

Supporting Information

Synergistic Steric Pairing Effects of Terfluorenes with Ternary Side Groups on β -Conformation Transition: Experiments and Computations

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1 Experimental Section

1.1 Preparation of thin films for optical analysis: Pristine films of four terfluorenes were spin-coated on quartz substrates from its toluene solution (10 mg/mL) using KW-4A (from the institute of micro-electronics of Chinese Academy of Science) at 1500 rpm/min for 30 s in the Figure 1 and 3. Terfluorenes were spin-coated from toluene solution (10 mg/mL) on quartz plates and then thermally annealed in N₂ at 220 °C for 10 min (Figure 1b and 3). The quartz cells of 10 mm thickness were used to measure the spectra of the dilute solutions (Figure 1a). The reported absorbances of the samples have been corrected for the solvent background.

1.2 Synthesis

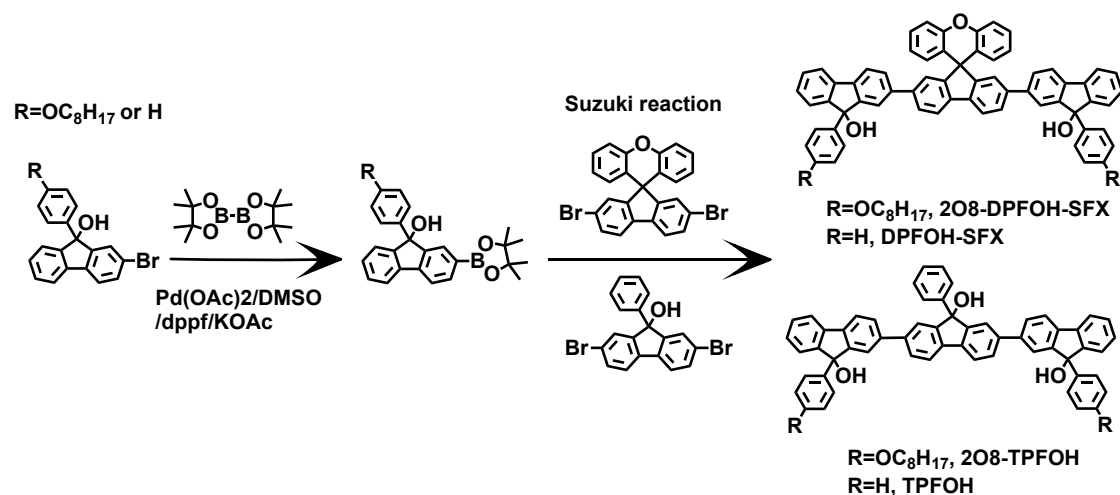


Figure S1. Synthetic routes to 2O8-DPFOH-SFX, DPFOH-SFX, 2O8-TPFOH and TPFOH.

The synthesis and optical properties including ¹H, ¹³C-NMR, MALDI-TOF-MS, UV-vis absorption and photoluminescence spectrum of TPFOH have been reported in our previous work, which be found in reference 36 in the manuscript.

1.2.1 Synthesis of 2O8-DPFOH-SFX

Under N₂ atmosphere, 2,7-dibromo-spiro[fluorene-9,9'-xanthene] (1.47 g, 3 mmol, 1 eq), 9-(4-(octyloxy)phenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-fluorene-9-ol (TMB-PFOHO8) (3.84 g, 7.5 mmol, 2.5 eq), tetrakis(triphenyl)phosphine palladium (0) (35 mg, 0.03 eq) were added to a three-necked Schlenk flask (150 mL).

The flask was evacuated and back-filled with nitrogen atmosphere more than three times before injecting with degassed toluene/THF (30 mL, 1:1 v/v) and an aqueous K_2CO_3 solution (5 mL, 10 eq) through a syringe. The mixture was heated to 90 °C and stirred for 48 h. The mixture was poured into water and extracted with dichloromethane. The combined extracts were dried by anhydrous $MgSO_4$, and then the solvent was removed under vacuum condition. The mixture was purified by silica gel chromatography to afford a pale yellow powder (1.5 g, 45%). MALDI-TOF-MS (m/z): calcd. For $C_{79}H_{54}O_5$: 1100.5 [M⁺]; Found: 896.9. ¹H NMR (400 MHz, $CDCl_3$, ppm, δ): 7.67 (dd, $J = 11.3, 5.5$ Hz, 7H), 7.60–7.55 (m, 4H), 7.52 (t, $J = 5.2$ Hz, 5H), 7.48–7.43 (m, 1H), 7.72–7.14 (m, 39H), 7.39 (dd, $J = 12.7, 7.3$ Hz, 5H), 7.31 (dd, $J = 12.2, 10.6, 5.8$ Hz, 7H), 7.29–7.18 (m, 10H), 6.76 (dd, $J = 15.1, 6.5$ Hz, 2H), 3.95–3.77 (m, 2H), 2.53 (d, $J = 4.2$ Hz, 3H), 1.71 (dt, $J = 14.5, 7.1$ Hz, 2H), 1.46–1.21 (m, 13H), 0.87 (dd, $J = 7.2, 3.6$ Hz, 3H).

1.2.2 Synthesis of DPFOH-SFX

Under N_2 atmosphere, 2,7-dibromo-spiro[fluorene-9,9'-xanthene] (1.47 g, 3 mmol, 1 eq), 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9-phenyl-fluoren-9-ol (TMB-PFOH) (2.9 g, 7.5 mmol, 2.5 eq), tetrakis(triphenylphosphine) palladium(0) (35 mg, 0.03 eq) were added to a three-necked Schlenk flask (150 mL). The flask was evacuated and back-filled with nitrogen atmosphere more than three times before injecting with degassed toluene/THF (30 mL, 1:1 v/v) and an aqueous K_2CO_3 solution (5 mL, 10 eq) through a syringe. The mixture was heated to 90 °C and stirred for 48 h. The mixture was poured into water and extracted with dichloromethane. The combined extracts were dried by anhydrous $MgSO_4$, and then the solvent was removed under vacuum condition. The product was purified with silica gel chromatography to afford a white powder (1.82 g, 72%). MALDI-TOF-MS (m/z): calcd. For $C_{63}H_{40}O_3$: 844.3 [M⁺]; Found: 896.9. ¹H NMR (400 MHz, $CDCl_3$, ppm, δ): 7.67 (dd, $J = 11.3, 5.5$ Hz, 7H), 7.60–7.55 (m, 4H), 7.52 (t, $J = 5.2$ Hz, 5H), 7.48–7.43 (m, 1H), 7.72–7.14 (m, 39H), 7.39 (dd, $J = 12.7, 7.3$ Hz, 5H), 7.31 (dd, $J = 12.2, 10.6, 5.8$ Hz, 7H), 7.29–7.18 (m, 10H), 6.76 (dd, $J = 15.1, 6.5$ Hz, 2H), 3.95–

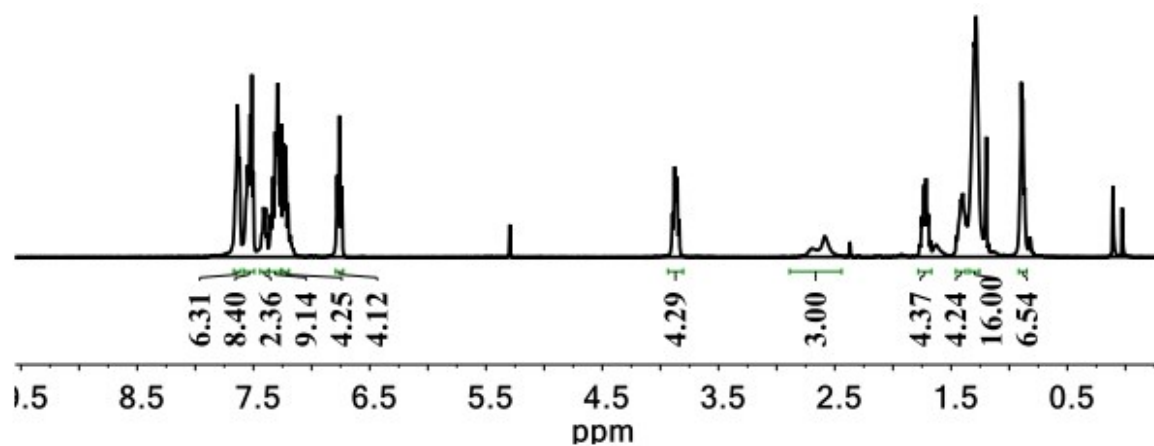
3.77 (m, 2H), 2.53 (d, $J = 4.2$ Hz, 3H), 1.71 (dt, $J = 14.5, 7.1$ Hz, 2H), 1.46–1.21 (m, 13H), 0.87 (dd, $J = 7.2, 3.6$ Hz, 3H).

1.2.3 Synthesis of 2O8-TPFOH

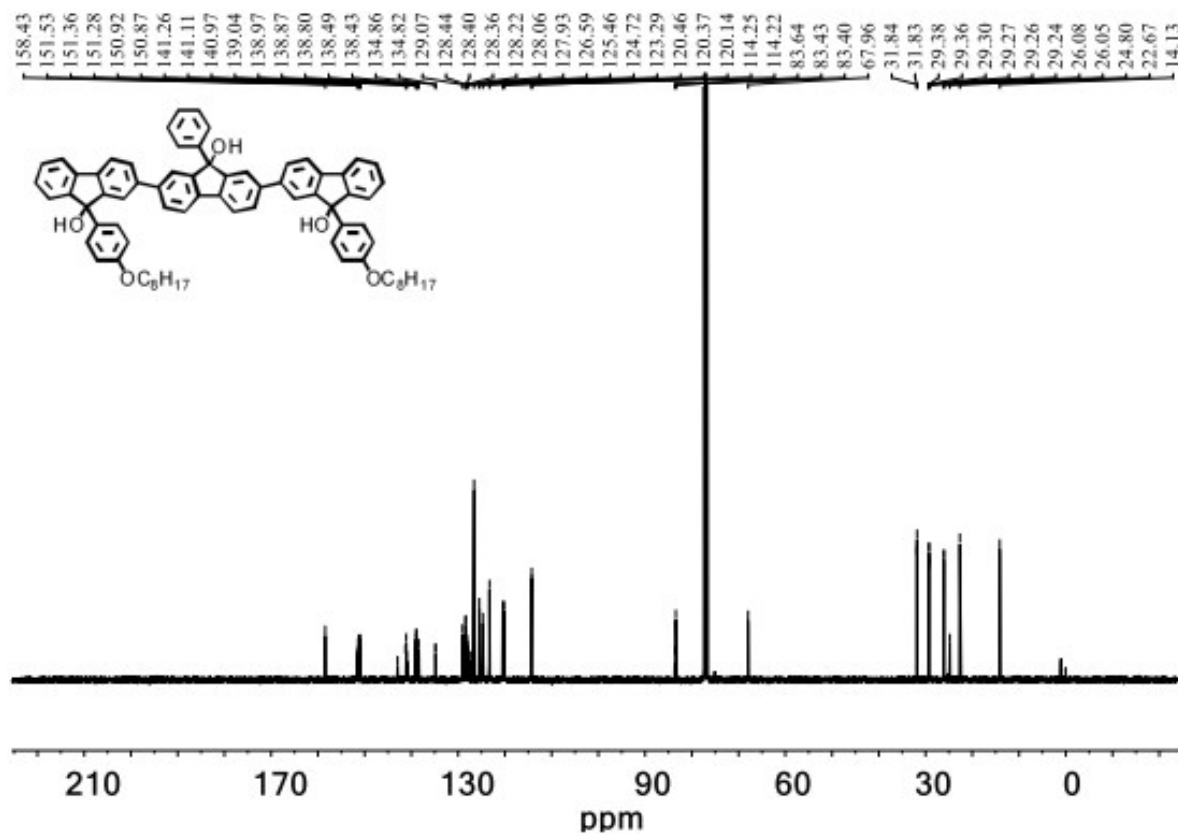
Under N₂ atmosphere, 2,7-dibromo-9-phenyl-fluoren-9-ol (1.25 g, 3 mmol, 1 eq), 9-(4-(octyloxy)phenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-fluoren-9-ol (TMB-PFOHO8) (3.84 g, 7.5 mmol, 2.5 eq), tetrakis(triphenylphosphine) palladium (0) (35 mg, 0.03 eq) were added to a three-necked Schlenk flask (150 mL). The flask was evacuated and back-filled with nitrogen atmosphere more than three times before injecting with degassed toluene/THF (30 mL, 1:1 v/v) and an aqueous K₂CO₃ solution (5 mL, 10 eq) through a syringe. The mixture was heated to 90 °C and stirred for 48 h, and then poured into water, extracted with dichloromethane. The combined extracts were dried by anhydrous MgSO₄, and then the solvent was removed under vacuum condition. The mixture was purified by silica gel chromatography to afford a pale yellow powder (2.1 g, 68%). MALDI-TOF-MS (m/z): calcd. For C₇₃H₇₀O₅: 1026.52 [M⁺]; Found: 1028.1. ¹H NMR (400 MHz, CDCl₃, ppm, δ): 7.64 (t, $J = 7.4$ Hz, 6H), 7.58-7.44 (m, 9H), 7.40 (dd, $J = 12.2, 5.2$ Hz, 2H), 7.36-7.27 (m, 9H), 7.25-7.19 (m, 4H), 6.76 (t, $J = 8.2$ Hz, 4H), 3.87 (dt, $J = 9.9, 6.5$ Hz, 4H), 2.64 (d, $J = 44.7$ Hz, 3H), 1.78-1.67 (m, 4H), 1.46- 1.37 (m, 4H), 1.29 (d, $J = 5.6$ Hz, 16H), 0.92-0.85 (m, 7H).

1.3 ^1H , ^{13}C -NMR, MALDI-TOF-MS, UV-*vis* absorption and photoluminescence spectrum of 2O8-TPFOH, DPFOH-SFX and 2O8-DPFOH-SFX

(a)



(b)



(c)

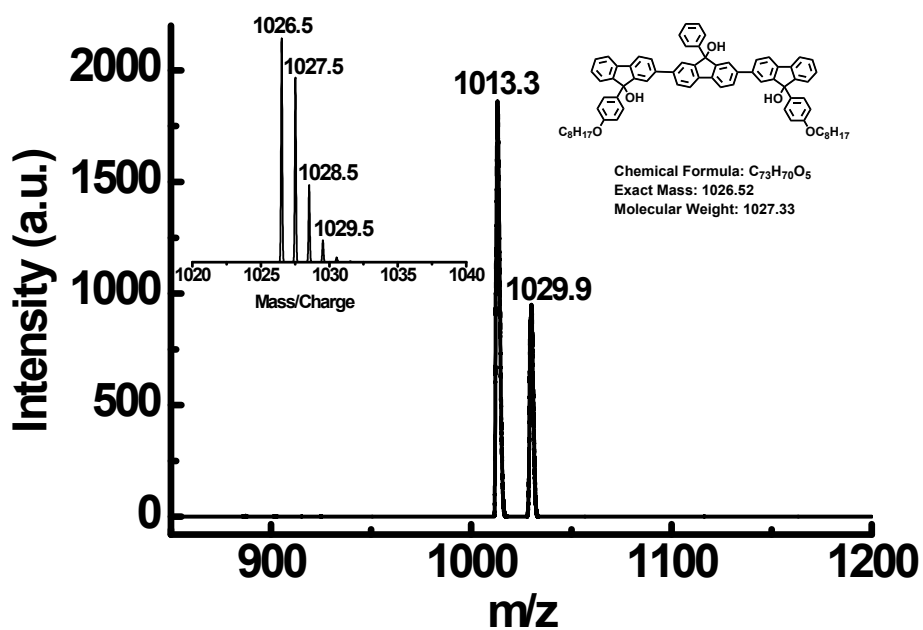
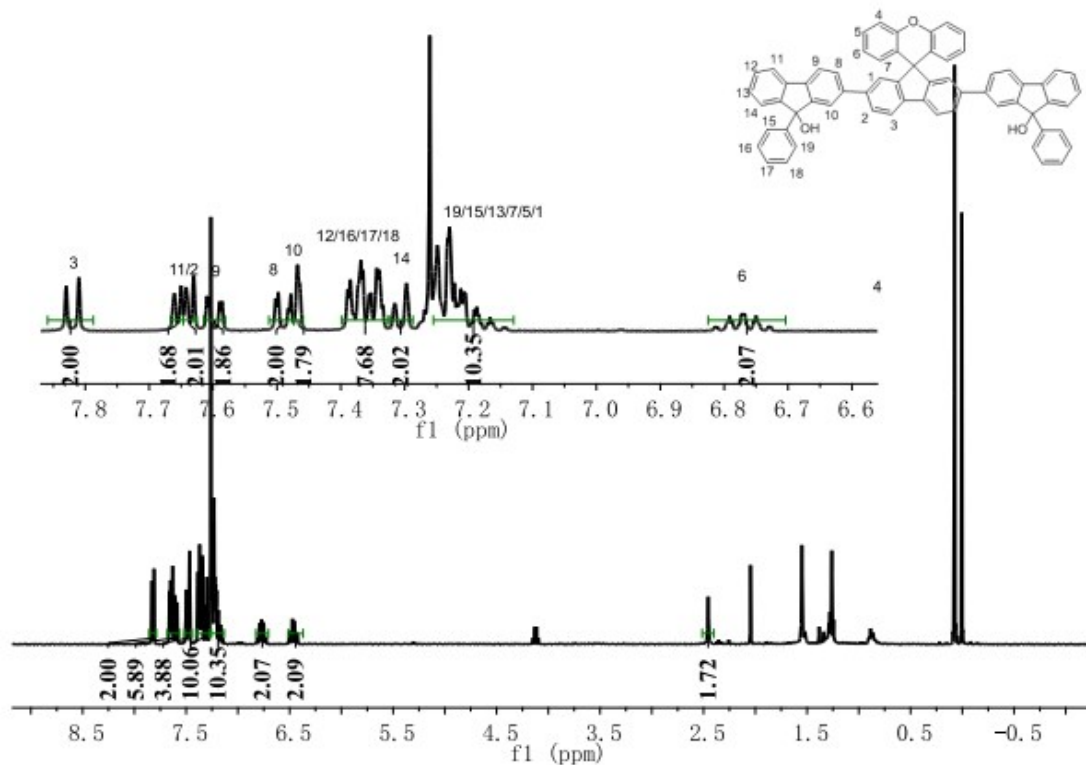


Figure S2. (a) ¹H, (b) ¹³C-NMR and (c) MALDI-TOF-MS spectra of 2O8-TPFOH.

