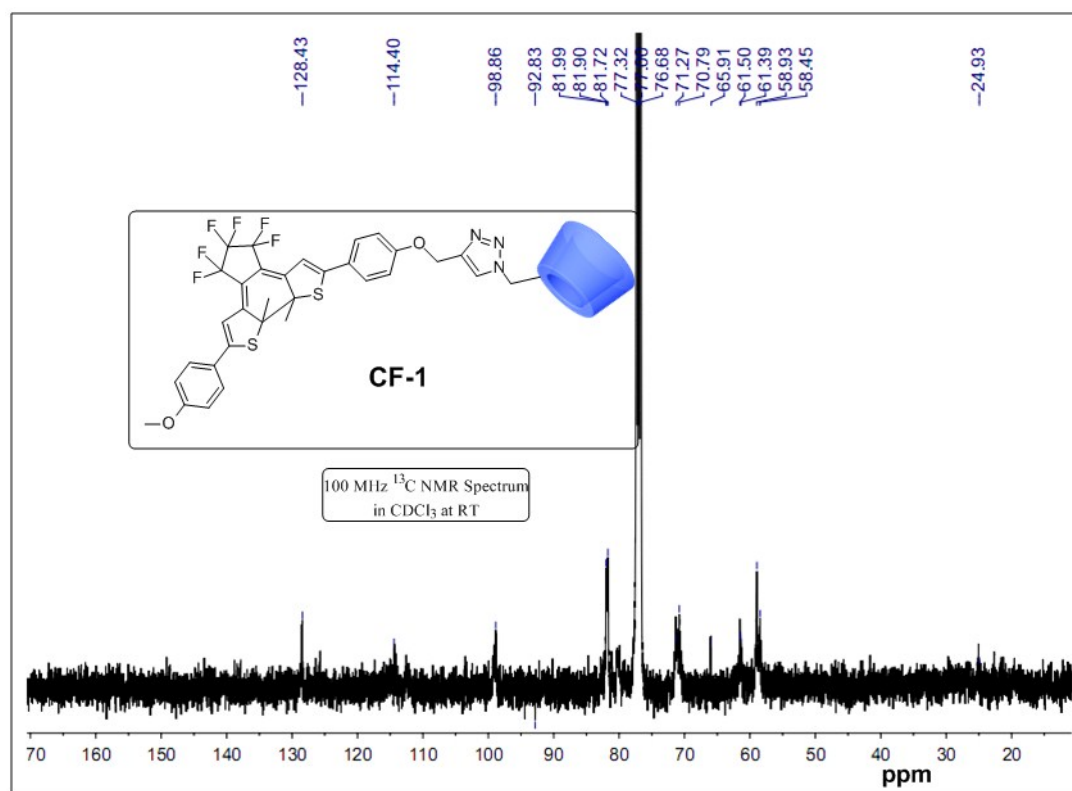
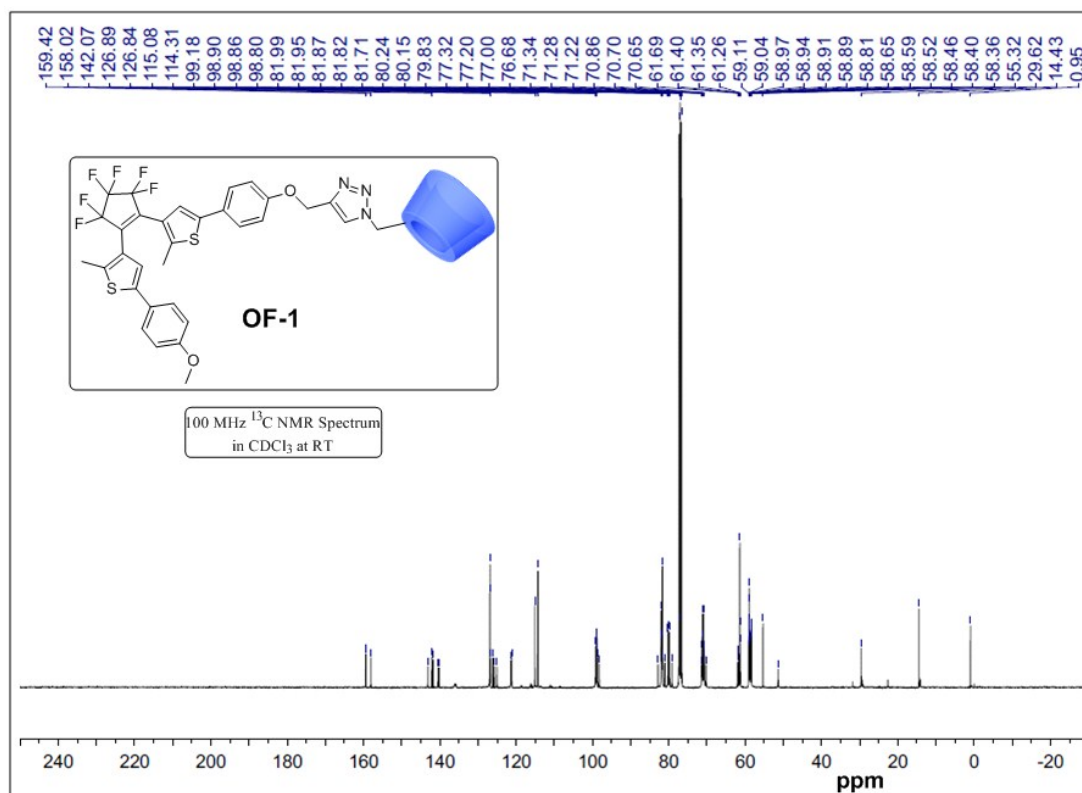


Figure S9. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **OF-1** and **CF-1**.

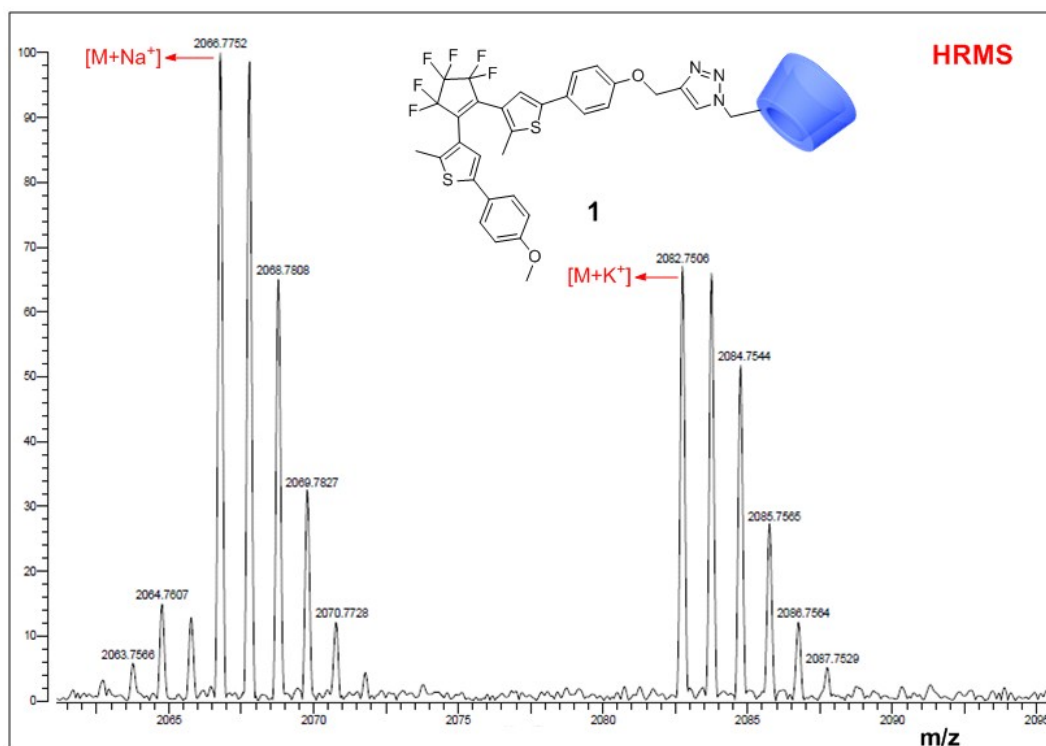


Figure S10. HR-MS of **1**.

Synthesis of **9**.

In a 100 mL two-necked, round-bottom flask equipped with a magnetic stirrer was placed a mixture of **6** (0.55 g, 1.00 mmol), 3-bromoprop-1-yne (0.24 g, 2.00 mmol), KI (0.01 g, 0.06 mmol), benzo-18-crown-6 (0.02 g, 0.06 mmol) and potassium carbonate (0.55 g, 4.00 mmol), then 60 mL of acetone was added. The reaction mixture was refluxed for 24 h under an argon atmosphere. The resulting mixture was cooled to ambient temperature and filtered. After that, the solvent was removed under vacuum, and the residue was extracted by ethyl acetate, dried over anhydrous Na_2SO_4 . After removing solvent under a reduced pressure, the residue was purified on a silica gel column using petroleum ether / ethyl acetate (7:1) as the eluent to obtain compound **9** as a light-green solid. Yield: 0.55 g, 88%. Compound **9**: 1H NMR (400 MHz, $CDCl_3$) δ ppm = 7.48 (d, J = 12 Hz, 4H), 7.16 (s, 2H), 6.99 (d, J = 8 Hz, 4H), 4.72 (d, J = 2.4 Hz, 4H), 2.53 (t, J = 4 Hz, 2H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm = 157.36, 141.88, 140.51, 127.10, 126.89, 125.78, 121.58, 115.43, 78.28, 75.75, 55.89, 14.44. HRMS (FTMALDI): m/z = 628.10; calculated exact mass: 628.10.

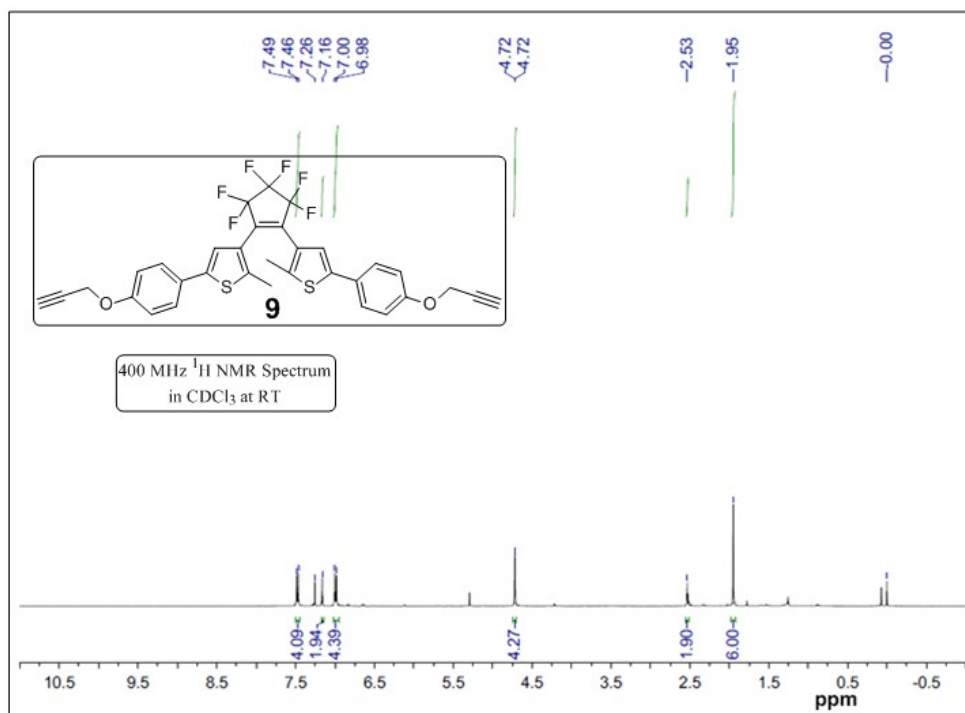


Figure S11. ^1H NMR spectrum (400 MHz, CDCl_3) of **9**.

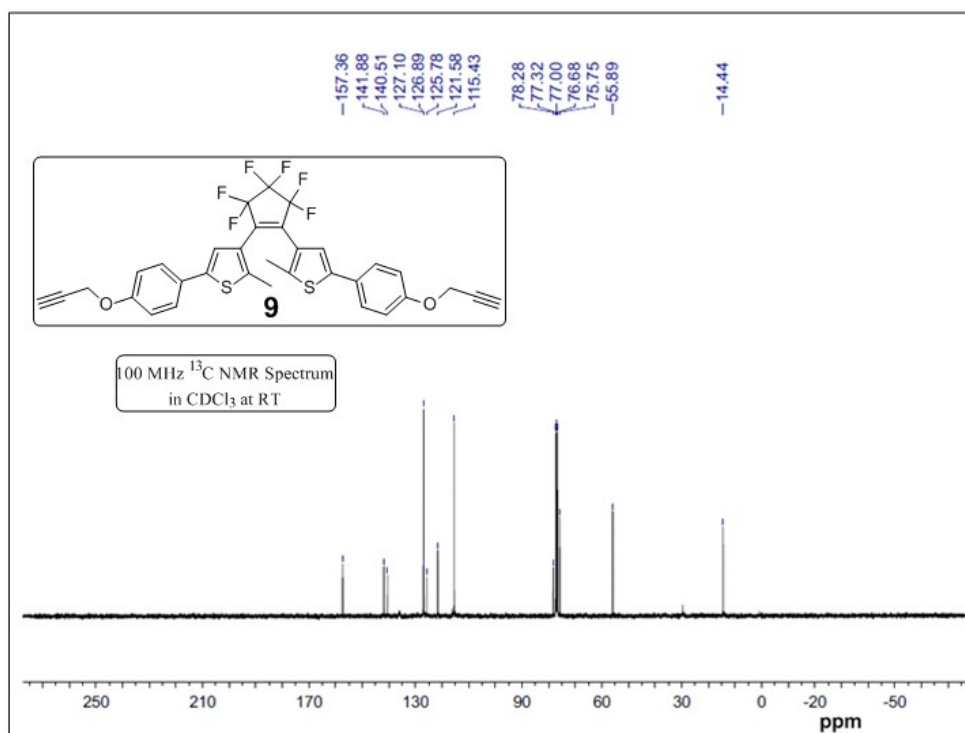


Figure S12. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **9**.

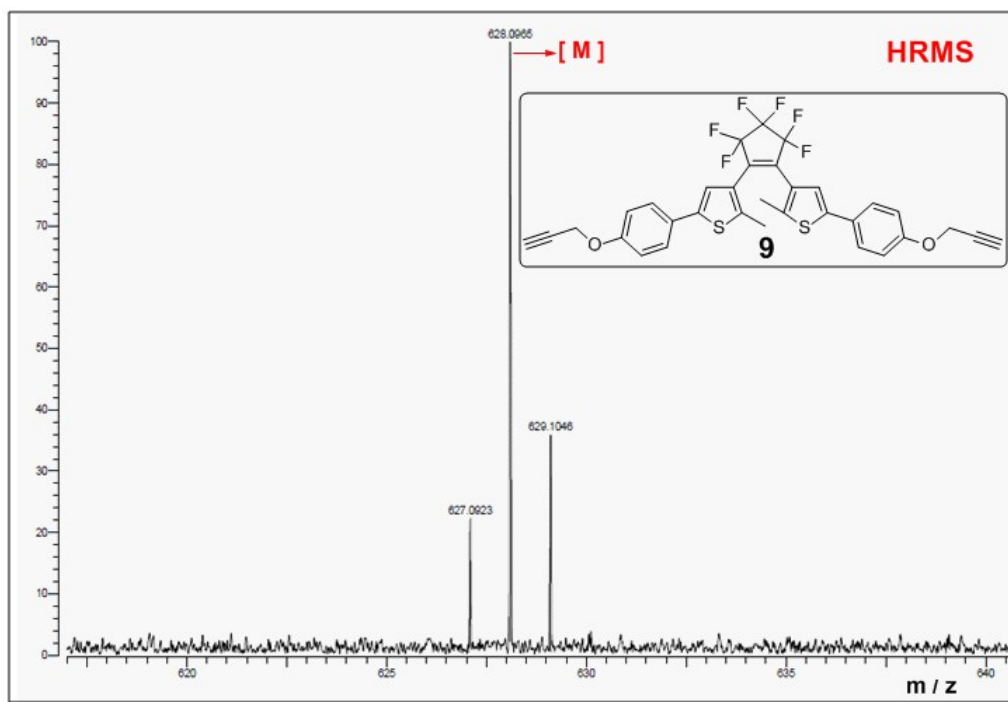


Figure S13. HR-MS of **9**.

Synthesis of **2**.

5 (0.40 mmol, 0.58 mg) and **9** (0.10 mmol, 0.06 mg) were dissolved in 20 mL of DMF, to which CuI (0.40 mmol, 0.08 mg) was added under nitrogen atmosphere. The solution was stirred at 70 °C for 24 h. After cooled to room temperature, the mixture was filtered in order to remove any insoluble copper salt, and the filtrate was evaporated under a reduced pressure to remove excess DMF. The residue was purified by silica gel column by using chloroform-methanol (v/v = 25:1) to obtain compound **OF-2** as a light-green solid. Yield: 0.17 mg, 49%. Compound **OF-2**: ^1H NMR (400 MHz, CDCl_3): δ ppm = 7.74 (s, 2H), 7.45 (d, J = 8 Hz, 4H), 7.16 (s, 2H), 6.98 (d, J = 8 Hz, 4H), 5.26 (s, 2H), 5.19 (s, 4H), 5.11 (br, 12H), 4.99 (d, J = 12 Hz, 4H), 3.54 (m, 3.64-3.29, 200H), 1.90 (s, 6H). ^{19}F NMR (400 MHz, CDCl_3) δ ppm = 110.01 (s, 4F), 131.82 (s, 2F). ^{13}C NMR (100 MHz, CDCl_3) δ ppm = 158.01, 141.77, 140.33, 126.83, 126.65, 125.67, 121.25, 115.07, 99.11, 98.83, 98.79, 98.74, 98.63, 98.15, 82.74, 81.96, 81.84, 81.68, 81.54, 81.04, 80.18, 80.10, 79.80, 79.10, 77.20, 71.42, 71.31, 71.20, 70.83, 70.67, 70.61, 70.19, 61.98, 61.58, 61.30, 61.24, 61.17, 58.95, 58.89, 58.86, 58.82, 58.38, 58.28, 51.30, 29.53, 14.34. HRMS (FT-MALDI): m/z = 3530.47 [$\text{M} + \text{Na}^+$]; calculated exact mass: 3507.48.

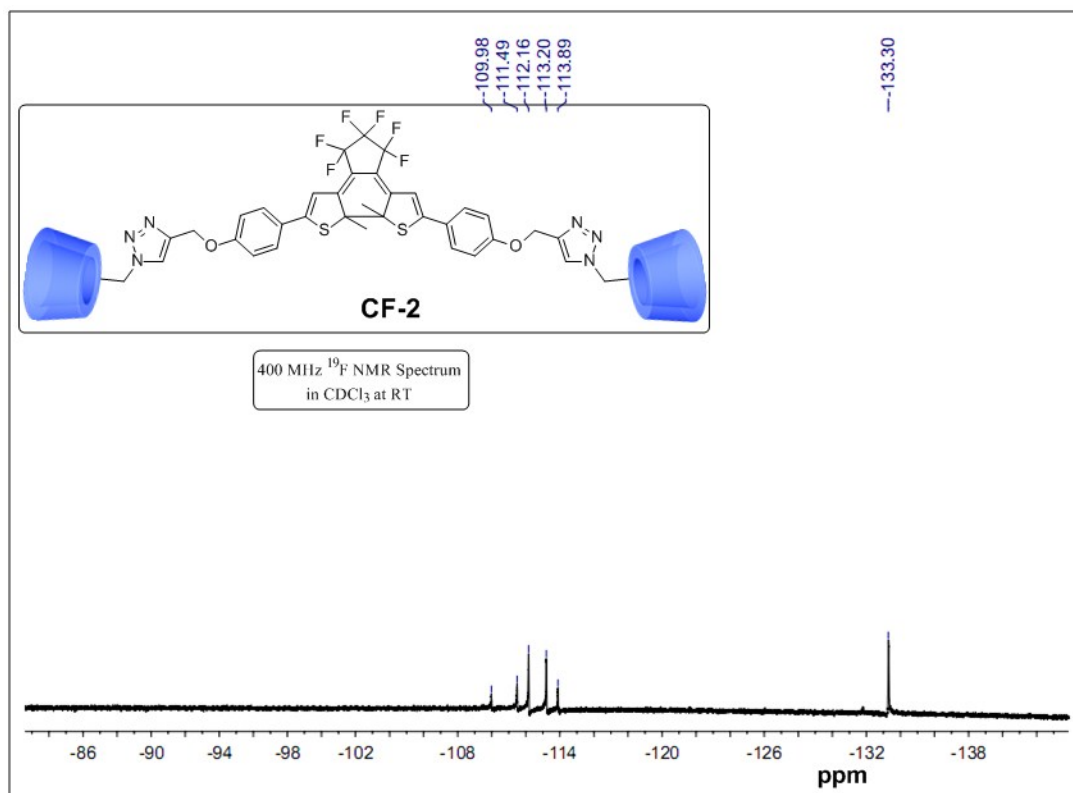
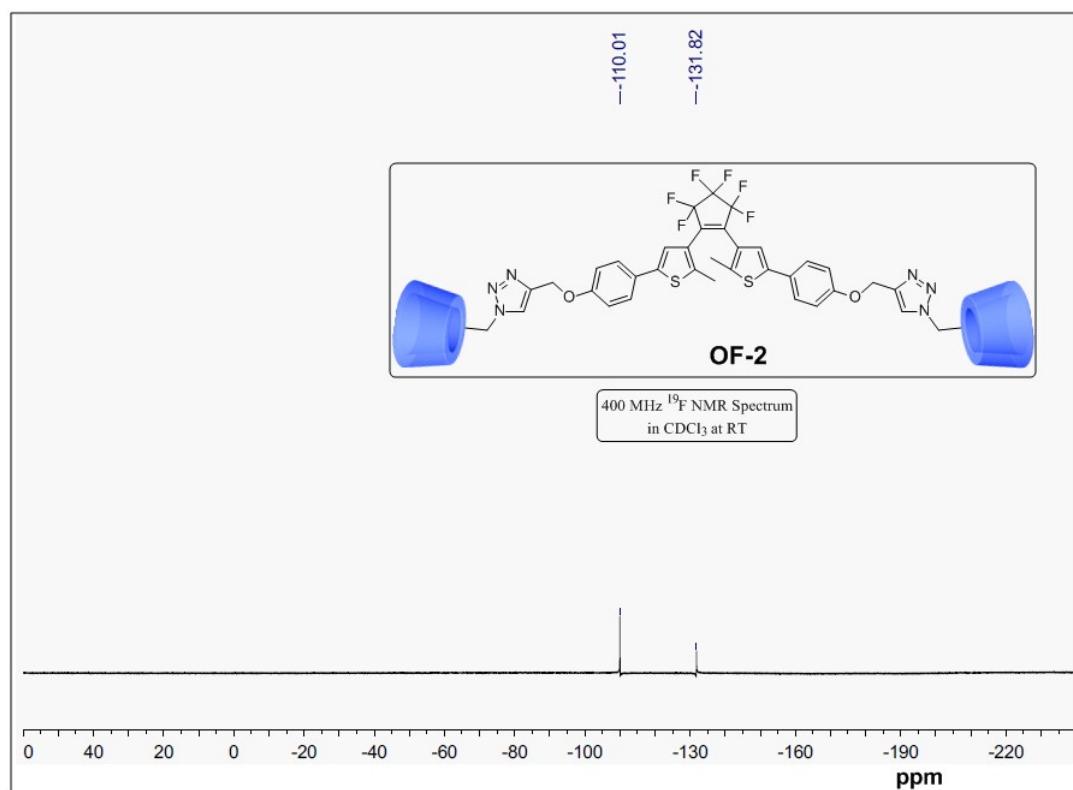


Figure S15. ^{19}F NMR spectrum (400 MHz, CDCl_3) of **OF-1** and **CF-1**.

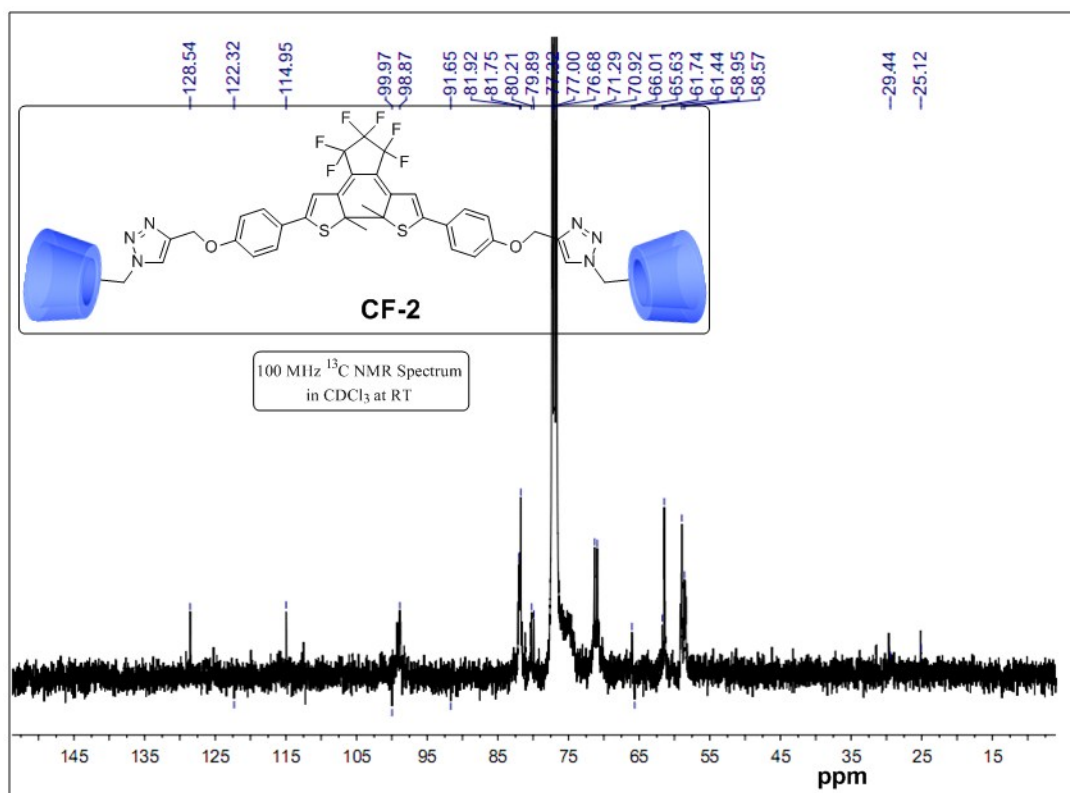
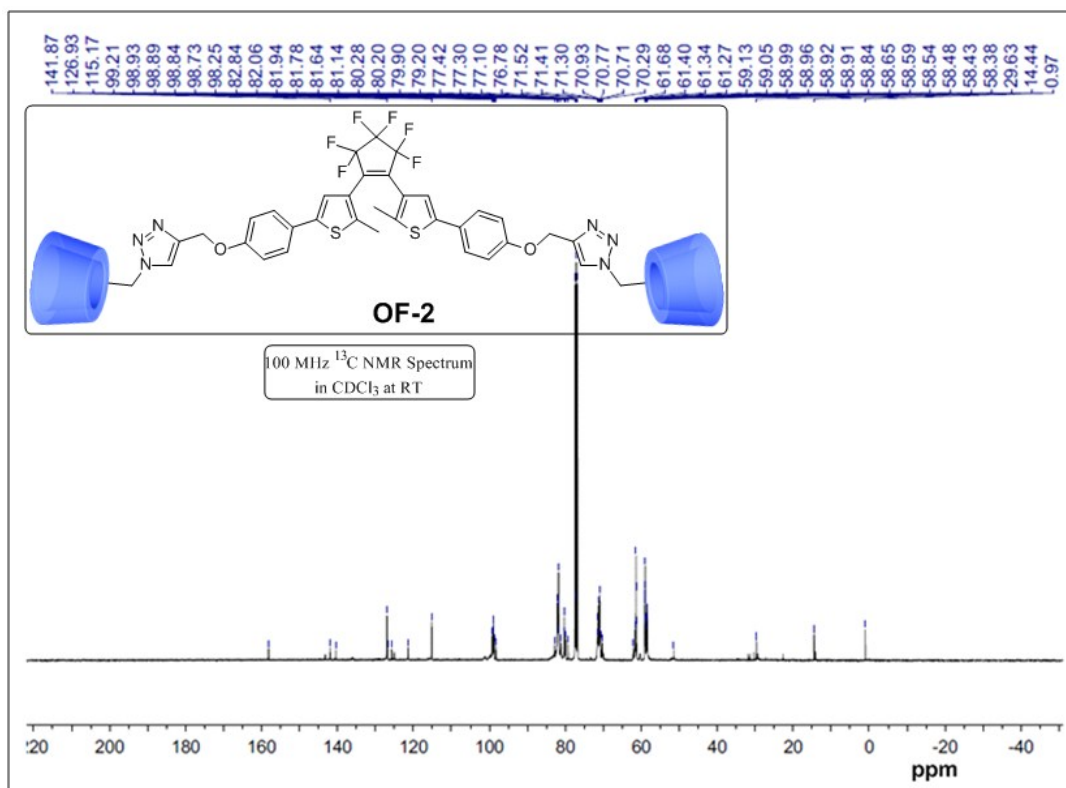


Figure S16. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **OF-1** and **CF-1**.

