Supporting Information

Binaphthyl-Derived Armchair-type Molecular Carbon Rings with Chirality: Synthesis, and Optical Properties

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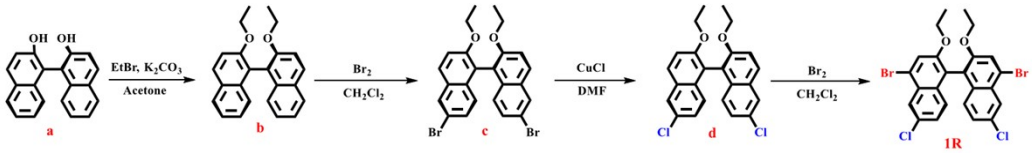
General. All the air-sensitive reactions were performed in an oven-dried vessel under argon atmosphere. NMR spectra were collected on a Bruker BioSpin (^{1}H 400 MHz, ^{13}C 100 MHz) spectrometer for $CDCl_3$ solution of a sample. Chemical shift values were expressed in parts per million (ppm) relative to $CDCl_3$ (δ 7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR). Flash chromatography was performed on silica gel (200-300 mesh). High-resolution MALDI-TOF mass spectra were measured on a Bruker Daltonics Inc. LTQ Orbitrap XL hybrid Fourier Transform high-resolution Mass Spectrometer. UV-vis spectra were collected on a UNIC-3802 spectrophotometer in standard glass cuvettes. Circular dichroism (CD) spectra were obtained on a spectropolarimeter (JASCO, Jasco-810).

Materials. All reagents were obtained from Innochem or Sigma Aldrich and used without further purification unless otherwise indicated. All organic solvents (THF, Toluene, $CHCl_2$, MeOH, EtOH, Et_2O, and 1,4-dioxane) were purchased from China Medicine Shanghai Chemical Reagent Co.

1. Synthesis

(R/S)-4,4′-dibromo-6,6′-dichloro-2,2′-diethoxy-1,1′-binaphthalene (1 (R/S)). The material **1 (R/S)** was synthesized according to literature reports.[S1-S2]



(R/S)-2,2'-(6,6'-dichloro-2,2'-diethoxy-[1,1'-binaphthalene]-4,4'-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (2 (R/S)). A 250-mL flask containing **1 (R/S)** (1.50 g, 2.65 mmol), Pd(dppf)Cl_2 (95 mg, 130 μmol), dried KOAc (1.30 g, 13.3 mmol), and bis(pinacolato)diboron (2.64 g, 10.4 mmol) was evacuated and filled with argon three times, dry 1,4-dioxane (10 mL) was transferred to the flask *via* syringe under nitrogen at room temperature. The mixture was then stirred at 90 °C for 48 h. After cooling down to room temperature, solvent was removed and residual was purified by silica gel column chromatography (*n*-hexane/CH_2Cl_2 = 0.3), affording **2 (R/S)** as white powder (1.3 g, 74%). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ 8.82 (s, 2H), 8.01 (s, 2H),

7.13 (dd, J = 10 Hz, 1.2 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 4.14-4.08 (m, 4H), 1.49 (s, 24H), 1.07 (t, J = 6.9 Hz, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ 153.68, 133.51, 132.46, 130.03, 127.35, 127.26, 126.75, 125.59, 124.07, 84.24, 65.27, 25.13, 15.16. HR-MS (MALDI-TOF) m/z calcd. for $C_{36}H_{42}B_2Cl_2O_6$ $[M]^+$: 662.2545, found: 662.2504. FT-IR (KBr): ν_{max} 3092, 3073, 2979, 2933, 2885, 1905, 1775, 1727, 1578, 1500, 1455, 1379, 1354, 1333, 1313, 1255, 1218, 1187, 1165, 1142, 1114, 1091, 1062, 1010, 978, 954, 924, 896, 874, 854, 822, 810, 773, 747 cm^{-1}.

Synthesis of compound 3. Compound **3** were prepared according to the published procedures.[S3]

Synthesis of compound 4 (R/S). To a degassed suspension of **2 (R/S)** (133 mg, 201 μmol), **3** (174 mg, 201μmol), and KOH (56 mg, 1.00 mmol) in THF/H_2O (150 mL/15 mL) was added $Pd(PPh_3)_4$ (10 mg, 8.65 μmol), then the mixture was further degassed for 0.5 h. The mixture was then heated up to 80 °C for 48 h under nitrogen atmosphere. After cooling down to room temperature, water was added and the mixture was extracted with DCM. The combined organic layer was dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to afford crude product **4 (R/S)** as a white solid for the next step without further purification.