(a)



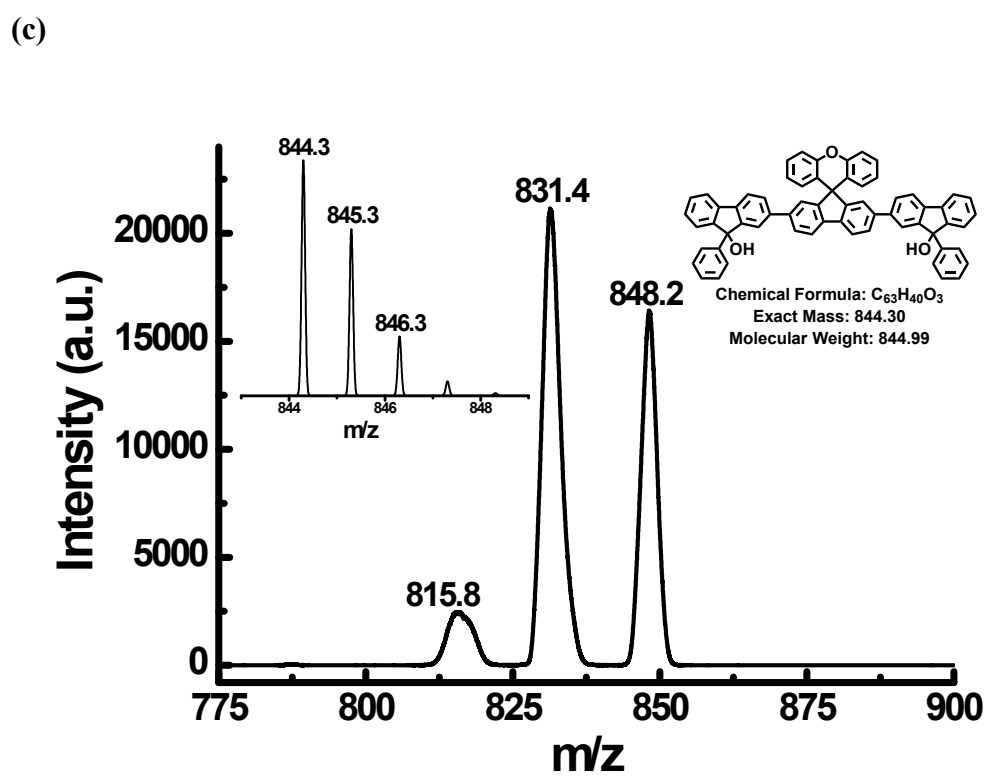
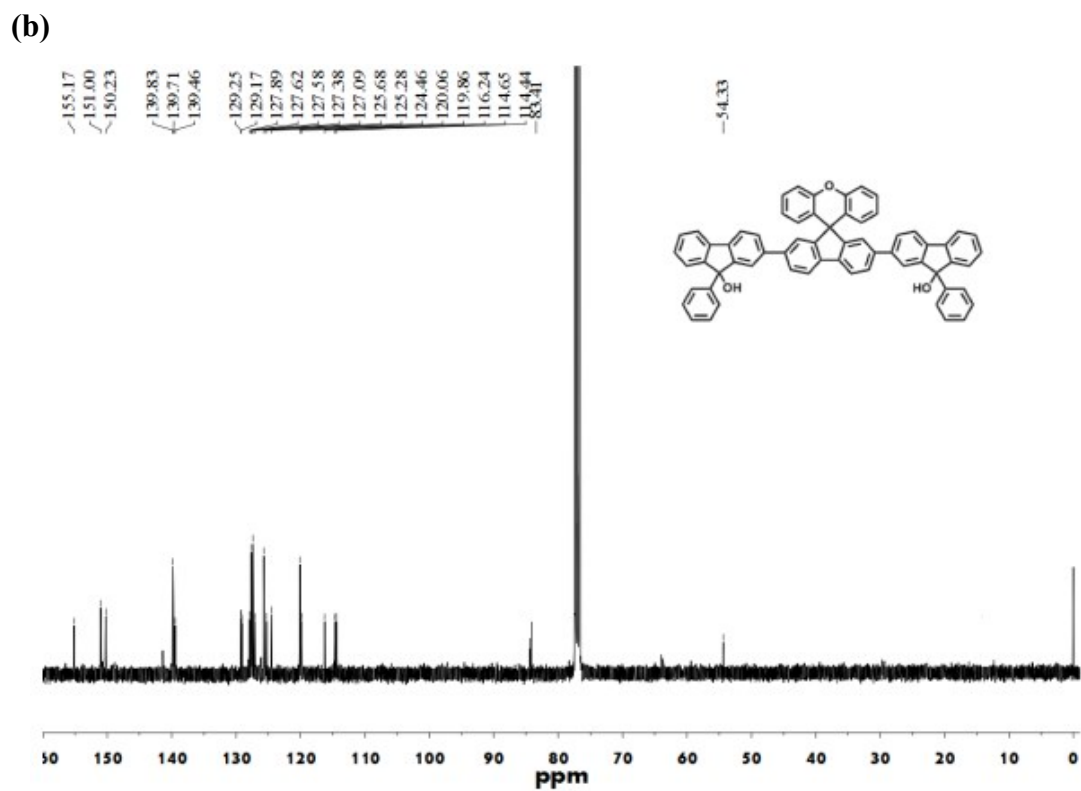
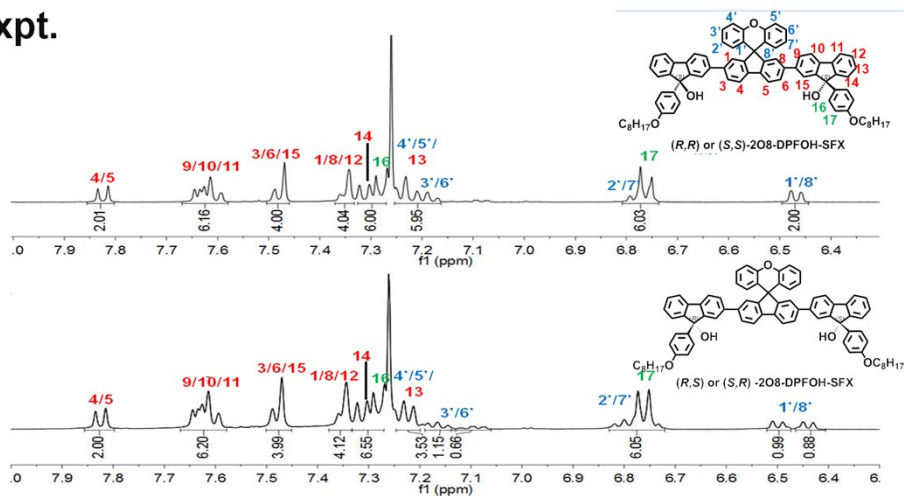


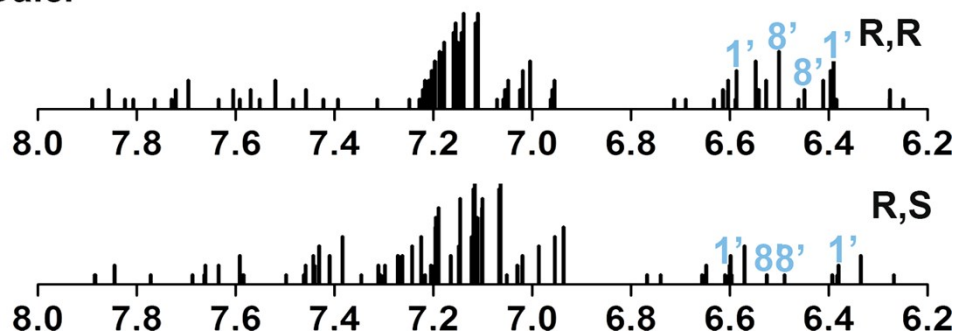
Figure S3. (a) ^1H , (b) ^{13}C -NMR and (c) MALDI-TOF-MS spectra of DPFOH-SFX.

(a)

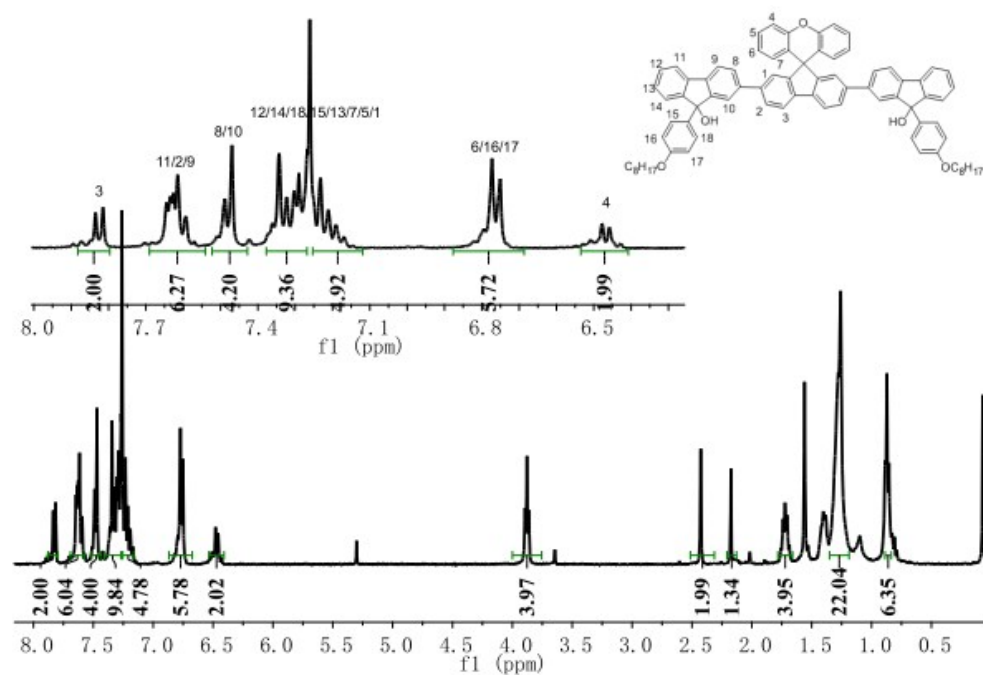
Expt.



Calc.



(b)



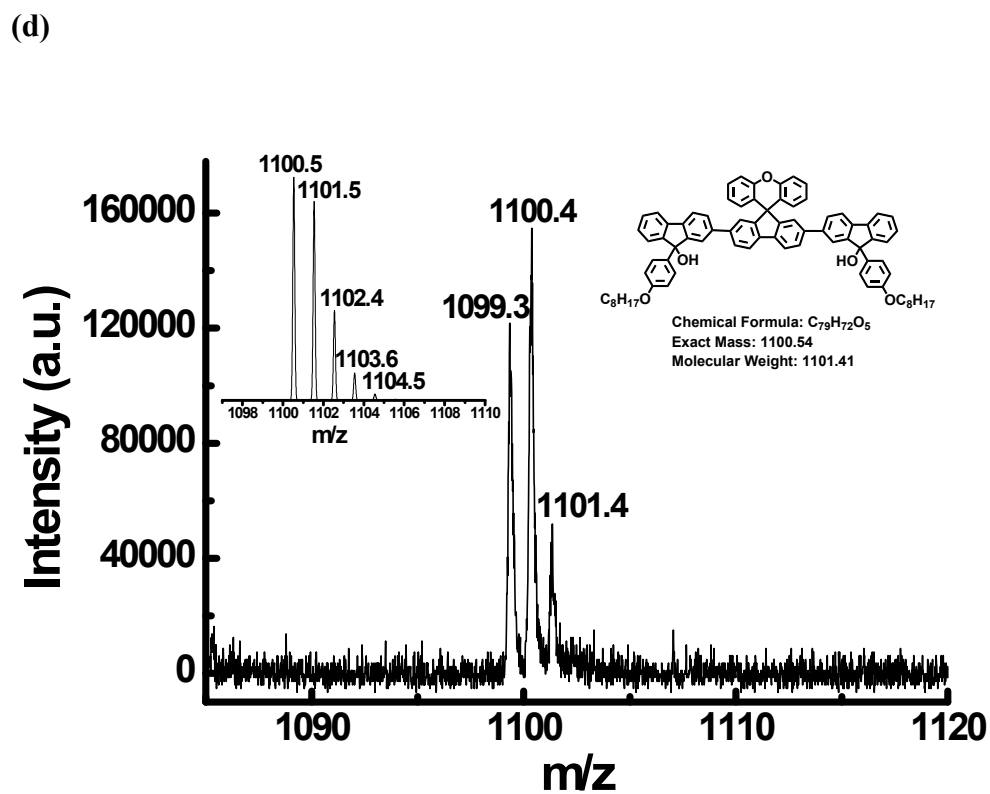
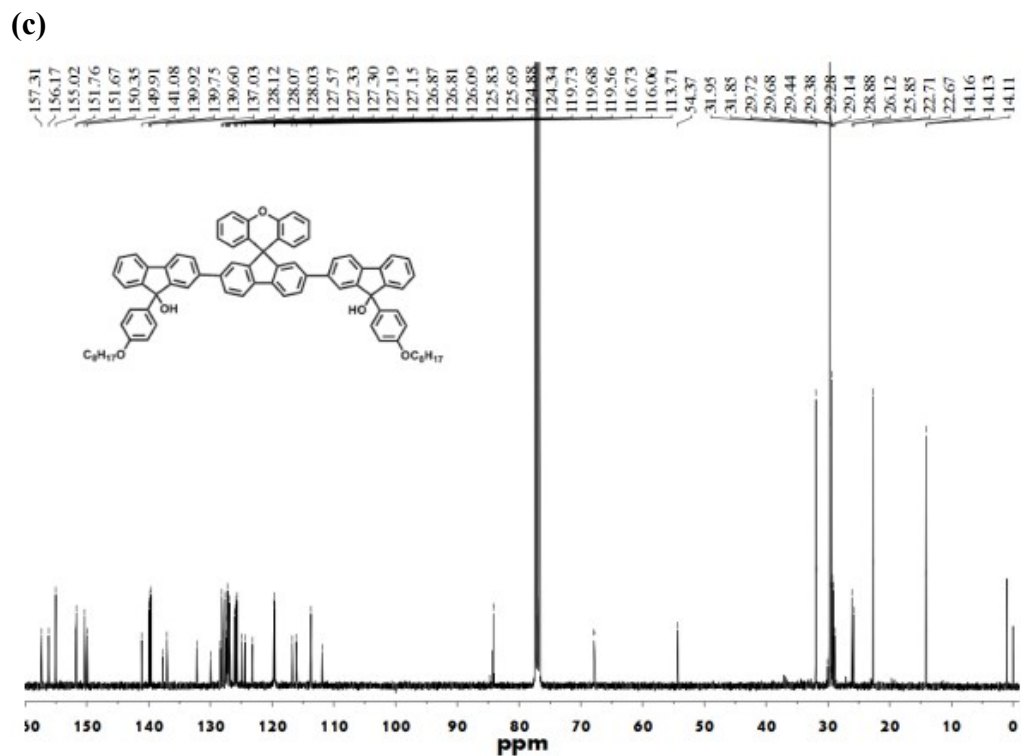


Figure S4. (a) The calculated and experimental ^1H -NMR of all the isomers of 2O8-DPFOH-SFX, (b) ^1H , (c) ^{13}C -NMR and (d) MALDI-TOF-MS spectra of 2O8-DPFOH-SFX.

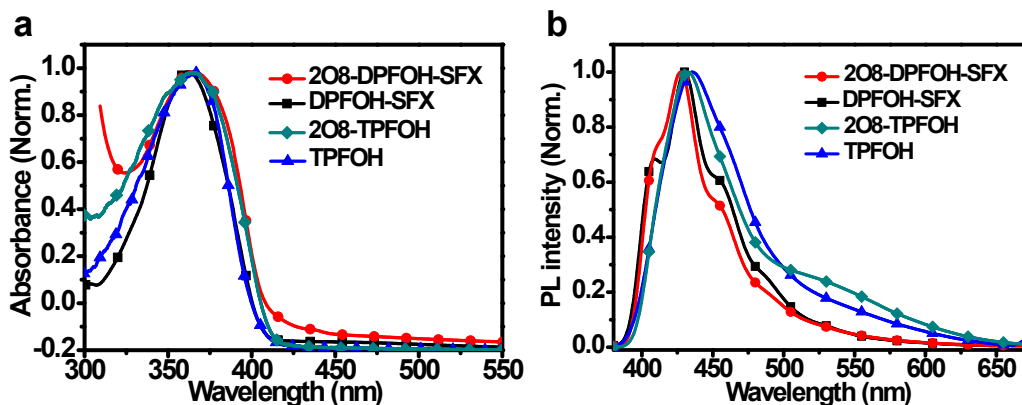


Figure S5. The experimental (a) UV-*vis* absorption and (b) photoluminescence spectra of pristine films spin-coated from toluene solution without annealing treatment.