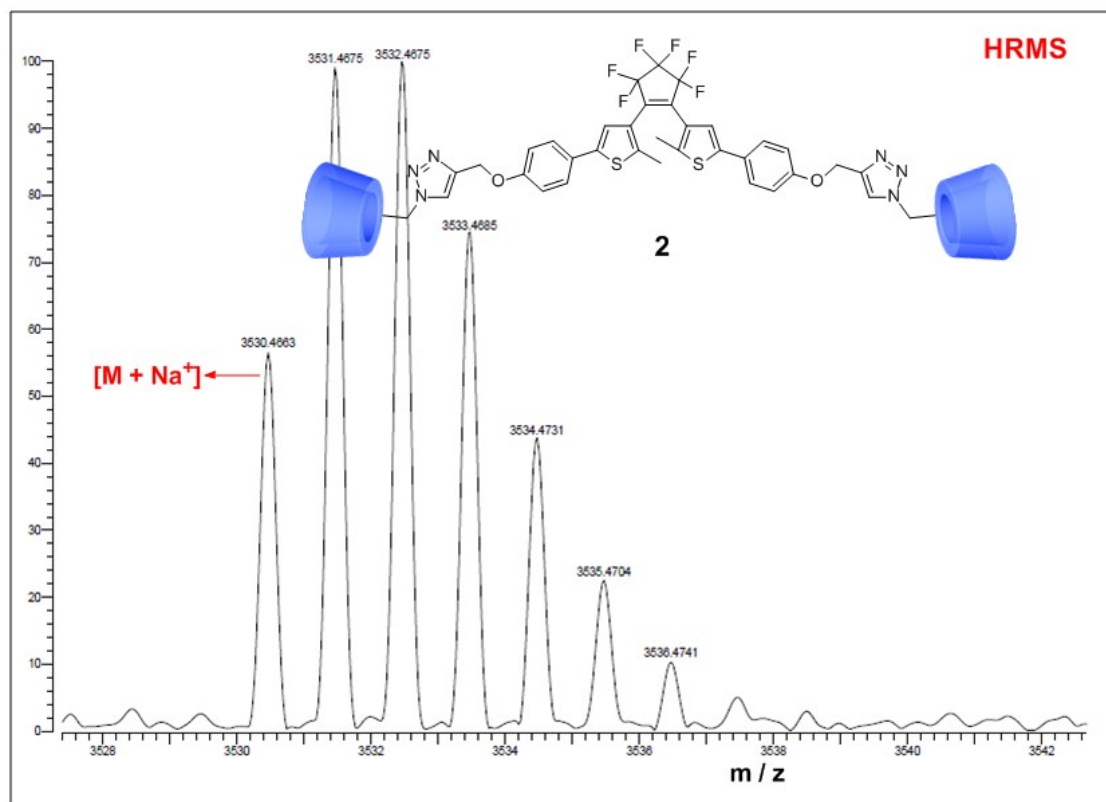


Figure S17. HR-MS of 2.

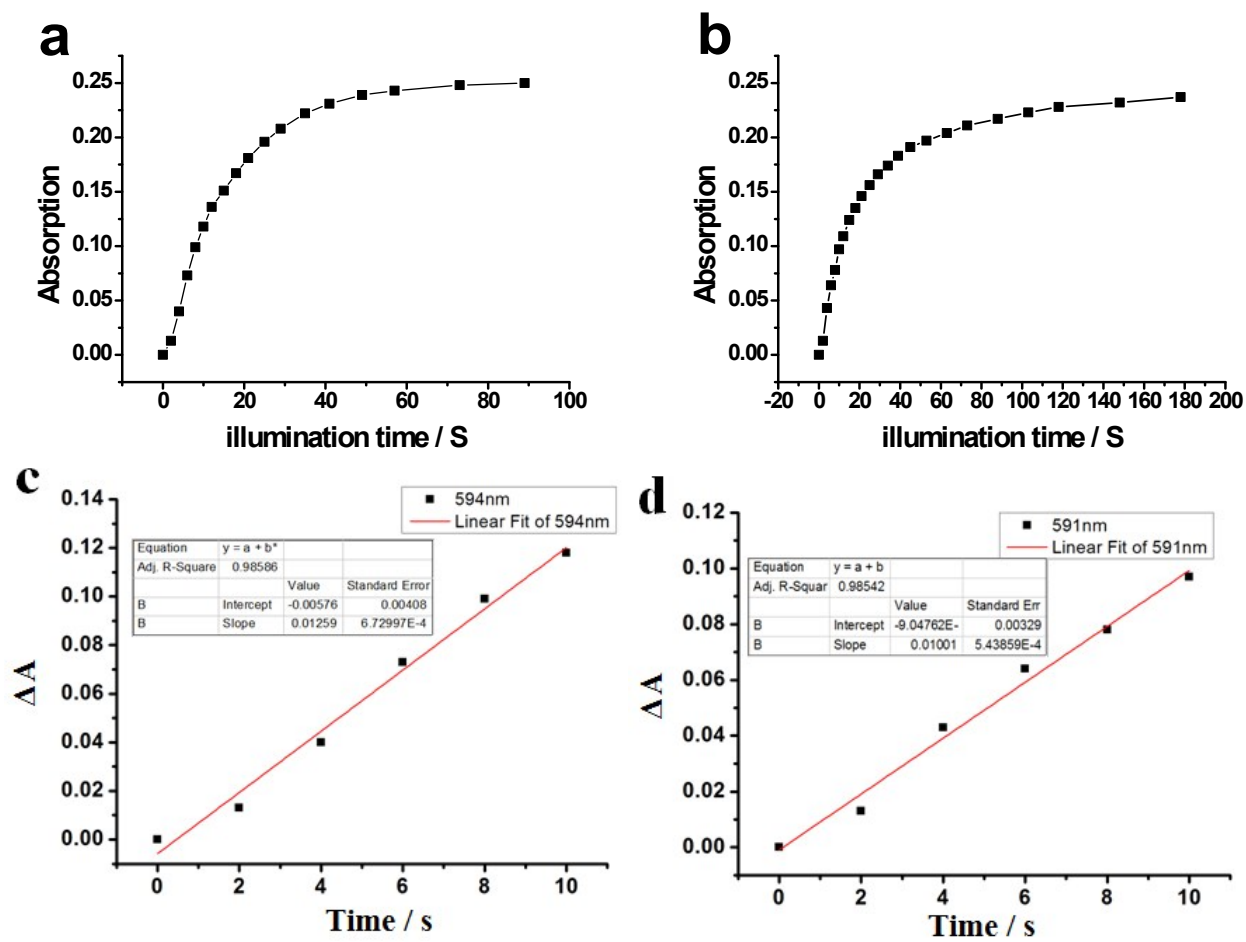


Figure S18. (a) Absorbance variation of **1** at 594nm over time upon irradiation by 254 nm light.(b) Absorbance variation of **2** at 591nm over time upon irradiation by 254 nm light. (c) Cyclization reaction rate constant of **1**. (d) Cyclization reaction rate constant of **2**.

Table S1 Photochromic parameters of **1** and **2** in 5% EtOH aqueous solution ($2.0 \times 10^{-5} \text{ mol L}^{-1}$)

Comps	$\lambda_{\text{max}} / \text{nm}^{\text{a}} (\varepsilon \times 10^{-4})$	$\lambda_{\text{max}} / \text{nm}^{\text{b}} (\varepsilon \times 10^{-4})$	$\Phi_{\text{o-c}} (\lambda / \text{nm})^{\text{c}}$
	(open)	(PSS)	
1	291(3.38)	594 (1.25)	0.5
2	295(3.32)	592(1.2)	0.42

^a Absorption maxima of open-ring isomers. ^b Absorption maxima of closed-ring isomers. ^c Quantum yields of closed-ring isomers.

$$\Phi_{\text{x}} = \varepsilon_0 k_{\text{x}} \Phi_0 / \varepsilon_{\text{x}} k_0$$

ε_0 : molar absorption coefficient of reference, ε_{x} : molar absorption coefficient of sample;

k_0 : reaction rate constant of reference, k_{x} : reaction rate constant of sample;

Φ_0 : Quantum yield of reference, Φ_{x} : Quantum yield of sample.

The quantum yields were determined by comparing the reaction yields of diarylethenes **1** and **2** against 1,2-bis(2-methyl-5-phenyl-3-thienyl)perfluorocyclopentene (reference substance) at room temperature.⁸⁻

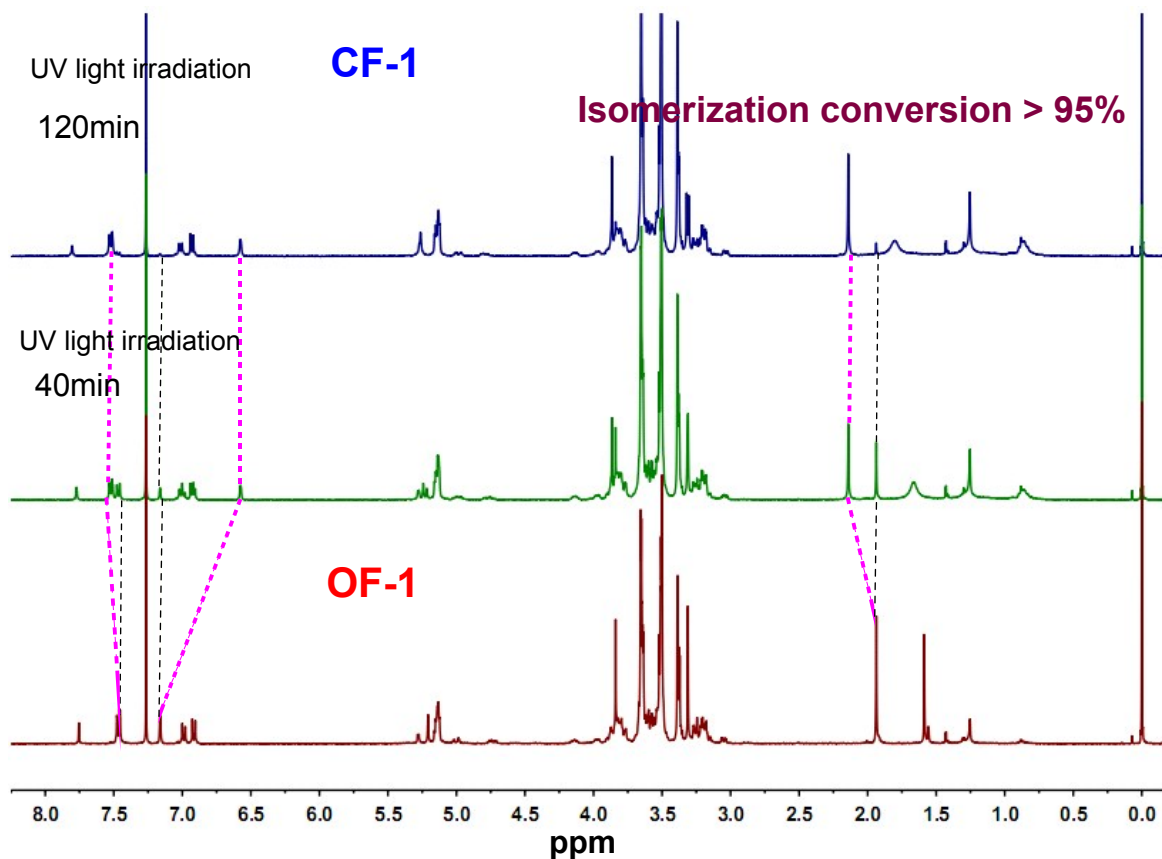


Figure S19. ¹H NMR (400 MHz, CDCl₃) comparison diagram of compound **OF-1** and **CF-1**. Cyclization conversion is determined exceeding 95% through the calculation of nuclear magnetic integral area.

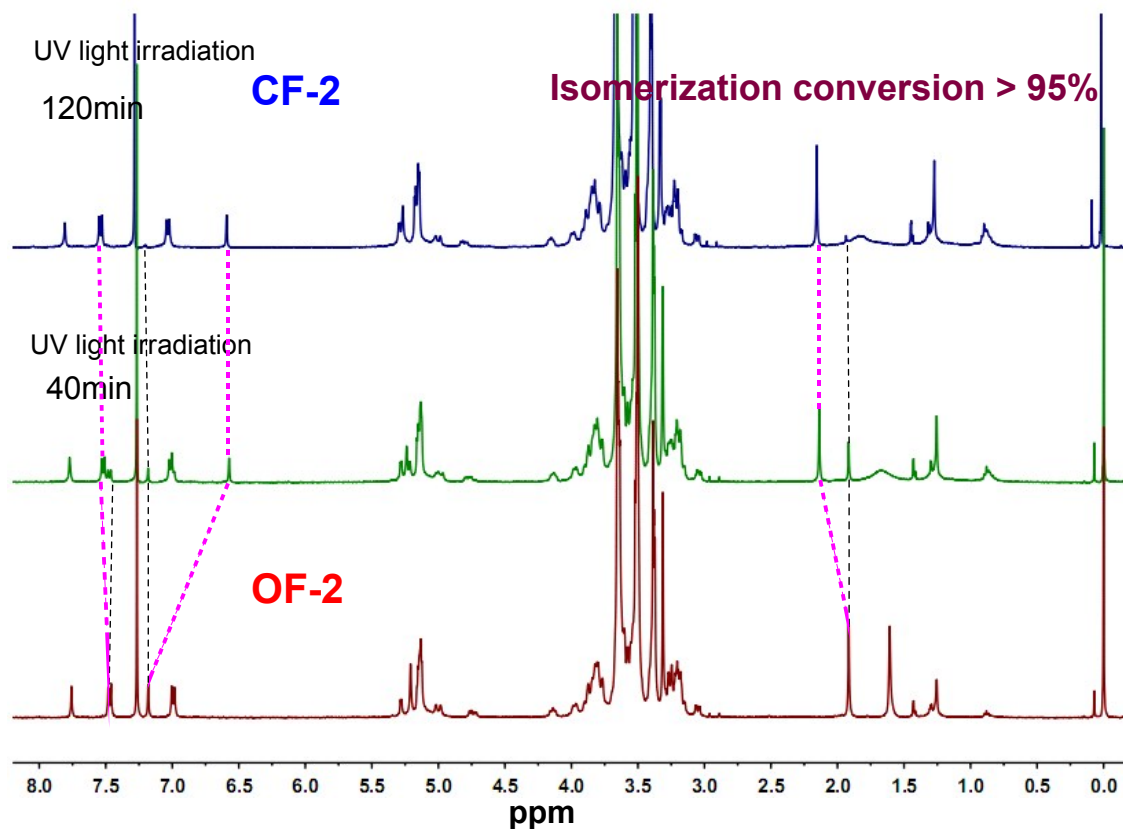


Figure S20. ^1H NMR (400 MHz, CDCl_3) comparison diagram of compound **OF-2** and **CF-2**. Cyclization conversion is determined exceeding 95% through the calculation of nuclear magnetic integral area.

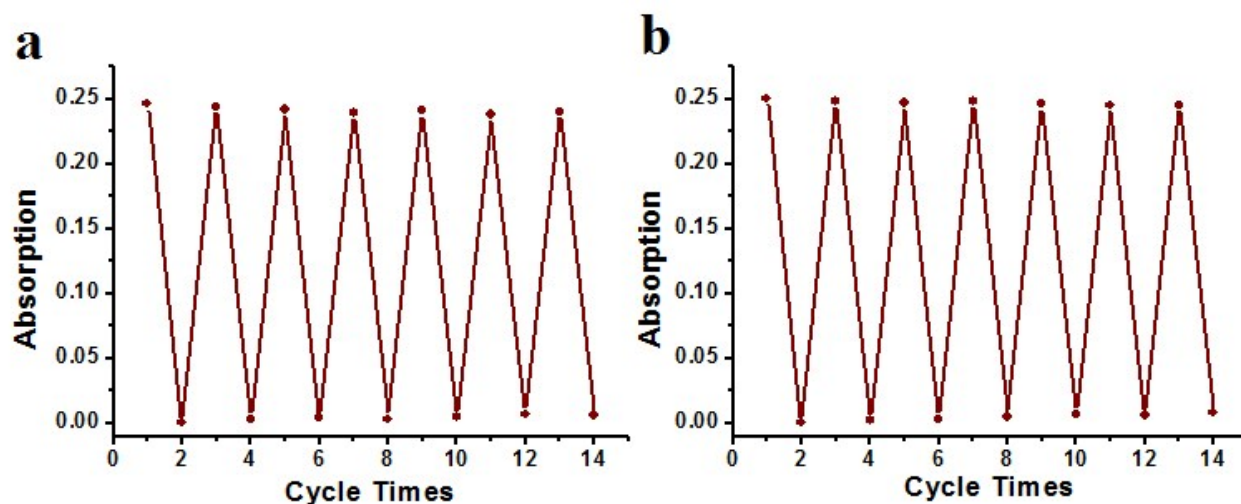


Figure S21. (a) Fatigue resistance of **1** monitored by the changes in absorbance at 594 over seven cycles, respectively. (b) Fatigue resistance of **2** monitored by the changes in absorbance at 591 nm over seven cycles, respectively.

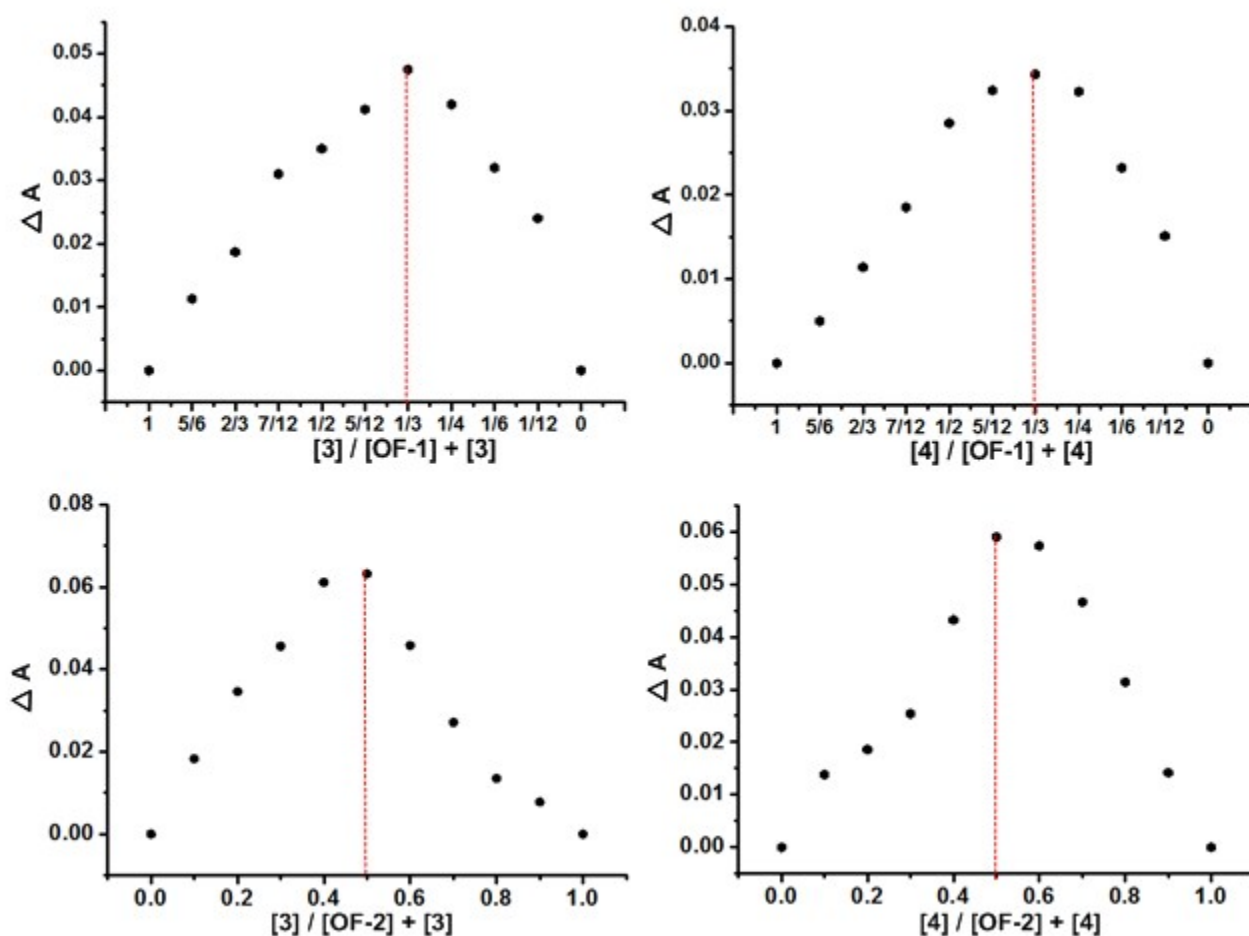


Figure S22. Job's plots of **3**, **4** and **OF-1** (**OF-2**).

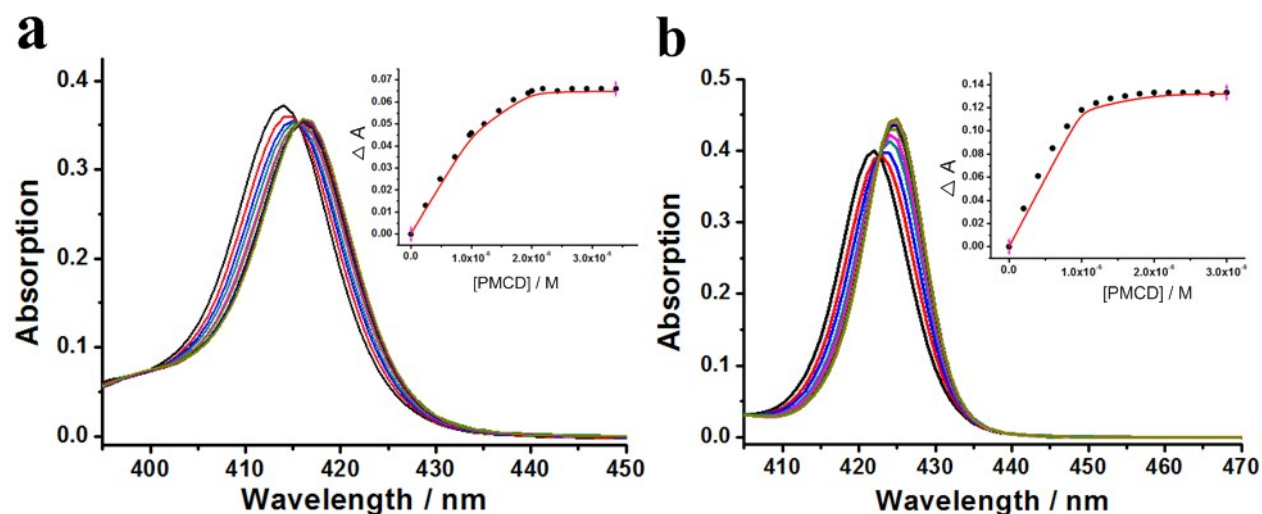


Figure S23. (a) UV/ vis titration spectra of **3** (1 μM) upon addition of PMCD (0–3 μM) in 5% EtOH PBS (pH 7.2). (b) UV/ vis titration spectra of **4** (1 μM) upon addition of PMCD (0–3 μM) in 5% EtOH PBS (pH 7.2). Insert: Nonlinear least-squares analysis of the differential absorbance (ΔA , $\lambda=417.0$ nm, 425.0nm) to calculate the complex binding constant (K_S).¹⁰