Synthesis of RCR and SCR To a round-bottom flask (50 mL, vessel A) containing a magnetic stirring bar were added sodium metal (274 mg, 11.9 mmol), dry THF (12 mL) and naphthalene (1.00 g, 7.81 mmol), and the resultant mixture was stirred at room temperature for 1 day. To a 250-mL round-bottom flask (vessel B) containing a magnetic stirring bar were added the dry crude product **4 (R/S)** and dry THF (20 mL). Then a solution of sodium naphthalide in vessel A was added at -78 °C. After stirring at -78 °C for 2 h, 1.5 mL of I_2 solution (1 M in THF) was added. After warming up to room temperature, the mixture was quenched with aqueous saturated sodium thiosulfate, extracted with CH_2Cl_2, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The crude product was purified by column chromatography with hexane/CH_2Cl_2 as the eluent (v/v, 1:1), the cyclic product was collected, further purification by recrystallization from MeOH and *n*-hexane to afford the pure **RCR/SCR**. (17 mg, 9.7 %) as a yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm):

δ 8.33-8.29 (m, 2H), 7.96-7.93 (m, 2H), 7.67-7.42 (m, 32H), 6.50 (s, 2H), 3.35-3.28 (m, 2H), 2.78-2.71 (m, 2H), 0.25 (t, J = 6.8 Hz, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ 154.14, 141.41, 140.75, 138.55, 138.28, 138.12, 137.97, 137.86, 137.34, 128.22, 127.59, 127.54, 127.46, 127.43, 127.34, 127.20, 126.51, 126.23, 125.81, 124.00, 121.88, 120.37, 65.27, 14.43. HR-MS (MALDI-TOF) *m/z* calcd. for $C_{66}H_{48}O_2$ $[M]^+$: 872.3654, found 872.3649. FT-IR (KBr): ν_{max} 2965, 2924, 2850, 1738, 1625, 1462, 1389, 1262, 1095, 1018, 813 cm^{-1}.

2. MALDI-TOF-MS spectrum

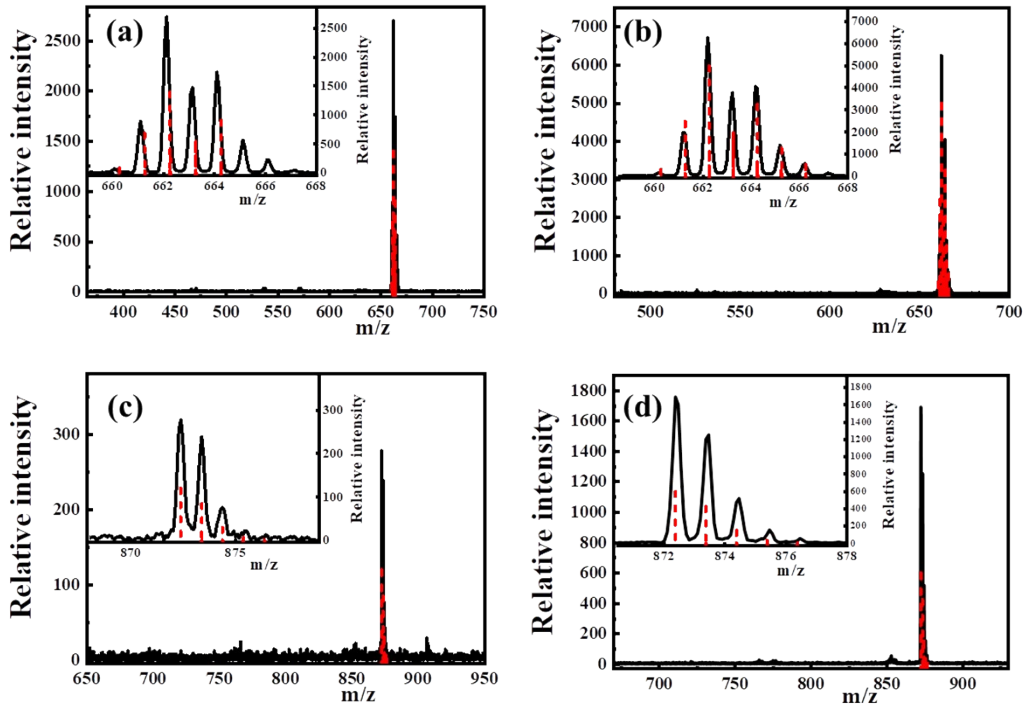


Figure S1. MALDI-TOF-MS spectrum and simulated data for **2R** (a), **2S** (b), **RCR** (c), and **SCR** (d).