1.4 TLC photographs of 2O8-DPFOH-SFX and MALDI-TOF-MS spectra of two isomers of 2O8-DPFOH-SFX

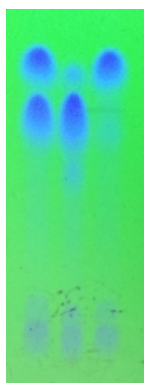
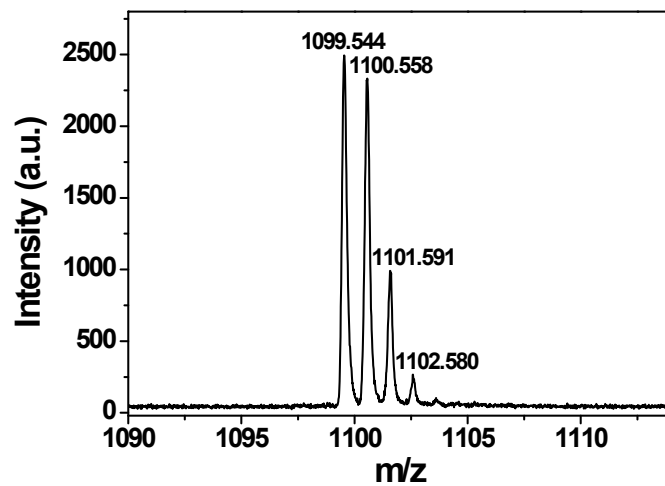


Figure S6. TLC photographs of 2O8-DPFOH-SFX under the UV lamp with irradiation wavelength of 254 nm (using dichloromethane as developing solvent). Left: mixed compound, middle and right: the separated compounds.

(a)



(b)

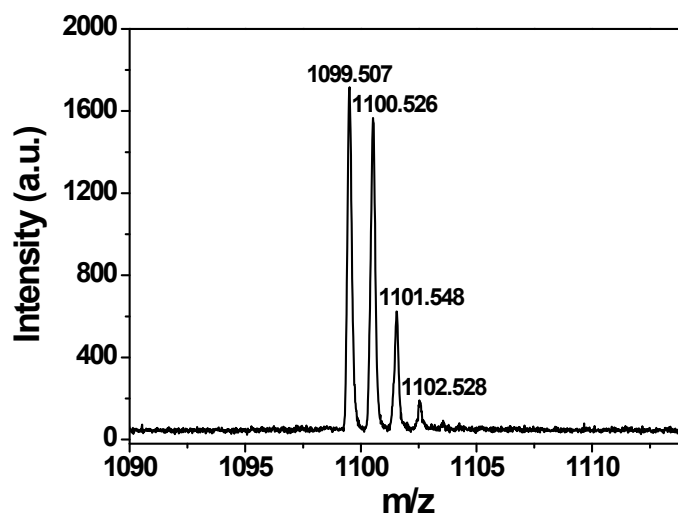


Figure S7. MALDI-TOF-MS spectra of (a) (*R,R*) or (*S,S*)-configuration and (b) (*R,S*) and (*S,R*)-configuration of 2O8-DPFOH-SFX.

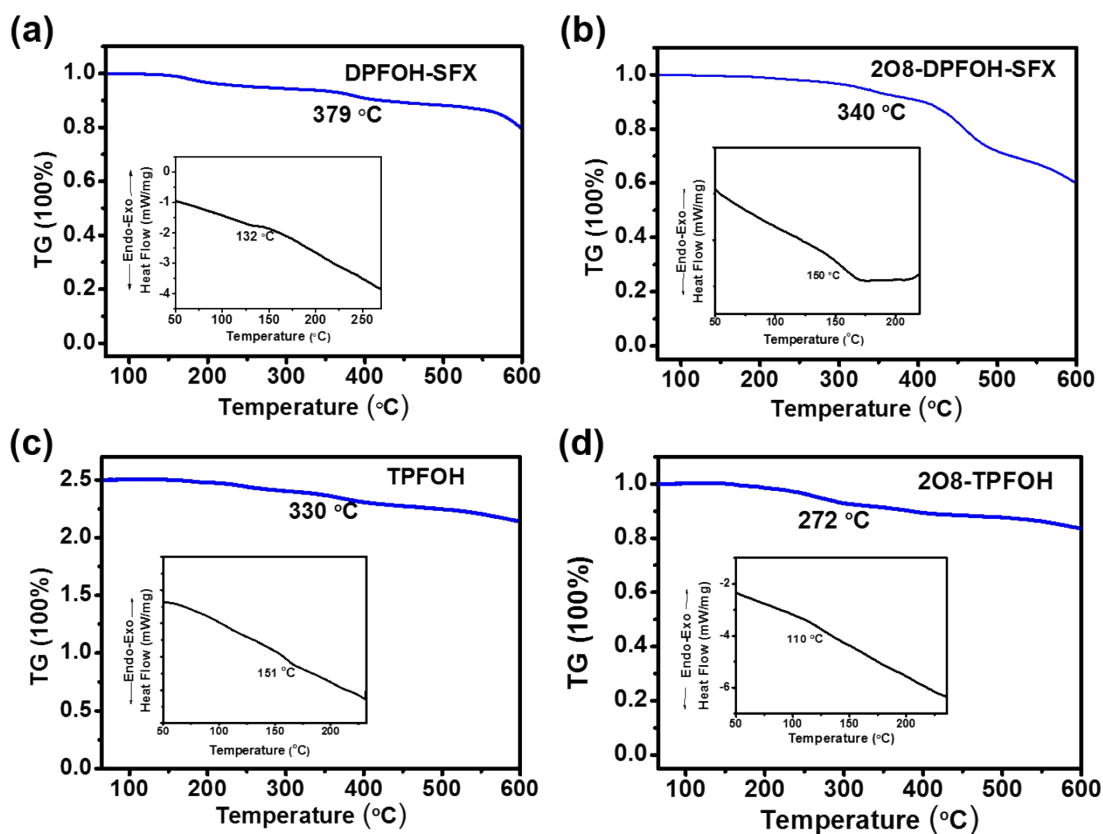


Figure S8. TG and DSC curves of (a) DPFOH-SFX, (b) 2O8-DPFOH-SFX, (c) TPFOH and (d) 2O8-TPFOH.

2. Computational Section

2.1 The heating and cooling process in simulation annealing and the comparison between crystals structures and calculation results using PCFF

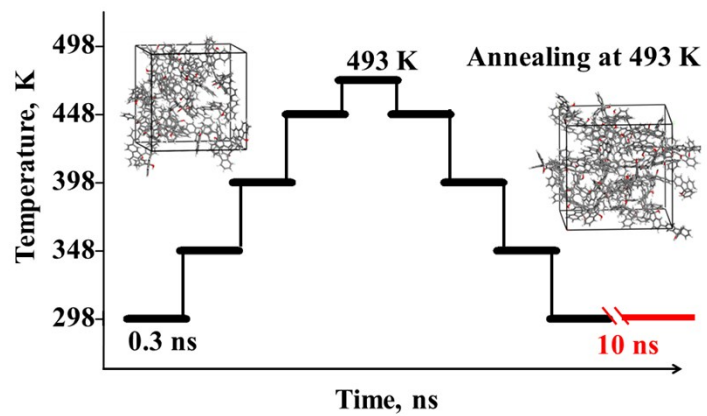
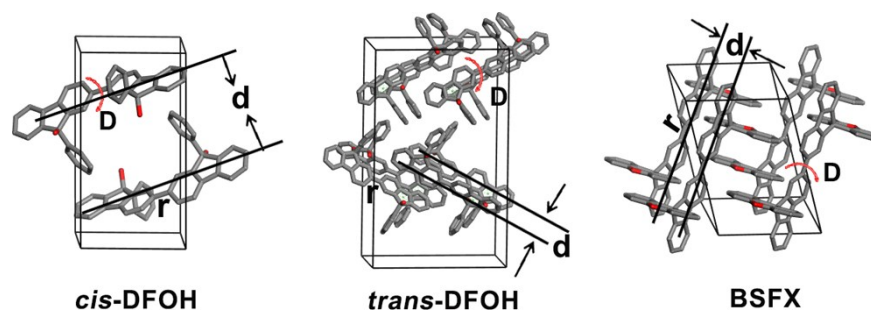


Figure S9. The heating and cooling process in simulation annealing at 493 K.

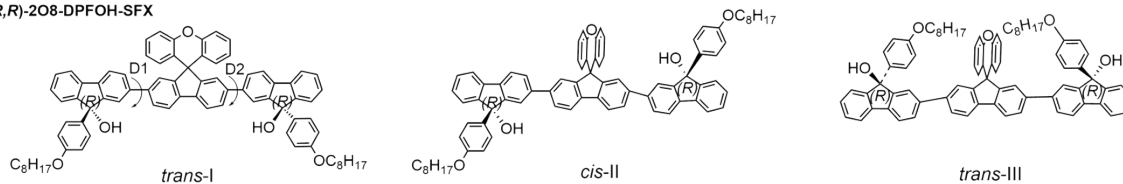
Table S1. The torsion angle (D), bond length (r) between two adjacent fluorene units and intermolecular distance (d) in crystal calculated at polymer consistent force field (PCFF).



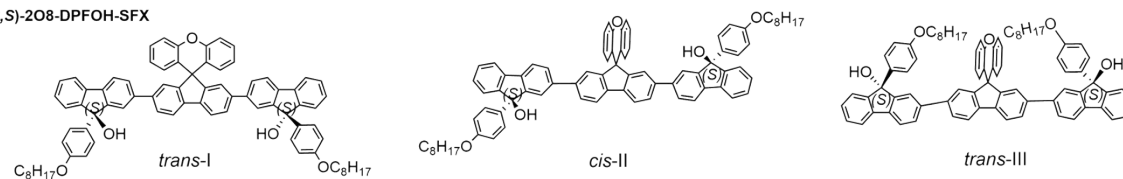
system	CCDC number/Sym.	Torsion angle D (°)		Bond length (Å)		Distance d (Å)	
		PCFF	Expt.	PCFF	Expt.	PCFF	Expt.
<i>cis</i> DFOH ⁴⁴	1061803/triclinic	29.3	25.3	1.45	1.48	1.45	1.48
<i>trans</i> DFOH ⁴⁴	1061802/orthorhomibic	22.4	28.4	1.45	1.46	1.45	1.46
BSFX ³³	1497103/triclinic	-3.3	-1.4	1.47	1.50	1.47	1.50

2.2 The optimized geometries, packing structures and relative energies of the different isomers of 2O8-DPFOH-SFX

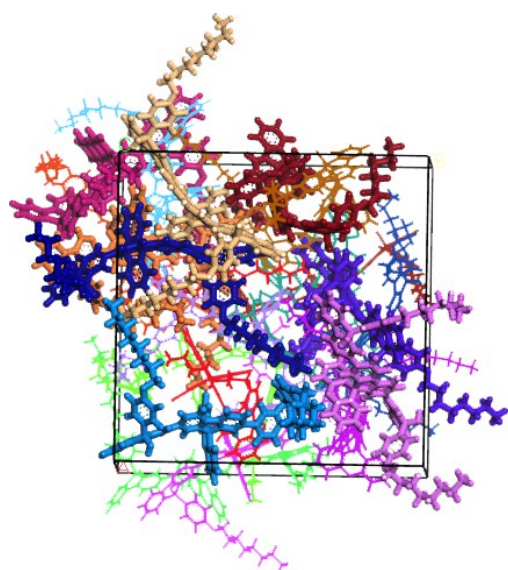
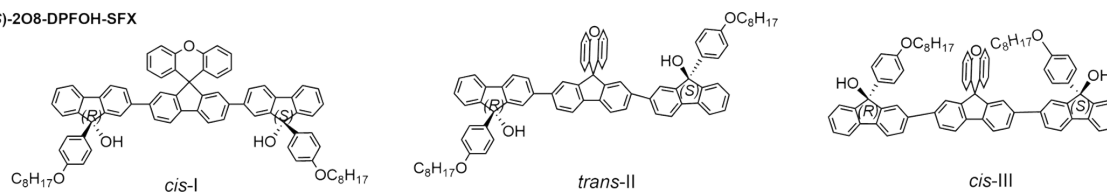
(R,R)-2O8-DPFOH-SFX



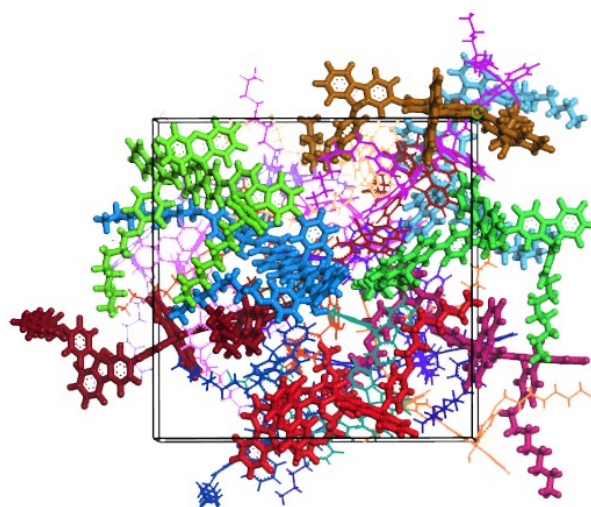
(S,S)-2O8-DPFOH-SFX



(R,S)-2O8-DPFOH-SFX



raceme



mesomer

Table S2. The torsion angle, D1/D2, relative energy ΔE of isomers of 2O8-DPFOH-SFX calculated at B3LYP/6-31+G(d) level and polymer consistent force field (PCFF).

isomers		B3LYP			PCFF		
		$\Delta E^a/\text{kcal/m}$	D1/ $^\circ$	D2/ $^\circ$	$\Delta E^b/\text{kcal/mol}$	D1/ $^\circ$	D2/ $^\circ$
S,S	<i>trans</i> -I	0.0	37.6	-37.6	0.0	34.7	-38.4
	<i>cis</i> -II	0.1	38.7	-37.1			
	<i>trans</i> -III	0.3	37.4	-38.5			
R,R	<i>trans</i> -I	0.7	37.0	-39.4	2.2	38.4	-34.2
	<i>cis</i> -II	0.9	-38.4	38.4			
	<i>trans</i> -III	1.0	37.3	-38.2			
R,S	<i>cis</i> -I	1.1	36.4	-39.2	2.8	34.6	-37.8
	<i>trans</i> -II	1.1	-37.4	38.9			
	<i>cis</i> -III	1.4	38.2	-36.8			

a the energy difference relative to S,S isomer of 2O8-DPFOH-SFX at B3LYP/6-31+G(d) level. b the energy difference relative to S,S isomer of 2O8-DPFOH-SFX at PCFF.

2.3 The experimental and calculated $^1\text{H-NMR}$ and UV-*vis* absorption spectra in

vacuum and amorphous state, typical planar conformations, their percentage and the maximum absorption peak in 10 ns MD-simulation, of TPFOH, 2O8-TPFOH, DPFOH-SFX and 2O8-DPFOH-SFX

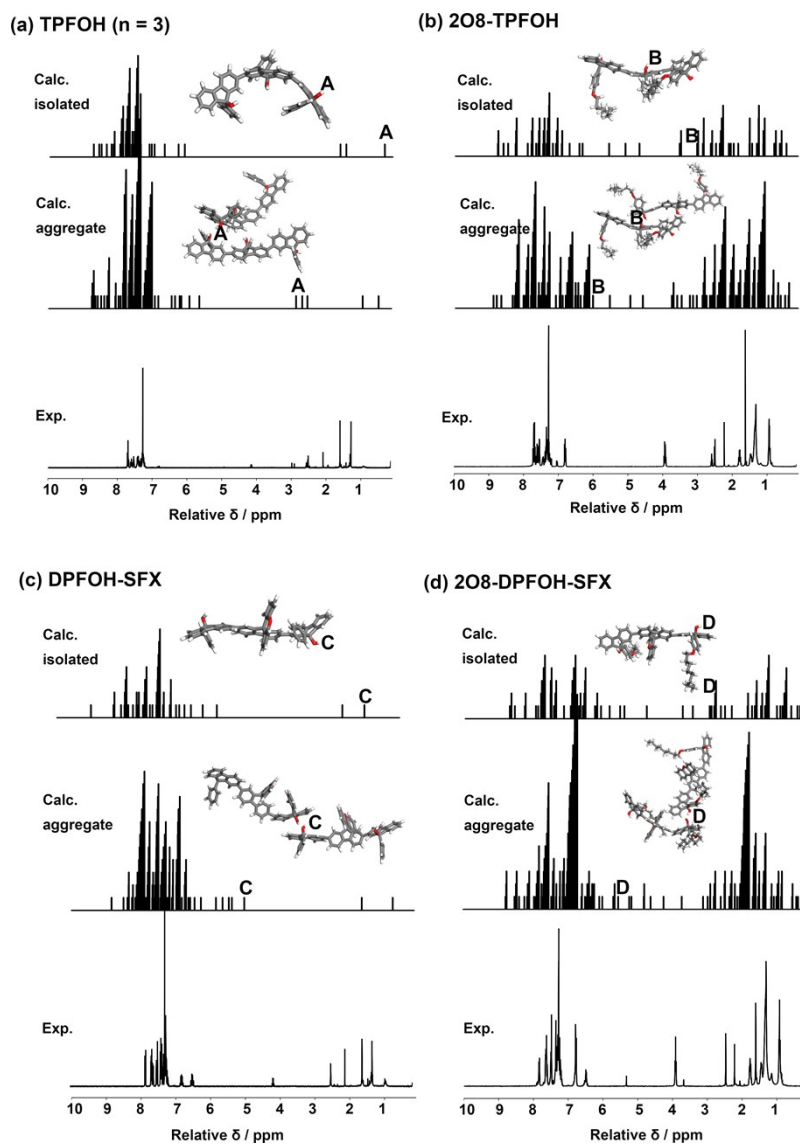


Figure S10. The experimental and calculated $^1\text{H-NMR}$ of aggregates and monomer in (a) TPFOH, (b) 2O8-TPFOH, (c) DPFOH-SFX and (d) 2O8-DPFOH-SFX at CAM-B3LYP/6-31+G(d) level.