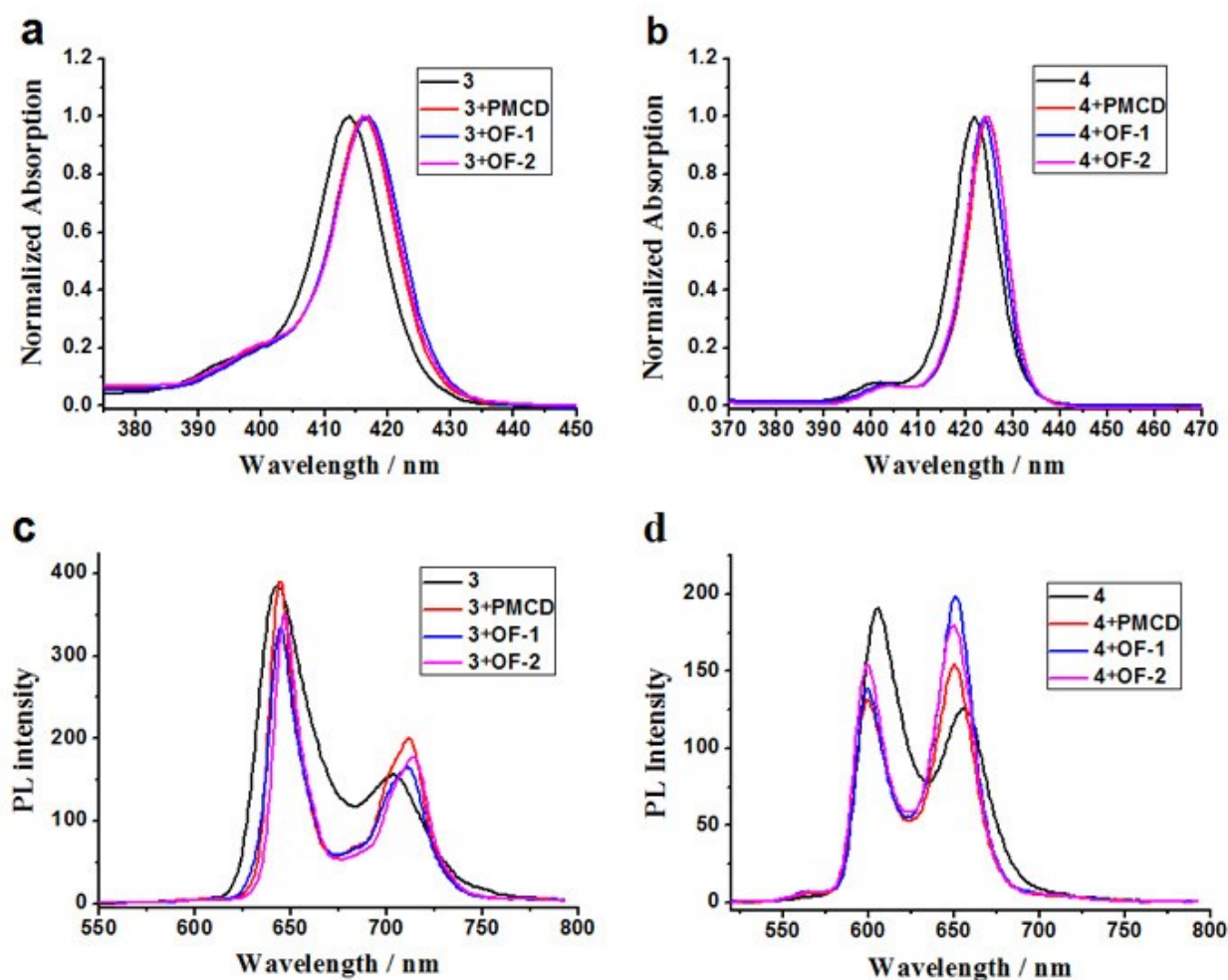


Figure S24. (a) Absorption spectrum of **3** and **3** with PMCD, **OF-1** and **OF-2** (b) Absorption spectrum of **4** and **4** with PMCD, **OF-1** and **OF-2**. (c) Emission spectra of **3** and **3** with PMCD, **OF-1** and **OF-2**. (d) Emission spectra of **4** and **4** with PMCD, **OF-1** and **OF-2**. ($2[\mathbf{3}] = 2[\mathbf{4}] = 2[\mathbf{OF-2}] = [\mathbf{OF-1}] = [\mathbf{PMCD}] = 4\mu\text{M}$ in 5% ETOH PBS (pH 7.2) aqueous solution)

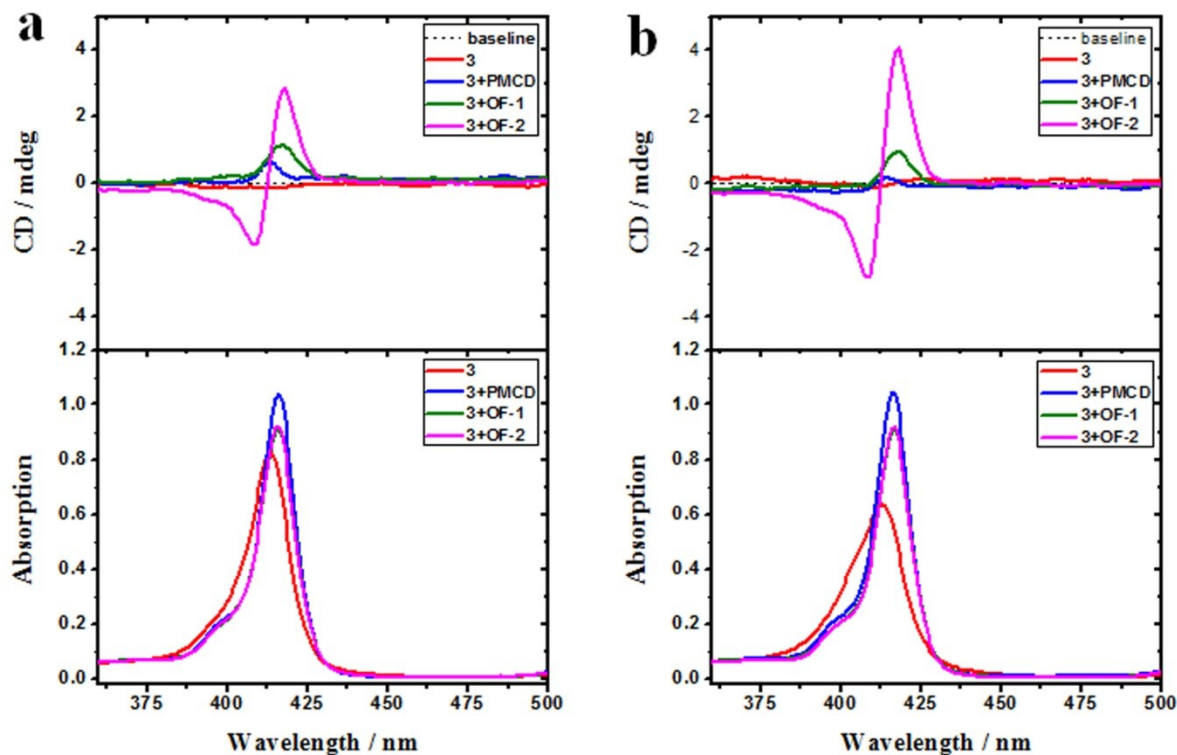


Figure S25. (a) Circular dichroism and corresponding absorption spectra of **3**, **3**⊂PMCD, **3**⊂**OF-1** and **3**⊂**OF-2** in dilute 5% EtOH PBS (pH 7.2). ($2\mu\text{M}$; light path, 10 mm) (b) Circular dichroism and corresponding absorption spectra of **3**, **3**⊂PMCD, **3**⊂**OF-1** and **3**⊂**OF-2** in concentrated 5% EtOH PBS (pH 7.2). ($20\mu\text{M}$; light path, 1 mm)

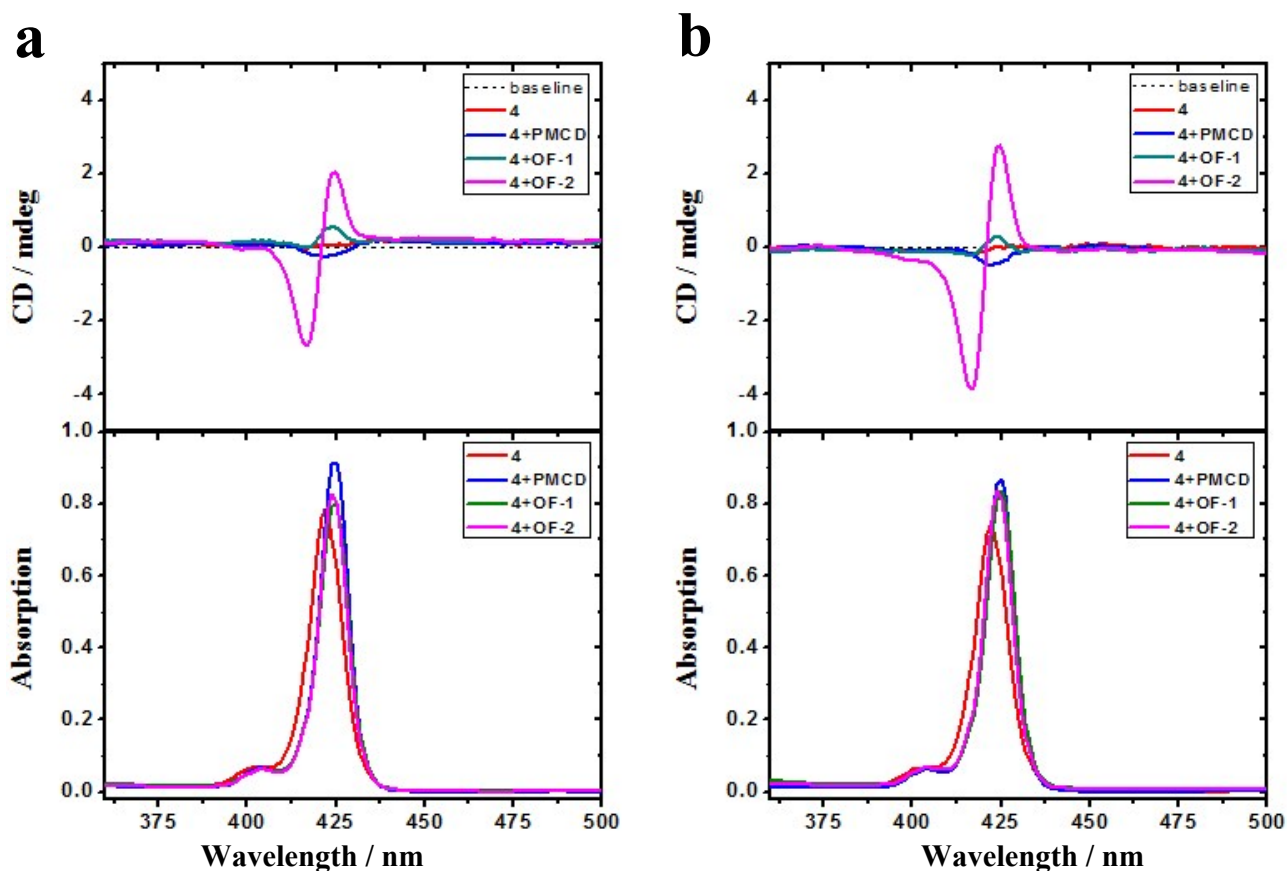
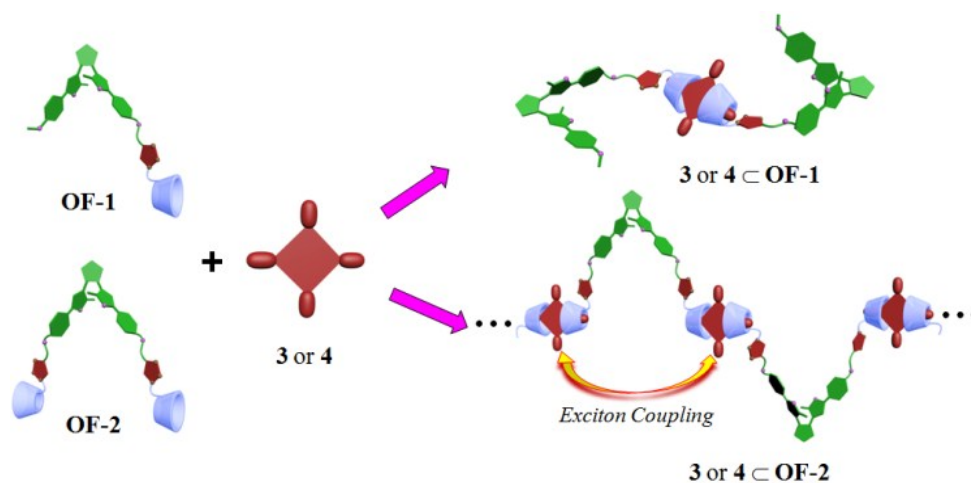


Figure S26. (a) Circular dichroism and corresponding absorption spectra of **4**, **4**+PMCD, **4**+OF-1 and **4**+OF-2 in dilute 5% ETOH PBS (pH 7.2). (2 μ M; light path, 10 mm) (b) Circular dichroism and corresponding absorption spectra of **4**, **4**+PMCD, **4**+OF-1 and **4**+OF-2 in concentrated 5% ETOH PBS (pH 7.2). (20 μ M, light path, 1 mm)



Scheme S2. Schematic representation of the assembly mode between **3** (or **4**) and **1** (or **2**).

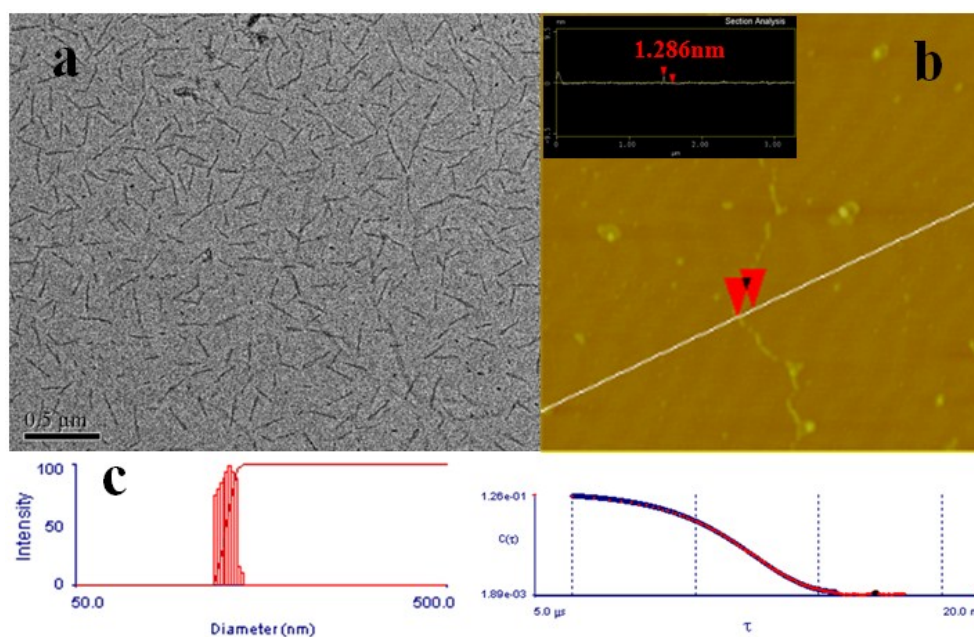


Figure S27. (a) TEM (b) AFM and (c) the DLS result of the **3@OF-2** assembly.

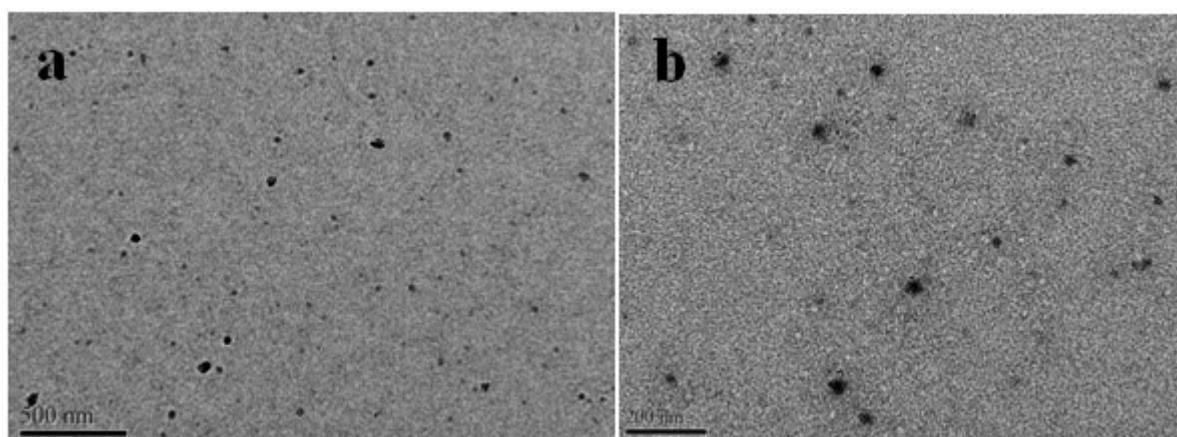


Figure S28. Typical TEM images of the **3@OF-1** assembly.

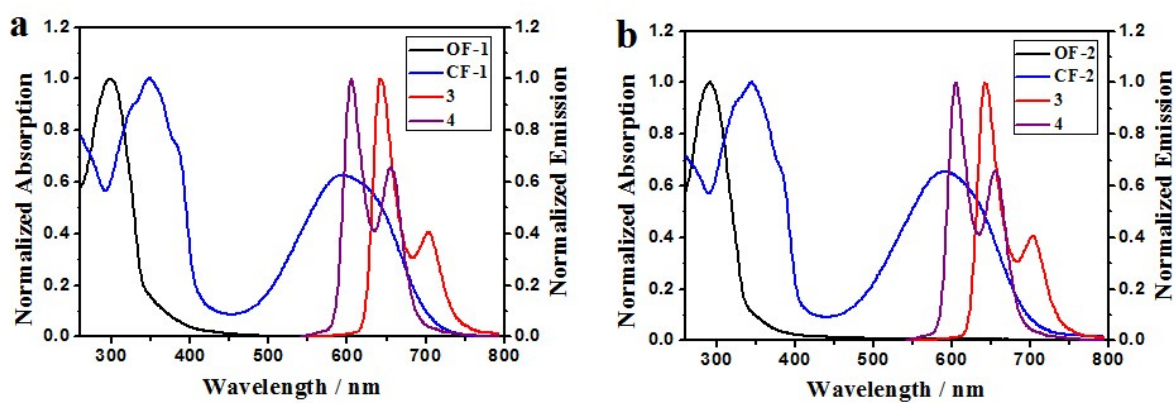


Figure S29. (a) Normalized absorption spectra of **OF-1**, **CF-1** and emission spectra of **3** and **4**. (b)

Normalized absorption spectra of **OF-2**, **CF-2** and emission spectra of **3** and **4**.

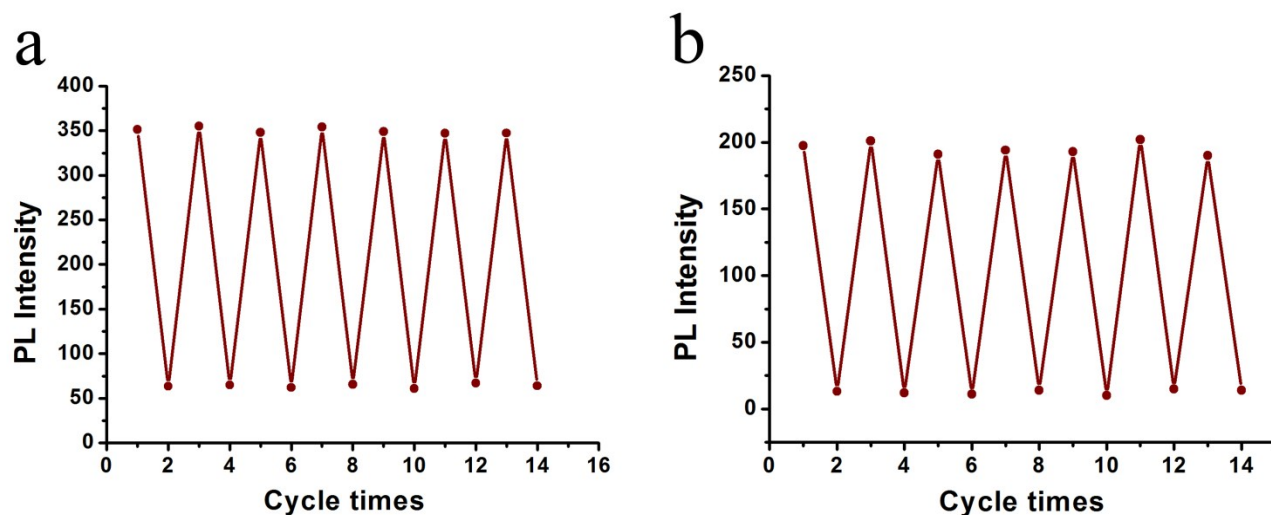


Figure S30. (a) The reversibility of fluorescence quenching for **3<OF-2** monitored by the change of emission intensity at 644 nm over seven cycles under irradiation of 254nm (50s) and >420nm light (50s), respectively. (b) The reversibility of fluorescence quenching for **4<OF-2** monitored by the change of emission intensity at 650 nm over seven cycles under irradiation of 254nm (50s) and >420nm light (50s), respectively.

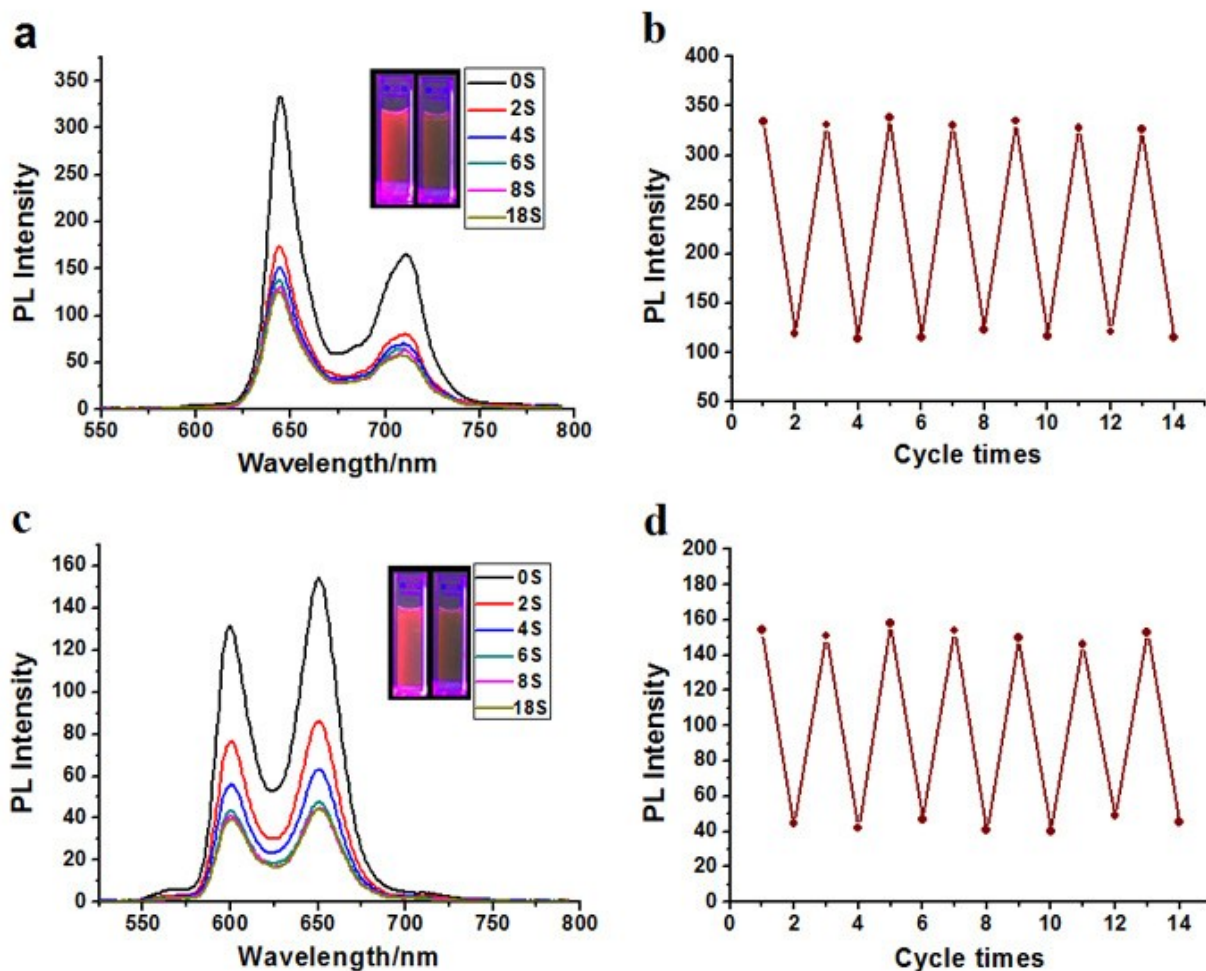


Figure S31. (a) Fluorescence spectral change of assembly **3<OF-1** upon irradiation with 254 nm UV light. (b) The reversibility of fluorescence quenching for **3<OF-1** monitored by the change of emission intensity at 644 nm over seven cycles under irradiation of 254nm (8s) and >420nm light (50s), respectively. (c) Fluorescence spectral change of assembly **4<OF-1** upon irradiation with 254 nm UV light. (d) The reversibility of fluorescence quenching for **4<OF-1** monitored by the change of emission intensity at 650 nm over seven cycles under irradiation of 254nm (8s) and >420nm light (50s), respectively. ($[\text{OF-1}] = 2[\mathbf{3}] = 2[\mathbf{4}] = 4\mu\text{M}$, in 5% EtOH pH 7.2 PBS)

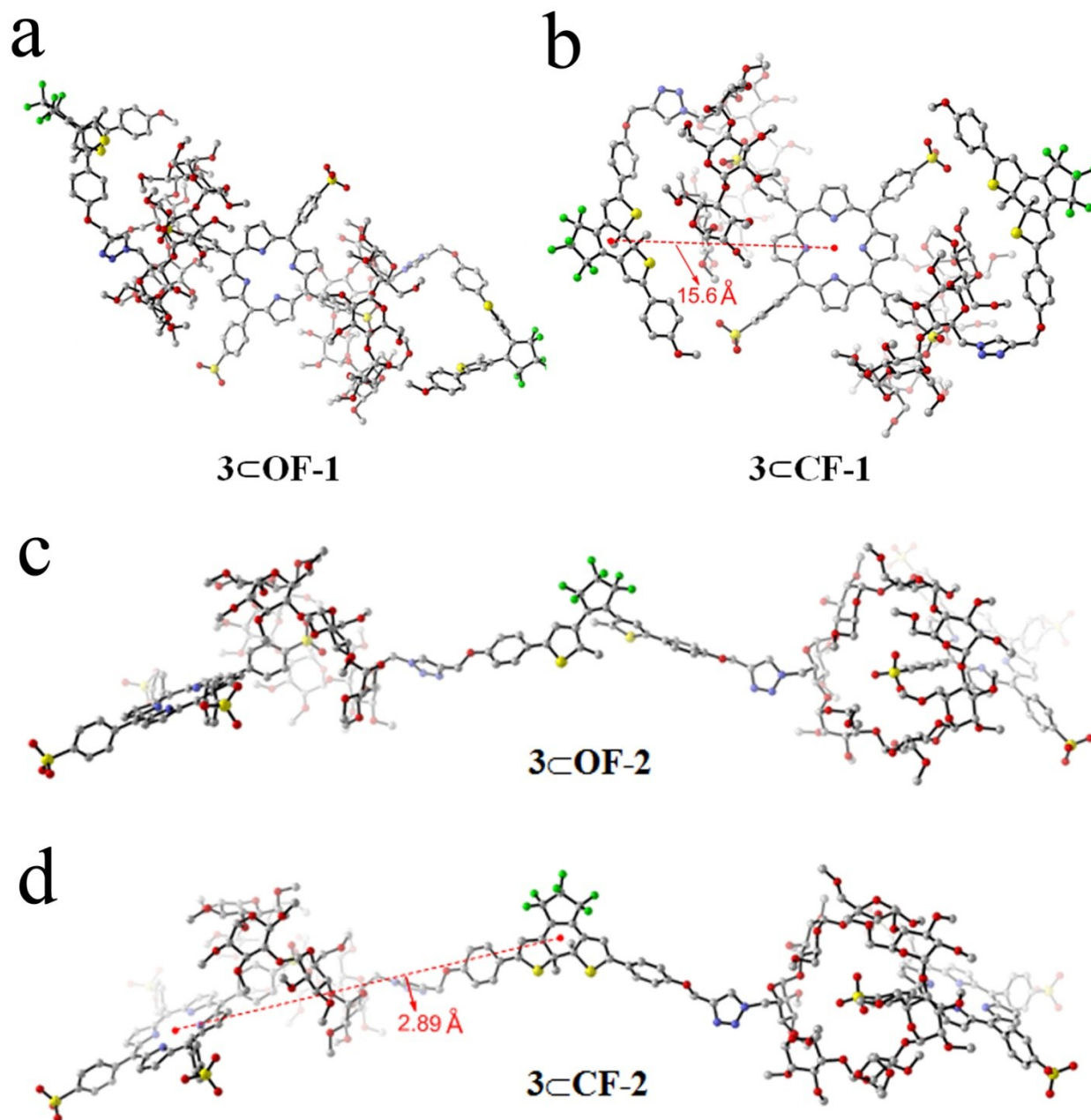


Figure S32. Optimizing geometries of the species **3C=OF-1**, **3C=CF-1**, **3C=OF-2** and **3C=CF-2**.