3. ^{1}H NMR and ^{13}C NMR copies for new compounds

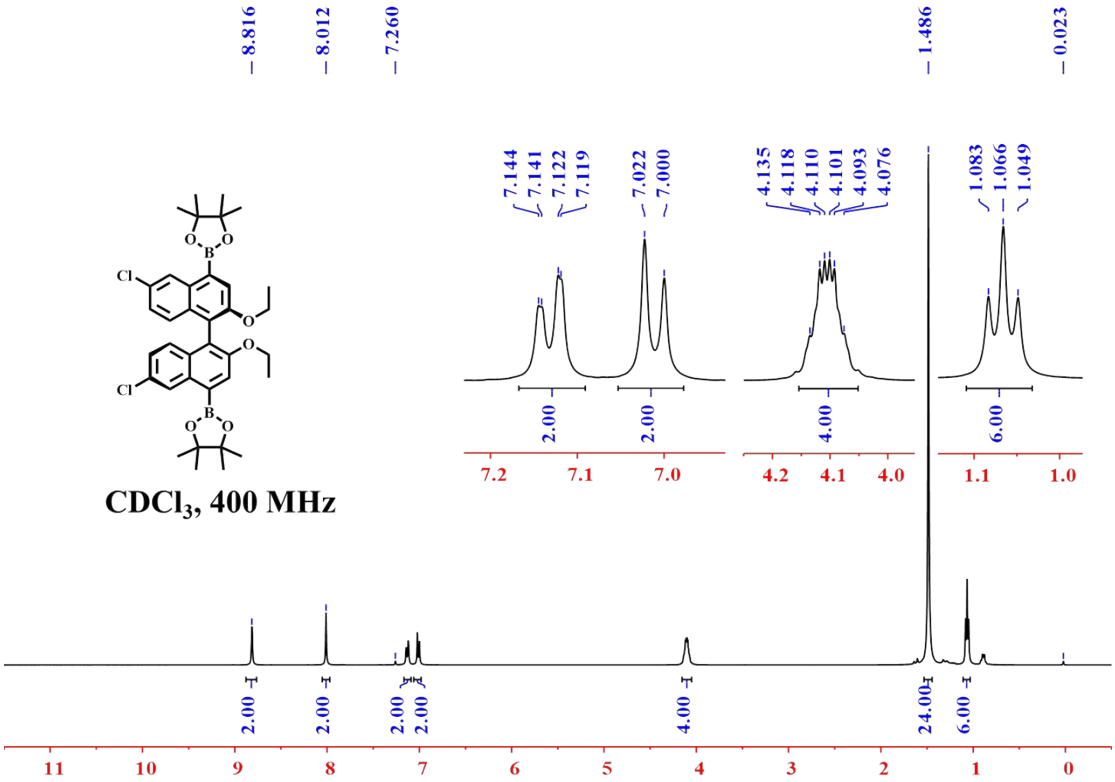


Figure S2. ^{1}H NMR spectrum of **2R**.