isolated molecule in vacuum

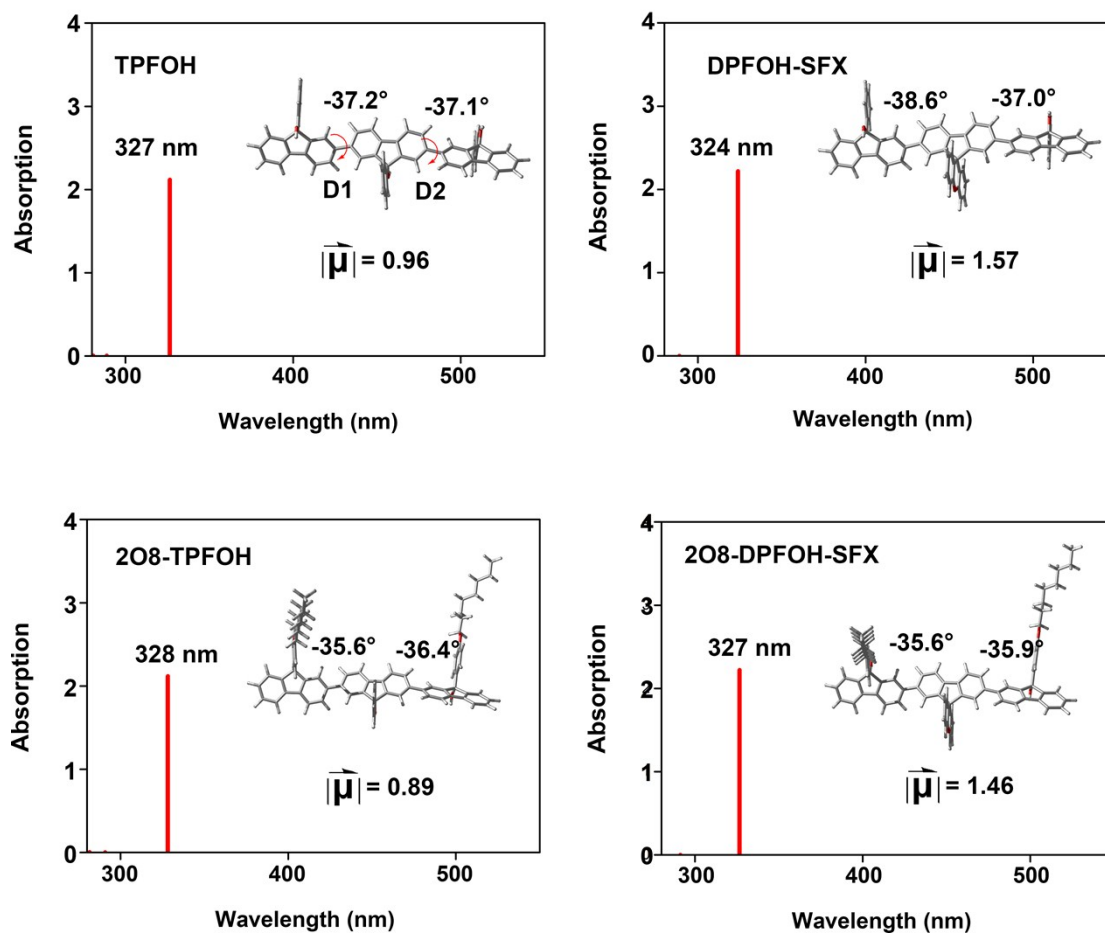


Figure S11. The calculated UV-*vis* absorption spectra at CAM-B3LYP/6-31+G(d) level and optimized structures at B3LYP/6-31+G(d) level of TPFOH, 2O8-TPFOH, DPFOH-SFX and 2O8-DPFOH-SFX in vacuum.

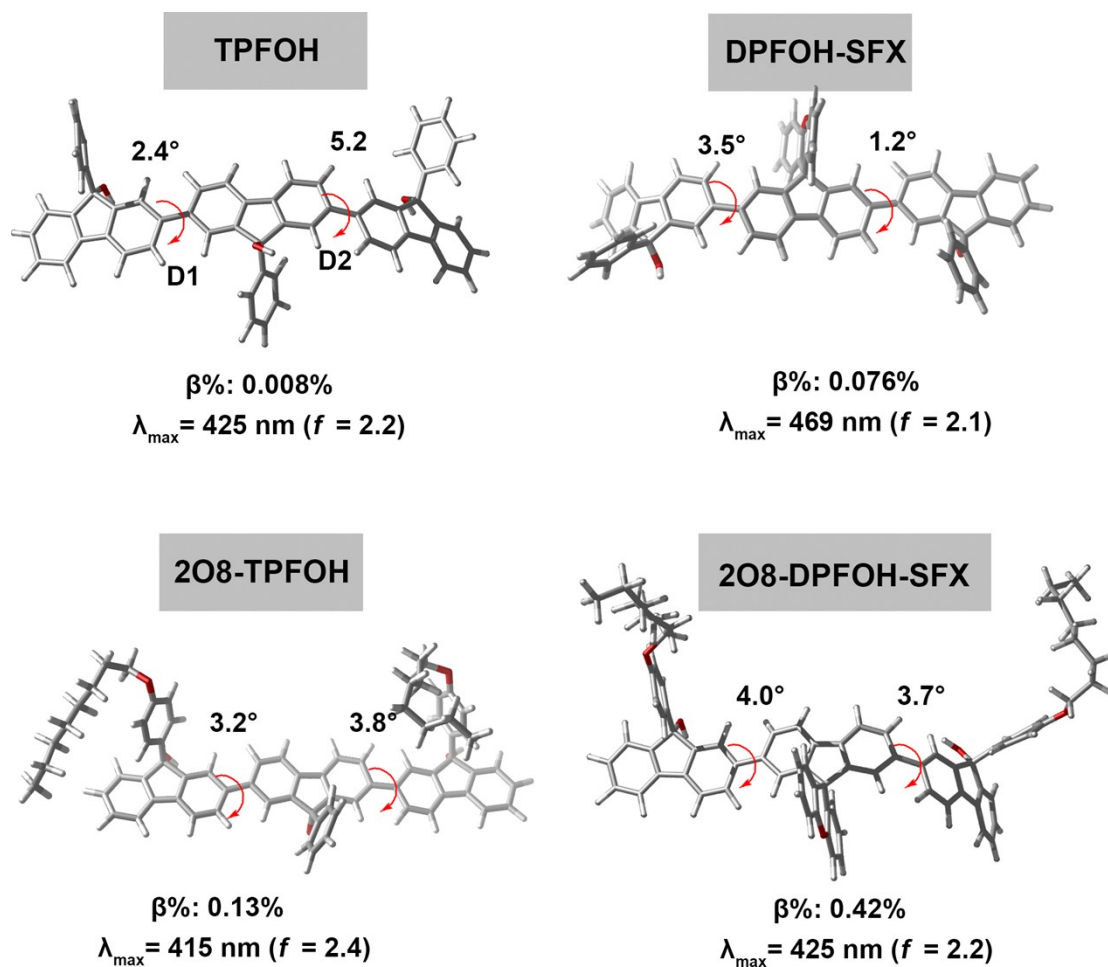


Figure S12. Typical planar conformations, their percentage in 10 ns MD-simulation, and the maximum absorption peak of TPFOH, 2O8-TPFOH, DPFOH-SFX and 2O8-DPFOH-SFX sampled from the 10 ns MD-simulated trajectories in amorphous after annealing at 493 K. The UV-*vis* absorption spectra was calculated at CAM-B3LYP/6-31+G(d) level.

2.4 The major molecular orbital contributions for λ_{\max} in UV-*vis* absorption spectra of different conformations (all-twist, twist-planar and all-planar) in 2O8-DPFOH-SFX.

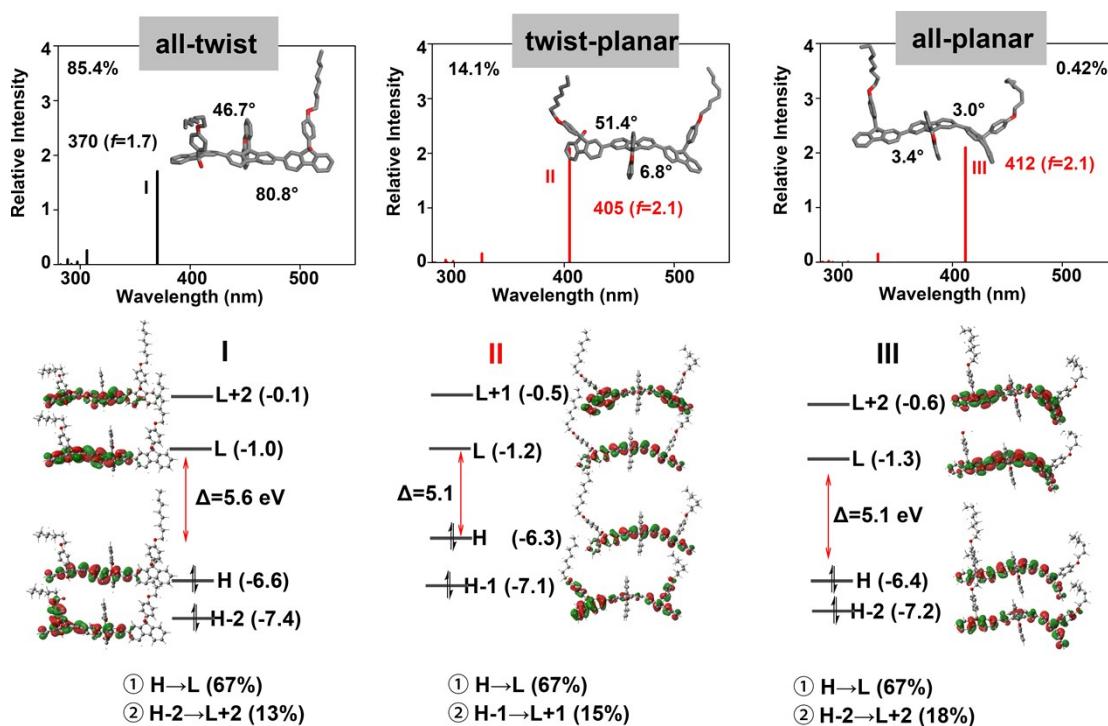


Figure S13. The percentage of different conformations (all-twist, twist-planar and all-planar) in 2O8-DPFOH-SFX, UV-*vis* absorption spectra of selected snapshots, and the major molecular orbital contributions for λ_{\max} .

Aggregates in amorphous films

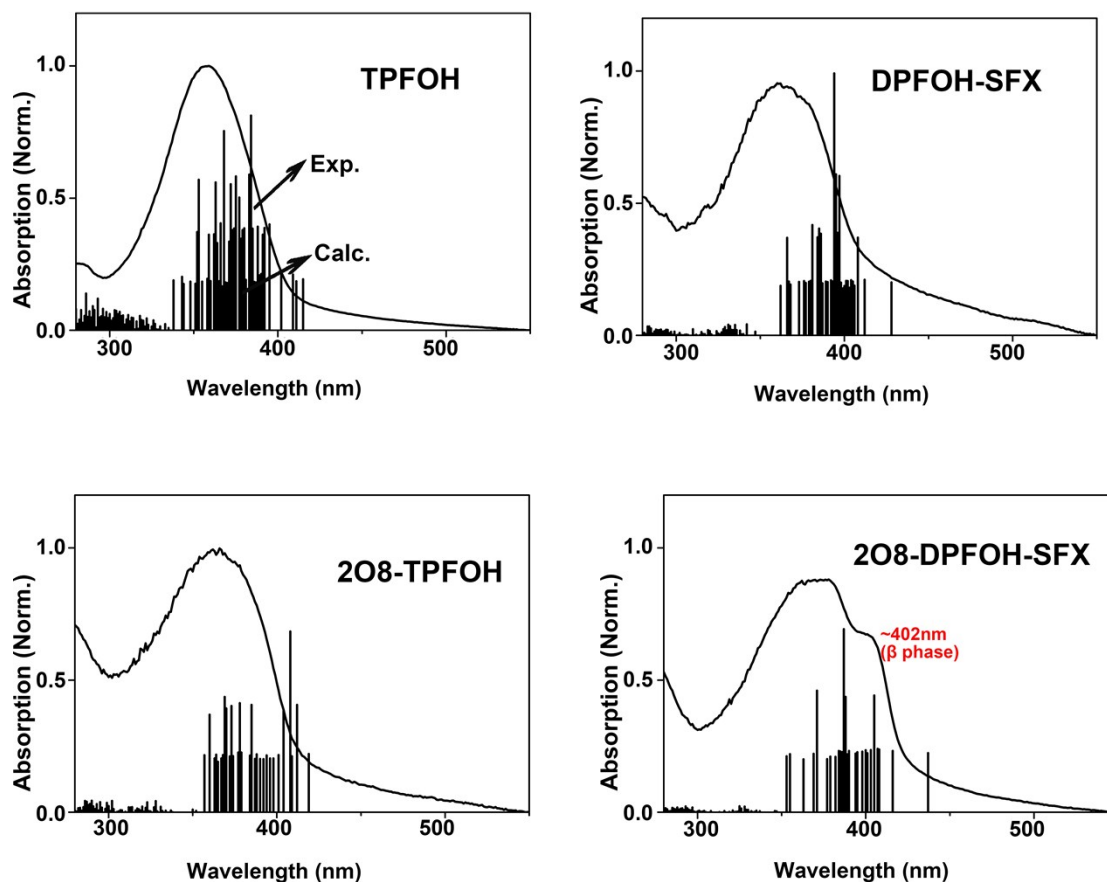


Figure 14. The experimental (solid curve line) and calculated UV-vis absorption spectra (solid column) of TPF OH, 2O8-TPF OH, DPFOH-SFX and 2O8-DPFOH-SFX after annealing at 493 K under N₂ environment. The absorption spectra were calculated at CAM-B3LYP/6-31+G(d) level on the basis of 50 conformations which were evenly sampled from 10ns-MD simulations in amorphous state.

2.5 The coordination of optimized structures

The optimized structures of all isomers of 2O8-DPFOH-SFX

Trans-(R,R)-2O8-DPFOH-SFX-I

C	10.38803700	-3.75121200	-4.34181700
C	10.71294300	-2.41099900	-4.58700300
C	9.86538500	-1.38254200	-4.15117100
C	8.69740000	-1.71863000	-3.47824700
C	8.36401000	-3.06499600	-3.23523800
C	9.21103400	-4.08971700	-3.66382300
C	7.07277000	-3.10765000	-2.52663900
C	6.62178500	-1.78952100	-2.33039800
C	5.41653400	-1.52928500	-1.69693200
C	4.62054900	-2.60050000	-1.23937400
C	5.08345300	-3.91668300	-1.43941600
C	6.29899000	-4.17896900	-2.07629500
C	7.61007800	-0.77976600	-2.93349300
C	-2.44844600	-1.23427400	2.53625900
C	-3.18177000	-2.29044900	1.95617600
C	-2.53396600	-3.12647700	1.02393800
C	-1.20353000	-2.90363800	0.70101200
C	-0.48205800	-1.84751800	1.28827700
C	-1.11094100	-1.00641300	2.21121000
C	0.88657100	-1.85990400	0.76004700
C	1.01031100	-2.92638600	-0.15004000
C	2.20963800	-3.17360700	-0.80170900
C	3.32610800	-2.34875400	-0.55636300
C	3.18874000	-1.28027100	0.35373400
C	1.98391800	-1.03089500	1.01189400
C	-0.32014800	-3.69091200	-0.28484700
C	-5.11589700	-3.82551800	2.44157300
C	-4.60255000	-2.51781700	2.32346200
C	-5.47032600	-1.43082400	2.56153400
C	-6.79108800	-1.66703900	2.90987400
C	-7.29004600	-2.97673000	3.03098200
C	-6.44743800	-4.06363800	2.79080000
C	-8.70779900	-2.90801400	3.42631700
C	-9.07532800	-1.55354700	3.54161300
C	-10.36152200	-1.19267700	3.92308300
C	-11.29410500	-2.20429800	4.19325500
C	-10.93441000	-3.55269600	4.07338900
C	-9.63857000	-3.91614700	3.68842600

C	-7.88594000	-0.63564700	3.22234300
H	11.05713800	-4.53772300	-4.68184200
H	11.63101000	-2.16683700	-5.11528000
H	10.11744500	-0.34083100	-4.33340700
H	8.96627100	-5.13294200	-3.47878000
H	5.07593600	-0.50427200	-1.57575600
H	4.49182000	-4.74796700	-1.06543200
H	6.63158000	-5.20606900	-2.20641100
H	-2.92965100	-0.59760000	3.27357700
H	-3.08633300	-3.92920400	0.54192100
H	-0.56959600	-0.18953700	2.68256900
H	2.28501400	-3.98579500	-1.52058700
H	4.04978100	-0.65268300	0.56675800
H	1.91127400	-0.20519800	1.71578000
H	-4.45278900	-4.67152400	2.28280300
H	-5.11391900	-0.41077500	2.44500500
H	-6.80863300	-5.08529700	2.88175900
H	-10.63899700	-0.14492400	4.00738700
H	-12.30501600	-1.94077700	4.49352700
H	-11.66959900	-4.32602300	4.28166900
H	-9.36756400	-4.96548500	3.59953400
C	-1.59002300	-2.26217900	-3.61981800
C	-1.09821200	-2.36251100	-2.32208900
C	-0.86561000	-3.60737800	-1.71383900
C	-1.14778000	-4.75303400	-2.46262700
C	-1.64342800	-4.67225000	-3.77068600
C	-1.86376800	-3.42758000	-4.34864500
C	-0.49411200	-6.21078200	-0.70507500
C	-0.17027100	-5.15211000	0.14816800
C	0.30355800	-5.47514100	1.43084200
H	0.56097800	-4.66610700	2.10969000
C	0.44830500	-6.79505600	1.84726800
C	0.11540600	-7.83777200	0.97150800
C	-0.35513500	-7.54642100	-0.30348100
H	-1.75993700	-1.28433600	-4.06149000
H	-0.88593400	-1.45860600	-1.75698100
H	-1.84636200	-5.59459700	-4.30692300
H	-2.24831600	-3.36453700	-5.36311400
H	0.81703800	-7.01187500	2.84593000
H	0.22276400	-8.87337300	1.28317500
H	-0.62199600	-8.33003500	-1.00649300
O	-0.96591100	-6.02939800	-1.98300900