Table S2. The efficiency of energy transfer (E) of **3** and **4** in the presence of **1** and **2**.

Complex	λ_{ex}/nm	λ_{em}/nm	E
3 ⊂ 1	413nm	644nm	63.7%
3 ⊂ 2	413nm	644nm	81.7%
4 ⊂ 1	422nm	650nm	71.2%
4 ⊂ 2	422nm	650nm	93.4%

Remarks: $E = 1 - F_{PS} / F_0$, where F_{PS} is the fluorescence intensity of the chromophore at photostationary equilibrium and F_0 is its original fluorescence intensity without light irradiation.¹¹⁻¹²

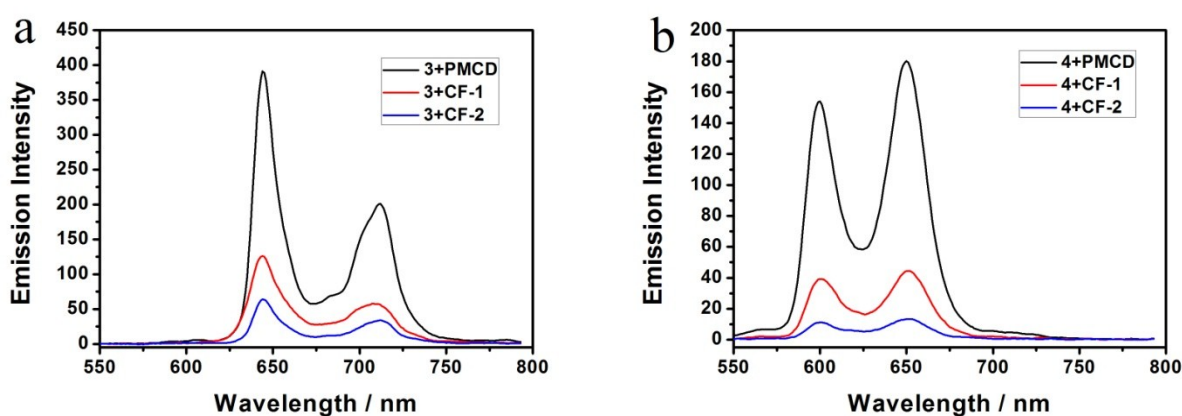


Figure S33. (a) The Fluorescence spectra of **3**⊂**PMCD**, **3**⊂**CF-1** and **3**⊂**CF-2**. (b) The Fluorescence spectra of **4**⊂**PMCD**, **4**⊂**CF-1** and **4**⊂**CF-2**. ($[\text{CF-1}] = [\text{PMCD}] = 2[\text{CF-2}] = 2[\text{3}] = 2[\text{4}] = 4\mu\text{M}$, in 5% EtOH pH 7.2 PBS) The efficiency of energy transfer (E) were calculated to be 68% (**3**⊂**CF-1**), 83.6% (**3**⊂**CF-2**), 75.5% (**4**⊂**CF-1**) and 92.7% (**4**⊂**CF-2**), respectively.

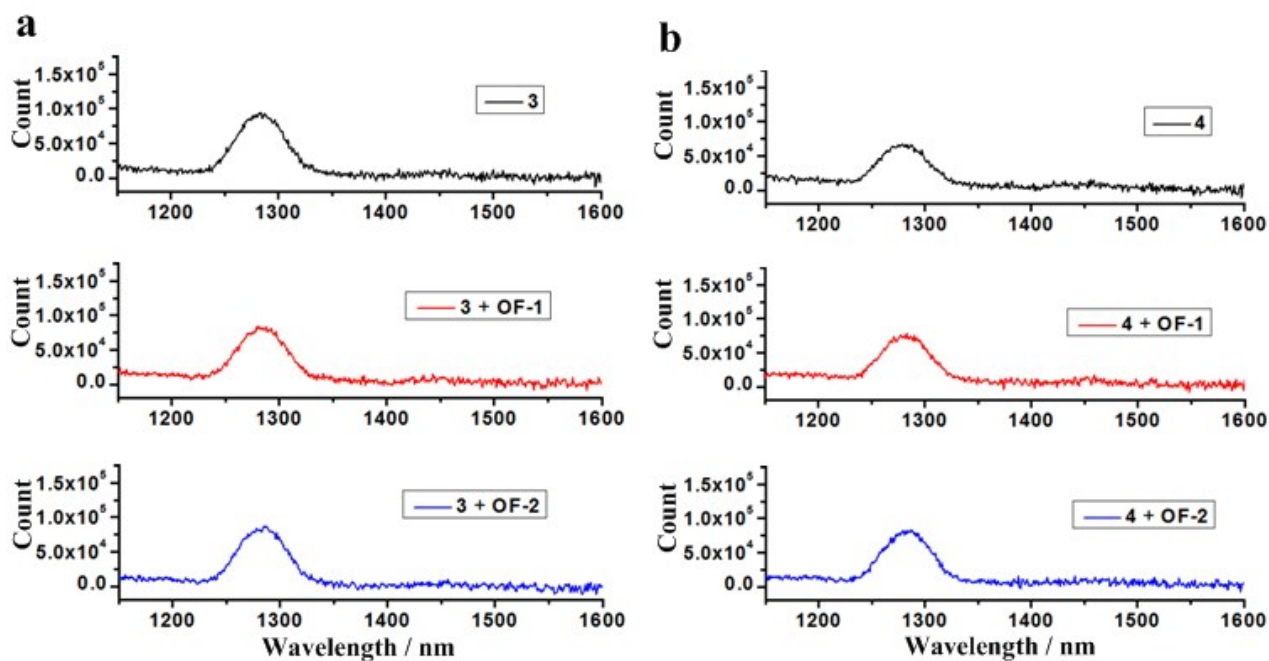


Figure S34. (a) NIR emission spectra of $^1\text{O}_2$ generated by **3** and **3** in the presence of **1** and **2** in O_2 equilibrated EtOH / D_2O (v/v, 1:100). (b) NIR emission spectra of $^1\text{O}_2$ generated by **4** and **4** in the presence of **1** and **2** in O_2 equilibrated EtOH / D_2O (v/v, 1:100). ($[\mathbf{1}] = [\mathbf{2}] = 5[\mathbf{3}] = 5[\mathbf{4}] = 10 \mu\text{M}$; **3**, excitation at 413nm; **4**, excitation at 422nm.)

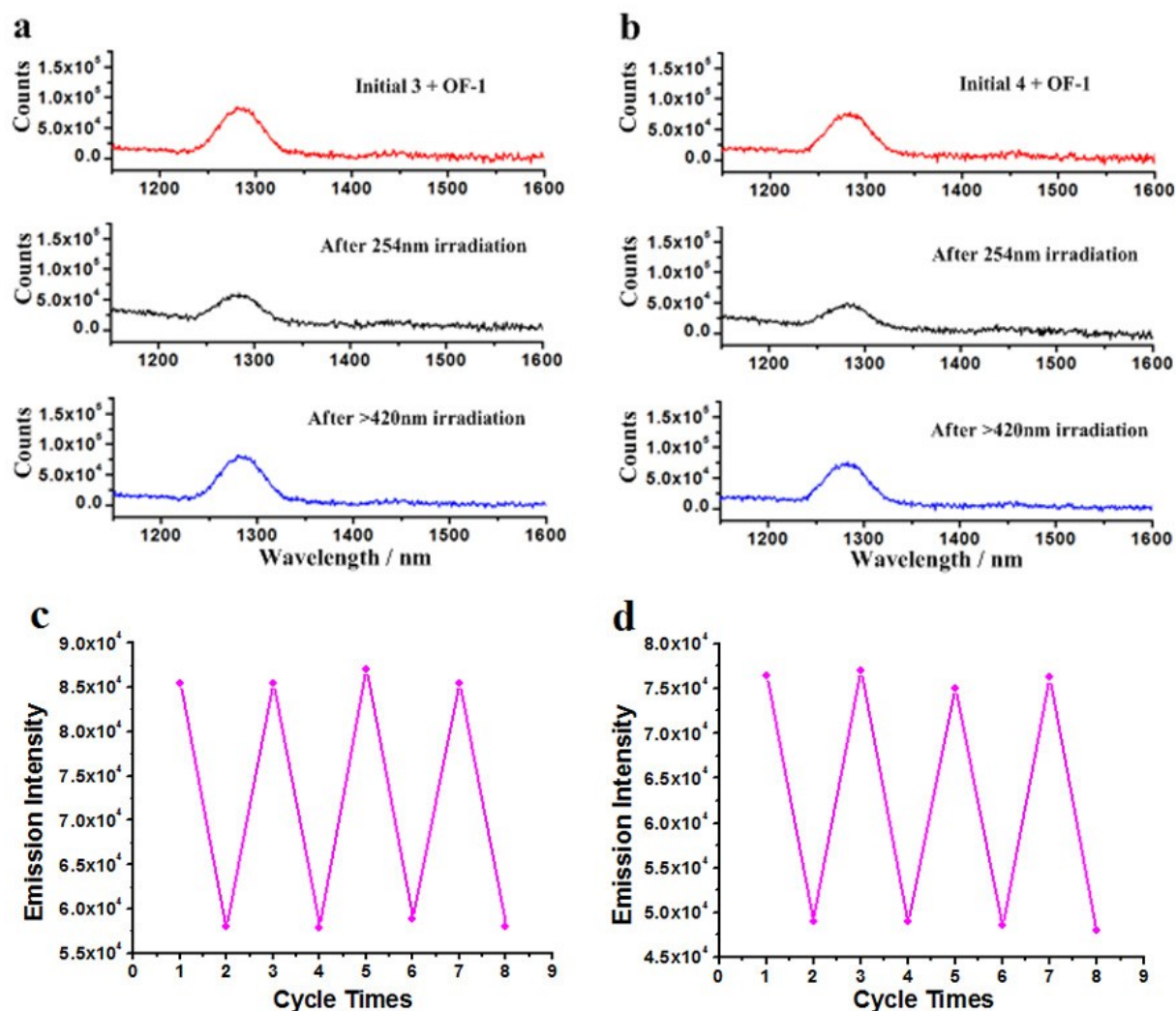


Figure S35. (a) NIR emission spectra changes of $^1\text{O}_2$ generated by **3** in the presence of **1**. (b) NIR emission spectra changes of $^1\text{O}_2$ generated by **4** in the presence of **1**. (c) The reversibility of $^1\text{O}_2$ generation by **3** + **1** was monitored by the change of emission intensity at 1283 nm over four cycles. (d) The reversibility of $^1\text{O}_2$ generation by **4** + **1** was monitored by the change of emission intensity at 1283 nm over four cycles. (The experiments were performed in O_2 equilibrated EtOH / D_2O (v/v, 1:100) alternatively irradiated with UV and visible light. **3**, excitation at 413 nm; **4**, excitation at 422 nm; $[\mathbf{1}] = 5[\mathbf{3}] = 5[\mathbf{4}] = 10\mu\text{M}$)

Table S3. Calculated energies of these switches and Zn-TSPP 4.

	Zn-TSPP 4 ^{6d}	OF-1' ($\approx$ OF-1)	CF-1' ($\approx$ CF-1)	OF-2' ($\approx$ OF-2)	CF-2' ($\approx$ CF-2)
S ₁ (eV)	2.05	3.34 (3.41)	2.05	3.35	2.05
T ₁ (eV)	1.53	2.87 (3.04)	1.20	2.95	1.20

Remarks: On account of optimizing calculation of **OF-1**, **CF-1**, **OF-2** and **CF-2** modified with PMCD using DFT [B3LYP/6-31G(d)] is greatly time-consuming, so we only optimized **OF-1** and calculated its lowest singlet energy and triplet energy. Meanwhile, **OF-1'** is the corresponding molecule of **OF-1** without PMCD, as show in Scheme S3. Table S2 manifests the lowest singlet and triplet energy of **OF-1** is approximately equal to **OF-1'**, respectively (column 3), which indicates the PMCD group has little influence on the transition energy of the photo-switched framework. Therefore, we calculate the singlet and triplet energy of the dithienylethene skeleton **OF-1'**, **CF-1'**, **OF-2'** and **CF-2'** with removing PMCD, which should be approximately equal to the singlet and triplet energy of **OF-1**, **CF-1**, **OF-2** and **CF-2**, respectively. The structures of **OF-1'**, **CF-1'**, **OF-2'** and **CF-2'** are listed in Scheme S3.

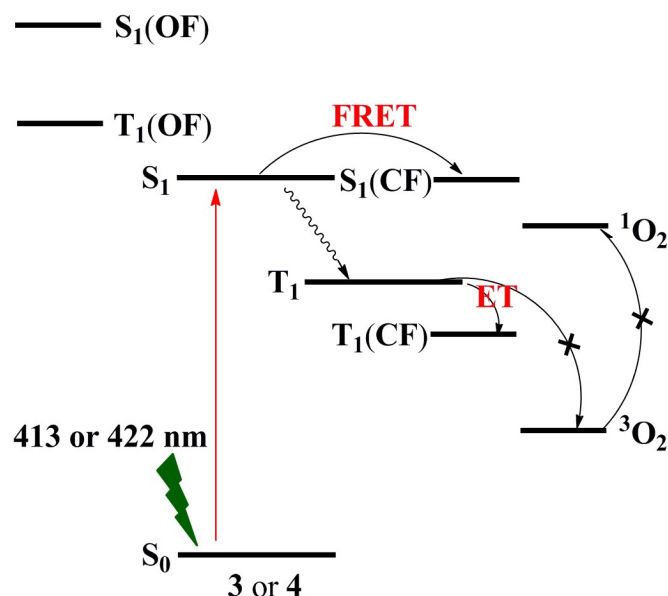
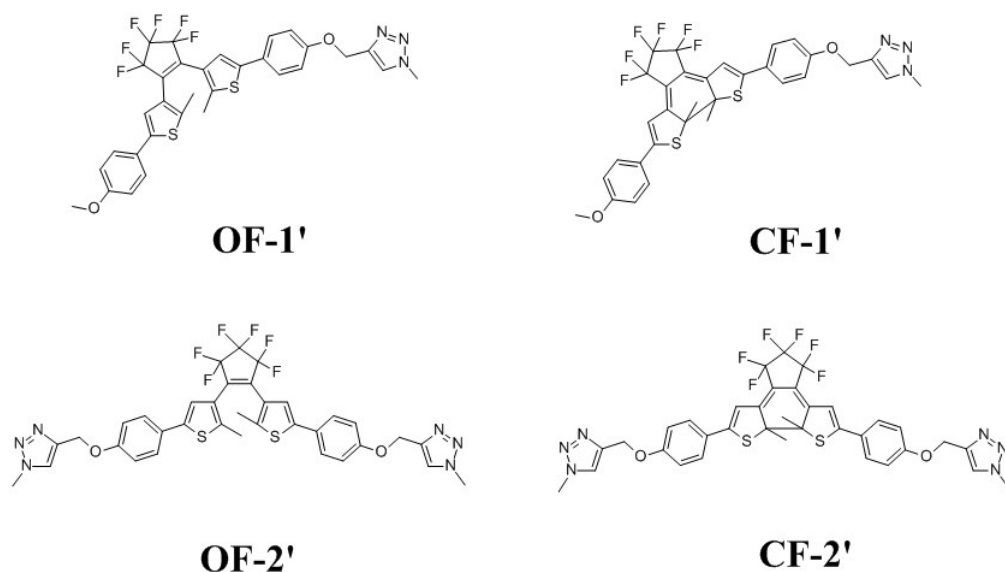


Figure S36. Proposed mechanism of energy transfer (ET) in these assemblies.



Scheme S3. chemical structures of **OF-1'**, **CF-1'**, **OF-2'** and **CF-2'**.

Computational data

The Cartesian coordinates (Å) for the optimized structures of **CF-1**, **OF-1**, **CF-2** and **OF-2**.

CF-1

Cartesian coordinates

ATOM	X	Y	Z
O	-8.85551500	-2.13371100	5.53807100
O	-10.54330000	-5.35631700	5.68281400
O	-8.37715400	-3.08292500	8.29138500
O	-7.98534000	-5.90765100	8.28177800
O	-12.16800100	-3.11268100	5.05054700
O	-8.58796000	-6.47168100	5.53932700
O	-9.08569600	-9.17248900	3.08440500
O	-6.59757000	-8.44092100	6.22417800
O	-5.51842400	-9.57579400	3.86521900
O	-11.60107200	-8.27627700	2.78198000
O	-7.28935300	-8.36601500	1.97419800
O	-7.79203000	-8.81548900	-1.65511200
O	-4.64657700	-8.02682800	0.89338300
O	-4.71166500	-6.87942700	-1.77596500
O	-8.83721400	-10.88157400	0.19739900
O	-7.36935100	-6.69501500	-2.27760100
O	-9.79009000	-5.09499900	-4.47013500
O	-6.09500500	-6.66362900	-4.94729600
O	-6.67052500	-4.08722500	-6.14445000

O	-11.34147700	-6.92997900	-3.38225700
O	-8.61280400	-3.17200500	-4.25513300
O	-10.80495700	-0.46032800	-3.10079900
O	-7.63989700	-0.84912300	-5.65302600
O	-7.75407200	1.42211300	-3.92736100
O	-9.28382400	0.46155900	-1.71736100
O	-10.91084900	1.09199600	1.51446900
O	-8.58978200	3.18006500	-1.15586700
O	-8.40889200	3.73140800	1.71807100
O	-8.99969600	1.16410400	2.67566000
O	-9.99718100	-0.22883400	5.95739900
O	-6.54155400	1.18739500	4.08479600
O	-6.46579400	-0.98819900	6.10741800
O	-11.49130300	2.06946200	4.92820200
C	-9.53489300	-3.20220700	6.20619000
H	-10.41120100	-2.81156800	6.78907100
C	-8.53058000	-3.91168000	7.13725200
H	-7.55377600	-4.05394500	6.59814700
C	-9.06687000	-5.27475500	7.60443600
H	-9.91410300	-5.11639800	8.33098600
C	-9.62086100	-6.11180500	6.43474500
H	-10.20524500	-6.99713700	6.81350400

C	-10.00384500	-4.16282600	5.10010500	C	-5.85472100	-7.73052100	0.19386300
H	-9.13157200	-4.42842100	4.43640900	H	-6.19375300	-6.67381900	0.37366100
C	-11.10824700	-3.59280200	4.21700300	C	-5.52609100	-7.94260800	-1.29327500
H	-10.68319200	-2.75871000	3.59463200	H	-5.00107800	-8.93262300	-1.41074500
H	-11.49942900	-4.39601400	3.53630300	C	-6.78485100	-7.97828500	-2.17966600
C	-7.03230000	-2.98482500	8.73808200	H	-6.53086500	-8.41109300	-3.19034200
H	-6.61868300	-4.00024800	8.95644600	C	-8.17380200	-8.55519700	-0.29548900
H	-7.09609500	-2.37469700	9.67311600	H	-8.57210400	-7.49816600	-0.19934900
H	-6.40982300	-2.46258600	7.96724400	C	-9.29713700	-9.54816600	0.00522800
C	-8.28723200	-7.20986400	8.75336600	H	-9.77068000	-9.27490300	0.99265400
H	-9.26921400	-7.23315900	9.28619200	H	-10.05689100	-9.50886300	-0.81869100
H	-7.45212200	-7.44957000	9.45857300	C	-4.43709000	-7.22129200	2.04371900
H	-8.28398100	-7.93126200	7.89568700	H	-4.38444000	-6.14056900	1.76179200
C	-13.19573300	-2.50387500	4.29211300	H	-3.45499700	-7.57326300	2.44756700
H	-12.79487800	-1.64087700	3.70041300	H	-5.25331100	-7.39488900	2.78871700
H	-13.93606500	-2.14705600	5.05043300	C	-3.31852700	-7.13917300	-1.66953500
H	-13.66787400	-3.24475200	3.59993200	H	-3.03958900	-7.40535500	-0.61982400
C	-8.60531900	-7.82266800	5.05982800	H	-2.83815400	-6.17223000	-1.96796000
H	-9.07994500	-8.50771200	5.81463500	H	-3.02448400	-7.96004200	-2.36907600
C	-7.11114700	-8.18380700	4.91583700	C	-8.59109100	-11.58823700	-1.00500300
H	-6.56992500	-7.33690700	4.41127100	H	-9.52858900	-11.67110300	-1.60945200
C	-6.91817200	-9.47404900	4.10627100	H	-8.25207500	-12.60116200	-0.67303000
H	-7.27245300	-10.35776300	4.70654700	H	-7.79645500	-11.08252300	-1.60734700
C	-7.72801000	-9.42990800	2.79465600	C	-7.99094500	-6.43532000	-3.54269200
H	-7.73348700	-10.42702000	2.26865800	H	-8.28178500	-7.39434900	-4.05186800
C	-9.35008100	-7.91697000	3.71523300	C	-6.97589300	-5.67083800	-4.41425900
H	-9.03143900	-7.07849500	3.03271100	H	-6.42225300	-4.92425800	-3.78103500
C	-10.86899000	-7.90049100	3.93391600	C	-7.65598700	-4.95365400	-5.59245200
H	-11.15661300	-8.67432300	4.69572400	H	-7.96362300	-5.71408700	-6.36583400
H	-11.16825300	-6.87402900	4.27777900	C	-8.93423300	-4.20426800	-5.16083500
C	-5.72062200	-7.42599600	6.69286400	H	-9.52859300	-3.85449700	-6.04967800
H	-4.82010200	-7.35466100	6.03545900	C	-9.24142400	-5.59161500	-3.24641200
H	-5.43510500	-7.76378100	7.72030000	H	-8.96225900	-4.72311000	-2.57547400
H	-6.25802700	-6.44441400	6.74052100	C	-10.33667100	-6.39217900	-2.53784600
C	-5.11721200	-10.84613800	3.38264800	H	-9.84860100	-7.20758000	-1.93585800
H	-5.40960200	-11.65501100	4.09735600	H	-10.90427900	-5.69440800	-1.85764200
H	-4.00332800	-10.77001300	3.30632800	C	-4.74418600	-6.23313200	-5.03260900
H	-5.56185900	-11.04461700	2.37600400	H	-4.67142500	-5.27353300	-5.60130600
C	-11.60587300	-7.28722200	1.75907000	H	-4.22497300	-7.05813800	-5.58099700
H	-12.04238200	-6.33171100	2.14244500	H	-4.31640500	-6.11438600	-4.00419000
H	-12.25691400	-7.72345900	0.96159000	C	-7.08850300	-3.43620500	-7.33289000
H	-10.56955900	-7.10579300	1.37267600	H	-7.46945000	-4.17243600	-8.08273900
C	-6.95653700	-8.71878600	0.62769700	H	-6.16228300	-2.93278200	-7.70885700
H	-6.56882200	-9.77271200	0.57841700	H	-7.87054100	-2.67006500	-7.09807500

C	-10.88557100	-7.93310200	-4.26952000	H	-6.74027800	3.69234400	-0.30114400
H	-10.24481200	-7.47979500	-5.06685000	H	-7.18010800	4.38579600	-1.94552100
H	-11.81766700	-8.35943400	-4.71755300	H	-6.68916400	2.61846100	-1.79709800
H	-10.31559600	-8.72621000	-3.72374900	C	-8.44547000	5.11451100	1.38275500
C	-9.33972500	-1.94227500	-4.38308800	H	-8.41504400	5.25167100	0.27381300
H	-9.92296800	-1.90034500	-5.33894900	H	-7.52720900	5.55463900	1.85529200
C	-8.24960300	-0.84890700	-4.36022000	H	-9.36919800	5.58463500	1.80127000
H	-7.50670600	-1.07676000	-3.54758400	C	-9.01279400	1.00779700	4.09764700
C	-8.85345000	0.54555600	-4.14257700	H	-9.10537800	2.00866700	4.60027800
H	-9.41054100	0.84286800	-5.07856200	C	-7.64751300	0.35166300	4.39359100
C	-9.87621800	0.59674200	-2.99329600	H	-7.50419700	-0.53795000	3.70856200
H	-10.49959900	1.53369200	-3.08255800	C	-7.56163900	-0.11593700	5.85319600
C	-10.25129200	-1.77788100	-3.15597600	H	-7.47837000	0.78352900	6.52684300
H	-9.63390900	-1.98515100	-2.22769000	C	-8.81039900	-0.92145100	6.26864600
C	-11.43800200	-2.75745700	-3.12136500	H	-8.83761300	-1.08252700	7.38311300
H	-11.08401300	-3.75134500	-3.52113500	C	-10.15712300	0.09729000	4.57135800
H	-11.72459600	-2.90341800	-2.03678100	H	-10.15172100	-0.85052500	3.95949800
C	-6.22014300	-0.81234300	-5.60490300	C	-11.55609000	0.71089400	4.49246400
H	-5.86843300	0.03071700	-4.96102900	H	-11.92912600	0.66461900	3.43339800
H	-5.91239200	-0.65396200	-6.66879100	H	-12.25026200	0.13731600	5.16522700
H	-5.83098100	-1.79210500	-5.22945900	C	-6.68845300	2.56971800	4.36348200
C	-8.04763600	2.77565500	-4.23659700	H	-7.40976200	3.03676900	3.64527900
H	-8.40627200	2.87573300	-5.29098600	H	-5.66136800	2.98792800	4.19752600
H	-7.07014100	3.30410500	-4.10175200	H	-7.01239100	2.73862300	5.41949000
H	-8.80740600	3.18171200	-3.52267800	C	-5.19538700	-0.48082100	5.72759100
C	-9.91087600	1.23411300	-0.68472100	H	-5.07659600	-0.53659800	4.61655200
H	-10.80253400	1.79577700	-1.07149700	H	-4.46950800	-1.16242400	6.23850700
C	-8.85636000	2.21873100	-0.13509300	H	-5.06299800	0.57408300	6.07064900
H	-7.92889100	1.65515300	0.15767900	C	-12.74560300	2.71954500	4.84200000
C	-9.42547100	2.96696200	1.08280300	H	-13.11619400	2.72450500	3.78606900
H	-10.27193100	3.62565200	0.73853200	H	-12.54724100	3.76266200	5.19313300
C	-10.00342600	1.99072100	2.12682800	H	-13.49632700	2.21980800	5.50342800
H	-10.59764300	2.54695300	2.90480500	C	1.71333900	-2.43001700	0.26933500
C	-10.34586300	0.30088300	0.46156300	N	1.34426800	-1.16616600	0.50732100
H	-9.43943900	-0.25056200	0.84468800	C	2.53943400	-0.40125900	0.65525900
C	-11.39962900	-0.73694100	0.08180200	C	3.70556500	-1.31794600	0.48757400
H	-11.08204800	-1.22504700	-0.88211100	C	3.20276600	-2.56183600	0.25190800
H	-11.46134600	-1.51239700	0.89442000	C	0.84773200	-3.56613400	0.05002000
C	-13.50692500	-0.00846000	0.92690100	C	-2.67860600	-2.74941800	0.36250300
H	-14.52136000	0.20861600	0.50655400	N	-1.32221200	-2.38776200	0.35153200
H	-13.14439800	0.85414900	1.53985800	C	-0.51765200	-3.51359500	0.11397100
H	-13.53532800	-0.93258800	1.55710300	C	-1.44620300	-4.66669900	-0.05024200
O	-12.68041600	-0.18957900	-0.20920200	C	-2.72191700	-4.21807100	0.10567200
C	-7.20443000	3.47556800	-1.29554400	C	-3.75748700	-1.92498700	0.55927100