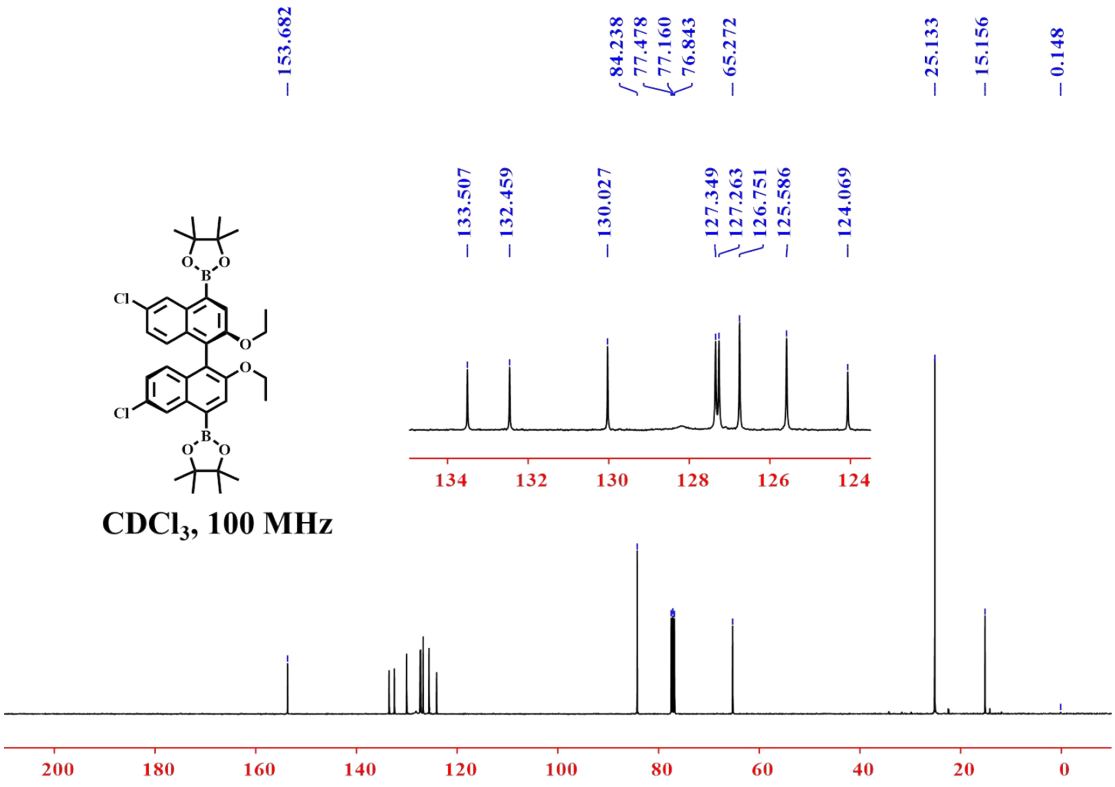


Figure S3. ^{13}C NMR spectrum **2R**.

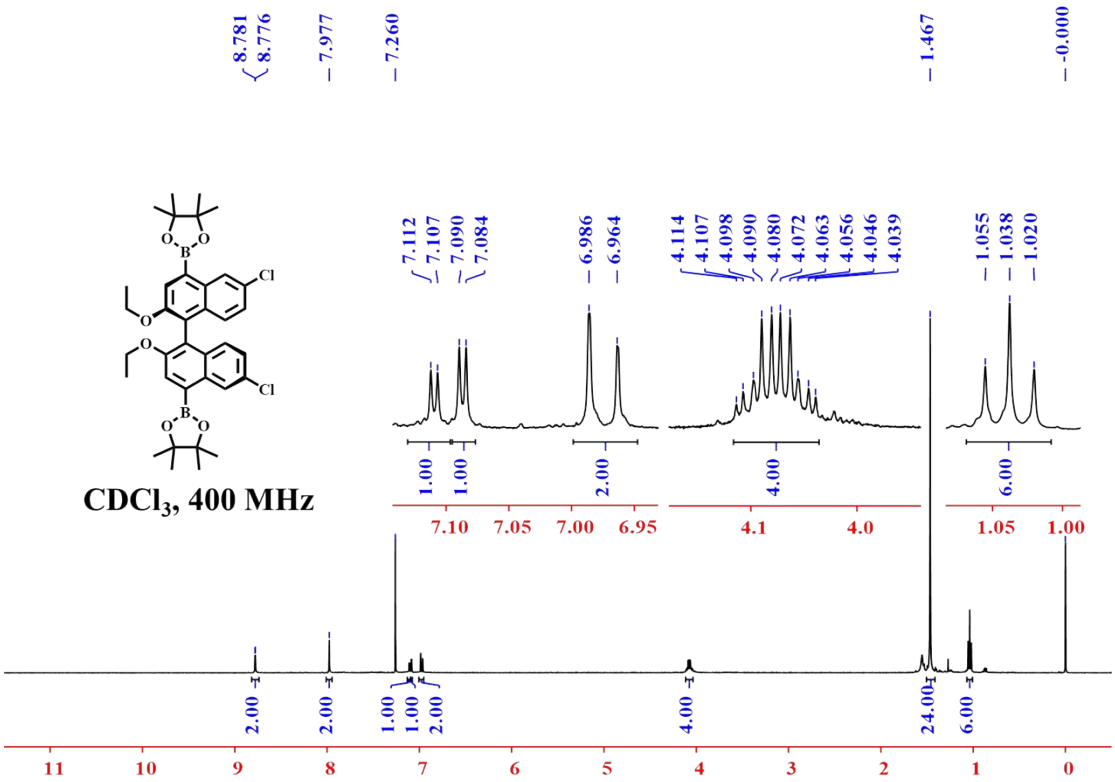


Figure S4. ^{1}H NMR spectrum of **2S**.