O	7.00033200	-0.01877300	-3.99083900
H	6.66439600	-0.64691800	-4.65035400
C	8.14205500	0.22347300	-1.91154500
C	8.03609600	1.60009900	-2.11055300
C	8.76236500	-0.23107000	-0.73428300
C	8.53052300	2.51262600	-1.16700200
H	7.56131200	1.97385500	-3.01070200
C	9.25648400	0.65977100	0.20885600
H	8.85937300	-1.29862400	-0.55140800
C	9.14311100	2.04460300	-0.00053600
H	8.42807000	3.57486600	-1.35950500
H	9.73442100	0.30615900	1.11783300
O	9.65646800	2.84043500	0.98622000
C	9.57568000	4.25941400	0.84110700
C	10.20446100	4.89675800	2.07326800
H	8.52236100	4.56140900	0.74201500
H	10.10651000	4.56815300	-0.07175300
C	10.16022400	6.43141400	2.01474400
H	9.67813100	4.52611200	2.96105000
H	11.24548900	4.55537700	2.15490700
C	10.85858800	7.13233200	3.19349200
H	10.63353600	6.76640300	1.08011300
H	9.11320400	6.76736300	1.96510100
H	10.89346200	8.21128600	2.98425900
H	11.90593500	6.79802100	3.24316000
C	10.19087700	6.91778200	4.56017600
C	10.87129300	7.69660200	5.69476800
H	10.18914000	5.84839700	4.81358600
H	9.13391400	7.21996700	4.49624900
C	10.20949600	7.49268100	7.06471900
H	11.92904400	7.39783800	5.75633300
H	10.87195400	8.76995200	5.44995800
C	10.89674000	8.27356300	8.19138800
H	9.15290000	7.79217900	7.00411400
H	10.20916500	6.42072500	7.31065400
H	10.40065200	8.10654500	9.15515500
H	11.94637500	7.97123300	8.30022100
H	10.88238400	9.35295300	7.99196700
C	-8.16040900	0.31626700	2.05931900
C	-8.07817400	1.70068800	2.20830000
C	-8.50980200	-0.19615900	0.79723300
C	-8.33301500	2.56508300	1.13349600

H	-7.81166400	2.11860000	3.17252000
C	-8.76465000	0.64655900	-0.27584900
H	-8.58143400	-1.27126300	0.65062400
C	-8.67651700	2.03973600	-0.11588100
H	-8.25899500	3.63541300	1.29101000
H	-9.03216500	0.24836300	-1.25029500
O	-7.53260400	0.17608900	4.35628000
H	-7.37489100	-0.41906200	5.10673800
O	-8.94160500	2.78553100	-1.23119900
C	-8.85186200	4.20872500	-1.14687400
C	-9.15698800	4.78383300	-2.52356800
H	-7.84107800	4.49634600	-0.82131300
H	-9.56946600	4.58071400	-0.40035100
C	-9.08489100	6.31708000	-2.54538000
H	-8.44436200	4.36344300	-3.24564900
H	-10.15579600	4.44879300	-2.83343200
C	-9.36524900	6.91533000	-3.93102300
H	-9.80375600	6.72995900	-1.82152400
H	-8.08906600	6.64244300	-2.20790300
H	-8.64642400	6.50254700	-4.65475200
H	-10.36063500	6.59219000	-4.27119400
C	-9.29151900	8.44812000	-3.96135100
C	-9.55868500	9.04851400	-5.34832100
H	-8.29814200	8.76979300	-3.61280100
H	-10.01528100	8.86082200	-3.24198100
C	-9.48306900	10.58130200	-5.38045500
H	-8.83514300	8.63571200	-6.06799900
H	-10.55219900	8.72848400	-5.69819800
C	-9.74879000	11.17189600	-6.77038100
H	-10.20733400	10.99445900	-4.66313300
H	-8.49074000	10.90178200	-5.03068000
H	-9.68827400	12.26689200	-6.75882100
H	-9.01816900	10.80548100	-7.50312600
H	-10.74763500	10.89721600	-7.13359500
Cis-(R,R)-2O8-DPFOH-SFX-II			
C	-8.88182800	-0.48594500	-6.95569600
C	-9.94421800	-0.88301100	-6.13374300
C	-9.71981800	-1.20648700	-4.78798800
C	-8.42562900	-1.13004700	-4.28860200
C	-7.35383100	-0.73774000	-5.11336100
C	-7.57758600	-0.41053500	-6.45287400
C	-6.11421300	-0.76851700	-4.31737200

C	-6.42860300	-1.17637900	-3.00821100
C	-5.44416800	-1.31078600	-2.04165000
C	-4.09949400	-1.03422700	-2.36753600
C	-3.79745000	-0.62022700	-3.68074200
C	-4.78945300	-0.48578200	-4.65522600
C	-7.93385800	-1.45260200	-2.86998800
C	1.76957900	-1.75141000	3.21290300
C	2.76945000	-2.28041400	2.37051800
C	2.46526400	-2.48164700	1.00877700
C	1.20392800	-2.16353100	0.52715400
C	0.21370100	-1.63812900	1.37825000
C	0.50022000	-1.43042200	2.73084800
C	-1.00544700	-1.40514600	0.59618800
C	-0.76668500	-1.78527400	-0.73771000
C	-1.75790700	-1.67188300	-1.70131900
C	-3.02686800	-1.16873600	-1.34945000
C	-3.25486900	-0.79302700	-0.00912200
C	-2.25939300	-0.90631700	0.96189300
C	0.66881100	-2.31625100	-0.90911500
C	4.25686900	-3.19416900	4.18356600
C	4.11298100	-2.61997900	2.90428800
C	5.27482100	-2.37455300	2.14199100
C	6.51863100	-2.70387200	2.65821500
C	6.64914600	-3.28242300	3.93406200
C	5.51025000	-3.52609100	4.70377200
C	8.07720000	-3.53387600	4.19574800
C	8.81946200	-3.10358200	3.07929400
C	10.20174600	-3.23889400	3.04586300
C	10.85046600	-3.81311200	4.14828100
C	10.11643100	-4.23590500	5.26381900
C	8.72367700	-4.09970300	5.29724100
C	7.89401200	-2.53050900	1.99563400
H	-9.07178300	-0.23362600	-7.99597200
H	-10.95039400	-0.93663600	-6.54150700
H	-10.54282200	-1.50904400	-4.14530200
H	-6.75855900	-0.10283100	-7.09862900
H	-5.70615500	-1.65062500	-1.04312400
H	-2.76993700	-0.37483400	-3.93524200
H	-4.52321800	-0.15662900	-5.65687100
H	2.00195000	-1.56387000	4.25769900
H	3.21298700	-2.90914700	0.34538800
H	-0.24645200	-1.01481900	3.40342500

H	-1.56768600	-1.99514400	-2.72175000
H	-4.22087700	-0.38017000	0.26833800
H	-2.46249100	-0.59883200	1.98499900
H	3.36784600	-3.41022100	4.77000500
H	5.19840100	-1.90427000	1.16512400
H	5.58503900	-3.97753900	5.69029300
H	10.76889000	-2.90278400	2.18142600
H	11.93144000	-3.92700300	4.13962000
H	10.63375500	-4.67505200	6.11319700
H	8.16160700	-4.43184300	6.16687800
C	-0.02348800	-6.09609700	-0.98738900
C	-0.01537900	-4.75734900	-0.60827100
C	0.67172900	-3.78268100	-1.35105000
C	1.35304800	-4.20608100	-2.49542400
C	1.35687700	-5.54985700	-2.89291300
C	0.66932900	-6.49372900	-2.13910400
C	2.10346900	-2.01162100	-3.00794400
C	1.46756300	-1.45726700	-1.89350000
C	1.59034600	-0.07107500	-1.69995800
H	1.10512300	0.37982200	-0.83807600
C	2.31393600	0.72958100	-2.57833700
C	2.94168500	0.14765700	-3.68828000
C	2.83666700	-1.22149100	-3.90352200
H	-0.56453900	-6.82568000	-0.39140600
H	-0.55240300	-4.44886600	0.28499200
H	1.90322800	-5.82404600	-3.79055000
H	0.67228800	-7.53594000	-2.44708300
H	2.39098700	1.79847500	-2.40016700
H	3.51121400	0.76035100	-4.38207600
H	3.31148700	-1.70415500	-4.75264900
O	2.06074000	-3.35245700	-3.30856300
O	-8.18700800	-2.82604000	-2.52688600
H	-7.75826400	-3.38203000	-3.19724400
C	-8.59847900	-0.59472000	-1.79433500
C	-9.25245200	-1.16403900	-0.70163200
C	-8.55428400	0.80791200	-1.88447000
C	-9.85383900	-0.36687100	0.28340500
H	-9.29843500	-2.24338600	-0.61078600
C	-9.14417600	1.61005400	-0.91714400
H	-8.05222800	1.28039500	-2.72541300
C	-9.80203200	1.02643900	0.17882300
H	-10.35350700	-0.84899700	1.11629400

H	-9.11010800	2.69322600	-0.98973200
O	-10.35297000	1.89883500	1.07661500
C	-11.04916600	1.37613400	2.20935000
C	-11.56607000	2.55054300	3.02974300
H	-10.36706000	0.75379800	2.80781600
H	-11.88134700	0.74113200	1.87069600
C	-12.31783100	2.08774800	4.28724200
H	-10.71466200	3.18738300	3.29842200
H	-12.22993200	3.15690000	2.39831400
C	-12.95824300	3.22594200	5.10123800
H	-13.10933400	1.38362500	3.99144200
H	-11.63260100	1.52224500	4.93703200
H	-13.56813700	2.77930600	5.89985800
H	-13.65791300	3.78048300	4.45768900
C	-11.96110900	4.20824600	5.73359000
C	-12.63024800	5.26080800	6.62874600
H	-11.39057100	4.72189500	4.94719000
H	-11.22550000	3.64338100	6.32740300
C	-11.64105100	6.25539900	7.25173400
H	-13.37808200	5.81519100	6.04094600
H	-13.18833300	4.75459700	7.43145000
C	-12.31551300	7.29989300	8.14911200
H	-10.89099200	5.70201600	7.83572700
H	-11.08749800	6.76530200	6.44967900
H	-11.58239500	7.99589400	8.57452700
H	-13.04925800	7.89179200	7.58661200
H	-12.84541100	6.82312500	8.98397800
C	8.21005600	-1.07580500	1.65035200
C	8.51590800	-0.68009600	0.34830000
C	8.19707300	-0.09423000	2.65711900
C	8.80332400	0.65832900	0.04271700
H	8.53096200	-1.41960300	-0.44430900
C	8.47910600	1.23418600	2.37005900
H	7.96208000	-0.37301300	3.68159500
C	8.78480600	1.62264900	1.05482800
H	9.03615100	0.92489900	-0.98230400
H	8.46727600	1.99109400	3.14893700
O	7.98722600	-3.28319500	0.77425800
H	7.79146800	-4.21067000	0.98353100
O	9.04548900	2.95295600	0.87258000
C	9.33941700	3.42610800	-0.44275100
C	9.56195200	4.93069200	-0.36280800

H	8.50089100	3.19211100	-1.11540200
H	10.23707900	2.91897300	-0.82676600
C	9.87109000	5.55132100	-1.73226200
H	8.66467800	5.39572800	0.06693100
H	10.38589500	5.12910600	0.33555000
C	10.09312300	7.06914000	-1.66976600
H	10.76518200	5.07320300	-2.16042700
H	9.04573400	5.33651200	-2.42793100
H	9.20114800	7.54717100	-1.23747300
H	10.92098500	7.28560400	-0.97790700
C	10.39467600	7.70058700	-3.03567400
C	10.61171000	9.21887600	-2.97531000
H	9.56731000	7.48049600	-3.72760200
H	11.28800600	7.22359200	-3.46717200
C	10.91019100	9.85299200	-4.34077700
H	9.71901800	9.69614100	-2.54257700
H	11.44004000	9.44037200	-2.28490600
C	11.12171100	11.37020600	-4.27101700
H	11.80397100	9.37900300	-4.77251000
H	10.08347700	9.63073600	-5.03139800
H	11.33554600	11.79086500	-5.26105100
H	10.23056500	11.87734500	-3.87899900
H	11.96280300	11.62345100	-3.61265800
Trans-(R,R)-2O8-DPFOH-SFX-III			
C	11.28134100	-0.22277000	-4.31711000
C	11.06123900	1.10930400	-3.94412700
C	9.80069200	1.52140800	-3.48908400
C	8.77596700	0.58589800	-3.42036800
C	8.99112000	-0.75267300	-3.80094800
C	10.24837300	-1.16505300	-4.24915700
C	7.72783600	-1.49423700	-3.64045900
C	6.74385100	-0.61077400	-3.16018100
C	5.44487700	-1.03702200	-2.93113800
C	5.09396700	-2.38022800	-3.18269700
C	6.08946900	-3.25764600	-3.65802400
C	7.39890700	-2.82830700	-3.88838100
C	7.32060500	0.80247600	-2.98186200
C	-2.47916700	-5.03058600	-1.86770500
C	-2.73425300	-4.30017400	-0.68825500
C	-1.72443100	-3.45084600	-0.19182200
C	-0.51316500	-3.35036700	-0.86019000
C	-0.26938800	-4.08740900	-2.03409200

C	-1.26086500	-4.93306100	-2.54064400
C	1.08532200	-3.78427800	-2.50836000
C	1.67702900	-2.85940600	-1.62742700
C	2.96890600	-2.39895000	-1.83637600
C	3.70852700	-2.85925700	-2.94476900
C	3.10389500	-3.78398200	-3.82146600
C	1.80475500	-4.24840100	-3.61365800
C	0.71166600	-2.49576600	-0.48362400
C	-4.70371500	-5.65893200	0.09549800
C	-4.03603600	-4.41996600	0.01626100
C	-4.63355800	-3.29432500	0.62248600
C	-5.84653900	-3.42907700	1.27988100
C	-6.50207100	-4.67175500	1.35438100
C	-5.92767500	-5.79425400	0.75526800
C	-7.74948300	-4.50346600	2.12036800
C	-7.85614800	-3.15497100	2.51134200
C	-8.93524700	-2.71403800	3.26715300
C	-9.92351800	-3.63778400	3.63580800
C	-9.82478100	-4.97862600	3.24291900
C	-8.73730600	-5.42285800	2.48163000
C	-6.65064200	-2.34433400	2.01358200
H	12.26542100	-0.52865800	-4.66345700
H	11.87515000	1.82728700	-4.00406100
H	9.62703500	2.55260800	-3.19197800
H	10.42803900	-2.19679700	-4.54199500
H	4.69507600	-0.33297200	-2.57987200
H	5.83909000	-4.30193200	-3.82446700
H	8.14509200	-3.53350700	-4.24688700
H	-3.26024200	-5.66485900	-2.27791800
H	-1.88861100	-2.89487000	0.72773300
H	-1.09779800	-5.50291000	-3.45238200
H	3.42289500	-1.70420000	-1.13418800
H	3.65415400	-4.12344000	-4.69488900
H	1.36239300	-4.95419600	-4.31286100
H	-4.24200400	-6.53860600	-0.34466100
H	-4.15975600	-2.31884300	0.55174500
H	-6.41119600	-6.76700100	0.80561500
H	-9.01173400	-1.67100000	3.56399700
H	-10.77483000	-3.31065400	4.22725100
H	-10.60113600	-5.68253800	3.53221400
H	-8.66853400	-6.46587900	2.18170400
C	2.18594800	-4.62987300	2.35274900

C	1.67321500	-4.23241200	1.12179900
C	1.27898700	-2.90601300	0.87855700
C	1.42113500	-1.98926600	1.92383000
C	1.93569400	-2.37074300	3.17016000
C	2.31725100	-3.68987400	3.38407000
C	0.56436800	-0.19362900	0.62721400
C	0.37038200	-1.00277200	-0.49572300
C	-0.15798000	-0.39653500	-1.64791400
H	-0.31658000	-1.00784200	-2.53266300
C	-0.48071500	0.95655800	-1.68096500
C	-0.27698200	1.74485300	-0.54014500
C	0.24516300	1.17085300	0.61285100
H	2.48245400	-5.66324500	2.50917600
H	1.57158200	-4.96136500	0.32181100
H	2.02603500	-1.61723600	3.94695600
H	2.71688700	-3.98561800	4.35043000
H	-0.88867700	1.39517400	-2.58726500
H	-0.52561000	2.80276900	-0.55115200
H	0.41521700	1.75263500	1.51396500
O	1.07313700	-0.66366300	1.81439100
O	6.65391100	1.75267700	-3.83113000
H	6.71054000	1.42429800	-4.74288900
C	7.19068600	1.31633500	-1.54883800
C	6.43647300	2.44896900	-1.24208800
C	7.82182800	0.63308500	-0.49425100
C	6.30686000	2.90158200	0.07892400
H	5.94136500	2.99144200	-2.03948700
C	7.70210700	1.06854900	0.81833900
H	8.41684600	-0.25296800	-0.70258600
C	6.93982200	2.21052800	1.11661300
H	5.71108700	3.78610200	0.27505700
H	8.19017400	0.53918000	1.63150500
O	6.88156100	2.55896200	2.43767700
C	6.12825700	3.71224200	2.81574000
C	6.23060900	3.86735500	4.32749500
H	5.07953800	3.58674400	2.50787300
H	6.53015300	4.59998100	2.30484900
C	5.44508600	5.08548000	4.83666100
H	5.86525100	2.94540100	4.79542700
H	7.29021300	3.96478700	4.60107600
C	5.59180600	5.35090700	6.34542500
H	5.78115400	5.97968600	4.29136900