C	-2.88283700	1.56652400	1.11908600	C	3.97920100	1.52920300	1.03056400
N	-2.51120000	0.20385900	0.92443000	C	4.85788200	1.50441500	-0.06076500
C	-3.64158400	-0.49756400	0.76963500	H	-3.57358900	3.25529300	3.44779200
C	-4.83843400	0.39772800	0.83301200	H	-4.75093900	5.41672300	3.88280000
C	-4.37117500	1.65747700	1.05708800	H	-3.08076500	7.06921800	0.27816400
C	-2.05268900	2.63435800	1.32287900	H	-1.86834300	4.92534400	-0.15547000
C	1.51699800	1.82561000	1.11526600	H	-5.61723900	-1.68841500	2.51644900
N	0.17138500	1.47142900	1.05836400	H	-7.94757600	-2.56787400	2.48431300
C	-0.61353600	2.59540700	1.30102000	H	-7.23956900	-4.32202500	-1.39207000
C	0.26576600	3.70066600	1.51948600	H	-4.93326200	-3.40851900	-1.39486200
C	1.58671800	3.22379500	1.40178000	H	3.02275200	-7.51158000	1.25067200
C	2.63418700	0.93725000	0.91792500	H	1.72885900	-5.44497900	1.80338800
H	4.74264500	-0.99098100	0.53745300	H	1.46412100	-4.50745300	-2.40830500
H	3.72629700	-3.49839000	0.07265900	H	2.74426200	-6.58358300	-2.94024600
H	-0.97850700	-1.47656900	0.53047200	H	6.85404400	1.94960200	-0.78163600
H	-1.08710800	-5.67484900	-0.25364700	H	6.07258800	2.92391000	3.34573800
H	-3.65684300	-4.77892900	0.05516900	H	3.71960900	2.12973600	3.09622800
H	-5.86347300	0.05368100	0.71514700	H	4.52107500	1.10800000	-1.03364000
H	-4.92257400	2.58831400	1.17596000	S	-4.98267500	7.80502600	2.33778900
H	-0.17464700	0.55900100	0.87515200	O	-4.35074600	8.84563300	1.59474500
H	-0.05604500	4.71617800	1.73514500	O	-4.99537600	8.03171000	3.73143100
H	2.50825800	3.79083800	1.50484700	O	-6.26383500	7.50527900	1.80018000
C	-3.46615600	4.09629200	2.74645300	S	8.26443400	2.96998000	1.51177000
C	-4.12831700	5.29863000	2.97961000	O	8.22423700	4.35768400	1.80027200
C	-4.02574700	6.36383300	2.08332900	O	8.95533500	2.71394500	0.28652400
C	-3.19486500	6.21951800	0.97240400	O	8.82636800	2.21748800	2.58214400
C	-2.51499500	5.02633000	0.72823000	S	-9.39578600	-4.05272400	0.49131900
C	-2.66953600	3.94353600	1.60217300	O	-9.93324200	-3.65390700	-0.77035100
C	-5.11562000	-2.48281300	0.55903700	O	-10.08063300	-3.42126400	1.56687800
C	-5.97314400	-2.26643500	1.64903400	O	-9.35841300	-5.46645400	0.61664600
C	-7.27549900	-2.76010000	1.62806300	S	3.97882400	-8.55599800	-1.25007200
C	-7.75940900	-3.48631300	0.53686700	O	5.26528400	-8.05251600	-1.60799100
C	-6.89061100	-3.72504500	-0.52985900	O	3.36946100	-9.19140100	-2.36315400
C	-5.58926500	-3.22619900	-0.53066800	O	4.00047800	-9.34571100	-0.07697900
C	2.68176200	-6.83822200	0.44479000	C	-13.68959700	8.81353300	-4.39512700
C	1.95481700	-5.68991500	0.75572100	C	-12.64567100	9.81852500	-4.28444700
C	1.52755400	-4.83230100	-0.26585500	C	-13.57645500	7.63186000	-3.75071500
C	1.80724100	-5.16651500	-1.59805800	C	-11.43582200	9.49405700	-3.76894700
C	2.53056200	-6.32131100	-1.89083800	C	-13.83454800	5.32682800	-3.34263500
C	2.99611200	-7.15856100	-0.87660500	S	-12.30540200	5.59875100	-2.63304900
C	6.16451700	1.96979700	0.08531800	C	-12.39555100	7.40800100	-2.81956600
C	6.62690500	2.45229400	1.31037800	S	-9.72067600	8.11308600	-2.29932700
C	5.72987300	2.51544100	2.37951500	C	-9.38985100	9.75493500	-2.62897200
C	4.41689000	2.06964400	2.24740800	C	-10.33975600	10.35315400	-3.41068200

C	-12.70755800	7.97040600	-1.44386000	H	-4.52390600	11.22790200	1.31783000
H	-12.83954200	9.07906100	-1.50167600	H	-3.60842700	10.38649600	-0.01413300
H	-13.64871500	7.51873500	-1.04735100	C	-14.51812500	10.85322100	-5.52247400
H	-11.86834500	7.74464700	-0.73949200	F	-12.23648200	11.75371400	-5.70253900
C	-10.68093100	7.30199400	-4.66413700	F	-13.24638700	12.13870400	-3.85835400
H	-11.49532700	7.27768400	-5.42936000	F	-14.49230700	11.15188100	-6.85837300
H	-9.79189100	7.81529900	-5.10434500	F	-15.51492500	11.65627200	-5.03620700
H	-10.40212100	6.25149700	-4.40048500	F	-14.96525700	8.62376700	-6.46003600
C	-14.83127600	9.28955000	-5.26312800	F	-16.08209800	9.13541400	-4.71043100
C	-13.09777700	11.15684400	-4.81104300	C	-14.40009900	6.44983000	-3.86660800
N	-12.63746900	-2.35175000	-3.83544300	H	-15.37411800	6.50039900	-4.36403700
C	-13.66806700	-1.60555800	-3.25712900	C	-11.14935600	8.04032500	-3.42162000
C	-14.57280500	-1.38716700	-4.31766000	O	7.95099300	-1.76196000	-0.83732200
H	-13.65540100	-1.28235900	-2.21312200	O	9.92851900	-2.24861200	2.15922100
N	-12.89538000	-2.53959200	-5.14980400	O	7.99535600	-4.69340600	-0.44112000
N	-14.00839800	-2.00562200	-5.46005500	O	7.67938200	-5.13637800	2.44818200
C	-15.88494600	-0.71153200	-4.31425800	O	10.88672500	-0.45170000	0.12642600
H	-16.05619900	-0.14853700	-5.27003700	O	8.30925000	-2.72802200	3.63322100
H	-16.71152400	-1.46161000	-4.15866900	O	9.42347500	-0.98225800	6.69480800
O	-16.04184600	0.16111300	-3.18684200	O	6.71135200	-3.83537100	5.75845300
C	-15.44581200	1.40620500	-3.31461600	O	5.91888300	-1.70029000	7.48477300
C	-14.44318600	1.75387500	-2.39616500	O	11.62567400	-0.23059700	5.12625900
C	-15.91077900	2.33575800	-4.25519100	O	7.62245300	0.36103100	6.53664300
C	-13.92427800	3.04276100	-2.41643400	O	8.70055500	3.69748500	7.70433400
H	-14.06630000	1.00538400	-1.67606000	O	5.15326700	1.81717600	6.82282900
C	-15.38318100	3.62323600	-4.26339400	O	5.55380900	4.65257200	6.17587800
H	-16.68563300	2.04633100	-4.97849800	O	9.52004200	1.29729800	9.32767400
C	-14.39085500	3.99266700	-3.34291900	O	8.23129700	4.61417700	5.69246900
H	-13.13107500	3.31943900	-1.69995400	O	11.00231600	6.27968700	4.02721400
H	-15.74247400	4.35545100	-5.00197500	O	7.75720400	7.45015300	6.24591400
H	-10.33145800	11.40198700	-3.72328300	O	8.65357800	9.11843600	4.12541100
C	-8.19981900	10.35411000	-2.08595000	O	12.15367600	3.93438200	4.10915200
C	-7.46446900	9.67471500	-1.09415200	O	9.68998400	7.11347000	2.38058400
C	-7.74022700	11.60369400	-2.53615400	O	10.93774500	6.12445500	-0.91546000
C	-6.29923700	10.21529700	-0.57049300	O	9.50241500	9.51679200	0.76362900
H	-7.81013900	8.69542500	-0.71322300	O	8.51486500	8.72908100	-1.82976200
C	-6.57802400	12.15991300	-2.02319200	O	8.85397900	5.91911100	-1.74085900
H	-8.30333100	12.14498100	-3.31113800	O	9.07662900	3.12204900	-4.15989400
C	-5.84998400	11.46178600	-1.03741900	O	6.31242800	5.93628100	-2.97830000
H	-5.73901300	9.65326400	0.20770900	O	5.47171200	3.26267500	-3.89118100
H	-6.21287000	13.13362300	-2.37515900	O	7.60441800	1.78291300	-3.08755400
O	-4.71261800	12.08855900	-0.59519400	O	9.07011900	-1.57504400	-2.80379900
C	-3.93626800	11.37953500	0.37996200	O	5.23678400	0.09313300	-3.34342500
H	-3.06545000	12.05971700	0.54956900	O	5.62929600	-2.51569000	-2.16886400

O	10.08007700	0.05496500	-4.94029700	H	6.01292300	-2.56772800	9.38930400
C	8.77707000	-2.49418600	0.06986500	H	4.61807600	-1.43689800	8.99253300
H	9.73283900	-2.80360200	-0.42899200	H	6.29466600	-0.75893700	9.31461400
C	7.99923300	-3.71605400	0.59694600	C	11.47844200	0.65111600	4.01962000
H	6.95190300	-3.40467400	0.86677700	H	11.87574500	0.17435000	3.08853400
C	8.68433100	-4.33942900	1.83158100	H	12.09213400	1.54672100	4.29556900
H	9.52800000	-4.99966700	1.47790000	H	10.40686900	0.94552700	3.87094300
C	9.30192400	-3.32697400	2.82147800	C	7.52538400	1.59854000	7.25045100
H	10.11494300	-3.82066100	3.42519400	H	7.22304400	1.41390700	8.31683600
C	9.05594500	-1.55810300	1.25545500	C	6.42222100	2.38885600	6.51191400
H	8.08378000	-1.31909300	1.77738600	H	6.62480600	2.37542200	5.40499900
C	9.70815500	-0.23251600	0.90319200	C	6.36373300	3.83956900	7.01661300
H	8.97414500	0.38173500	0.30900200	H	5.97137800	3.84861100	8.07180100
H	9.97268900	0.32395100	1.84538500	C	7.75883400	4.49655100	7.01730000
C	6.76167500	-5.40152400	-0.54256000	H	7.74180800	5.48245400	7.56192100
H	6.47944400	-5.84011300	0.44545900	C	8.85617100	2.36463900	7.19933500
H	6.95259400	-6.21618600	-1.28763000	H	9.20256500	2.41330200	6.12563000
H	5.96163000	-4.70895300	-0.90799600	C	9.96423400	1.74204700	8.05193800
C	8.15973700	-5.96221300	3.49455100	H	10.33504800	0.80543700	7.54638800
H	9.06540800	-6.53542800	3.17863300	H	10.80020900	2.48135100	8.16631400
H	7.30853200	-6.65726800	3.70778500	C	4.71578500	0.84594800	5.88079300
H	8.38368600	-5.33708600	4.39689700	H	4.68610200	1.28205600	4.85068200
C	11.52093400	0.77604200	-0.19692900	H	3.68679100	0.57630500	6.22613300
H	10.77436300	1.56673900	-0.47246300	H	5.39035700	-0.04699500	5.90762700
H	12.18890300	0.53396900	-1.06234600	C	4.16370600	4.56595000	6.44911200
H	12.13303500	1.12066900	0.67606900	H	3.79003400	3.52517100	6.28530400
C	8.61809400	-2.56768500	5.02316000	H	3.70231300	5.27406100	5.71522300
H	9.17472600	-3.46548300	5.40646800	H	3.94877900	4.88973000	7.49767100
C	7.21685000	-2.50297800	5.67817700	C	9.33634300	2.33819200	10.27120600
H	6.54956500	-1.83817800	5.06271900	H	10.30404100	2.86436100	10.46500000
C	7.26761000	-1.98192200	7.12179200	H	8.98147700	1.82041400	11.19683400
H	7.69387400	-2.78044500	7.79193500	H	8.57371600	3.07110700	9.90841700
C	8.15607500	-0.73110400	7.25860100	C	9.16649500	5.67690500	5.48791600
H	8.36001400	-0.48719500	8.34062900	H	9.76638500	5.86070500	6.41891900
C	9.42742600	-1.28763300	5.29403500	C	8.41501500	6.95731800	5.07748000
H	8.98464000	-0.42970900	4.71558900	H	7.69026000	6.72304300	4.24975900
C	10.92045300	-1.45189300	4.97878600	C	9.42293400	8.02322900	4.60911200
H	11.39489900	-2.13378800	5.73523100	H	10.04572200	8.35712000	5.48735700
H	11.04963700	-1.85837400	3.94364200	C	10.39781300	7.46724300	3.54532900
C	5.72377700	-4.12593800	4.77672400	H	11.25028600	8.17609800	3.35589800
H	4.82206500	-3.48510400	4.93237400	C	10.06700000	5.23483600	4.32024400
H	5.47794700	-5.20356500	4.94862600	H	9.41577100	5.04237400	3.41044100
H	6.14377300	-3.97885100	3.74890000	C	10.85069800	3.96847300	4.67094200
C	5.71743200	-1.61475400	8.88426600	H	10.89449100	3.83025400	5.78406600

H	10.31777000	3.09290900	4.18879800	C	10.96062200	4.18852900	-3.27051900
C	6.43022900	7.89190400	5.99569100	H	11.42226500	4.59286400	-2.32860500
H	6.42081000	8.66033700	5.18393900	H	11.47471700	3.23910100	-3.57728900
H	6.09926100	8.33883800	6.96590600	C	11.10426500	4.75830600	-5.58003700
H	5.78333300	7.01955300	5.72181100	H	11.28143400	5.67525000	-6.19539000
C	9.42504900	10.28269100	3.88155200	H	10.09444600	4.32672400	-5.79080400
H	10.03645000	10.55684700	4.77658400	H	11.89320200	3.99220300	-5.78670400
H	8.66552800	11.07648100	3.66799800	O	11.19170000	5.20605800	-4.23873700
H	10.08213200	10.13105300	2.98789200	C	5.95095600	6.52809000	-1.73651300
C	13.14448600	4.56745800	4.89928700	H	5.44323000	5.78324100	-1.07608900
H	12.91763800	5.65313800	5.03347500	H	5.24428300	7.34665900	-2.02273700
H	14.09170000	4.43346700	4.31958200	H	6.85857200	6.94599600	-1.23132900
H	13.22556400	4.06853500	5.89776500	C	4.38313700	4.14051300	-4.12866300
C	10.35114300	7.31606300	1.12393600	H	4.33777700	4.93579300	-3.34438700
H	11.33011300	7.84602200	1.24238200	H	3.48569700	3.47406400	-4.06778900
C	9.35836200	8.17051100	0.30195600	H	4.46369600	4.60744100	-5.14141600
H	8.31604200	7.78050200	0.47587100	C	7.70387900	0.38792300	-3.41323300
C	9.66451100	8.16139700	-1.20470400	H	7.72366500	0.22019600	-4.52378200
H	10.56242800	8.81305000	-1.40481000	C	6.47978500	-0.30772300	-2.78820000
C	9.99115500	6.75733600	-1.74980500	H	6.37887400	-0.00153900	-1.70248900
H	10.48867000	6.81913000	-2.76007700	C	6.66186000	-1.83221500	-2.86514100
C	10.51535800	5.94753300	0.43940300	H	6.71744200	-2.16750700	-3.93714200
H	9.50928700	5.41633500	0.47326700	C	7.98465500	-2.22390400	-2.17346500
C	11.52634500	5.00521800	1.10326800	H	8.19420400	-3.32701300	-2.25282500
H	11.42481000	5.11515900	2.22531100	C	9.00854600	-0.14733300	-2.79168100
H	11.23955500	3.95032300	0.81001900	H	9.08685900	0.21566000	-1.72424000
C	8.26147900	10.19140500	0.90985700	C	10.25268600	0.31896000	-3.54656600
H	7.66798200	10.13547300	-0.03577700	H	10.37992600	1.42039400	-3.36692600
H	8.54528400	11.24938000	1.13733600	H	11.15351400	-0.24604600	-3.18311100
H	7.68863900	9.74958300	1.76423900	C	5.16691900	0.13900300	-4.75550600
C	8.68916200	8.98530800	-3.21197700	H	5.67861300	1.06235800	-5.12924000
H	9.58390000	9.63217700	-3.38988900	H	4.07026800	0.19307400	-4.97462300
H	7.75262200	9.51717900	-3.51462700	H	5.61236800	-0.77129400	-5.22583600
H	8.78965900	8.02593500	-3.77806000	C	4.52990800	-2.87942400	-2.99027400
C	8.60832300	5.17161900	-2.93509800	H	4.07016900	-1.97429500	-3.45866800
H	8.78088400	5.81837800	-3.83855800	H	3.81279300	-3.36846300	-2.27959800
C	7.11859400	4.76724500	-2.84531100	H	4.85517800	-3.60137700	-3.78006900
H	6.92482900	4.23450900	-1.87341800	C	10.96947600	0.81070100	-5.74219800
C	6.75315800	3.85908900	-4.03048300	H	10.80672800	1.90891200	-5.58497800
H	6.79747500	4.46552000	-4.97924300	H	10.71839800	0.52162500	-6.79279400
C	7.73790300	2.67658100	-4.17036300	H	12.03063700	0.54452000	-5.50939100
H	7.60941400	2.18063400	-5.17449900	C	14.70013800	-3.72776500	-5.88947200
C	9.47534100	3.90655500	-3.02516700	C	13.78726300	-4.75537000	-6.35538600
H	9.35170300	3.30010100	-2.07652900	C	14.55037800	-3.18213300	-4.66378600

C	12.63431300	-4.99914200	-5.68731800
C	14.64259700	-1.53360600	-2.98516200
S	13.23506000	-2.37448000	-2.52115400
C	13.48177700	-3.72152000	-3.72689000
S	11.02332700	-5.10868500	-3.59407100
C	10.82016400	-6.24778500	-4.84390700
C	11.70005000	-6.07441800	-5.87830800
C	14.03662500	-4.89994100	-2.94474500
H	14.26991300	-5.74601200	-3.63715200
H	14.97345400	-4.60410800	-2.41387200
H	13.28432300	-5.24701000	-2.19339400
C	11.48214200	-2.89576900	-5.03095500
H	12.17188800	-2.20226300	-5.57145000
H	10.67684600	-3.21667200	-5.73591200
H	11.00447600	-2.33565700	-4.18323300
C	15.76637800	-3.42038400	-6.91544400
C	14.29414400	-5.43418300	-7.60203200
N	12.92996600	5.17242000	0.75936200
C	13.74536000	4.13637800	0.29569000
C	14.99734700	4.75063600	0.07914500
H	13.40561800	3.10656500	0.18330400
N	13.63751200	6.32061500	0.80186900
N	14.83674200	6.11393400	0.42324600
C	16.26524700	4.17758000	-0.41750500
H	16.29617400	4.21937500	-1.53909800
H	17.15073800	4.72815400	0.00820900
O	16.46558600	2.83621500	0.04948800
C	15.95857600	1.83282800	-0.75943500
C	15.10494000	0.89155800	-0.16266300
C	16.36860200	1.67925900	-2.09113200
C	14.67761600	-0.20709500	-0.89996500
H	14.78317300	1.02894800	0.88112200
C	15.93303000	0.57595200	-2.81832300
H	17.03156500	2.42235100	-2.55559400
C	15.09046000	-0.38150800	-2.23269000
H	13.99383600	-0.94191700	-0.43688600
H	16.24984300	0.45613900	-3.86561000
H	11.74383700	-6.69017000	-6.78209200
C	9.81018200	-7.27119800	-4.75102700
C	8.77313000	-7.17497100	-3.80280000
C	9.84040000	-8.38219700	-5.61240000
C	7.78268100	-8.14498100	-3.71750100
H	8.73711700	-6.31073300	-3.11451000
C	8.86509200	-9.36341500	-5.54018100

H	10.64991700	-8.47972100	-6.35128000
C	7.82685600	-9.24462600	-4.59253800
H	6.96899800	-8.04341700	-2.96586800
H	8.88434200	-10.23272500	-6.21071200
O	6.91523100	-10.26753000	-4.60990800
C	5.81895200	-10.16427500	-3.69378500
H	5.21964600	-11.08383200	-3.90609700
H	6.18822700	-10.15536300	-2.63937100
H	5.21380300	-9.24382900	-3.88752600
C	15.57650900	-4.55552500	-8.04893300
F	13.38872700	-5.51425700	-8.63434600
F	14.65880900	-6.75190400	-7.44161100
F	15.41241700	-4.00955600	-9.29357700
F	16.70073500	-5.32576600	-8.18591600
F	15.68863700	-2.16590100	-7.47549800
F	17.05544400	-3.43544500	-6.43250300
C	15.24498800	-2.05064600	-4.09287900
H	16.15561700	-1.66705100	-4.56396500
C	12.24069300	-4.10792000	-4.51916900

OF-1

Cartesian coordinates

ATOM	X	Y	Z
O	-8.46496300	2.52267400	4.18618400
O	-11.06813700	0.00261100	4.58641600
O	-7.89604900	1.31886400	6.81649500
O	-8.48111100	-1.48650800	6.74721400
O	-11.99138500	2.61386900	4.20713500
O	-9.66762400	-1.72248900	4.19266500
O	-11.15640000	-3.91327500	1.65977400
O	-8.92752200	-4.44081000	5.00399900
O	-8.22419300	-5.89399800	2.65165600
O	-13.07581700	-2.00101100	1.37167300
O	-9.09393400	-3.88316200	0.72830700
O	-9.43778400	-3.97704500	-2.95662300
O	-6.39242400	-4.29732100	-0.16900800
O	-5.88190500	-3.24267100	-2.78651900
O	-11.21395100	-5.73214100	-1.31520600
O	-8.30014100	-2.06038900	-3.30362700
O	-10.04524300	0.42506400	-5.32239500
O	-6.78305000	-1.97494900	-5.80816300
O	-6.66810200	0.74306500	-6.75612400
O	-12.08981900	-0.94486700	-4.56190200

O	-8.48725900	2.01691500	-4.95863700	C	-10.00848600	-4.70517200	1.42250600
O	-10.05509700	5.10733000	-3.75086700	H	-10.37748700	-5.57884000	0.81360000
O	-7.34368800	4.05176600	-6.63347100	C	-10.91537000	-2.68823000	2.35684400
O	-6.96799800	6.48707200	-5.22634100	H	-10.25335100	-2.02608100	1.72925200
O	-8.17189200	5.82519700	-2.71866200	C	-12.29505700	-2.04608500	2.55110200
O	-9.28026000	7.14470800	0.54504100	H	-12.91588200	-2.66747500	3.25343500
O	-6.12004400	7.71798500	-2.05124200	H	-12.14049500	-1.01074100	2.96280000
O	-5.77588800	8.03867300	0.82542900	C	-7.56790600	-4.46719400	5.41689300
O	-7.62615900	5.96127400	1.48786300	H	-6.94049600	-5.01317100	4.66999600
O	-8.80144000	4.68699900	4.73643700	H	-7.58616000	-5.01286300	6.39324000
O	-5.19180800	4.99312400	2.65134800	H	-7.19845100	-3.42059800	5.56179500
O	-5.81342400	2.66789800	4.40993000	C	-8.38468300	-7.15057300	2.01612800
O	-9.48045100	7.41445900	3.95716100	H	-9.15979600	-7.76587700	2.53712600
C	-9.33796700	1.68124400	4.94772700	H	-7.37689800	-7.63008800	2.09996100
H	-9.94885500	2.29260200	5.66465900	H	-8.66176800	-7.01543000	0.94129500
C	-8.48887500	0.64140600	5.70629700	C	-12.52493600	-1.18089600	0.34616800
H	-7.70774600	0.21620300	5.01878100	H	-12.11309700	-0.22439500	0.75771900
C	-9.37247700	-0.48535400	6.26539500	H	-13.38345800	-0.98270700	-0.34183600
H	-9.98679500	-0.08222300	7.12075500	H	-11.70816700	-1.73603300	-0.18350000
C	-10.35950900	-1.03720500	5.21907500	C	-8.79459500	-4.27437400	-0.61652400
H	-11.14989300	-1.66953500	5.71456100	H	-8.75001500	-5.39422900	-0.69631700
C	-10.24856000	0.97770300	3.92705100	C	-7.41274100	-3.65785900	-0.92784500
H	-9.62579600	0.47724100	3.12854500	H	-7.43604400	-2.54740200	-0.73810100
C	-11.20643200	1.93223100	3.22319600	C	-7.05894100	-3.93854100	-2.39876000
H	-10.59851800	2.66049000	2.62254300	H	-6.93199600	-5.04865200	-2.54057700
H	-11.87953700	1.35254200	2.53725500	C	-8.18022700	-3.46783700	-3.34573400
C	-6.56271300	0.90634200	7.08163300	H	-8.00399900	-3.85600500	-4.38869800
H	-6.52224500	-0.19706300	7.25633800	C	-9.82732300	-3.70281000	-1.60039200
H	-6.28101100	1.46438700	8.00897200	H	-9.89088300	-2.57979100	-1.44273800
H	-5.89551000	1.19420300	6.22920600	C	-11.22020100	-4.31611100	-1.45785300
C	-9.12599100	-2.50890800	7.48740400	H	-11.68480000	-3.94697700	-0.49938800
H	-9.75531100	-2.07984600	8.30554600	H	-11.84805700	-4.01642200	-2.33791800
H	-8.28494300	-3.11316400	7.91193200	C	-6.20504600	-3.76390600	1.13397500
H	-9.74594200	-3.14549500	6.80601700	H	-6.31018300	-2.65173300	1.14732100
C	-12.81439500	3.60737400	3.62835700	H	-5.16218700	-4.06552900	1.40803600
H	-12.19744200	4.37183100	3.09097600	H	-6.94986800	-4.22734200	1.82864800
H	-13.34855300	4.07541300	4.49200800	C	-4.68564800	-3.98200800	-2.57987400
H	-13.54639300	3.14950200	2.91701400	H	-4.54097500	-4.20526200	-1.49322200
C	-10.26724800	-2.93939100	3.73261800	H	-3.88041200	-3.29865400	-2.95082300
H	-11.03751200	-3.31747200	4.46024700	H	-4.70207800	-4.92999800	-3.17187700
C	-9.10382400	-3.95026300	3.67230300	C	-11.01173100	-6.43759100	-2.52671500
H	-8.18138500	-3.43147600	3.29083100	H	-11.82636900	-6.20340300	-3.25637600
C	-9.43373100	-5.15545100	2.77928000	H	-11.04867900	-7.51660800	-2.23444300
H	-10.21596300	-5.79414600	3.28280700	H	-10.01918300	-6.18098400	-2.97305200