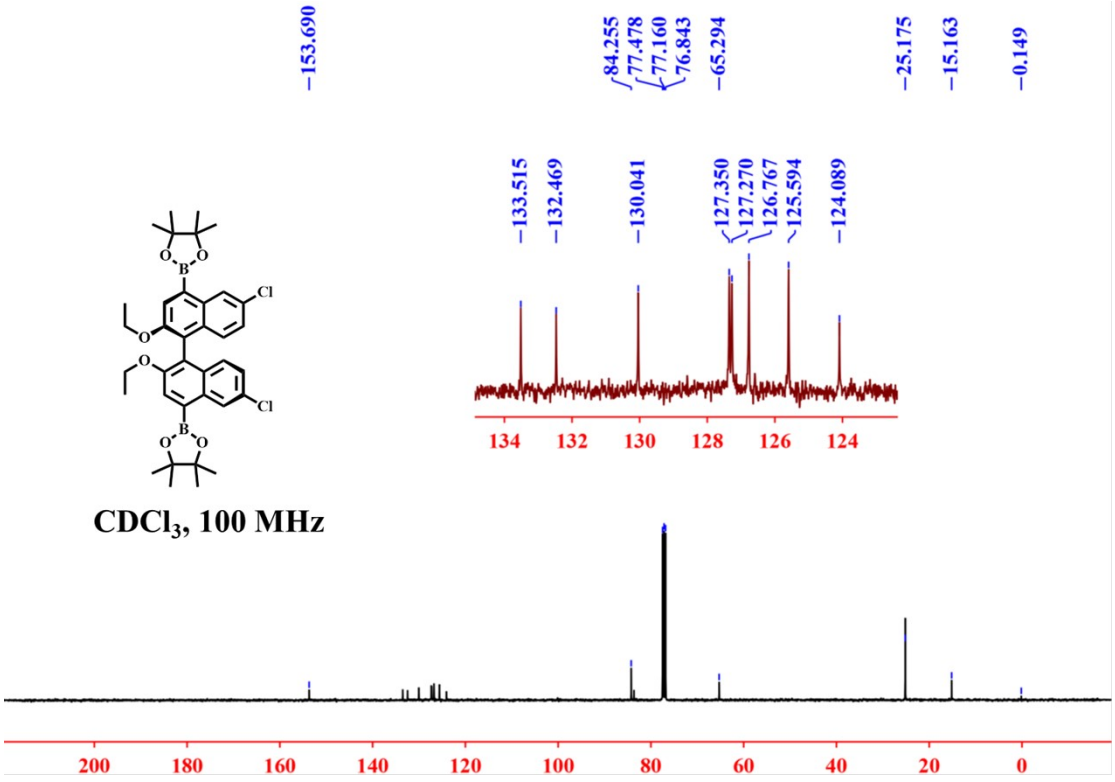


Figure S5. ^{13}C NMR spectrum **6S**.

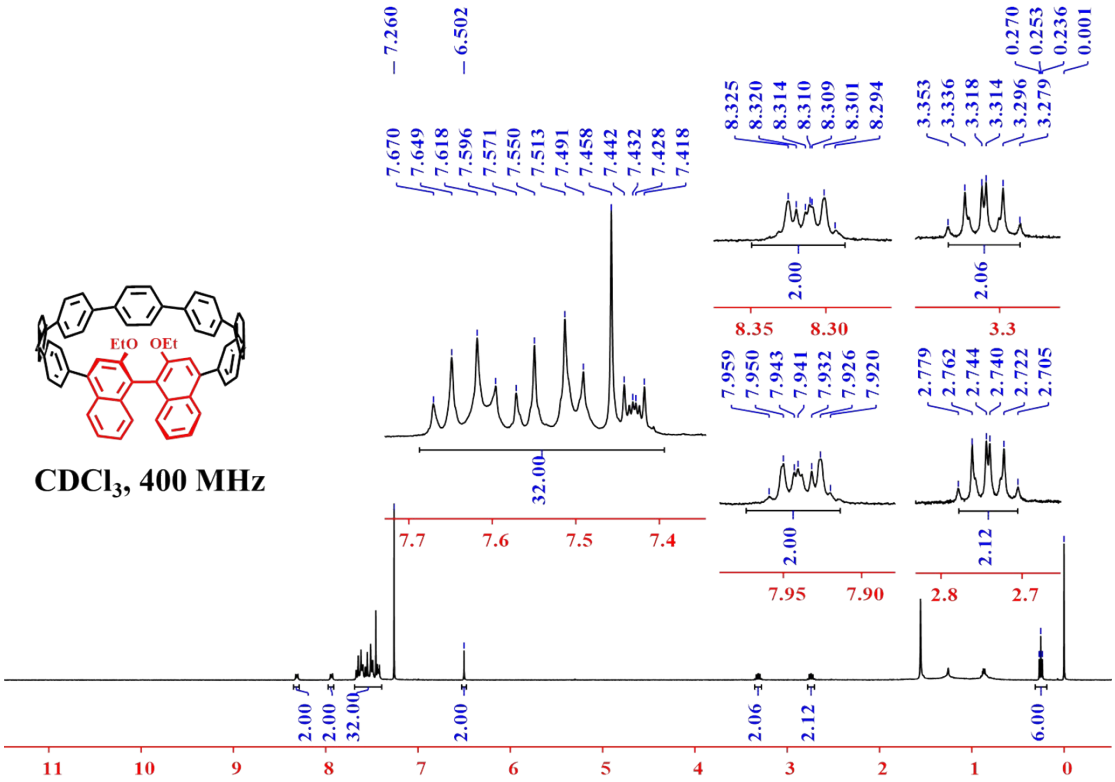


Figure S6. ^{1}H NMR spectrum of **RCR**.