H	4.37839000	4.96229600	4.59482500
H	5.11386700	6.31402100	6.57623900
H	6.65816000	5.47446800	6.58811600
C	4.98493000	4.27098800	7.25360000
C	5.07559000	4.61636900	8.74668800
H	5.48560400	3.30820500	7.07947100
H	3.92890900	4.12185200	6.97941400
C	4.46224000	3.54960600	9.66423000
H	6.13123000	4.76566100	9.02109500
H	4.57499300	5.58003000	8.92795200
C	4.55915200	3.90319600	11.15317400
H	3.40695200	3.40180800	9.39161200
H	4.96153900	2.58630400	9.48408900
H	4.11065500	3.12316200	11.78027300
H	5.60485100	4.02134400	11.46551800
H	4.04025800	4.84558400	11.37167700
C	-7.04251800	-1.17784700	1.10805400
C	-6.62576200	0.12690900	1.37155000
C	-7.83485300	-1.40437700	-0.03148200
C	-6.98228000	1.18970800	0.52873300
H	-6.01442600	0.32559800	2.24447900
C	-8.19550800	-0.36263900	-0.87520000
H	-8.17583500	-2.41087200	-0.26231900
C	-7.77015200	0.94801400	-0.60065700
H	-6.63673900	2.18896600	0.76930000
H	-8.80790800	-0.53957000	-1.75463900
O	-5.90319100	-1.79152000	3.11088900
H	-5.63666600	-2.52610100	3.68682000
O	-8.17649100	1.90493200	-1.48954200
C	-7.77911400	3.25981400	-1.27345300
C	-8.36124400	4.10875200	-2.39590200
H	-6.68099500	3.32616700	-1.26525800
H	-8.14897700	3.60207300	-0.29543200
C	-7.98756800	5.59143600	-2.25874300
H	-8.00242400	3.71727400	-3.35708600
H	-9.45337500	3.99383700	-2.39535300
C	-8.56630500	6.46749800	-3.37868800
H	-8.33858200	5.97048000	-1.28692400
H	-6.89188000	5.69478600	-2.25025900
H	-8.21777300	6.08930500	-4.35150200
H	-9.66212100	6.36764500	-3.38692200
C	-8.19289100	7.95055000	-3.24774500

C	-8.77069900	8.83100000	-4.36425000
H	-7.09654200	8.04883400	-3.23973400
H	-8.53977500	8.32692900	-2.27321500
C	-8.39569000	10.31382600	-4.23386400
H	-8.42504900	8.45515500	-5.33950700
H	-9.86729500	8.73488800	-4.37225800
C	-8.97738500	11.18684400	-5.35222500
H	-8.74085800	10.68967800	-3.25950200
H	-7.30002900	10.41053200	-4.22727800
H	-8.69178200	12.23856500	-5.22905200
H	-8.62174700	10.85838300	-6.33742800
H	-10.07396000	11.13865500	-5.36345400
Trans-(S,S)-2O8-DPFOH-SFX-I			
C	10.67393500	-3.90822000	4.58301500
C	11.07675500	-2.58154700	4.78185500
C	10.20907800	-1.52214000	4.48052600
C	8.94332900	-1.81393900	3.98778400
C	8.53183900	-3.14647800	3.79297300
C	9.39830200	-4.20210500	4.08703000
C	7.14739900	-3.14025800	3.28807200
C	6.71261800	-1.80670600	3.18035600
C	5.43247400	-1.50125500	2.74549800
C	4.54162800	-2.54066500	2.40330900
C	4.99146000	-3.87264800	2.50655500
C	6.28226700	-4.18049100	2.94353100
C	7.82180900	-0.83497100	3.61095100
C	-3.01896300	-0.86933900	-0.07827400
C	-3.12572500	-1.87919000	-1.05718200
C	-2.02654200	-2.73824200	-1.26086000
C	-0.87501300	-2.58029700	-0.50411400
C	-0.78045800	-1.56891900	0.46994800
C	-1.86072900	-0.70742700	0.68271400
C	0.54171900	-1.64480300	1.10097100
C	1.26192500	-2.70415900	0.51763600
C	2.55331200	-3.00138000	0.92804400
C	3.16206600	-2.23774900	1.94471900
C	2.43042700	-1.17776300	2.52012500
C	1.13205600	-0.87597000	2.10864100
C	0.42842300	-3.40082300	-0.57185500
C	-4.84729200	-3.31268000	-2.20412600
C	-4.36821800	-2.03338400	-1.85579400
C	-5.09793900	-0.90318000	-2.28133800

C	-6.25301200	-1.07056800	-3.02911100
C	-6.71659800	-2.35206900	-3.37827900
C	-6.01045400	-3.48134900	-2.95943400
C	-7.93826600	-2.20760300	-4.18972700
C	-8.21734700	-0.83536500	-4.33824700
C	-9.30951800	-0.40491500	-5.08106400
C	-10.13620100	-1.36398600	-5.68346600
C	-9.86647200	-2.73012600	-5.53217400
C	-8.76547200	-3.16364000	-4.78417500
C	-7.16587600	0.01768000	-3.61387900
O	-6.45253900	0.86285500	-4.53284000
C	-7.76559500	0.93080100	-2.54406400
C	-7.54774700	2.31607700	-2.55335200
C	-8.09623300	3.13311200	-1.56688600
C	-8.87851000	2.58258000	-0.54324800
C	-9.10486600	1.19893100	-0.52109800
C	-8.54827600	0.39256700	-1.51730800
H	11.35921300	-4.71920000	4.81669600
H	12.07098000	-2.37214400	5.16811900
H	10.52064600	-0.49088500	4.62666600
H	9.09343300	-5.23518100	3.93776800
H	5.12721200	-0.46328400	2.64278400
H	4.30840600	-4.68272300	2.26574900
H	6.59393700	-5.21937200	3.02141200
H	-3.86822500	-0.21689200	0.10476200
H	-2.07493600	-3.50581900	-2.02921400
H	-1.81179200	0.07612000	1.43516200
H	3.10745500	-3.80468000	0.44905300
H	2.88038600	-0.59716900	3.32080200
H	0.59067500	-0.05758400	2.57730500
H	-4.31170100	-4.19180100	-1.85631900
H	-4.74370500	0.09690000	-2.04557800
H	-6.35543900	-4.48280500	-3.20562900
H	-9.51921700	0.65620700	-5.19037300
H	-10.99481400	-1.04563700	-6.26913600
H	-10.51874500	-3.46242800	-6.00144800
H	-8.56259500	-4.22627200	-4.67385200
H	-6.05447500	0.29372000	-5.21098000
H	-6.94530900	2.75570900	-3.33992400
H	-7.92799600	4.20630400	-1.57521400
H	-9.70659400	0.74073400	0.25589700
H	-8.73492600	-0.67832500	-1.48373800

O	-9.37170000	3.46602200	0.37714700
C	-10.17743800	2.97453500	1.44948400
C	-10.58052300	4.16185800	2.31390500
H	-9.60500200	2.24151300	2.03727700
H	-11.06569800	2.46811100	1.04324400
C	-11.44921600	3.75131600	3.51131000
H	-9.66996200	4.66495300	2.66551300
H	-11.11990900	4.88565400	1.68864700
C	-11.85690000	4.94121800	4.39146800
H	-12.35551800	3.24075000	3.15197100
H	-10.90636300	3.01712500	4.12570000
H	-10.95071800	5.45378300	4.74786300
H	-12.40130300	5.67494700	3.77821100
C	-12.72213000	4.54592000	5.59615000
C	-13.12630200	5.73719900	6.47547500
H	-12.17761100	3.81116300	6.20872200
H	-13.62912000	4.03398600	5.23989600
C	-13.98997800	5.34694400	7.68308000
H	-12.21932300	6.25025400	6.83051900
H	-13.67168200	6.47188000	5.86342700
C	-14.38756600	6.54463000	8.55420600
H	-14.89695600	4.83525500	7.32913800
H	-13.44513600	4.61373800	8.29564100
H	-15.00313300	6.23355800	9.40690700
H	-13.50179200	7.05691300	8.95174200
H	-14.96381700	7.27990700	7.97774300
C	2.10055600	-1.90140600	-3.69250500
C	1.52797400	-2.03632100	-2.43130000
C	1.08521800	-3.27982300	-1.95034700
C	1.24201700	-4.38761700	-2.78788200
C	1.81620200	-4.27170300	-4.06052600
C	2.24407500	-3.02876000	-4.51245100
C	0.37654600	-5.88957900	-1.16501000
C	0.16860700	-4.87120800	-0.23015800
C	-0.31958100	-5.24203600	1.03392200
H	-0.48818900	-4.46574800	1.77575700
C	-0.59202300	-6.56911000	1.35311200
C	-0.37645600	-7.57013800	0.39607100
C	0.10823600	-7.23126800	-0.86195200
H	2.43365500	-0.92589400	-4.03534700
H	1.41639300	-1.16160300	-1.79588500
H	1.91621800	-5.16585100	-4.66872700

H	2.69021100	-2.93802100	-5.49923900
H	-0.96954600	-6.82331300	2.33960900
H	-0.58395900	-8.61055600	0.63189900
H	0.29001200	-7.98212800	-1.62526800
O	0.85009400	-5.65816000	-2.43445500
O	7.41437900	-0.04270600	4.74012900
H	7.16907000	-0.65241100	5.45450100
C	8.22441300	0.13769200	2.50338400
C	8.13955200	1.51974100	2.67222800
C	8.69175000	-0.35327100	1.27125900
C	8.50876500	2.40277800	1.64673200
H	7.78253300	1.92126500	3.61391200
C	9.06148100	0.50795600	0.24761300
H	8.76771100	-1.42591600	1.10954300
C	8.97328100	1.89864400	0.42818900
H	8.42775500	3.47055500	1.81791100
H	9.42268400	0.12664900	-0.70308700
O	9.36381200	2.66245900	-0.63668400
C	9.29130100	4.08532300	-0.53240400
C	9.79666200	4.67804200	-1.84122100
H	9.90752900	4.42692800	0.31246500
H	8.25116300	4.38901600	-0.34151200
C	9.74737200	6.21226000	-1.84957700
H	10.82590100	4.33349900	-2.00853700
H	9.19163100	4.27790100	-2.66564000
C	10.27581400	6.82346700	-3.15509000
H	8.71205200	6.54802200	-1.68680300
H	10.33372500	6.60482900	-1.00494300
H	11.31398100	6.49468400	-3.31321900
H	9.69691900	6.42458100	-4.00165000
C	10.21993100	8.35702700	-3.18067000
C	10.75949000	8.96817400	-4.48122700
H	10.79182600	8.75562700	-2.32875400
H	9.18000500	8.68492300	-3.03019400
C	10.70000700	10.50163200	-4.51223500
H	11.80088000	8.64371200	-4.62984000
H	10.19098000	8.56710400	-5.33434100
C	11.24562800	11.10251000	-5.81330100
H	9.65912500	10.82651300	-4.36789100
H	11.26601100	10.90310100	-3.65884900
H	11.18772400	12.19768200	-5.80409600
H	12.29660200	10.82577000	-5.96761600

Cis-(S,S)-2O8-DPFOH-SFX-II

C	8.58912700	-2.34039600	-6.71934700
C	9.66002300	-2.34754400	-5.81661600
C	9.42626500	-2.42987000	-4.43652200
C	8.11528100	-2.51089700	-3.98398500
C	7.03605300	-2.51095800	-4.88857900
C	7.26818100	-2.42158800	-6.26318300
C	5.78261600	-2.62568800	-4.12250700
C	6.09550500	-2.69780600	-2.75280900
C	5.10207500	-2.82195900	-1.79403000
C	3.74895800	-2.88045700	-2.19004600
C	3.44779500	-2.80430300	-3.56518800
C	4.44869200	-2.67632800	-4.53123700
C	7.61490300	-2.63242100	-2.53670500
C	-2.18247000	-3.63661900	3.32111800
C	-3.13276600	-2.80680100	2.69091400
C	-2.78714500	-2.19348000	1.46960300
C	-1.53485300	-2.41325200	0.91512900
C	-0.59497200	-3.24479800	1.55257000
C	-0.92211800	-3.85965200	2.76494300
C	0.62410900	-3.28942000	0.73744500
C	0.43571400	-2.48533800	-0.40225300
C	1.43734000	-2.34465300	-1.35122900
C	2.66602700	-3.01517200	-1.18300400
C	2.84301100	-3.81755500	-0.03650000
C	1.83774400	-3.95911500	0.92069000
C	-0.96161600	-1.83833700	-0.39378000
C	-4.61580100	-2.42465400	4.68970300
C	-4.46972200	-2.58041500	3.29642900
C	-5.62222300	-2.50617500	2.48589400
C	-6.86053500	-2.28584100	3.06856500
C	-6.99452700	-2.13412000	4.46068100
C	-5.86402100	-2.20274700	5.27707400
C	-8.41863300	-1.92775000	4.77859900
C	-9.15419700	-1.95655800	3.57804100
C	-10.53511000	-1.80384700	3.58344900
C	-11.18891100	-1.61791600	4.80985400
C	-10.46016000	-1.58189200	6.00546300
C	-9.06881800	-1.73648200	6.00007600
C	-8.22903300	-2.19845800	2.37609500
O	-8.55695300	-3.42747000	1.70512700
C	-8.29601300	-1.08740800	1.32841400

C	-8.64645900	-1.35087000	-0.00356900
C	-8.69070600	-0.32664700	-0.94738400
C	-8.38325900	0.99016300	-0.58114600
C	-8.03609700	1.26907900	0.74850300
C	-7.99687000	0.23185800	1.68359900
H	8.78545700	-2.27104300	-7.78637200
H	10.67931800	-2.28376800	-6.18879100
H	10.25464700	-2.42726800	-3.73244400
H	6.44302300	-2.41607600	-6.97138600
H	5.36532000	-2.84429300	-0.73984800
H	2.41161400	-2.87169500	-3.88529200
H	4.18135200	-2.62847500	-5.58421500
H	-2.44821300	-4.13592400	4.24906800
H	-3.49484900	-1.53046000	0.97822800
H	-0.21447100	-4.51351200	3.26925400
H	1.28733400	-1.69732200	-2.21156400
H	3.77636100	-4.35869300	0.09257500
H	2.00168200	-4.59214300	1.78962000
H	-3.73144200	-2.44975300	5.32085700
H	-5.54342700	-2.64176300	1.41040500
H	-5.94108200	-2.07679900	6.35447900
H	-11.09693900	-1.82630200	2.65298200
H	-12.26893700	-1.49718600	4.83304400
H	-10.98039800	-1.43246600	6.94831300
H	-8.51105500	-1.70834700	6.93323100
H	-8.51863500	-4.14207100	2.36089800
H	-8.88129000	-2.36590700	-0.30288400
H	-8.95906500	-0.53215300	-1.97977600
H	-7.79385300	2.27679500	1.06663800
H	-7.72215100	0.46737700	2.70922100
O	-8.44738100	1.92352400	-1.57915500
C	-8.12509000	3.28170000	-1.27579700
C	-8.23904900	4.09446000	-2.55875700
H	-7.10358400	3.33798100	-0.87137900
H	-8.81703400	3.66360400	-0.51021400
C	-7.92147800	5.57968000	-2.33578400
H	-7.55503900	3.67067400	-3.30604300
H	-9.25507400	3.98223400	-2.95986700
C	-7.99942700	6.41610900	-3.62071200
H	-8.61685400	5.99600200	-1.59124300
H	-6.91433700	5.67872000	-1.90307300
H	-7.29842200	6.00524400	-4.36279000

H	-9.00324900	6.31470100	-4.05994300
C	-7.69030400	7.90314400	-3.39947300
C	-7.74980500	8.74184700	-4.68350600
H	-6.69102900	8.00210100	-2.94848200
H	-8.39843200	8.31498100	-2.66422100
C	-7.44583100	10.22978000	-4.46022700
H	-7.03805400	8.33361500	-5.41742600
H	-8.74721900	8.64118300	-5.13833400
C	-7.50095400	11.05964100	-5.74851400
H	-8.15992700	10.63919600	-3.73069400
H	-6.45080900	10.33074100	-4.00251800
H	-7.28169400	12.11650800	-5.55414000
H	-6.77141200	10.69792000	-6.48466200
H	-8.49410800	11.00538600	-6.21299900
C	-0.03964200	1.71206900	0.75409800
C	-0.13904900	0.32613200	0.68153100
C	-0.86788300	-0.31061400	-0.33680700
C	-1.49673800	0.50189700	-1.28415600
C	-1.40793300	1.89933100	-1.22760700
C	-0.67995800	2.50339600	-0.20925700
C	-2.37077200	-1.35677200	-2.47667400
C	-1.79013200	-2.28067300	-1.60329300
C	-2.00044400	-3.64428700	-1.86877600
H	-1.55802400	-4.37952400	-1.20139800
C	-2.75738000	-4.07016000	-2.95593500
C	-3.33020900	-3.12203300	-3.81483100
C	-3.13708600	-1.76654100	-3.57606500
H	0.53298500	2.17393600	1.55345500
H	0.35888800	-0.28750900	1.42784100
H	-1.91538000	2.48257000	-1.99035100
H	-0.61004700	3.58706300	-0.16577100
H	-2.90291300	-5.13204500	-3.13338100
H	-3.92649500	-3.43998400	-4.66592200
H	-3.56875400	-1.00618700	-4.22015100
O	-2.23851700	0.00363500	-2.32888400
O	8.10624100	-3.83214900	-1.91284800
H	7.85987300	-4.58036200	-2.48014800
C	8.04774300	-1.46121800	-1.65633300
C	8.83716900	-1.64855100	-0.52166300
C	7.66032200	-0.15033900	-1.98657600
C	9.23698400	-0.56498900	0.27427700
H	9.14756000	-2.65045800	-0.24734700