C	-8.71768400	-1.45856700	-4.53288500	H	-6.14423200	8.31614800	-5.35613100
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C	-7.46863400	-0.87043100	-5.21484800	C	-8.32112900	6.81603500	-1.69100200
H	-6.83052700	-0.34170400	-4.45544400	H	-8.68637600	7.78962500	-2.11845500
C	-7.86501500	0.09526600	-6.34282300	C	-6.91143800	7.01828000	-1.09314400
H	-8.29321300	-0.50614300	-7.19655000	H	-6.46000200	6.02749300	-0.81673000
C	-8.95546400	1.10005400	-5.92248600	C	-7.01675500	7.91163900	0.15351500
H	-9.39235200	1.60350300	-6.83173700	H	-7.41634800	8.92084100	-0.14558900
C	-9.71398200	-0.34583600	-4.16334300	C	-8.00916900	7.28092800	1.15341500
H	-9.24854400	0.31978400	-3.37474200	H	-8.17259300	7.94164700	2.04994900
C	-11.02868000	-0.90974300	-3.61540500	C	-9.30353200	6.31262900	-0.62107300
H	-10.83820100	-1.93419500	-3.19456500	H	-9.02368500	5.26044200	-0.32768000
H	-11.41048700	-0.23715300	-2.79677500	C	-10.76112100	6.32162100	-1.08495100
C	-5.36901500	-1.88656800	-5.69688100	H	-10.93044800	5.43976000	-1.76020500
H	-5.00301400	-0.91543300	-6.11228300	H	-11.44353700	6.26510000	-0.19548400
H	-4.99100700	-2.74557700	-6.30518600	C	-12.15370500	7.45075800	-2.62499800
H	-5.06283700	-1.99859100	-4.62578000	H	-12.24362500	8.46555300	-3.08579100
C	-6.75287900	1.30626600	-8.05502000	H	-13.07103600	7.21153500	-2.03254900
H	-7.05133100	0.53504200	-8.80770500	H	-11.98907300	6.67000400	-3.41048700
H	-5.71627200	1.67511600	-8.26054700	O	-11.02261600	7.54512300	-1.77433900
H	-7.47369200	2.16204900	-8.06233600	C	-5.13012300	6.90579100	-2.66851600
C	-11.93019700	-1.92093800	-5.57527800	H	-4.42558300	6.49638100	-1.90424000
H	-11.10866000	-1.61970500	-6.27232400	H	-4.59831300	7.60495700	-3.36129500
H	-12.91288300	-1.93473000	-6.11078900	H	-5.61907400	6.07985700	-3.24487100
H	-11.70904600	-2.92509300	-5.13532800	C	-4.97909400	9.12805500	0.37158500
C	-9.00401800	3.35093500	-5.07624400	H	-4.68574800	8.97254000	-0.69525200
H	-9.70397400	3.44871500	-5.94786200	H	-4.07692400	9.12216900	1.04243400
C	-7.78384900	4.26959100	-5.29167700	H	-5.53818700	10.09005900	0.47793200
H	-6.98131600	4.01796200	-4.54569900	C	-7.55604500	5.66100300	2.88424000
C	-8.18189900	5.74848300	-5.15358300	H	-7.25515000	6.56522500	3.47948400
H	-8.84265600	6.04207200	-6.01891400	C	-6.49505800	4.55066800	2.99743700
C	-8.97833200	6.01308600	-3.86213500	H	-6.70317200	3.74446600	2.22992700
H	-9.47471100	7.02719600	-3.88904300	C	-6.49590000	3.91840600	4.39794100
C	-9.71094500	3.72003700	-3.76087200	H	-6.01197300	4.62479400	5.12997300
H	-9.03694300	3.47457400	-2.88417500	C	-7.91508800	3.60456100	4.91656900
C	-11.02462900	2.96519200	-3.51382600	H	-7.89903500	3.41657100	6.02778300
H	-10.77219500	1.86343000	-3.47483700	C	-8.91414400	5.14513400	3.38597400
H	-11.41181700	3.27982800	-2.50192400	H	-9.25486100	4.29275700	2.73048300
C	-5.92942600	4.08557600	-6.76915700	C	-10.01000100	6.21001800	3.40122400
H	-5.50738700	5.01282000	-6.30945900	H	-10.35547600	6.38643300	2.34616900
H	-5.75748200	4.07932100	-7.87466600	H	-10.86609600	5.86627600	4.04123400
H	-5.48480300	3.17213500	-6.29979600	C	-4.75716700	6.21455500	3.22684900
C	-7.13813200	7.88739500	-5.07204700	H	-5.28022700	7.07900100	2.74676100
H	-7.94176300	8.27268000	-5.74618600	H	-3.66107100	6.25044800	2.98568100

H	-4.91204400	6.22689300	4.33296200	C	-1.12272100	7.38786000	2.75778300
C	-4.40208500	2.76848800	4.28422100	C	-0.55323300	8.28745100	1.85672000
H	-4.12187800	3.11276600	3.25499100	C	0.20262600	7.78166300	0.79975700
H	-4.04353400	1.72307800	4.46213100	C	0.35859900	6.40772800	0.61623400
H	-3.98350700	3.46544200	5.05108500	C	-0.25928100	5.51027000	1.49590600
C	-10.30401500	8.53534900	3.68889100	C	-4.97217200	0.53555300	0.22729000
H	-10.40757000	8.69263900	2.58513800	C	-5.80479800	1.05767800	1.22838700
H	-9.76916600	9.39629200	4.16141800	C	-7.18467400	1.11867200	1.03844500
H	-11.31356800	8.40146000	4.15082900	C	-7.77576200	0.65695500	-0.14024000
C	1.32442500	-2.11719900	0.54518500	C	-6.94398000	0.10561300	-1.11809200
N	1.47391200	-0.79969200	0.72623900	C	-5.56285100	0.04649300	-0.94729400
C	2.86566900	-0.55729200	0.91717700	C	0.48634400	-6.51057800	1.01587400
C	3.58303300	-1.86315600	0.83880900	C	0.21816200	-5.15541800	1.20377600
C	2.64141200	-2.82191200	0.61235900	C	0.22793500	-4.28186500	0.10874900
C	0.09007900	-2.83100400	0.30958400	C	0.44419400	-4.79866200	-1.17558800
C	-2.83273600	-0.67312400	0.29360500	C	0.71188700	-6.15605000	-1.34441000
N	-1.44890100	-0.87706200	0.40803600	C	0.77094100	-7.01966400	-0.25088800
C	-1.14194400	-2.23996000	0.26188200	C	7.12665800	0.16367800	0.41469800
C	-2.43579000	-2.94016300	0.02999300	C	7.73120600	0.54854000	1.61340500
C	-3.43398100	-2.01496500	0.04700200	C	6.91539800	1.01968900	2.64364800
C	-3.51225600	0.51515100	0.39112800	C	5.53047200	1.09167600	2.49602600
C	-1.37064600	3.39156300	1.03175400	C	4.93151700	0.67766300	1.29978200
N	-1.55234500	1.99185900	0.83059400	C	5.74523500	0.22661800	0.25013100
C	-2.86193500	1.78499300	0.63354400	H	-1.45931400	5.31331400	3.29013500
C	-3.61814000	3.07263900	0.68702200	H	-1.69324100	7.77975200	3.61619100
C	-2.70413300	4.05245100	0.93514200	H	0.67807500	8.49047000	0.09978700
C	-0.19788400	4.05552200	1.26780000	H	0.95239100	6.02328100	-0.22554600
C	2.77676000	1.90899000	1.27209200	H	-5.36808500	1.43675600	2.16801400
N	1.40336900	2.10687300	1.13729400	H	-7.82513900	1.53900800	1.83776900
C	1.11016400	3.45458800	1.32140000	H	-7.39350500	-0.29853200	-2.04390600
C	2.34008000	4.13584500	1.58113400	H	-4.93056600	-0.38134900	-1.73969500
C	3.37302000	3.17866200	1.54816300	H	0.48412400	-7.19868800	1.87812200
C	3.46551500	0.65054800	1.15217700	H	0.02129700	-4.76396600	2.21183100
H	4.66061600	-1.96728200	0.95271000	H	0.42515900	-4.12537500	-2.04403600
H	2.75784000	-3.89755900	0.49503400	H	0.89038600	-6.56334800	-2.35401800
H	-0.78786400	-0.16815600	0.60973100	H	7.75062500	-0.22459700	-0.41069000
H	-2.49079200	-4.01790100	-0.11872300	H	7.37776900	1.32669800	3.60226100
H	-4.50638600	-2.16014800	-0.09490100	H	4.90886800	1.46813500	3.32349100
H	-4.69450400	3.16381000	0.55865600	H	5.29178700	-0.09450600	-0.70300000
H	-2.86434300	5.12251200	1.05934000	S	-0.84667600	10.02176300	2.03278100
H	0.73762400	1.39647100	0.94402800	O	0.07674800	10.65238900	1.16514900
H	2.42977400	5.20295600	1.76879200	O	-0.63345500	10.30512800	3.40213100
H	4.43532500	3.34599100	1.71147900	O	-2.19858500	10.19335800	1.63748400
C	-0.98774000	6.01235300	2.58411300	S	9.44353300	0.40643600	1.80860300

O	10.05832300	1.32651600	0.91655100	C	-17.52254300	0.89918300	-6.07885800
O	9.76786300	-0.94150300	1.46570000	C	-15.80866700	-0.93026400	-4.84529300
O	9.73783300	0.69946200	3.17072400	H	-14.17240300	0.22288100	-5.63987700
S	-9.47742500	0.77476900	-0.40732900	C	-18.04501700	-0.15091100	-5.33684700
O	-9.68616300	1.73291400	-1.44242400	H	-18.17999900	1.63456300	-6.56211700
O	-10.07579300	1.15281900	0.82521900	C	-17.19798400	-1.08092200	-4.71312800
O	-9.93026300	-0.50629500	-0.84198200	H	-15.12529500	-1.63584800	-4.34335200
S	1.29073900	-8.69274600	-0.45399700	H	-19.13535800	-0.25714200	-5.23386600
O	0.63505200	-9.42481300	0.56429300	H	-18.66830300	-5.52289600	1.30894300
O	2.70014900	-8.64119600	-0.28423300	C	-16.20115600	-4.88171900	2.65747100
O	0.90206800	-9.05747400	-1.76557100	C	-14.82164500	-4.64735100	2.54812000
C	-20.18768900	-3.59430600	-1.55919200	C	-16.65656800	-5.92277300	3.48180800
C	-20.12164700	-3.63334700	-0.21193700	C	-13.90873500	-5.43194800	3.24792300
C	-19.09008700	-3.38101500	-2.47075000	H	-14.44056200	-3.83555900	1.89859100
C	-18.94827000	-3.43268500	0.60127200	C	-15.75929800	-6.71131400	4.18976700
C	-17.73361700	-2.16343600	-3.92527000	H	-17.73710800	-6.11163700	3.56812800
S	-16.92449800	-3.63067100	-3.75074000	C	-14.37907100	-6.46214400	4.07137500
C	-18.05687800	-4.28018300	-2.71091900	H	-12.83184500	-5.22652100	3.12811700
C	-18.27265900	-2.22440100	0.76291600	H	-16.10815500	-7.52438900	4.84015400
S	-16.90461200	-2.41931100	1.68652700	O	-13.57168100	-7.29643300	4.82060500
C	-17.13464500	-4.06414900	1.91999800	C	-12.16825700	-7.09549700	4.68365600
C	-18.29210000	-4.49788400	1.29504000	H	-11.72697200	-7.85690100	5.37509300
C	-17.91730100	-5.62294100	-2.13933800	H	-11.84658400	-7.28597400	3.63043700
H	-17.93538400	-5.56943600	-1.01817600	H	-11.88046500	-6.06312900	5.00048500
H	-18.76029700	-6.28088300	-2.47163400	C	-22.50199300	-4.04804300	-0.78547200
H	-16.95387100	-6.09758900	-2.45236500	F	-21.89307000	-2.98292500	1.34621800
C	-18.66380200	-0.92686700	0.20268900	F	-21.48912900	-5.08525600	1.20087500
H	-18.76761100	-1.00065500	-0.91214700	F	-23.52620900	-3.14625700	-0.68632900
H	-19.64762500	-0.59780800	0.62427700	F	-23.13897800	-5.25889200	-0.81456900
H	-17.90072100	-0.14130500	0.43248400	F	-22.09393900	-2.74878800	-2.83402300
C	-21.60379000	-3.80448700	-2.10461900	F	-21.73031800	-4.85806500	-2.97590700
C	-21.47051800	-3.93405100	0.45159600	C	-18.90704800	-2.15781100	-3.19393500
N	-12.08072900	3.15172600	-4.49931900	H	-19.61574900	-1.32781900	-3.14635100
C	-12.51626400	2.16246600	-5.38140000	O	9.94341300	4.69403100	3.21259300
C	-13.53873900	2.78766600	-6.13008600	O	12.56431700	4.44455800	0.71286500
H	-12.09964600	1.14767500	-5.39021200	O	10.75599400	7.51915600	2.67863900
N	-12.79880600	4.28362300	-4.70255700	O	11.25659000	7.78554200	-0.12993400
N	-13.64612100	4.10872400	-5.63447700	O	13.23633500	3.31912400	3.21809300
C	-14.32106400	2.23675500	-7.24997200	O	11.02207800	5.00047500	-0.84144000
H	-14.32910300	2.95444900	-8.12008200	O	11.36303800	2.67390500	-3.67200900
H	-13.89477900	1.24914800	-7.57069400	O	9.93580300	6.43261400	-3.07691400
O	-15.72024900	2.10282900	-6.97393100	O	8.46751600	4.66103600	-4.74267600
C	-16.12511400	1.03417200	-6.20651700	O	13.02909700	1.25976400	-1.99343400
C	-15.26852900	0.11543100	-5.58558900	O	9.16715700	2.19040000	-3.53247300

O	8.78062100	-1.37602200	-4.39195400	H	12.70595200	2.21502700	4.91547800
O	6.32731400	1.87477700	-3.93330100	H	14.41192600	2.89137900	4.79755800
O	5.50632100	-0.78274900	-2.94739000	H	13.92229900	1.43120800	3.79585700
O	10.61729400	0.30999000	-6.08248500	C	11.21853000	4.59748300	-2.19909800
O	7.92924000	-1.85565400	-2.36605900	H	12.08545500	5.14202400	-2.66202500
O	9.15731000	-4.54434000	-0.24878600	C	9.90686000	5.01614000	-2.90283500
O	6.11924900	-4.11669900	-2.93230800	H	9.02854800	4.68517000	-2.28242500
O	5.62799300	-5.56564000	-0.45802900	C	9.79973700	4.40801500	-4.30893900
O	11.40927200	-3.78999200	-1.22345500	H	10.53555000	4.91117900	-4.99725100
O	7.49979900	-4.23549900	1.23947200	C	10.11709500	2.89952400	-4.29847800
O	8.85976900	-3.69501800	4.59108000	H	10.24059000	2.49473900	-5.34421000
O	6.00165600	-6.05063100	2.97657000	C	11.43014800	3.07644900	-2.29644200
O	5.36142300	-4.54763000	5.36940000	H	10.64354300	2.53837700	-1.69425800
O	7.13665500	-2.33043900	5.10221500	C	12.83214700	2.65743400	-1.84279500
O	8.58772200	0.39136200	7.12988700	H	13.60884300	3.11655600	-2.51269300
O	4.86940700	-1.22915400	6.42996700	H	12.98025500	2.97571900	-0.77703300
O	5.17934400	1.61094000	7.08681100	C	9.04907300	7.12400800	-2.20652500
O	7.63099200	1.97405900	5.82808300	H	7.99012000	6.85261000	-2.43642400
O	10.20230500	4.59466600	5.45249900	H	9.23996600	8.20425100	-2.42518100
O	6.06522900	4.10473600	4.81244600	H	9.29742300	6.89374900	-1.13887000
O	7.63890400	6.12503400	3.39162600	C	8.27692800	4.46715200	-6.13296800
O	9.97465900	3.12865500	7.97878100	H	8.96758900	5.11693000	-6.72571600
C	11.12271400	5.16858500	2.55402500	H	7.21180500	4.76312600	-6.30662400
H	11.92700100	5.40262500	3.30218400	H	8.43067900	3.39373600	-6.40656900
C	10.75701400	6.43245500	1.74858700	C	12.56438400	0.49574400	-0.88528800
H	9.74499400	6.29697300	1.27570600	H	13.29764000	0.58370200	-0.04505500
C	11.80365200	6.73745900	0.66519300	H	12.52640700	-0.55646900	-1.26361800
H	12.75419200	7.10201900	1.14895500	H	11.55071800	0.82988900	-0.54319300
C	12.15990400	5.48062200	-0.15144100	C	8.58239600	1.04499800	-4.16247500
H	13.04139900	5.66893600	-0.82576900	H	8.42823800	1.23357000	-5.25954300
C	11.55424200	4.01246200	1.63534100	C	7.21991600	0.86849500	-3.45793500
H	10.66442600	3.61284200	1.06099800	H	7.35550700	0.92713800	-2.34166800
C	12.15820100	2.84377400	2.40786000	C	6.57626400	-0.47586000	-3.83271000
H	11.34556900	2.38025000	3.03500500	H	6.21342100	-0.42834300	-4.89712700
H	12.55589400	2.08453600	1.68149600	C	7.56913100	-1.64939400	-3.71611800
C	9.74302800	8.48059200	2.42251600	H	7.15084900	-2.57387600	-4.20738200
H	9.84384300	8.89082700	1.38750600	C	9.46400300	-0.19582800	-3.95648600
H	9.92256700	9.28033500	3.18342400	H	9.70810800	-0.28804800	-2.85901400
H	8.73130900	8.02048800	2.56393900	C	10.77115400	-0.16906100	-4.75181400
C	12.06240300	8.14905500	-1.23752600	H	11.47842500	0.56715300	-4.27358400
H	13.13462400	8.26213600	-0.94390500	H	11.22104700	-1.19665300	-4.75711900
H	11.64299200	9.12967100	-1.57623900	C	6.23099600	3.00525400	-3.07627900
H	11.95251900	7.38391600	-2.04896500	H	5.88247800	2.69847800	-2.05959000
C	13.57823600	2.39912100	4.23816900	H	5.47119900	3.65861900	-3.57310200

H	7.22027300	3.52541100	-3.01461100	C	10.15078600	-3.43430300	2.62749200
C	4.26016800	-0.21424700	-3.32377400	H	10.07387800	-3.18184500	1.52671500
H	4.32920900	0.90107100	-3.35848800	H	10.67378700	-2.58191100	3.15102200
H	3.56021000	-0.54654300	-2.51513000	C	4.60443300	-6.06254600	2.70913700
H	3.93401600	-0.61217100	-4.31626500	H	4.03759100	-5.67226500	3.58952500
C	10.07115900	-0.64254200	-6.98016100	H	4.36973200	-7.14112600	2.52288700
H	10.75284700	-1.52415500	-7.07216500	H	4.38395100	-5.45658400	1.79385400
H	9.99894800	-0.10069900	-7.95578200	C	5.30343000	-4.50798800	6.78503400
H	9.06192500	-0.97717100	-6.63416200	H	5.90434000	-5.33183500	7.24202000
C	8.11287900	-3.23258500	-2.00852200	H	4.21700200	-4.63718500	7.02012100
H	8.59215000	-3.79275500	-2.85700400	H	5.66066500	-3.50985400	7.14740600
C	6.74410300	-3.85461100	-1.67309500	C	7.26867700	-1.42156800	6.19997800
H	6.13452800	-3.13869300	-1.05668300	H	7.25227500	-1.97401800	7.17965100
C	6.91133900	-5.19029700	-0.93033000	C	6.04406500	-0.48240300	6.12120900
H	7.30628800	-5.95851400	-1.65638400	H	5.98208200	-0.00762100	5.10253300
C	7.93753400	-5.10052400	0.21645100	C	6.17380500	0.60254500	7.20354800
H	8.20552600	-6.12915900	0.58835400	H	6.12258400	0.11906400	8.21904900
C	9.03585700	-3.22159700	-0.77754800	C	7.53323700	1.32871000	7.08154900
H	8.59926200	-2.53102600	0.00579500	H	7.71266800	2.01894700	7.95303500
C	10.45394500	-2.74455900	-1.10727000	C	8.56382500	-0.60104800	6.09239700
H	10.42706300	-2.13378300	-2.04950000	H	8.63094400	-0.08807100	5.08483400
H	10.83982700	-2.12028100	-0.24861000	C	9.83426900	-1.42414000	6.29615900
C	4.70142300	-4.00891100	-2.89542300	H	10.04111800	-2.00224300	5.35503000
H	4.27611900	-4.63257800	-2.07057000	H	10.69613300	-0.74305700	6.52683500
H	4.37137800	-4.39351900	-3.89236300	C	10.57935500	-3.38153200	7.38982300
H	4.40979800	-2.93493500	-2.76858500	H	10.30886700	-4.00002600	8.28110800
C	5.48378300	-6.96521800	-0.24024700	H	11.62349100	-2.99420000	7.48906600
H	5.85403800	-7.55030500	-1.11682000	H	10.47942800	-3.97794600	6.44697700
H	4.37798700	-7.12652700	-0.11122500	O	9.65075400	-2.30927700	7.40379500
H	6.03625400	-7.25786600	0.68726000	C	4.15237000	-1.66222500	5.27952400
C	11.24132300	-4.60696500	-2.36810500	H	3.80945900	-0.78290500	4.68113600
H	10.30203800	-5.20805100	-2.28125300	H	3.28010700	-2.22308100	5.69849000
H	12.13847700	-5.27682300	-2.36731800	H	4.79092200	-2.34069400	4.65880400
H	11.21531500	-3.98980000	-3.30035800	C	3.91931800	1.25560900	7.63354400
C	7.85008100	-4.62449800	2.57583800	H	3.47694500	0.38955700	7.08240000
H	8.38589900	-5.61038700	2.59565900	H	3.29672700	2.17485600	7.49149500
C	6.50592400	-4.76118300	3.32179700	H	4.01695800	1.00917100	8.72001800
H	5.80937300	-3.93956800	2.99731400	C	8.16999600	3.29891800	5.84598200
C	6.67601900	-4.71934300	4.84969600	H	7.96313700	3.80770200	6.82626700
H	7.08854200	-5.70746400	5.20441100	C	7.47658700	4.05010600	4.69119000
C	7.65405100	-3.62867900	5.32309000	H	7.62658800	3.48568400	3.72202100
H	7.96847600	-3.79834700	6.39442000	C	8.09196300	5.45182400	4.56143800
C	8.72057300	-3.51339500	3.18085900	H	7.86405300	6.06184300	5.47906400
H	8.24435600	-2.51085200	2.96599600	C	9.62752600	5.36048600	4.41881000

H	10.10259500	6.37857400	4.49789100	N	12.12973100	-6.20032400	3.66719900
C	9.68669800	3.26393400	5.58891900	C	12.69650500	-7.66245300	1.64536800
H	9.88862300	2.67317700	4.64457500	H	12.43213400	-8.59324200	2.22560900
C	10.49015100	2.64899400	6.73403500	H	12.34252400	-7.75905100	0.58509900
H	10.40333700	1.53053600	6.67317800	O	14.12929700	-7.68342200	1.69892400
H	11.56577400	2.96147300	6.65599700	C	14.81787500	-7.00582900	0.72074000
C	5.55836900	4.53280000	6.06330800	C	14.24693800	-6.12851900	-0.21119500
H	5.77102600	3.77048200	6.85412200	C	16.20518700	-7.25999400	0.69955100
H	4.45448000	4.61210500	5.89253500	C	15.05348200	-5.54021100	-1.18094500
H	5.97905000	5.52677000	6.35429100	H	13.17578000	-5.87120400	-0.16718500
C	6.39580900	6.79146600	3.55132400	C	16.99583500	-6.65828800	-0.26787900
H	5.58380500	6.06847400	3.81058600	H	16.64004300	-7.92890800	1.45463300
H	6.20706300	7.25372500	2.54980000	C	16.42897500	-5.80732600	-1.23120400
H	6.47528800	7.58184100	4.33906200	H	14.59918700	-4.84503800	-1.90543500
C	10.35812000	2.30847700	9.06827400	H	18.07899300	-6.85083900	-0.28814200
H	9.96584000	1.26815300	8.93316600	H	18.85054600	-0.79754700	-5.19195000
H	9.89475000	2.79267200	9.96337100	C	16.68799200	0.98844600	-4.58180900
H	11.47145600	2.28740300	9.17177500	C	15.36952100	1.19751300	-4.14902300
C	20.27876500	-3.38682200	-3.35036600	C	17.06487800	1.42826300	-5.86108400
C	20.42909500	-2.05322500	-3.22435800	C	14.43737800	1.81971300	-4.97394600
C	19.03857500	-4.12368400	-3.29210700	H	15.04545900	0.86501000	-3.14563800
C	19.37562400	-1.08275600	-3.04805100	C	16.14836200	2.05302500	-6.69627400
C	17.26140300	-5.21707900	-2.25252000	H	18.09898100	1.27450200	-6.20376800
S	16.84655500	-5.23484300	-3.88417900	C	14.82678300	2.24373400	-6.25086000
C	18.22507800	-4.42905100	-4.37631900	H	13.40652400	1.96138700	-4.59980800
C	18.90194500	-0.60247700	-1.83152300	H	16.43713700	2.39929800	-7.69745600
S	17.62233100	0.44247400	-2.05577300	O	13.99101900	2.87553100	-7.14938200
C	17.63576600	0.31034700	-3.73074000	C	12.61149100	2.91801800	-6.78988100
C	18.64135200	-0.54287100	-4.15114400	H	12.12891900	3.40119800	-7.67611000
C	18.48805500	-4.09210500	-5.77873200	H12.20811900	1.88642200	-6.62734700	
H	18.40366900	-2.98494400	-5.93465200	H	12.46156400	3.53714000	-5.87015000
H	19.52423600	-4.40726400	-6.06686900	C	22.71762100	-2.96399700	-3.54114000
H	17.76019900	-4.59840900	-6.46043400	F	22.34937400	-0.94099400	-2.19273100
C	19.40800000	-0.96135600	-0.50285700	F	22.15054500	-0.69996900	-4.31529500
H	19.17059200	-2.03283000	-0.27344600	F	23.65637100	-3.16993400	-2.56744500
H	20.52053700	-0.83384400	-0.46123400	F	23.45081500	-2.93100500	-4.69615300
H	18.94699800	-0.32331300	0.29200700	F	21.88130200	-5.08613700	-2.62016300
C	21.60191700	-4.13066400	-3.56510000	F	21.67138100	-4.83822400	-4.74064300
C	21.89068900	-1.59650000	-3.30863000	C	18.47670700	-4.58868000	-2.05882200
N	10.96501800	-4.63215700	2.75591800	H	18.95687800	-4.44181200	-1.08889300
C	11.34464500	-5.43994000	1.68269000				
C	12.10193100	-6.47314400	2.27820300				
H	11.07097900	-5.20999600	0.64568200				
N	11.46920400	-5.14077500	3.90660900				