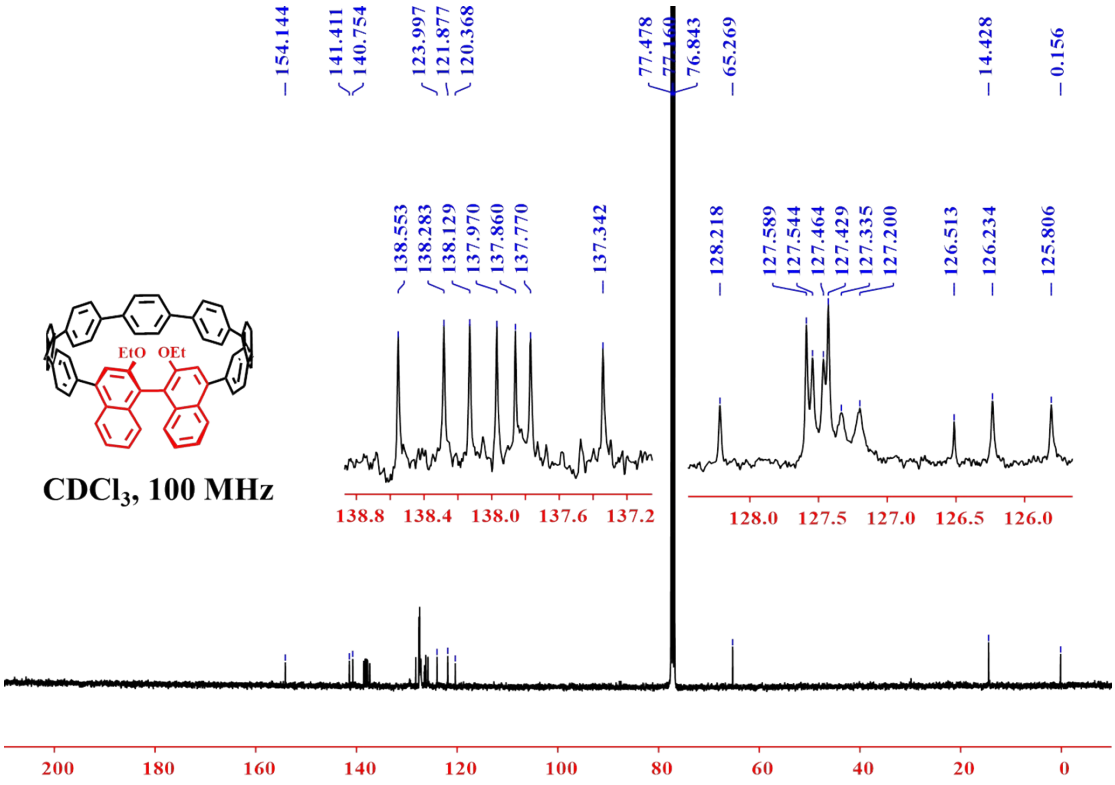


Figure S7. ^{13}C NMR spectrum **RCR**.