C	8.04756500	0.93187700	-1.20833600
H	7.04505500	0.02705800	-2.86544600
C	8.84257000	0.73227000	-0.06720400
H	9.85054900	-0.75300200	1.14847600
H	7.74551400	1.94323500	-1.46439900
O	9.17177300	1.85947200	0.63402000
C	9.99185100	1.73399300	1.79688800
C	10.20982400	3.12668300	2.37350500
H	10.95169900	1.27112800	1.52314100
H	9.49565600	1.08195300	2.53107100
C	11.10227000	3.10886300	3.62240600
H	10.65955000	3.76199800	1.59894800
H	9.23259500	3.56572000	2.61462900
C	11.32666500	4.50339300	4.22396300
H	10.65439200	2.45485200	4.38592400
H	12.07685500	2.66371300	3.37091900
H	11.76809800	5.16055700	3.45966200
H	10.35335100	4.94679300	4.48271500
C	12.22727000	4.49519400	5.46678200
C	12.45082200	5.88788700	6.07196200
H	13.20097800	4.05297000	5.20601300
H	11.78705100	3.83495800	6.22965500
C	13.35454900	5.88208300	7.31269300
H	12.88895900	6.54952200	5.30898500
H	11.47768700	6.32995800	6.33555100
C	13.57180500	7.27773200	7.90967600
H	12.91706700	5.22195200	8.07596600
H	14.32743200	5.44161900	7.04962600
H	14.21988000	7.23932000	8.79361400
H	14.04120500	7.95179300	7.18142300
H	12.61962200	7.73138200	8.21403200
Trans-(S,S)-2O8-DPFOH-SFX-III			
C	9.64964800	-6.41706500	-0.88747900
C	9.71455800	-5.85965900	0.39594200
C	8.78910300	-4.88516600	0.79581500
C	7.80562500	-4.48849700	-0.10180700
C	7.73234700	-5.05190600	-1.39019400
C	8.65829400	-6.01777300	-1.79157700
C	6.58390000	-4.45785100	-2.09682400
C	5.95192000	-3.53958400	-1.23854000
C	4.82441200	-2.83992100	-1.63956400
C	4.29497100	-3.04580800	-2.93123100

C	4.94025200	-3.96349100	-3.78452200
C	6.07652700	-4.66883800	-3.38023500
C	6.67912400	-3.46811800	0.11367200
C	-2.29655700	1.04088100	-5.37250200
C	-3.00536600	1.00264600	-4.15377400
C	-2.41566100	0.34885600	-3.05255000
C	-1.16566100	-0.23750400	-3.18436600
C	-0.46850700	-0.19383300	-4.40633600
C	-1.03962100	0.45018900	-5.50791000
C	0.81226600	-0.89037900	-4.24351700
C	0.90518600	-1.36333800	-2.92118100
C	2.02361800	-2.06088400	-2.48891000
C	3.08799400	-2.30627900	-3.38008500
C	2.98233800	-1.82874800	-4.70300300
C	1.85885400	-1.12631600	-5.14023900
C	-0.35581500	-1.00040100	-2.11750000
C	-5.26784500	1.58710100	-5.09138000
C	-4.34152200	1.63889600	-4.02996400
C	-4.71446100	2.30534200	-2.84340100
C	-5.96612700	2.89371200	-2.74823700
C	-6.87784300	2.84493000	-3.81849800
C	-6.52798500	2.18297500	-4.99690300
C	-8.09833300	3.57540400	-3.43396700
C	-7.92937100	4.07288700	-2.12754100
C	-8.92519300	4.82393800	-1.51557700
C	-10.10872200	5.07973900	-2.22263600
C	-10.28357200	4.58054200	-3.51958700
C	-9.27993500	3.82429800	-4.13629900
C	-6.55270900	3.68252000	-1.56806500
O	-5.76012000	4.84297200	-1.26465000
C	-6.64426800	2.85748000	-0.28406100
C	-6.08268500	3.30560500	0.92012400
C	-6.18132900	2.54358000	2.08252000
C	-6.84530800	1.30996600	2.06831800
C	-7.41366600	0.85037700	0.87178900
C	-7.30680600	1.62573300	-0.28549000
H	10.37686900	-7.16843400	-1.18500800
H	10.49073600	-6.18227100	1.08515500
H	8.84014400	-4.44529900	1.78867600
H	8.61425400	-6.45709000	-2.78535800
H	4.36768700	-2.11422700	-0.97174400
H	4.52822900	-4.14762900	-4.77313000

H	6.54429000	-5.37775000	-4.05939400
H	-2.72764900	1.56704000	-6.21993900
H	-2.95286200	0.28598500	-2.10955200
H	-0.51377000	0.50551400	-6.45824300
H	2.07255600	-2.43859200	-1.47067400
H	3.80880500	-1.98666200	-5.39064600
H	1.81202500	-0.76048800	-6.16328200
H	-5.00520400	1.04821200	-5.99778100
H	-4.01554900	2.37771900	-2.01431200
H	-7.22154800	2.11888800	-5.83204000
H	-8.78905200	5.20349900	-0.50595900
H	-10.89832200	5.66598800	-1.75961000
H	-11.20855600	4.78291700	-4.05382400
H	-9.42343100	3.44272200	-5.14449300
H	-5.69874200	5.37889000	-2.07161200
H	-5.56161900	4.25575300	0.94422100
H	-5.74309300	2.88965100	3.01431800
H	-7.93451700	-0.09937000	0.82555400
H	-7.75176100	1.25133900	-1.20448000
O	-6.88392300	0.63384400	3.25685100
C	-7.53229000	-0.63789500	3.30927000
C	-7.40621600	-1.17318400	4.72957100
H	-7.05849200	-1.32470800	2.59233300
H	-8.59007300	-0.52623800	3.02768400
C	-8.08756900	-2.53787300	4.90255300
H	-6.34055900	-1.24926500	4.98342600
H	-7.84501900	-0.44268100	5.42213800
C	-7.94947200	-3.10561600	6.32224700
H	-9.15539100	-2.45047100	4.65105700
H	-7.66125000	-3.25532000	4.18502300
H	-6.88177500	-3.19971700	6.57128300
H	-8.36884800	-2.38699100	7.04237400
C	-8.63533700	-4.46633300	6.50620300
C	-8.48679700	-5.04206000	7.92124400
H	-8.22210000	-5.18193400	5.77896300
H	-9.70485200	-4.36936100	6.26468200
C	-9.17485900	-6.40140000	8.10814300
H	-7.41725100	-5.14194600	8.16189200
H	-8.89723500	-4.32629100	8.64999700
C	-9.01773100	-6.96999800	9.52358300
H	-10.24420200	-6.30137500	7.87097000
H	-8.76633900	-7.11695200	7.37950800

H	-9.51740800	-7.94120400	9.62308100
H	-7.95945800	-7.11195100	9.77834400
H	-9.45047600	-6.29442300	10.27281100
C	-2.13470500	-4.40849800	-2.15361000
C	-1.43297300	-3.27515400	-2.55319400
C	-1.10382500	-2.25224900	-1.64840600
C	-1.50472700	-2.41340900	-0.31917300
C	-2.21206000	-3.54755000	0.10182900
C	-2.52740100	-4.54340000	-0.81501500
C	-0.48377500	-0.38115000	0.36250700
C	-0.02319000	-0.09741000	-0.92618800
C	0.74434800	1.06655100	-1.09864000
H	1.11347900	1.30555600	-2.09268700
C	1.03950800	1.91269500	-0.03402900
C	0.56273700	1.60548900	1.24753500
C	-0.19773600	0.45928300	1.44653700
H	-2.37463100	-5.18178300	-2.87801600
H	-1.12837300	-3.17035800	-3.59131900
H	-2.49827500	-3.62165900	1.14682500
H	-3.07555900	-5.42321400	-0.48850800
H	1.63646500	2.80511700	-0.19969600
H	0.78399400	2.25808600	2.08789700
H	-0.58218800	0.19200400	2.42634800
O	-1.24160300	-1.48863100	0.66270500
O	5.81634700	-3.85927800	1.19540600
H	5.46877200	-4.74244400	0.99151400
C	7.18817400	-2.06325600	0.43335800
C	6.69864400	-1.33595600	1.51840900
C	8.15537200	-1.45908300	-0.38921700
C	7.15345900	-0.03725100	1.78886100
H	5.95353900	-1.78233600	2.16718700
C	8.61508000	-0.17423500	-0.13435300
H	8.55578000	-2.00219000	-1.24191200
C	8.11493500	0.55008000	0.96067400
H	6.74843300	0.49412200	2.64291800
H	9.36294500	0.29039800	-0.77038600
O	8.62921700	1.80637500	1.12923300
C	8.14351600	2.61126800	2.20473800
C	8.86080300	3.95366100	2.15293900
H	8.33497500	2.10421000	3.16216900
H	7.05653100	2.74652900	2.10178000
C	8.38513300	4.91185900	3.25397500

H	9.94157400	3.78119500	2.24345200
H	8.69403900	4.40384100	1.16526300
C	9.10120700	6.26943100	3.22570200
H	7.30110000	5.07404100	3.15471400
H	8.53598700	4.44533400	4.23936200
H	8.96292600	6.73112100	2.23640400
H	10.18408900	6.11063300	3.33989200
C	8.61309900	7.23974300	4.31017800
C	9.32949300	8.59688100	4.28839000
H	8.74626600	6.77554600	5.29940200
H	7.53043200	7.39950900	4.19186900
C	8.83438600	9.57124800	5.36622900
H	10.41172600	8.43890900	4.41368900
H	9.20220000	9.05914000	3.29739700
C	9.55706200	10.92329300	5.33908100
H	7.75366200	9.73177900	5.23958800
H	8.96003300	9.10945800	6.35662600
H	9.17948100	11.59520500	6.11936300
H	10.63598400	10.79985600	5.49948500
H	9.42188800	11.42608000	4.37265200
Cis-(R,S)-2O8-DPFOH-SFX-I			
C	11.29033300	-4.21036300	1.22130800
C	11.73651300	-3.43411000	0.14416200
C	10.82830500	-2.68354000	-0.61605900
C	9.48002900	-2.72933300	-0.28405800
C	9.02642100	-3.51472000	0.79307200
C	9.93160300	-4.25756000	1.55474900
C	7.56171800	-3.38174300	0.88585200
C	7.12238000	-2.51244800	-0.12920600
C	5.77717600	-2.21973900	-0.29179400
C	4.82457300	-2.79907000	0.57287200
C	5.27690300	-3.66416200	1.58959900
C	6.63272900	-3.95929000	1.75341800
C	8.30603400	-2.02044800	-0.97579500
C	-3.08856900	-1.11778400	-0.23280800
C	-3.58708100	-2.41104900	0.03047200
C	-2.66670700	-3.44209900	0.30965400
C	-1.30629200	-3.17171600	0.32387100
C	-0.82160300	-1.87799700	0.05580800
C	-1.72058700	-0.84456100	-0.22450500
C	0.64303900	-1.89693100	0.13504000
C	1.06195100	-3.20122800	0.45785700

C	2.40803900	-3.50428200	0.60157800
C	3.37842600	-2.49812700	0.41970800
C	2.94676500	-1.19659000	0.08955500
C	1.59337400	-0.88876200	-0.05234300
C	-0.14629400	-4.14666800	0.59894800
C	-5.62535800	-3.58837700	0.92252600
C	-5.04759900	-2.67956100	0.01260500
C	-5.89036200	-2.02781300	-0.91264900
C	-7.25045700	-2.29492300	-0.91291700
C	-7.81338600	-3.21402900	-0.00889500
C	-6.99536200	-3.86201800	0.91854800
C	-9.26023500	-3.30911900	-0.27131500
C	-9.58009000	-2.44484900	-1.33599100
C	-10.88164800	-2.34998400	-1.81247900
C	-11.87882300	-3.13150200	-1.21165900
C	-11.56638100	-3.98644100	-0.14701900
C	-10.25467300	-4.08277600	0.33217400
C	-8.32870200	-1.71115900	-1.83906500
O	-8.06008300	-2.00964200	-3.21900300
C	-8.43736800	-0.18987300	-1.72465400
C	-8.18659400	0.65116600	-2.81840700
C	-8.27274400	2.03621600	-2.69010100
C	-8.61090000	2.61572200	-1.46010000
C	-8.86455400	1.78680100	-0.35796000
C	-8.77577700	0.40004800	-0.50252700
H	12.00672800	-4.78345400	1.80463700
H	12.79514700	-3.41048800	-0.10139500
H	11.17186100	-2.07489500	-1.44881200
H	9.59375400	-4.86462800	2.39132000
H	5.45678400	-1.56478600	-1.09786700
H	4.55536100	-4.09276700	2.27990700
H	6.94911800	-4.62452200	2.55335300
H	-3.78766500	-0.30819600	-0.42303500
H	-3.02386800	-4.45344700	0.48702000
H	-1.36816000	0.16442100	-0.42510400
H	2.71891000	-4.52124200	0.82792900
H	3.68508900	-0.40859100	-0.03123100
H	1.29105000	0.12663000	-0.29739200
H	-4.99295600	-4.07224300	1.66174600
H	-5.47356000	-1.33559900	-1.63930100
H	-7.40882100	-4.56607500	1.63679100
H	-11.12112500	-1.68019500	-2.63461700

H	-12.90260200	-3.07099800	-1.57189500
H	-12.35098500	-4.58290200	0.31187600
H	-10.02080000	-4.75098800	1.15758200
H	-7.96459800	-2.97214900	-3.30092100
H	-7.92523400	0.21660100	-3.77652800
H	-8.08087600	2.68715700	-3.53839400
H	-9.13011200	2.20155100	0.60796400
H	-8.97747900	-0.22652500	0.36309100
O	-8.66922700	3.98223200	-1.43383200
C	-9.00925100	4.63589500	-0.21001000
C	-9.00913100	6.13829800	-0.45947400
H	-8.27684500	4.37014200	0.56683900
H	-10.00107100	4.29893900	0.12629200
C	-9.36695800	6.93796600	0.80123100
H	-8.01760400	6.43592900	-0.82565100
H	-9.72341100	6.36212100	-1.26293000
C	-9.38308200	8.45567000	0.57063400
H	-10.35352200	6.61957700	1.17074300
H	-8.64933700	6.70228200	1.60167900
H	-8.39823800	8.77655900	0.19928800
H	-10.10257100	8.69293800	-0.22740600
C	-9.73794700	9.26006300	1.82883500
C	-9.76341900	10.77772900	1.60116100
H	-9.01536600	9.02484400	2.62520100
H	-10.72043000	8.93349500	2.20260700
C	-10.11906900	11.58207700	2.85932300
H	-8.78145900	11.10614800	1.22743000
H	-10.48643900	11.01368800	0.80531600
C	-10.14707600	13.09679900	2.62237200
H	-11.09929700	11.25243400	3.23382200
H	-9.39509400	11.34953300	3.65401800
H	-10.40373500	13.64110300	3.53927300
H	-9.17053400	13.46293500	2.27992900
H	-10.88751800	13.36486100	1.85758800
C	0.00143300	-5.97176400	-2.78045400
C	-0.04870600	-4.97043700	-1.81562600
C	-0.09971100	-5.26776800	-0.44343900
C	-0.09897200	-6.61611000	-0.07611200
C	-0.04832000	-7.63848500	-1.03303500
C	0.00192100	-7.31607500	-2.38414600
C	-0.22511200	-6.10977200	2.24108900
C	-0.23140500	-4.73097000	2.01188700

C	-0.31262800	-3.88820200	3.13317400
H	-0.31854900	-2.81248900	2.97691100
C	-0.38467100	-4.39540100	4.42704100
C	-0.37693000	-5.78257900	4.62850100
C	-0.29742600	-6.63929400	3.53684100
H	0.03975000	-5.70867300	-3.83377800
H	-0.04864500	-3.92798300	-2.12355300
H	-0.05062900	-8.66952000	-0.69184600
H	0.04069600	-8.10860400	-3.12670300
H	-0.44658300	-3.71686900	5.27325600
H	-0.43311400	-6.19289700	5.63329200
H	-0.28973200	-7.71860900	3.65735500
O	-0.14782900	-7.03948400	1.23178300
O	8.17802800	-2.43474800	-2.34672200
H	8.08482800	-3.40089300	-2.35643600
C	8.44497000	-0.49802200	-0.98231100
C	8.44760600	0.23570700	-2.17731800
C	8.57492300	0.20165300	0.22186000
C	8.57677100	1.62315500	-2.16452000
H	8.34718800	-0.28498400	-3.12274300
C	8.70516900	1.59257300	0.25073500
H	8.57569600	-0.33976700	1.16511200
C	8.70689400	2.31313000	-0.95212300
H	8.57891500	2.19092800	-3.09065800
H	8.80392800	2.09448700	1.20667800
O	8.82809300	3.67246900	-1.04423900
C	8.97006100	4.43923000	0.15268800
C	9.08678500	5.90638800	-0.23966200
H	9.86670000	4.11002400	0.69889900
H	8.09636500	4.27800500	0.80164100
C	9.26004100	6.81947600	0.98322900
H	9.93365300	6.01329000	-0.92806400
H	8.18521800	6.19401500	-0.79788700
C	9.27476800	8.32345100	0.65758600
H	8.44240400	6.62523800	1.69294700
H	10.19036300	6.55634900	1.50942400
H	9.27694500	8.88252600	1.60449400
H	8.33709800	8.59219600	0.14787400
C	10.46659600	8.79008800	-0.19170400
C	10.49530400	10.30962900	-0.40855900
H	10.44900000	8.29083400	-1.17066800
H	11.40240600	8.47599400	0.29646600