CF-2
Cartesian coordinates

ATOM	X	Y	Z				
O	22.32251600	-0.16749400	4.55593300	C	20.50283700	-2.53925600	4.72442600
O	22.49984300	-3.79886800	4.77776300	H	20.01980800	-1.63022300	4.27474400
O	24.94886500	-0.71546900	5.77763800	H	20.03694900	-3.46213700	4.28658300
O	26.09074400	-3.02136500	4.48218600	C	26.09084100	-0.05420500	5.25091200
O	20.34329000	-2.54960100	6.14736600	H	26.80691400	-0.79375700	4.81507500
O	23.85523700	-4.01914000	2.99089900	H	26.54332100	0.46044800	6.13473600
O	22.87219500	-7.05709400	1.13627300	H	25.77760100	0.69263200	4.47712300
O	26.20250900	-4.71164100	1.50471500	C	26.74581400	-4.26904300	4.63658600
O	25.55035200	-5.96684700	-1.04788500	H	26.66426500	-4.64361100	5.68637600
O	20.72115400	-7.10604400	2.88780100	H	27.81265000	-4.05353600	4.37558600
O	22.77533900	-5.86636300	-0.78696900	H	26.31902200	-5.01241600	3.91573000
O	19.75148400	-7.02458300	-2.55390500	C	18.98112000	-2.50932200	6.52349700
O	23.23085500	-5.08621800	-3.54589500	H	18.48195100	-1.59355000	6.11536300
O	20.67905000	-4.34157300	-4.80906600	H	18.99299100	-2.48108100	7.64126500
O	21.44321700	-9.04541300	-1.07257900	H	18.44391200	-3.42148000	6.16145000
O	18.95511300	-4.92194700	-2.79986700	C	24.02089400	-5.29010600	2.34769800
O	15.60112100	-3.89724100	-1.82841500	H	24.58454600	-6.00116800	3.01266900
O	17.37802000	-5.09789200	-5.30374900	C	24.86937600	-5.00494400	1.08844600
O	15.50918800	-2.90039400	-5.37026600	H	24.41507500	-4.15661000	0.50607600
O	16.53632400	-6.20200500	-0.56468400	C	24.95471200	-6.26256700	0.20682300
O	15.89754800	-1.87016600	-2.74895000	H	25.53825300	-7.05657900	0.75032200
O	14.33143300	0.51734200	-0.40751200	C	23.54325800	-6.81921800	-0.08387100
O	15.91235200	0.62483100	-4.17026800	H	23.58874400	-7.82273000	-0.59262300
O	16.44465900	2.80366600	-2.25472900	C	22.66253500	-5.90653200	1.96198000
O	16.38313600	1.35050600	0.05599600	H	22.02511800	-5.15425100	1.41098500
O	17.39948000	1.42241900	3.54301300	C	21.94006600	-6.45140900	3.19914500
O	15.74389500	4.07053500	0.95396400	H	22.55783400	-7.25718500	3.68003900
O	17.97994800	4.94106600	2.65552400	H	21.75920300	-5.60616100	3.91483100
O	19.27277500	2.63824100	3.38389800	C	26.52102300	-3.32679800	1.46885900
O	21.21336500	1.04392600	6.10282800	H	26.48625200	-2.94529200	0.41689900
O	21.81282500	4.04435600	3.45806200	H	27.56223300	-3.27688300	1.87510000
O	23.89838400	1.93322300	3.84653600	H	25.82023100	-2.75090100	2.12557300
O	18.67035500	2.43929900	6.80419400	C	26.96591100	-6.10120600	-1.05999700
C	22.77341600	-1.40863900	5.11106900	H	27.43439400	-5.41921900	-0.30845500
H	22.57720400	-1.44624300	6.21603300	H	27.25697800	-5.80666000	-2.09971000
C	24.28153200	-1.54365600	4.82158200	H	27.25899900	-7.16013900	-0.85525500
H	24.49620000	-1.20891700	3.76921400	C	19.66713400	-6.21452300	2.54922700
C	24.77481300	-2.98652300	5.02305500	H	19.52575900	-5.44666400	3.34998700
H	24.82368000	-3.20540400	6.12911800	H	18.76389800	-6.87187200	2.47922600
C	23.83790800	-4.04324900	4.40605300	H	19.87455500	-5.71219900	1.56814900
H	24.07274600	-5.06341600	4.82583200	C	22.01734300	-6.36555700	-1.89578900
C	21.99005400	-2.51666200	4.39036900	H	22.52903400	-7.24991600	-2.36361000
H	22.07905000	-2.38636100	3.27281900	C	21.95977600	-5.19853300	-2.90462900
				H	21.67235000	-4.25065900	-2.37292000

C	20.95917000	-5.50133900	-4.02963400	H	16.37155800	-8.06279200	0.18848600
H	21.37794400	-6.31772400	-4.68306700	H	16.58615600	-6.74699600	1.45205600
C	19.59810100	-5.97813600	-3.48417500	C	15.10002000	-0.75053500	-2.35370000
H	18.96679300	-6.40609100	-4.31446100	H	14.13430000	-0.73388700	-2.92436600
C	20.60306800	-6.74654400	-1.43286700	C	15.98467300	0.45799100	-2.75415300
H	20.17661200	-5.88596400	-0.83328500	H	17.04068000	0.26943700	-2.41088300
C	20.57213300	-8.02720600	-0.59405200	C	15.47136900	1.77079300	-2.14697600
H	20.95918900	-7.79786100	0.44087600	H	14.51547900	2.07163000	-2.65926200
H	19.52005800	-8.41443800	-0.54510600	C	15.18520000	1.61984500	-0.63979300
C	24.08423400	-4.11898000	-2.95222100	H	14.63401300	2.51705100	-0.23922700
H	23.69033200	-3.09114300	-3.15037800	C	14.85251600	-0.74467300	-0.83743600
H	25.07054300	-4.27273700	-3.45703900	H	15.83947700	-0.94384100	-0.31689200
H	24.17972500	-4.29885600	-1.85136100	C	13.85349500	-1.78571700	-0.30737000
C	21.66060100	-4.05418100	-5.79178500	H	14.21686700	-2.81125200	-0.60773800
H	22.65064300	-3.84285900	-5.31738500	H	13.87208900	-1.70785400	0.82139300
H	21.26634700	-3.14335200	-6.30897900	C	16.97123900	-0.01062600	-4.87378800
H	21.75524100	-4.90417500	-6.51259900	H	17.95801900	0.40303600	-4.55047800
C	20.96331300	-9.72293800	-2.21965900	H	16.77311300	0.23739400	-5.94624400
H	20.00750700	-10.25573600	-1.98742700	H	16.93692700	-1.11800000	-4.71010200
H	21.76817700	-10.45746200	-2.47171000	C	16.44182700	3.47417400	-3.50456600
H	20.79996700	-9.00816900	-3.06404700	H	16.68046700	2.76476200	-4.33510000
C	17.53020800	-4.90649100	-2.93366100	H	17.24457800	4.24684100	-3.39616800
H	17.11988000	-5.95190900	-2.94906600	H	15.45106000	3.95907600	-3.68870500
C	17.16294800	-4.16847000	-4.23684700	C	16.38981100	1.81806400	1.40893600
H	17.81154200	-3.25702900	-4.35012100	H	15.37334600	1.70243600	1.87030800
C	15.67899900	-3.76923500	-4.25245200	C	16.84510000	3.28923500	1.42590700
H	15.04795900	-4.69291400	-4.39086500	H	17.74342300	3.40986100	0.75845800
C	15.23486700	-3.10439000	-2.93537900	C	17.18720800	3.77285100	2.84737000
H	14.11395200	-3.02128800	-2.89140200	H	16.23055100	4.04659700	3.37797800
C	17.00957900	-4.14029200	-1.70541300	C	17.90760500	2.72952400	3.72731200
H	17.56249000	-3.15821000	-1.58970600	H	17.74358500	2.96429600	4.81766900
C	17.18688900	-4.93754700	-0.41632000	C	17.42555900	0.98306200	2.17854500
H	18.29091100	-5.06196700	-0.22855600	H	18.45099300	1.15499700	1.74103500
H	16.70943600	-4.38694200	0.43756600	C	17.17664500	-0.51765900	2.17520100
C	17.87680700	-4.49318800	-6.48658300	H	17.33332800	-0.91112200	1.13062700
H	17.19617900	-3.67421500	-6.82718100	H	17.90622500	-1.01937400	2.86997400
H	17.89882600	-5.32436200	-7.23471300	C	15.60435400	-2.15795800	2.79881400
H	18.90899600	-4.09593100	-6.30868800	H	14.53036100	-2.22834400	3.10344800
C	14.15278700	-2.61528700	-5.66625100	H	16.26626500	-2.55243300	3.60937000
H	13.56049900	-3.55594700	-5.78582600	H	15.78427500	-2.73258700	1.85451000
H	14.19259500	-2.05076600	-6.63120100	O	15.83168400	-0.77581400	2.59307700
H	13.70371900	-1.97830900	-4.86411300	C	16.14250800	5.16426200	0.13806200
C	16.90982100	-7.11750600	0.44694500	H	16.91463500	5.78375000	0.65774800
H	18.01786800	-7.28229000	0.44606600	H	15.20325600	5.75055700	-0.01815300

H	16.53694100	4.78251300	-0.83831800	C	28.02205600	-0.48603100	-2.31736000
C	18.20155100	5.68826700	3.83903700	C	27.33375300	-1.80505000	-2.17221500
H	17.23121000	5.99728900	4.30105400	C	26.06205100	-1.53761900	-1.75992500
H	18.77830500	6.58311100	3.49260500	C	24.81977800	0.61359700	-1.22984700
H	18.80478700	5.09439200	4.56987700	C	25.15967900	4.26934200	-1.32879300
C	20.20779000	2.55820200	4.46923700	N	25.63998200	2.98525200	-1.57304700
H	20.06437400	3.43484800	5.15764600	C	24.69739700	2.04881900	-1.15116800
C	21.57279500	2.66639700	3.74807300	C	23.58299700	2.76800300	-0.61756100
H	21.55163100	2.04636500	2.80948700	C	23.86693500	4.14277300	-0.73220000
C	22.74832100	2.22481400	4.63226100	C	25.83169600	5.51001600	-1.63052700
H	22.97553900	3.04343800	5.37238100	H	27.31129600	7.88319000	-2.29032600
C	22.44721000	0.93930900	5.42651200	H	29.84210100	7.26219800	-3.19759000
H	23.22112000	0.77790700	6.22949700	H	28.59723200	2.31758400	-2.55877700
C	20.07920900	1.24417000	5.25093800	H	32.62223600	2.79132200	-3.89878500
H	20.00425100	0.39080900	4.51560700	H	32.09500100	0.10577800	-3.60382300
C	18.88585600	1.15861700	6.20662200	H	27.81478300	-2.75838100	-2.37852700
H	17.96661800	0.84826100	5.64082900	H	25.24299200	-2.22804500	-1.56450700
H	19.11054400	0.40413600	7.00914800	H	26.51906000	2.77006900	-1.98086300
C	21.35294100	4.45519700	2.17771100	H	22.68994100	2.31336100	-0.19510000
H	21.87641900	3.88104500	1.37181600	H	23.23533500	4.97536300	-0.43017300
H	21.62716300	5.53899900	2.12500400	C	23.75364000	-1.14902500	0.17248500
H	20.24384800	4.32173700	2.10053300	C	22.63575600	-1.87395600	0.58058800
C	24.62123800	3.08183700	3.42914600	C	21.37218200	-1.62547800	0.04152600
H	23.97946900	3.75065000	2.80397200	C	21.26300400	-0.64641900	-0.94841000
H	25.46499700	2.66324000	2.82453600	C	22.37361600	0.08027600	-1.37659900
H	25.00884000	3.64186000	4.31599900	C	23.63479600	-0.15687800	-0.81142200
C	17.64585400	2.40813500	7.77958100	C	30.14610900	-1.63612300	-2.91760800
H	16.67425800	2.09407100	7.32242600	C	30.35103700	-2.49311100	-1.82704300
H	17.58040100	3.45936300	8.15544100	C	31.08498400	-3.66750800	-1.98607100
H	17.91296000	1.71212500	8.61336800	C	31.62814300	-4.02061600	-3.22154900
C	29.14620400	5.11652800	-2.85057500	C	31.40670400	-3.17249900	-4.30651300
N	28.00605100	4.56041600	-2.42062300	C	30.67899100	-1.99185400	-4.16471300
C	27.10129700	5.62213700	-2.12657700	C	33.21775900	6.87357100	-3.14715600
C	27.78549100	6.91352600	-2.42756900	C	32.10613300	6.12825700	-2.75605600
C	29.03676400	6.60758700	-2.87335600	C	31.50510900	5.23440500	-3.65315700
C	30.35053100	4.42108500	-3.24593200	C	32.03967900	5.11255900	-4.94388800
C	30.02438200	0.80744400	-3.01399900	C	33.14874700	5.86901300	-5.31912000
N	29.48439900	2.10112000	-2.94119900	C	33.75332400	6.75786400	-4.43010700
C	30.46862200	3.05498600	-3.25237100	C	24.00524800	8.76910000	-2.15925200
C	31.70230200	2.29153300	-3.59627100	C	23.64535000	9.12375500	-0.85941900
C	31.44131200	0.96428000	-3.45172600	C	23.98904600	8.26206900	0.18206900
C	29.39599300	-0.38323400	-2.75242700	C	24.68713800	7.07940500	-0.05868300
C	25.94353300	-0.05645200	-1.63544200	C	25.06230500	6.73955500	-1.36541400
N	27.19374700	0.52011500	-2.00833400	C	24.71115700	7.59499500	-2.41854200

H	24.73496600	-1.34965800	0.63113400	C	-0.64749600	-0.40357800	2.46864100
H	22.75635400	-2.66514000	1.34337100	S	1.84821300	-0.05013500	1.16201700
H	20.27172700	-0.44758400	-1.39271100	C	3.18117400	-0.11788700	2.23281200
H	22.26366700	0.84859700	-2.15655300	C	2.82614000	0.01587900	3.54058200
H	29.92939800	-2.23108600	-0.84609000	C	-0.38582000	-1.89066700	2.31110400
H	31.23551500	-4.34172300	-1.12633900	H	0.28683100	-2.25208300	3.12795300
H	31.81077200	-3.45590600	-5.29335100	H	-1.34568200	-2.45958800	2.36239200
H	30.51535300	-1.33509100	-5.03112600	H	0.10580200	-2.09014700	1.32693400
H	33.69862100	7.56054400	-2.43036900	C	0.38518700	1.88921600	2.31142800
H	31.69655200	6.23478000	-1.74119500	H	-0.28746100	2.25049100	3.12834100
H	31.57721900	4.41636300	-5.65814300	H	1.34504900	2.45812900	2.36281200
H	33.57279900	5.75839700	-6.33135400	H	-0.10643800	2.08886600	1.32729400
H	23.71436400	9.43212200	-2.99173500	C	-1.28766700	0.13060400	6.31710600
H	23.68858100	8.52365000	1.21078800	C	1.28705000	-0.13273700	6.31707900
H	24.95022800	6.41128900	0.77402700	N	-12.46818000	1.62229500	-0.71556000
H	24.99500700	7.33411100	-3.44823900	C	-11.57635500	0.70837400	-0.14947100
S	19.98001700	-2.48728300	0.63028900	C	-10.34812100	0.97868100	-0.79214200
O	18.85633700	-2.04028600	-0.11720900	H	-11.88389300	-0.02554000	0.59553200
O	19.85445200	-2.16086000	2.01022700	N	-11.81878600	2.37334000	-1.64083000
O	20.23132100	-3.87692100	0.45509000	N	-10.59728900	2.03316400	-1.70484600
S	22.78383800	10.63696500	-0.53838100	C	-9.02213300	0.36621600	-0.58308100
O	22.05184500	10.90577100	-1.72124800	H	-9.10973600	-0.74305700	-0.43484400
O	23.79021900	11.59843400	-0.28025800	H	-8.32856100	0.59184400	-1.43644900
O	21.97223500	10.37036200	0.59123200	O	-8.50041400	0.94314800	0.63344700
S	32.57752400	-5.49778600	-3.40320300	C	-7.18424400	0.69230500	0.92548800
O	32.48399700	-5.83971600	-4.77637200	C	-6.30875800	-0.08290600	0.15214200
O	31.97136600	-6.44302300	-2.53812100	C	-6.73180800	1.29081900	2.12245800
O	33.89532700	-5.15903900	-3.00855400	C	-4.99068400	-0.25415700	0.56992200
S	35.15768500	7.70796900	-4.91882100	H	-6.64889500	-0.56078100	-0.77696500
O	35.89393100	7.93481100	-3.72791000	C	-5.42310200	1.09788200	2.53050900
O	34.64360800	8.90062800	-5.48408500	H	-7.43073200	1.90070900	2.71307200
O	35.84469400	6.90516800	-5.86534300	C	-4.53367000	0.32172400	1.76247200
N	12.46771400	-1.62279300	-0.71564000	H	-4.30227600	-0.85973800	-0.04122700
C	11.57578800	-0.70902700	-0.14945900	H	-5.06915300	1.56016000	3.46546900
C	10.34759400	-0.97938100	-0.79218900	H	3.52071600	0.00526300	4.38868300
H	11.88323700	0.02482200	0.59564200	C	4.53303400	-0.32309600	1.76240300
N	11.81842100	-2.37377600	-1.64102500	C	4.99008500	0.25306700	0.57000400
N	10.59688700	-2.03372000	-1.70502000	C	5.42242300	-1.09948300	2.53025600
C	-0.72625100	-0.00795000	4.92010400	C	6.30815400	0.08185300	0.15219000
C	0.72562900	0.00605200	4.92010200	H	4.30171500	0.85884000	-0.04099800
C	-1.40624600	-0.14846300	3.76202300	C	6.73112200	-1.29238400	2.12216500
C	1.40562000	0.14676400	3.76204400	H	5.06844800	-1.56196600	3.46510600
C	-3.18181100	0.11644600	2.23284700	C	7.18359200	-0.69360600	0.92534000
S	-1.84885000	0.04888000	1.16203300	H	6.64832500	0.55995400	-0.77678900

H	7.43001300	-1.90245200	2.71263400	O	-21.21403000	-1.04307300	6.10358500
O	8.49973000	-0.94450400	0.63320600	O	-21.81329900	-4.04367700	3.45900400
C	9.02154400	-0.36707600	-0.58304500	O	-23.89881800	-1.93239800	3.84703400
H	8.32807300	-0.59244300	-1.43656500	O	-18.67108200	-2.43830400	6.80532000
H	9.10906300	0.74214700	-0.43439800	C	-22.77391700	1.40948600	5.11153100
C	-0.00030700	-0.00115000	7.28596100	H	-22.57791500	1.44711600	6.21653100
F	2.23847100	0.80248100	6.64992400	C	-24.28197500	1.54455700	4.82175700
F	1.94699300	-1.31594000	6.55477300	H	-24.49646800	1.20974700	3.76937700
F	0.11033100	1.06921600	8.13092200	C	-24.77521400	2.98746400	5.02302600
F	-0.11094200	-1.07166200	8.13073800	H	-24.82421300	3.20646100	6.12905900
F	-1.94760400	1.31377000	6.55500100	C	-23.83816200	4.04406500	4.40603100
F	-2.23909100	-0.80466600	6.64979700	H	-24.07304700	5.06431100	4.82559100
C	-2.82676700	-0.01754300	3.54059100	C	-21.99034300	2.51742900	4.39093900
H	-3.52133800	-0.00708000	4.38870000	H	-22.07903800	2.38701300	3.27337900
C	0.64686400	0.40210000	2.46870800	C	-20.50321200	2.54002900	4.72539600
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O	-22.50018300	3.79969800	4.77805300	H	-20.03723800	3.46295400	4.28774100
O	-24.94951400	0.71647300	5.77775900	C	-26.09143200	0.05522700	5.25088400
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O	-20.34404600	2.55028200	6.14837700	H	-26.54410000	-0.45932500	6.13467000
O	-23.85521800	4.01971000	2.99087700	H	-25.77809300	-0.69169300	4.47721500
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O	-26.20237000	4.71209700	1.50448800	H	-26.66455100	4.64473900	5.68598600
O	-25.55015100	5.96709200	-1.04819500	H	-27.81293700	4.05457000	4.37524500
O	-20.72106700	7.10660000	2.88755600	H	-26.31925500	5.01333700	3.91530800
O	-22.77516500	5.86642000	-0.78737700	C	-18.98197100	2.51019100	6.52487300
O	-19.75145500	7.02424600	-2.55476300	H	-18.48251200	1.59459400	6.11670600
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O	-17.37826400	5.09676800	-5.30426500	H	-24.41495500	4.15688300	0.50592400
O	-15.50967000	2.89904600	-5.37039400	C	-24.95446800	6.26285500	0.20648400
O	-16.53657600	6.20176800	-0.56541800	H	-25.53793700	7.05695700	0.74993000
O	-15.89801300	1.86941100	-2.74884000	C	-23.54297600	6.81936900	-0.08427800
O	-14.33198800	-0.51770400	-0.40694600	H	-23.58840600	7.82285800	-0.59308500
O	-15.91302900	-0.62594200	-4.16957800	C	-22.66231700	5.90679500	1.96166600
O	-16.44572500	-2.80417200	-2.25339600	H	-22.02491400	5.15437300	1.41083000
O	-16.38368000	-1.35062600	0.05700500	C	-21.93983900	6.45168300	3.19882300
O	-17.39977000	-1.42198500	3.54411900	H	-22.55770800	7.25725800	3.67991400
O	-15.74463900	-4.07060800	0.95525200	H	-21.75874100	5.60633700	3.91434600
O	-17.98043800	-4.94076000	2.65724700	C	-26.52093300	3.32726100	1.46883300
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H	-27.56195900	3.27739000	1.87555700	H	-17.56280200	3.15780800	-1.58985900
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H	-27.43424700	5.41977000	-0.30866300	H	-16.70950800	4.38683500	0.43714900
H	-27.25680200	5.80691300	-2.09997800	C	-17.87712400	4.49188300	-6.48697700
H	-27.25867200	7.16058800	-0.85573400	H	-17.19657300	3.67278700	-6.82743100
C	-19.66728700	6.21544700	2.54725100	H	-17.89908400	5.32291900	-7.23526200
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H	-19.87442300	5.71603500	1.56462900	H	-13.56080200	3.55414700	-5.78586400
C	-22.01731500	6.36549600	-1.89635300	H	-14.19318400	2.04907000	-6.63120900
H	-22.52902300	7.24985600	-2.36415600	H	-13.70444700	1.97658600	-4.86408200
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C	-20.95932900	5.50087200	-4.03018000	H	-16.37143400	8.06250300	0.18780700
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C	-24.08476300	4.11943900	-2.95266100	H	-14.63468000	-2.51735600	-0.23820700
H	-23.69144300	3.09146200	-3.15126600	C	-14.85302500	0.74425400	-0.83709700
H	-25.07119300	4.27383400	-3.45704800	H	-15.83996500	0.94358200	-0.31657300
H	-24.17975600	4.29904100	-1.85171500	C	-13.85393700	1.78535200	-0.30726400
C	-21.66092400	4.05351000	-5.79209300	H	-14.21728200	2.81085000	-0.60779700
H	-22.65108700	3.84266600	-5.31773400	H	-13.87248500	1.70769000	0.82151500
H	-21.26691500	3.14238600	-6.30895500	C	-16.97184200	0.00944500	-4.87327200
H	-21.75520200	4.90330600	-6.51318700	H	-17.95865600	-0.40413800	-4.54995900
C	-20.96285900	9.72276500	-2.22087300	H	-16.77365400	-0.23875300	-5.94567500
H	-20.00691400	10.25536800	-1.98877400	H	-16.93750600	1.11684400	-4.70976700
H	-21.76757400	10.45744300	-2.47294900	C	-16.44313000	-3.47501800	-3.50305300
H	-20.79974100	9.00785700	-3.06518900	H	-16.68166600	-2.76577500	-4.33376100
C	-17.53041200	4.90584500	-2.93413600	H	-17.24604800	-4.24747500	-3.39439300
H	-17.11998000	5.95121900	-2.94975300	H	-15.45248500	-3.96019300	-3.68712800
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H	-17.81194800	3.25613400	-4.35026900	H	-15.37371900	-1.70244000	1.87124900
C	-15.67935000	3.76814000	-4.25275600	C	-16.84570400	-3.28912900	1.42722200
H	-15.04822300	4.69172600	-4.39139700	H	-17.74412100	-3.40974600	0.75990000
C	-15.23523300	3.10354100	-2.93555600	C	-17.18769200	-3.77249900	2.84879400
H	-14.11432400	3.02035100	-2.89159700	H	-16.23099500	-4.04611700	3.37939200
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H	-17.74417000	-2.96365000	4.81895300	C	-29.14537100	-5.11612200	-2.85126300
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H	-18.45129000	-1.15452600	1.74215500	C	-27.10058000	-5.62180500	-2.12698900
C	-17.17659500	0.51791600	2.17613300	C	-27.78475000	-6.91316600	-2.42815700
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H	-15.78404700	2.73253300	1.85512600	C	-31.70134600	-2.29105500	-3.59710600
O	-15.83157800	0.77585400	2.59397100	C	-31.44037800	-0.96381600	-3.45239800
C	-16.14346300	-5.16442500	0.13957200	C	-29.39516600	0.38363100	-2.75266200
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C	-18.20185100	-5.68777100	3.84091500	C	-27.33301900	1.80539200	-2.17197700
H	-17.23143200	-5.99681500	4.30275700	C	-26.06137000	1.53791600	-1.75955000
H	-18.77876100	-6.58261200	3.49473900	C	-24.81915800	-0.61335200	-1.22955500
H	-18.80486500	-5.09374400	4.57181500	C	-25.15906500	-4.26908600	-1.32882500
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C	-21.57325200	-2.66569900	3.74891300	C	-23.58247100	-2.76780900	-0.61726400
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C	-22.74886800	-2.22399600	4.63292300	C	-25.83105200	-5.50973300	-1.63073900
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C	-21.35324300	-4.45466700	2.17876200	H	-22.68947100	-2.31320600	-0.19464400
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H	-21.62737900	-5.53849600	2.12618000	C	-23.75324600	1.14924800	0.17296700
H	-20.24415100	-4.32114300	2.10167600	C	-22.63544400	1.87422100	0.58121300
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H	-22.75619600	2.66544100	1.34393400
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O	-34.64242300	-8.89995800	-5.48589900
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OF-2

Cartesian coordinates

ATOM	X	Y	Z
O	22.85177700	-1.66715700	4.48042800
O	22.90947400	-5.20856700	3.63125000
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O	20.79887500	-4.34671800	5.33316500
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O	25.87500300	-5.67051900	-2.60985400
O	21.01890400	-7.76236100	0.87400700
O	23.10496400	-5.56566900	-2.30036200
O	20.04285300	-6.06232000	-4.29607600
O	23.58608000	-4.03192000	-4.71684600
O	21.06127900	-2.87278400	-5.68720300
O	21.66465700	-8.47979300	-3.48414400
O	19.31970600	-3.95389700	-3.91366500
O	16.00588100	-3.12468400	-2.66016100
O	17.73837500	-3.34836900	-6.34995800
O	15.96725100	-1.14447500	-5.76233900
O	16.85036500	-5.73336300	-2.12158000
O	16.39272100	-0.93303900	-2.95987900
O	14.91234300	0.73743100	-0.01777800
O	16.54306700	1.86443100	-3.58746400
O	17.15596100	3.35689500	-1.11819000
O	16.99391400	1.30015400	0.66687400
O	17.97904200	0.30938000	4.02056600
O	16.45646300	3.66660300	2.31747200
O	18.68495800	3.91187500	4.21218800
O	19.89698200	1.45030700	4.20554500
O	21.78485200	-0.92455100	6.32446900
O	22.48183900	2.69577800	4.66338900
O	24.49645900	0.49712600	4.39665800
O	19.28766100	0.28172000	7.42509700
C	23.26203600	-3.02974100	4.64461700
H	23.06688000	-3.38180700	5.69286500
C	24.76435500	-3.12087400	4.31110800
H	24.98807200	-2.49862300	3.40093400