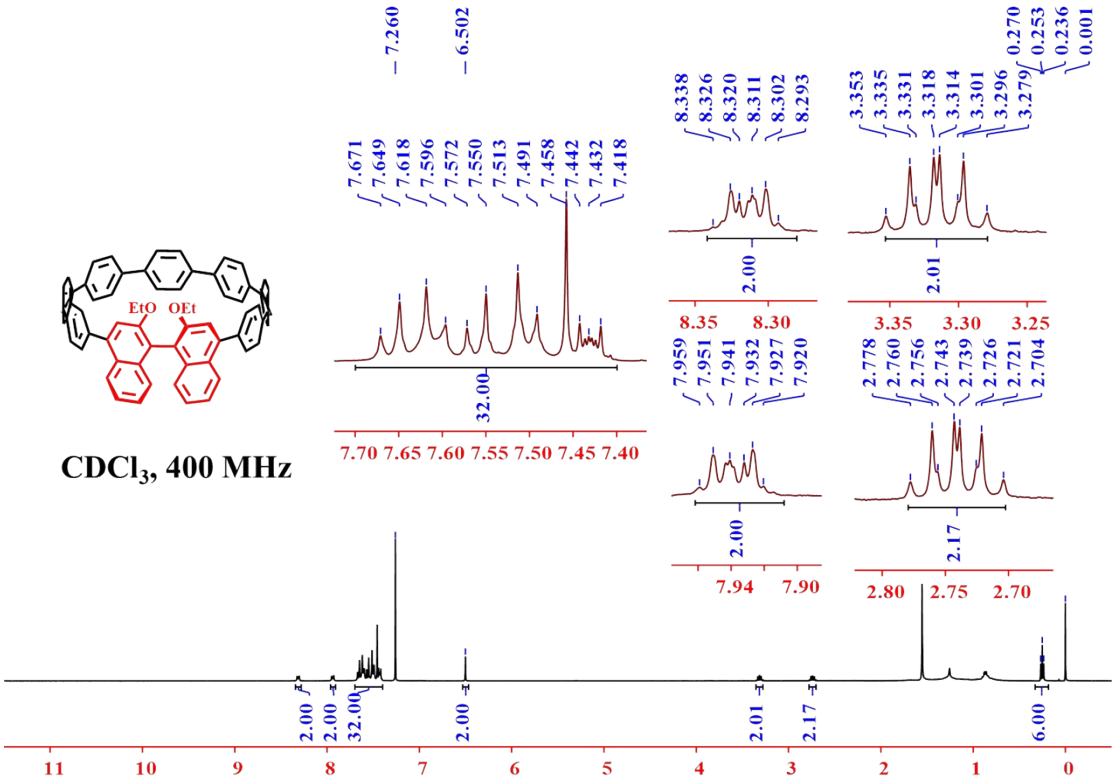


Figure S8. ^{1}H NMR spectrum of **SCR**.

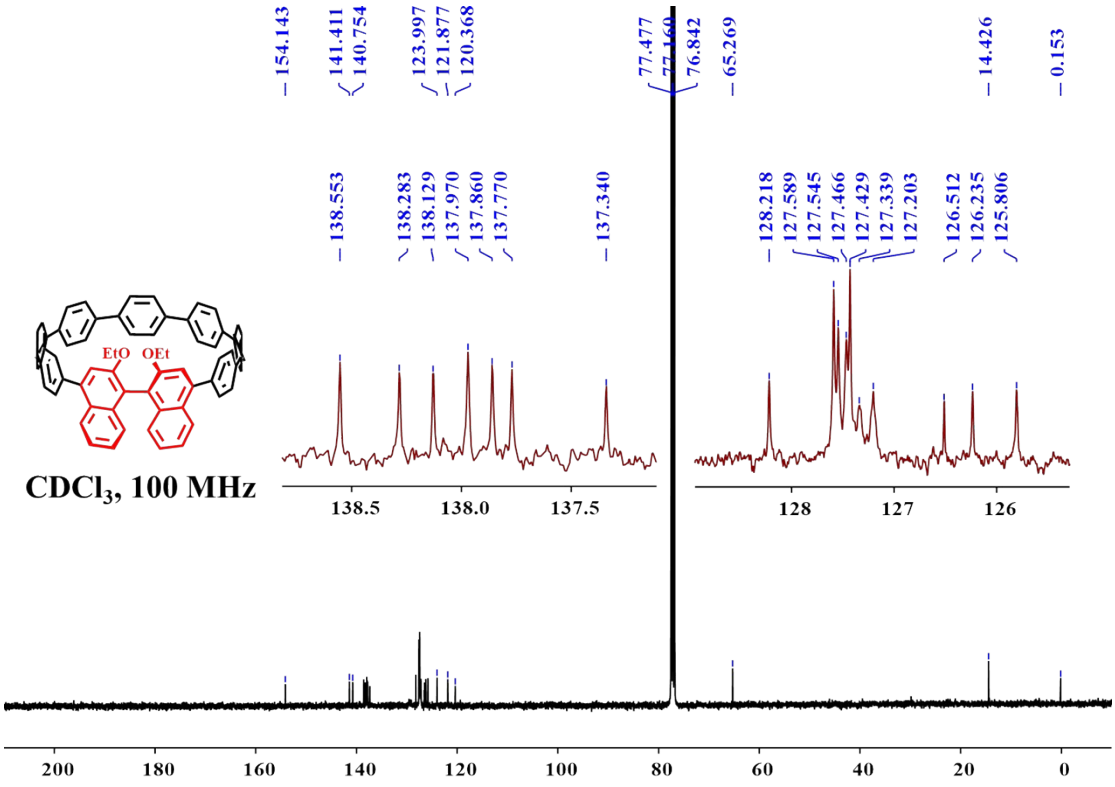


Figure S9. ^{13}C NMR spectrum **SCR**.