C	11.68070000	10.78870200	-1.25786900
H	9.55608600	10.62547900	-0.88830700
H	10.52295200	10.81576800	0.56873400
C	11.70187500	12.30802700	-1.46451500
H	12.61946500	10.47171800	-0.78026200
H	11.65148500	10.28702000	-2.23614700
H	12.56070200	12.61803600	-2.07208900
H	10.79219200	12.65161600	-1.97384300
H	11.76385000	12.83773000	-0.50501200
Trans-(R,S)-2O8-DPFOH-SFX-II			
C	-7.63918000	7.13405600	1.57800300
C	-8.56307800	6.83181200	0.56949900
C	-8.40937400	5.67904400	-0.21377900
C	-7.32179500	4.84823800	0.02522200
C	-6.38663400	5.15268900	1.03286200
C	-6.54308500	6.29725400	1.81824400
C	-5.34240800	4.11334500	1.03250800
C	-5.64083700	3.17329100	0.02932500
C	-4.80479000	2.09506900	-0.21634800
C	-3.63284300	1.92766400	0.55147100
C	-3.35105400	2.86951600	1.56196900
C	-4.19199200	3.95747500	1.80782900
C	-6.93561600	3.55294800	-0.70522400
O	-6.70010500	3.78562100	-2.10394900
C	-8.01569200	2.47602900	-0.60619300
C	-8.61460300	1.92828700	-1.74059900
C	-9.61503700	0.95017100	-1.63582300
C	-10.02762700	0.50967500	-0.37465700
C	-9.42728700	1.05185200	0.77426200
C	-8.43866900	2.01861400	0.65449400
C	1.38600000	-4.32688400	-0.79580600
C	2.60042000	-3.64664400	-0.56875200
C	2.55301400	-2.28117200	-0.22170700
C	1.32934800	-1.63684000	-0.11419700
C	0.12364800	-2.32604800	-0.34414100
C	0.15368300	-3.68146200	-0.68628000
C	-0.99470800	-1.39384100	-0.16193600
C	-0.47802600	-0.12945900	0.17705400
C	-1.31998900	0.94852300	0.40632500
C	-2.71650700	0.78552800	0.30390300
C	-3.22258200	-0.48604700	-0.03747200
C	-2.37727800	-1.57141600	-0.27090200

C	1.06153000	-0.16134300	0.23202300
C	4.11717700	-5.29253600	-1.72076300
C	3.90243600	-4.34964600	-0.69525700
C	4.95619200	-4.08086600	0.20362500
C	6.16554300	-4.74423700	0.06467400
C	6.36696600	-5.68655500	-0.96035500
C	5.33625600	-5.96070800	-1.86125300
C	7.73097300	-6.23124600	-0.84069000
C	8.36062300	-5.62308000	0.26227300
C	9.65878800	-5.96439800	0.62053100
C	10.33682600	-6.92930900	-0.13793900
C	9.71596200	-7.53273400	-1.23899100
C	8.40790100	-7.18879300	-1.59980700
C	7.41538600	-4.62563600	0.94944600
O	7.13674000	-5.02102400	2.30419100
C	7.97978800	-3.20645400	1.00831400
C	8.21691300	-2.56041200	2.23022100
C	8.73996600	-1.26976600	2.26700200
C	9.03962700	-0.59107200	1.07856900
C	8.80915500	-1.22499700	-0.15064500
C	8.28412000	-2.51975000	-0.17149900
H	-7.77421500	8.02863700	2.18082800
H	-9.40783000	7.49359900	0.39638300
H	-9.12881700	5.43735200	-0.99216700
H	-5.82961800	6.54042100	2.60201600
H	-5.03966800	1.39656700	-1.01513100
H	-2.46878200	2.73363900	2.18137200
H	-3.94758300	4.66285800	2.59850700
H	-6.01665300	4.47099800	-2.17807500
H	-8.30253000	2.26440300	-2.72298400
H	-10.05577900	0.54917900	-2.54199300
H	-9.75420800	0.70156100	1.74899400
H	-7.98952600	2.42669500	1.55677900
H	1.40937600	-5.38631200	-1.03683800
H	3.47725700	-1.73032200	-0.06595100
H	-0.76622600	-4.23542900	-0.85794500
H	-0.90523500	1.92578700	0.64047800
H	-4.29791200	-0.63092200	-0.09427100
H	-2.79865300	-2.54170900	-0.52302200
H	3.32354200	-5.48499700	-2.43782900
H	4.81460800	-3.37311600	1.01624800
H	5.47216500	-6.67462100	-2.67026500

H	10.13976700	-5.48969300	1.47213800
H	11.35313400	-7.20868300	0.12782200
H	10.25555000	-8.27646700	-1.82007000
H	7.93313600	-7.66337800	-2.45533700
H	6.78697400	-5.92621300	2.28245600
H	7.98610100	-3.07221900	3.15738800
H	8.92050200	-0.76857800	3.21371700
H	9.02874900	-0.72798600	-1.08891100
H	8.11025200	-2.99452300	-1.13442000
O	9.54635700	0.67127400	1.22024500
O	-10.99466500	-0.43086800	-0.15112900
C	9.87064800	1.42585600	0.05151100
C	10.40972400	2.77697200	0.50279300
H	8.97135500	1.55208700	-0.56951100
H	10.62299100	0.88504100	-0.54183000
C	10.80025800	3.67947100	-0.67600400
H	9.64713500	3.27180600	1.11876400
H	11.27971700	2.60900600	1.15143800
C	11.34898400	5.04258300	-0.23135900
H	11.55513600	3.17100800	-1.29473700
H	9.92575400	3.83626100	-1.32551100
H	10.59449700	5.55190300	0.38687700
H	12.22196200	4.88569200	0.41994700
C	11.74687000	5.95525200	-1.39956700
C	12.29837400	7.31596200	-0.95222300
H	10.87335600	6.11371300	-2.05035000
H	12.50018600	5.44457000	-2.01871100
C	12.70070300	8.23156500	-2.11675600
H	11.54503800	7.82780000	-0.33389500
H	13.17081600	7.15731800	-0.29985600
C	13.25244600	9.58668500	-1.65773100
H	13.45352000	7.72089300	-2.73500200
H	11.82924400	8.39297200	-2.76804500
H	13.53072700	10.21641100	-2.51144300
H	12.50998600	10.13723000	-1.06556100
H	14.14565200	9.45942100	-1.03237400
C	-11.68164300	-1.00163500	-1.26621600
C	-12.73200800	-1.96091400	-0.72163900
H	-10.96463000	-1.52885400	-1.91312800
H	-12.15308500	-0.20314300	-1.85821300
C	-13.55359100	-2.62585600	-1.83639600
H	-12.22834000	-2.72938700	-0.11928800

H	-13.38435300	-1.40175200	-0.04054100
C	-14.58043500	-3.65661700	-1.33360700
H	-14.07612800	-1.85252400	-2.41985300
H	-12.86903900	-3.12718400	-2.53634600
H	-15.02080300	-4.16235200	-2.20512400
H	-14.05665200	-4.43722900	-0.76109700
C	-15.71391100	-3.07234100	-0.47773700
C	-16.76711900	-4.11276700	-0.07129100
H	-16.20449200	-2.25933900	-1.03561600
H	-15.29954900	-2.61337600	0.43067600
C	-17.89765500	-3.53670900	0.79202100
H	-17.19845000	-4.56790500	-0.97620000
H	-16.27571500	-4.93172700	0.47647500
C	-18.94517700	-4.58091000	1.19666900
H	-17.46651800	-3.08244700	1.69614500
H	-18.38984600	-2.71886800	0.24530400
H	-19.73690400	-4.13617900	1.81170800
H	-19.42101600	-5.02861900	0.31452000
H	-18.49091000	-5.39492400	1.77641600
C	1.93494600	1.45717700	-3.14369200
C	1.40615300	0.60386500	-2.18003400
C	1.67243200	0.77859100	-0.81173000
C	2.49628400	1.84702400	-0.44673100
C	3.03797900	2.71675400	-1.40274100
C	2.75650900	2.52218900	-2.74987700
C	2.39905000	1.29236200	1.86034100
C	1.57013900	0.19028500	1.63312500
C	1.19917800	-0.58198200	2.74658600
H	0.55529700	-1.44397700	2.59186000
C	1.63293500	-0.26969400	4.03140300
C	2.46281700	0.84198800	4.23105200
C	2.84593200	1.62263200	3.14670600
H	1.70940700	1.29557600	-4.19406100
H	0.76859700	-0.22177200	-2.48553000
H	3.67208400	3.53053400	-1.06343600
H	3.17612600	3.19664800	-3.49160500
H	1.32920300	-0.88743100	4.87187500
H	2.81189200	1.09586600	5.22838100
H	3.49190800	2.48745300	3.26571900
O	2.83251800	2.12626600	0.85661300
Cis-(R,S)-2O8-DPFOH-SFX-III			
C	11.31082300	-3.92457700	0.32586500

C	11.28531300	-3.09045400	-0.79908000
C	10.07957300	-2.52605100	-1.23912800
C	8.91268300	-2.81486400	-0.54256600
C	8.93283200	-3.65895400	0.58425800
C	10.13498800	-4.21556900	1.02746700
C	7.55652700	-3.79440400	1.09273000
C	6.69647800	-3.03863800	0.27526700
C	5.33142800	-2.99589000	0.51379100
C	4.78654100	-3.71904500	1.59617600
C	5.65902000	-4.46757900	2.41189000
C	7.03446500	-4.51153900	2.17084600
C	7.48376900	-2.33631700	-0.84121900
C	-3.19973000	-3.49669300	3.10405400
C	-3.64654900	-3.51532400	1.76621100
C	-2.68438000	-3.56288500	0.73678700
C	-1.33370700	-3.59098000	1.05154900
C	-0.90084000	-3.57469800	2.39062700
C	-1.84194300	-3.52733800	3.42342800
C	0.56542000	-3.61137700	2.41277600
C	1.03697000	-3.64745200	1.08717500
C	2.39635700	-3.68346800	0.81299900
C	3.32765700	-3.68569400	1.87125400
C	2.84268300	-3.65057900	3.19524500
C	1.47599200	-3.61407400	3.47374500
C	-0.13408000	-3.64666600	0.08695600
C	-6.03071100	-4.15967800	2.25656000
C	-5.09659500	-3.48085400	1.44778000
C	-5.57215000	-2.76325900	0.32942700
C	-6.92996800	-2.74341200	0.05049500
C	-7.85218900	-3.42633000	0.86438300
C	-7.39929300	-4.13756300	1.97704200
C	-9.20444000	-3.23384900	0.31172000
C	-9.10670400	-2.43123900	-0.84109200
C	-10.23637500	-2.10202200	-1.57973000
C	-11.48340700	-2.58304300	-1.15607000
C	-11.58588800	-3.37593800	-0.00597300
C	-10.44746900	-3.70781500	0.73800000
C	-7.64530700	-2.04647400	-1.11667900
O	-7.19968200	-2.56089000	-2.38353100
C	-7.41955000	-0.53494100	-1.14666300
C	-6.89946000	0.10805600	-2.27917600
C	-6.70540500	1.48763000	-2.29209400

C	-7.02833200	2.26073300	-1.16928100
C	-7.54901400	1.63155300	-0.02966100
C	-7.73748700	0.24696900	-0.03144900
H	12.25403600	-4.35138400	0.65774900
H	12.20809800	-2.87612200	-1.33210100
H	10.05692300	-1.87195900	-2.10717800
H	10.16366400	-4.86553800	1.89882100
H	4.68873900	-2.38391300	-0.11370500
H	5.24819400	-5.04785100	3.23378100
H	7.67819200	-5.10797200	2.81313400
H	-3.92966800	-3.42892400	3.90611000
H	-3.00407300	-3.59973900	-0.30159700
H	-1.52884900	-3.50236300	4.46461300
H	2.74584100	-3.73217900	-0.21529700
H	3.55145800	-3.62298300	4.01850000
H	1.13312600	-3.57667500	4.50513100
H	-5.67533600	-4.73765800	3.10535600
H	-4.88106800	-2.20499900	-0.29651200
H	-8.09151500	-4.68012800	2.61663500
H	-10.15370000	-1.48008600	-2.46751700
H	-12.37810800	-2.33588700	-1.72176500
H	-12.56017300	-3.73829900	0.31249900
H	-10.53610500	-4.32531400	1.62875200
H	-7.34054700	-3.52127000	-2.37946900
H	-6.64430900	-0.47743100	-3.15497900
H	-6.30099300	1.98493800	-3.16911700
H	-7.80906700	2.19940600	0.85661700
H	-8.14201400	-0.22310600	0.86197600
O	-6.80208700	3.60509000	-1.28117400
C	-7.11495300	4.45735000	-0.17853900
C	-6.77296100	5.88601800	-0.58071600
H	-6.53353500	4.15114300	0.70392300
H	-8.18342700	4.36714300	0.06790600
C	-7.06842000	6.89953400	0.53362700
H	-5.71069000	5.92870000	-0.85588600
H	-7.34330700	6.14274200	-1.48335500
C	-6.73010000	8.34331900	0.13590600
H	-8.13160400	6.84171300	0.81213100
H	-6.49961800	6.63101400	1.43671700
H	-5.66733100	8.40163300	-0.14343300
H	-7.29805900	8.61144100	-0.76765500
C	-7.02084800	9.36896800	1.24006400

C	-6.68396100	10.81173300	0.83881300
H	-6.45176800	9.10153200	2.14355100
H	-8.08367400	9.30943400	1.52030100
C	-6.97425800	11.84153000	1.93942500
H	-5.62107300	10.87194200	0.55866000
H	-7.25237800	11.07906900	-0.06521800
C	-6.63602100	13.27938800	1.52759100
H	-8.03622700	11.78182300	2.21960500
H	-6.40518600	11.57637500	2.84259100
H	-6.85650200	13.98953900	2.33376200
H	-5.57219300	13.38032900	1.27646000
H	-7.21431000	13.58569000	0.64627000
C	-0.02242600	0.01595800	-1.07212100
C	-0.05512700	-1.11992200	-0.26926200
C	-0.09255600	-2.41253600	-0.81878600
C	-0.09477300	-2.52080900	-2.21194400
C	-0.06259300	-1.38857100	-3.03680000
C	-0.02667700	-0.12153400	-2.46682100
C	-0.14938700	-4.89439900	-2.14861300
C	-0.15246400	-4.92833600	-0.75124300
C	-0.17658100	-6.18999200	-0.13368200
H	-0.17966500	-6.23880800	0.95224600
C	-0.19666800	-7.36769900	-0.87448100
C	-0.19279600	-7.30502300	-2.27466700
C	-0.16908600	-6.06990100	-2.91149600
H	0.00611500	1.00193200	-0.61702100
H	-0.05202300	-1.01300900	0.81249900
H	-0.06614400	-1.53036800	-4.11346000
H	-0.00158600	0.75684600	-3.10612000
H	-0.21525300	-8.32802800	-0.36680000
H	-0.20816300	-8.21656900	-2.86623500
H	-0.16536600	-5.98558800	-3.99420400
O	-0.12786200	-3.72655400	-2.87254000
O	7.04749800	-2.76505300	-2.14208300
H	7.13762100	-3.73070600	-2.18157400
C	7.34563200	-0.81403300	-0.80422000
C	6.90786100	-0.08707700	-1.92053000
C	7.66336100	-0.10774000	0.36037600
C	6.79236700	1.30067200	-1.86951300
H	6.65377800	-0.61315600	-2.83360300
C	7.55252200	1.28331300	0.42673200
H	8.00483000	-0.64420400	1.24263700

C	7.11296400	1.99729900	-0.69710700
H	6.45102800	1.86307300	-2.73394300
H	7.80844100	1.79042900	1.35018600
O	6.96666100	3.35672800	-0.74538400
C	7.26216700	4.12597400	0.42120500
C	7.01132800	5.59274400	0.09631000
H	8.31085700	3.96712600	0.71393800
H	6.62192300	3.79653900	1.25315500
C	7.30528900	6.50703500	1.29536700
H	7.63232500	5.86811300	-0.76449100
H	5.96458500	5.71030900	-0.21598600
C	6.98378900	7.99288800	1.05577100
H	6.72154400	6.15915200	2.16023900
H	8.36376700	6.40979500	1.58141800
H	7.09092800	8.52890900	2.00995100
H	5.92599000	8.09168100	0.76841600
C	7.86381400	8.68311900	0.00290200
C	7.56492000	10.18138300	-0.14727000
H	7.73521000	8.19491800	-0.97331200
H	8.92247600	8.55021200	0.27538200
C	8.44342200	10.88327300	-1.19203600
H	6.50596800	10.31448000	-0.41730800
H	7.69521200	10.67793000	0.82669500
C	8.13598800	12.37867600	-1.33577500
H	9.50153700	10.75231700	-0.92169400
H	8.31385900	10.38834400	-2.16564300
H	8.78117300	12.84989700	-2.08712300
H	7.09444300	12.54185900	-1.64166000
H	8.28862800	12.90810200	-0.38631300