C	25.21063400	-4.57365300	4.07464400	H	19.06989100	-7.36536800	0.56315400
H	25.25605400	-5.10873900	5.06725100	H	20.21517100	-6.02454700	0.01670700
C	24.23749700	-5.37382700	3.18705100	C	22.33001500	-5.69631800	-3.49842500
H	24.44000800	-6.47892300	3.28616100	H	22.81095500	-6.42273400	-4.20821200
C	22.44065000	-3.85426400	3.64149100	C	22.31166400	-4.28535100	-4.12439000
H	22.53053600	-3.40580200	2.60968600	H	22.05532000	-3.52408900	-3.33793000
C	20.95441300	-3.92868100	3.97251700	C	21.30186000	-4.21700600	-5.27941100
H	20.49909900	-2.91444700	3.81163400	H	21.69281000	-4.82249700	-6.14501800
H	20.45821300	-4.67064500	3.29148600	C	19.92534400	-4.78665700	-4.88157800
C	26.62309200	-1.88083900	5.13807000	H	19.27937000	-4.93450700	-5.79365700
H	27.31364400	-2.48275700	4.49737400	C	20.90383000	-6.14942400	-3.15137800
H	27.09333900	-1.66199100	6.12889100	H	20.50675900	-5.48699800	-2.32342100
H	26.33433900	-0.93071000	4.61989600	C	20.83036400	-7.61682600	-2.72011700
C	27.13723100	-5.74549200	3.30373900	H	21.22749200	-7.71073400	-1.66795700
H	27.04693600	-6.40904400	4.19847700	H	19.76562000	-7.96714400	-2.77272800
H	28.20968000	-5.49534800	3.10378100	C	24.47003400	-3.30504000	-3.87623700
H	26.68391200	-6.23121600	2.40210600	H	24.11068700	-2.25161900	-3.76652800
C	19.43963900	-4.37989900	5.72045100	H	25.45157300	-3.33841400	-4.41174400
H	18.96612500	-3.37216300	5.59968400	H	24.55779000	-3.79769900	-2.87478500
H	19.45584900	-4.67595300	6.79862000	C	22.05117600	-2.34594500	-6.55574200
H	18.87497100	-5.13383300	5.11678600	H	23.04886600	-2.31526300	-6.05219300
C	24.37336800	-5.96647900	0.85170800	H	21.68921900	-1.31133600	-6.78179600
H	24.91550300	-6.85804500	1.27207100	H	22.11403600	-2.95276700	-7.49321400
C	25.22677700	-5.35050200	-0.27930400	C	21.15875100	-8.77961800	-4.77227100
H	24.79597500	-4.35747100	-0.58501700	H	20.18518900	-9.32477800	-4.69263300
C	25.27180600	-6.29979200	-1.48885000	H	21.93664300	-9.43594900	-5.23593400
H	25.83046300	-7.23455800	-1.20525600	H	21.01908300	-7.84585800	-5.37156100
C	23.84281800	-6.70504100	-1.91376800	C	17.89671200	-3.84790100	-4.02585200
H	23.85530900	-7.51753900	-2.69320700	H	17.44737700	-4.82900600	-4.33734900
C	22.99486500	-6.40142100	0.31830000	C	17.56182800	-2.75403900	-5.05987500
H	22.38176900	-5.50192200	0.01672600	H	18.24913400	-1.87582500	-4.91600500
C	22.25608800	-7.25954100	1.35128700	C	16.09643500	-2.30579800	-4.94498600
H	22.84984900	-8.18666500	1.57495400	H	15.42680200	-3.12283100	-5.33814000
H	22.09936900	-6.65156600	2.28149500	C	15.67736600	-2.03144100	-3.48798100
C	26.92706300	-3.90150200	0.55588800	H	14.56100400	-1.91693200	-3.41169000
H	26.90073700	-3.22841800	-0.33831300	C	17.40302200	-3.44844900	-2.62460300
H	27.97018900	-4.00038600	0.94798900	H	17.99429800	-2.56381800	-2.23545800
H	26.24458300	-3.52410500	1.35951700	C	17.54584200	-4.58892400	-1.62088300
C	27.28561600	-5.83762700	-2.67485400	H	18.64404800	-4.80126000	-1.48452300
H	27.77622700	-5.41716000	-1.76277400	H	17.08570200	-4.29039200	-0.64142700
H	27.58455600	-5.26306000	-3.58753200	C	18.25930400	-2.45110200	-7.31794800
H	27.54549200	-6.91867400	-2.78879900	H	17.61085700	-1.54437100	-7.40357900
C	19.99169000	-6.78177000	0.81326600	H	18.24831400	-3.03530900	-8.27168900
H	19.87147000	-6.27286000	1.80188400	H	19.30631000	-2.15929800	-7.04680200

C	14.62497900	-0.73137600	-5.95307500	H	16.66196400	-3.46998700	2.88162800
H	13.99557200	-1.57224300	-6.33614000	H	16.17932900	-3.06429500	1.16498700
H	14.69231600	0.08675600	-6.71302400	O	16.32379300	-1.44447600	2.48130700
H	14.19814900	-0.33706200	-4.99751000	C	16.91140700	4.93202000	1.85607000
C	17.19602200	-6.91559100	-1.42588600	H	17.69968400	5.34012500	2.53581300
H	18.29744800	-7.10922900	-1.49177000	H	15.99900600	5.57817700	1.87436000
H	16.62281900	-7.72643500	-1.93974400	H	17.30507300	4.83369300	0.81205000
H	16.89129600	-6.84346400	-0.35155500	C	18.91105700	4.26763100	5.56508700
C	15.64408700	0.05893800	-2.25207500	H	17.94355400	4.45619900	6.09321400
H	14.68828800	0.28956100	-2.79247000	H	19.51772600	5.20645800	5.50247100
C	16.59023400	1.28659900	-2.28272100	H	19.48667300	3.46533800	6.09018300
H	17.63186200	0.95421900	-2.01241700	C	20.82901200	1.02992700	5.21194700
C	16.13261200	2.38791300	-1.31680600	H	20.71363600	1.67223400	6.12685200
H	15.19943300	2.87306400	-1.71743400	C	22.19675100	1.30141700	4.54069000
C	15.81925100	1.81720000	0.08032600	H	22.15501300	0.98387100	3.46211500
H	15.30411400	2.58402200	0.72540000	C	23.35753100	0.58409000	5.24544300
C	15.37520500	-0.36792100	-0.80088200	H	23.61311300	1.14404000	6.18919200
H	16.34199900	-0.76409300	-0.36208700	C	23.01418700	-0.86681400	5.63433400
C	14.31301200	-1.46230200	-0.60219100	H	23.78283400	-1.27970300	6.34734400
H	14.62722700	-2.37409800	-1.18820900	C	20.65798200	-0.45026100	5.57794600
H	14.31288900	-1.71917800	0.49971500	H	20.55650200	-1.04945000	4.62644300
C	17.57439100	1.40680500	-4.45166000	C	19.46138100	-0.77381100	6.47670200
H	18.57832800	1.64858400	-4.02386200	H	18.53320500	-0.87480900	5.85234300
H	17.40492500	1.97280600	-5.40134000	H	19.65980500	-1.73716600	7.02104600
H	17.47610700	0.30459200	-4.62400600	C	22.03281900	3.47729300	3.56463800
C	17.20284900	4.36314800	-2.11671900	H	22.53679000	3.14954500	2.62028000
H	17.41776100	3.91677400	-3.11898700	H	22.34060600	4.52036700	3.82884600
H	18.04084800	5.02850400	-1.78766100	H	20.91999100	3.40507800	3.46346600
H	16.23950800	4.93021200	-2.14926500	C	25.25466300	1.69510800	4.31979600
C	17.00389800	1.35295600	2.09740000	H	24.63342900	2.53452300	3.92049300
H	15.97835700	1.15036600	2.50559500	H	26.08373800	1.44338000	3.61129500
C	17.51754300	2.73473400	2.54359000	H	25.66126200	1.96417200	5.32610300
H	18.43061400	3.00594800	1.94393800	C	18.26018300	-0.00040500	8.35603600
C	17.85585400	2.76528800	4.04546200	H	17.27973500	-0.13432600	7.83410100
H	16.90143400	2.89837100	4.63092100	H	18.22921500	0.89585200	9.02416400
C	18.53606000	1.48537600	4.57513300	H	18.50153500	-0.91880000	8.94703300
H	18.37987000	1.39583800	5.68790700	C	29.77375700	5.38630100	-1.18246600
C	17.99631500	0.28622400	2.58720100	N	28.62185000	4.75729300	-0.91517000
H	19.03173100	0.53273600	2.21352200	C	27.74504100	5.71252900	-0.32264500
C	17.68149500	-1.13567700	2.14755400	C	28.46000100	7.02034800	-0.25306700
H	17.82813900	-1.21304000	1.03259200	C	29.70150600	6.82479500	-0.78071400
H	18.38253600	-1.85057900	2.66124100	C	30.95855800	4.80426500	-1.77226300
C	16.02481300	-2.80782100	2.24423200	C	30.54019600	1.28368400	-2.57819000
H	14.94724000	-2.91653400	2.52388400	N	30.03414900	2.51496400	-2.13268500

C	31.04153800	3.49438300	-2.16919700	C	24.72342900	8.80708800	0.56763500
C	32.25383500	2.83202500	-2.73018400	C	24.37914300	8.78866100	1.91893500
C	31.95911600	1.52545900	-2.96817100	C	24.70881300	7.66168100	2.67164600
C	29.88197300	0.08336400	-2.66162100	C	25.37773100	6.58043200	2.09939500
C	26.44347300	0.15876000	-1.45954500	C	25.73714500	6.61451500	0.74536400
N	27.70725400	0.78757500	-1.66455800	C	25.40028100	7.73914100	-0.02008100
C	28.50740000	-0.10688800	-2.25914600	H	25.20712200	-1.70367900	0.35010800
C	27.78479500	-1.39464800	-2.49205100	H	23.19471200	-3.11671000	0.67631200
C	26.52209800	-1.22629400	-2.00627300	H	20.76329700	-0.13964200	-1.27385500
C	25.33953700	0.71127000	-0.86605700	H	22.78827900	1.26944400	-1.65512900
C	25.77378500	4.23349200	0.08028600	H	30.37162900	-2.24678700	-1.37167400
N	26.21912800	3.06228900	-0.52736500	H	31.61991500	-4.21964100	-2.25988000
C	25.25564000	2.06605300	-0.37747300	H	32.20693500	-2.18827100	-6.00268400
C	24.16414000	2.62756700	0.35543300	H	30.96945800	-0.20079800	-5.12897400
C	24.48263800	3.97090500	0.63437600	H	34.38629800	7.50401000	-0.13133600
C	26.47508100	5.49330500	0.13510700	H	32.35421400	6.08299300	0.17247500
H	28.01052900	7.92190500	0.15815300	H	32.17752400	5.45754700	-4.09847000
H	30.52170200	7.52585400	-0.91493600	H	34.20357100	6.88976300	-4.38228200
H	29.15484600	2.63366600	-1.69346400	H	24.44340600	9.68357200	-0.04109500
H	33.18532300	3.37541000	-2.88718000	H	24.42047800	7.62924000	3.73598300
H	32.58985700	0.73104600	-3.36635400	H	25.63004900	5.69960300	2.70723700
H	28.23968000	-2.25956700	-2.96930800	H	25.67219800	7.77302900	-1.08488500
H	25.68559700	-1.92343600	-2.00910200	S	20.42106200	-2.66737700	0.07701600
H	27.08951700	2.95277600	-0.99192300	O	19.30831000	-1.99157300	-0.49448300
H	23.26261200	2.09148200	0.64278800	O	20.31114800	-2.75309000	1.49358700
H	23.87494800	4.69647600	1.17064100	O	20.62975800	-3.95195300	-0.49845200
C	24.23010500	-1.35369900	-0.01942500	S	23.55431900	10.16746900	2.66279200
C	23.09365600	-2.13623000	0.17554000	O	22.81430200	10.76752600	1.61416500
C	21.83560500	-1.70977700	-0.25379500	O	24.58400900	11.00166600	3.16049300
C	21.75032600	-0.48411800	-0.91787200	O	22.75044300	9.61132200	3.68768900
C	22.87937400	0.30601000	-1.13144400	S	32.92375300	-4.70573400	-4.78686600
C	24.13551100	-0.11699400	-0.67370400	O	32.81760400	-4.63566000	-6.19933100
C	30.59826100	-1.08723900	-3.18722600	O	32.29436600	-5.84427900	-4.22400000
C	30.78331900	-2.22625400	-2.39088800	O	34.25114900	-4.52804300	-4.32480600
C	31.48508000	-3.32327400	-2.88813900	S	35.84031100	8.32061700	-2.48970800
C	32.01502200	-3.31983800	-4.17858500	O	36.58574300	8.18252500	-1.29095500
C	31.81337500	-2.19045900	-4.97188300	O	35.35363800	9.63606500	-2.68716600
C	31.11793800	-1.08267900	-4.48941900	O	36.50431600	7.80511400	-3.63237300
C	33.88629900	7.06057200	-1.00900800	O	-22.85099800	1.66496500	4.48086200
C	32.75782700	6.26034100	-0.83484200	O	-22.90859700	5.20657200	3.63257100
C	32.13197800	5.67274300	-1.94301500	O	-25.45906300	2.62856700	5.46179100
C	32.65933000	5.91097500	-3.22041100	O	-26.52208800	4.48648000	3.53227700
C	33.78557600	6.71742600	-3.37617300	O	-20.79744500	4.34402900	5.33338200
C	34.41469500	7.30261200	-2.27723200	O	-24.25030100	4.93455100	1.84266900

O	-23.16651700	7.26751900	-0.80640700	C	-27.13645400	5.74387200	3.30608100
O	-26.56891100	5.22634600	0.19092700	H	-27.04601000	6.40715200	4.20100600
O	-25.87496900	5.67007600	-2.60793500	H	-28.20893700	5.49379800	3.10621600
O	-21.01870800	7.76136100	0.87599000	H	-26.68327900	6.22986500	2.40452300
O	-23.10494100	5.56607800	-2.29870100	C	-19.43808200	4.37636800	5.72030500
O	-20.04286200	6.06437100	-4.29409200	H	-18.96527300	3.36830200	5.59951900
O	-23.58556500	4.03299600	-4.71551600	H	-19.45381600	4.67254800	6.79844600
O	-21.06064500	2.87543700	-5.68708500	H	-18.87307300	5.12986200	5.11641000
O	-21.66536200	8.48107900	-3.48101800	C	-24.37319100	5.96551900	0.85362200
O	-19.31938400	3.95589000	-3.91265500	H	-24.91541900	6.85686000	1.27434500
O	-16.00562500	3.12644500	-2.65917400	C	-25.22664900	5.34975000	-0.27747300
O	-17.73770600	3.35166100	-6.34907800	H	-24.79578800	4.35683200	-0.58347200
O	-15.96650400	1.14763000	-5.76224700	C	-25.27194500	6.29930000	-1.48680900
O	-16.84988500	5.73481500	-2.11971300	H	-25.83088600	7.23383300	-1.20300100
O	-16.39235700	0.93492100	-2.95991500	C	-23.84310200	6.70510000	-1.91168100
O	-14.91209500	-0.73694600	-0.01854400	H	-23.85588000	7.51785800	-2.69084400
O	-16.54263600	-1.86219700	-3.58888400	C	-22.99484600	6.40088800	0.32017000
O	-17.15548900	-3.35601300	-1.12033700	H	-22.38165500	5.50161800	0.01813000
O	-16.99362100	-1.30023200	0.66577600	C	-22.25600400	7.25880400	1.35328300
O	-17.97874400	-0.31127100	4.01999400	H	-22.84961600	8.18603700	1.57689700
O	-16.45584600	-3.66744900	2.31518000	H	-22.09947400	6.65081200	2.28349900
O	-18.68441000	-3.91391700	4.20971400	C	-26.92671000	3.90040600	0.55760300
O	-19.89655200	-1.45246500	4.20466200	H	-26.90028900	3.22747400	-0.33670900
O	-21.78405500	0.92173900	6.32465300	H	-27.96985500	3.99908400	0.94970500
O	-22.48143400	-2.69795400	4.66224300	H	-26.24418700	3.52296100	1.36117300
O	-24.49596600	-0.49915400	4.39667300	C	-27.28563300	5.83677100	-2.67287800
O	-19.28700900	-0.28543300	7.42478100	H	-27.77609800	5.41602700	-1.76084700
C	-23.26112200	3.02754200	4.64544200	H	-27.58442500	5.26224500	-3.58563000
H	-23.06563900	3.37936900	5.69370700	H	-27.54583400	6.91775700	-2.78666200
C	-24.76351800	3.11889100	4.31234900	C	-19.99125100	6.78092200	0.81694400
H	-24.98752700	2.49685200	3.40210100	H	-19.87008700	6.27479900	1.80688600
C	-25.20973700	4.57176400	4.07630800	H	-19.06984800	7.36416100	0.56455700
H	-25.25496300	5.10660600	5.06905500	H	-20.21505700	6.02146500	0.02260200
C	-24.23671600	5.37212100	3.18874900	C	-22.32995000	5.69742900	-3.49665200
H	-24.43909400	6.47720400	3.28826600	H	-22.81104100	6.42400500	-4.20617200
C	-22.43995900	3.85220200	3.64224400	C	-22.31116200	4.28671700	-4.12317900
H	-22.53031400	3.40403700	2.61035300	H	-22.05434500	3.52525800	-3.33705900
C	-20.95358900	3.92626300	3.97272400	C	-21.30149200	4.21932600	-5.27836900
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H	-20.45748100	4.66823000	3.29162700	C	-19.92508300	4.78901400	-4.88021300
C	-26.62215400	1.87883200	5.13952200	H	-19.27907600	4.93741000	-5.79217700
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H	-27.09215100	1.65978600	6.13041800	H	-20.50664700	5.48807900	-2.32169500
H	-26.33360700	0.92880300	4.62104900	C	-20.83077800	7.61798100	-2.71745800

H	-21.22782800	7.71130500	-1.66521600	H	-15.19901400	-2.87175100	-1.71935100
H	-19.76613400	7.96861000	-2.77001300	C	-15.81890300	-1.81684900	0.07895400
C	-24.46899200	3.30523500	-3.87511300	H	-15.30370000	-2.58397800	0.72361200
H	-24.10885700	2.25206300	-3.76561700	C	-15.37502400	0.36877000	-0.80109700
H	-25.45053000	3.33798100	-4.41065800	H	-16.34189300	0.76460300	-0.36215700
H	-24.55715000	3.79761700	-2.87355800	C	-14.31296200	1.46315900	-0.60177100
C	-22.05056600	2.34892000	-6.55579300	H	-14.62722700	2.37520600	-1.18736600
H	-23.04805600	2.31725100	-6.05190600	H	-14.31297300	1.71949600	0.50026100
H	-21.68815500	1.31471300	-6.78295600	C	-17.57395300	-1.40416900	-4.45287800
H	-22.11408800	2.95659300	-7.49266700	H	-18.57789700	-1.64613700	-4.02520400
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H	-20.18625900	9.32687900	-4.68938500	H	-17.47565800	-0.30187600	-4.62471100
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H	-17.44713200	4.83142200	-4.33582900	H	-16.23919200	-4.92855200	-2.15273200
C	-17.56127200	2.75675700	-5.05924500	C	-17.00357900	-1.35376000	2.09627200
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C	-18.25841400	2.45478200	-7.31754300	H	-17.82835400	1.21261200	1.03273500
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C	-15.64376400	-0.05737800	-2.25252200	H	-17.94326500	-4.45895200	6.09064000
H	-14.68791100	-0.28771800	-2.79294400	H	-19.51720900	-5.20920200	5.49927300
C	-16.58987500	-1.28505500	-2.28383600	H	-19.48654500	-3.46833500	6.08775000
H	-17.63152100	-0.95284500	-2.01339000	C	-20.82844800	-1.03244100	5.21133800
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C	-23.35691700	-0.58644100	5.24526500	C	-26.47611300	-5.49356800	0.13408300
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C	-23.01342700	0.86432000	5.63455600	H	-30.52312500	-7.52537400	-0.91590100
H	-23.78199400	1.27708400	6.34772400	H	-29.15556700	-2.63330700	-1.69398200
C	-20.65724400	0.44757300	5.57796500	H	-33.18613400	-3.37439700	-2.88780200
H	-20.55564000	1.04715000	4.62672100	H	-32.59031300	-0.73005300	-3.36669500
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H	-18.53243000	0.87180600	5.85260600	H	-25.68573700	1.92340700	-2.00905800
H	-19.65896700	1.73367800	7.02172000	H	-27.09028900	-2.95279400	-0.99253500
C	-22.03258000	-3.47905200	3.56312500	H	-23.26306000	-2.09230500	0.64183800
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H	-24.63323300	-2.53641800	3.92003600	C	-21.75062500	0.48346100	-0.91850600
H	-26.08348600	-1.44504800	3.61136700	C	-22.87977800	-0.30650000	-1.13213300
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C	-18.25945600	-0.00389200	8.35581500	C	-30.59851000	1.08794700	-3.18733600
H	-17.27900600	0.13011600	7.83390700	C	-30.78352600	2.22684400	-2.39082000
H	-18.22860600	-0.90046100	9.02352900	C	-31.48519100	3.32399200	-2.88792400
H	-18.50064600	0.91426900	8.94724100	C	-32.01507200	3.32080200	-4.17839500
C	-29.77483900	-5.38592800	-1.18331500	C	-31.81345600	2.19154400	-4.97187300
N	-28.62281500	-4.75712900	-0.91603000	C	-31.11811900	1.08363600	-4.48955600
C	-27.74613500	-5.71255200	-0.32361600	C	-33.88766800	-7.05956500	-1.00996400
C	-28.46130800	-7.02025600	-0.25409300	C	-32.75908200	-6.25951100	-0.83572700
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C	-31.04237600	-3.49372200	-2.16980800	C	-24.72501300	-8.80769500	0.56621600
C	-32.25457900	-2.83114600	-2.73073900	C	-24.38057000	-8.78941100	1.91747800
C	-31.95968700	-1.52459400	-2.96858500	C	-24.70995300	-7.66241700	2.67029400
C	-29.88235600	-0.08280500	-2.66187700	C	-25.37874300	-6.58101300	2.09818500
C	-26.44384500	-0.15880100	-1.45987300	C	-25.73831400	-6.61494900	0.74419200
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C	-28.50775500	0.10722500	-2.25939400	H	-25.20711100	1.70299100	0.35032900
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H	-34.20481600	-6.88854400	-4.38323900	H	0.11018200	-3.10526200	2.29364000
H	-24.44521600	-9.68419300	-0.04259700	H	0.10266700	-2.77395700	0.50935900
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H	-25.63083300	-5.70017500	2.70610800	C	-1.19647100	-0.44285500	5.20655400
H	-25.67378100	-7.77336400	-1.08613500	N	12.94744500	-1.10597900	-0.95022500
S	-20.42097600	2.66632400	0.07670200	C	12.11535700	-0.30002600	-0.16967300
O	-19.30840600	1.99051900	-0.49513700	C	10.89009600	-0.28504300	-0.87147800
O	-20.31078800	2.75171300	1.49327200	H	12.46105800	0.18630000	0.74263900
O	-20.62967000	3.95103900	-0.49842800	N	12.26645800	-1.53285500	-2.04391300
S	-23.55590600	-10.16840800	2.66116100	N	11.07924600	-1.08260300	-2.02629000
O	-22.81626400	-10.76864800	1.61237500	C	9.62515500	0.38986500	-0.52503200
O	-24.58568300	-11.00235700	3.15910000	H	9.80852200	1.22138000	0.20662300
O	-22.75166900	-9.61244300	3.68587400	H	9.11052700	0.78421300	-1.44210200
S	-32.92371000	4.70684600	-4.78648500	O	8.78564500	-0.60014000	0.10479900
O	-32.81726300	4.63716400	-6.19894700	C	7.49497200	-0.21696800	0.37917400
O	-32.29447100	5.84524900	-4.22316800	C	6.96633200	1.06206100	0.15918200
O	-34.25119800	4.52899100	-4.32475600	C	6.68663500	-1.23044600	0.93692400
S	-35.84182200	-8.31925100	-2.49078200	C	5.64173800	1.32460600	0.50055500
O	-36.58723100	-8.18116700	-1.29201500	H	7.58349700	1.86261400	-0.27136500
O	-35.35533300	-9.63474800	-2.68836600	C	5.37205600	-0.94957700	1.27485900
O	-36.50575900	-7.80354800	-3.63339700	H	7.11614000	-2.22977800	1.09738100
N	-12.94732900	1.10714100	-0.94984300	C	4.83005800	0.33141100	1.06553400
C	-12.11528200	0.30084500	-0.16960200	H	5.23218500	2.33316800	0.33291500
C	-10.88993400	0.28630600	-0.87126500	H	4.74157900	-1.73775800	1.71423600
H	-12.46105500	-0.18595400	0.74243300	H	-3.23113400	0.64348500	3.23854500
N	-12.26623900	1.53462300	-2.04323300	C	-4.82985500	-0.33058100	1.06548200
N	-11.07900100	1.08444200	-2.02569200	C	-5.64153500	-1.32365900	0.50030300
C	0.62869200	0.24570600	3.78976900	C	-5.37187300	0.95034400	1.27513900
C	-0.62846000	-0.24558000	3.78968900	C	-6.96615000	-1.06106500	0.15905300
C	1.47638900	0.60867200	2.68120200	H	-5.23196300	-2.33217000	0.33240200
C	-1.47614800	-0.60821200	2.68100600	C	-6.68647400	1.23126100	0.93733400
C	3.47035800	0.62091300	1.45551000	H	-4.74139300	1.73843500	1.71467300
S	2.48228200	1.71476700	0.63621800	C	-7.49481400	0.21789700	0.37937700
C	1.18619000	1.52844900	1.68076200	H	-7.58331700	-1.86153200	-0.27165000
C	-1.18592500	-1.52766200	1.68027600	H	-7.11599500	2.23054400	1.09804800
S	-2.48202500	-1.71369200	0.63567900	O	-8.78551000	0.60110400	0.10517300
C	-3.47013000	-0.62014400	1.45533400	C	-9.62499600	-0.38870300	-0.52500400
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H	-0.94701700	1.63355800	1.64445300	C	0.00011400	-0.00031600	6.18860300

F	-1.59581800	-1.72786600	5.47728600	F	2.32713300	-0.29175600	5.47117500
F	-2.32690700	0.29133600	5.47126600	F	1.59605900	1.72745000	5.47784100
F	0.37366800	-1.01017400	7.03246000	C	2.80514900	0.08179300	2.53914500
F	-0.37344400	1.00927600	7.03277600	H	3.23133200	-0.64325800	3.23833700

Reference

1. M. J. S. Dewar, E. G. Zoebisch, E. F. Healy and J. J. P. Stewart, *J. Am. Chem. Soc.*, 1985, **107**, 3902-3909.
2. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
3. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
4. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.
5. P. C. Hariharan and J. A. Pople, *Theoret. Chimica Acta*, 1973, **28**, 213-222.
6. M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654-3665.
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09*, revision B.01., Gaussian, Inc. Wallingford, CT; **2010**.
8. M. Irie, T. Lifka, S. Kobatake, N. Kato, *J. Am. Chem. Soc.*, 2000, **122**, 4871-4876.
9. Z. Li, C. Zhang, Y. Ren, J. Yin, S. H. Liu, *Org. Lett.*, 2011, **13**, 6022-6025.
10. H. Bakirci and W. M. Nau, *J. photoch. Photobio. A*, 2005, **173**, 340-348.
11. K. K. Jensen, S. B. van Berlekom, J. Kajanus, J. Martensson and B. Albinsson, *J. Phys. Chem. A*, 1997, **101**, 2218-2220.
12. K. Kilså, J. Kajanus, J. Mårtensson and B. Albinsson, *J. Phys. Chem. B*, 1999, **103**, 7329-7339.