4. Additional photophysical data

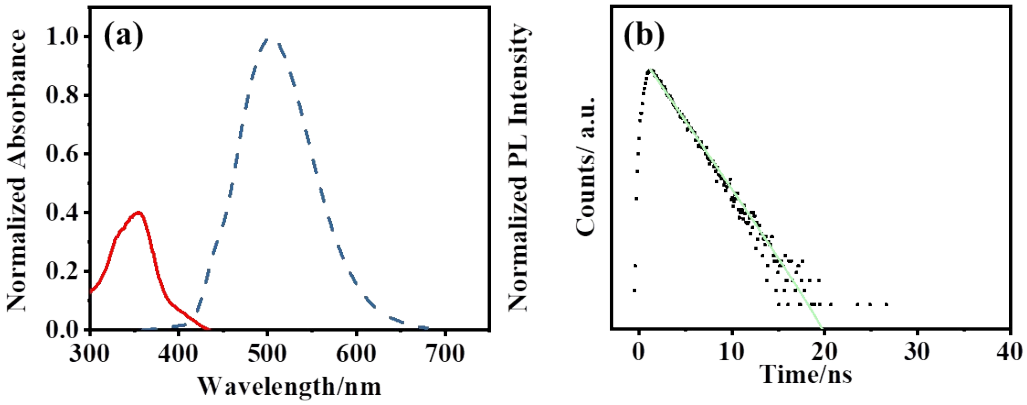


Figure S10. (a) UV-*vis* absorption (solid lines) and fluorescence spectra (dash lines) of **SCR** in CH_2Cl_2 at 298 K. (b) Emission lifetime measured at 500 nm for **SCR** in CH_2Cl_2.

Computational details

Geometrical optimization were carried out in the theoretical level of D3BJ-B3LYP/def2TZVP and further validated by frequency analysis. Transition states were located by QST3 strategy using the STQN method[S4] and further validated by frequency analysis (one imaginary frequency). For enantiomerization reaction path, intrinsic reaction coordinate (IRC)[S5] was further validated. All calculations were performed by using Gaussian 09 software.[S6]

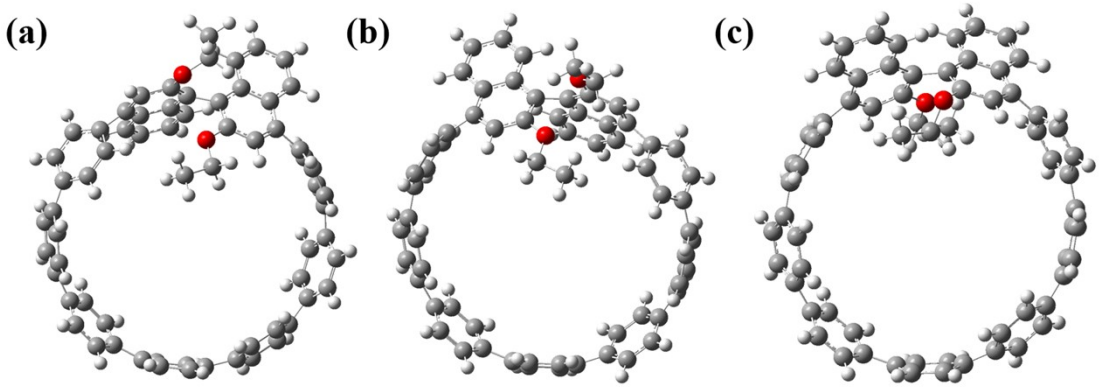


Figure S11. Relaxed structure of **RCR** (a), **SCR** (b) and **TS** (c).

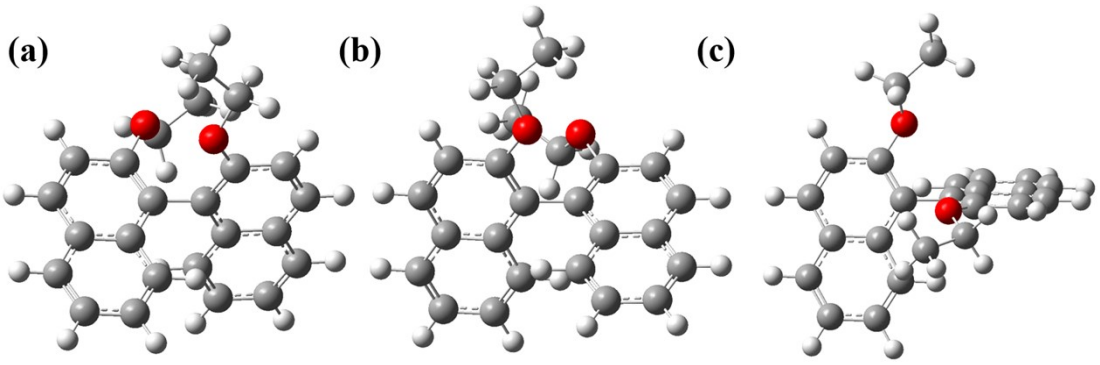


Figure S12. Relaxed structure of **5R** (a), **5S** (b) and **TS** (c).

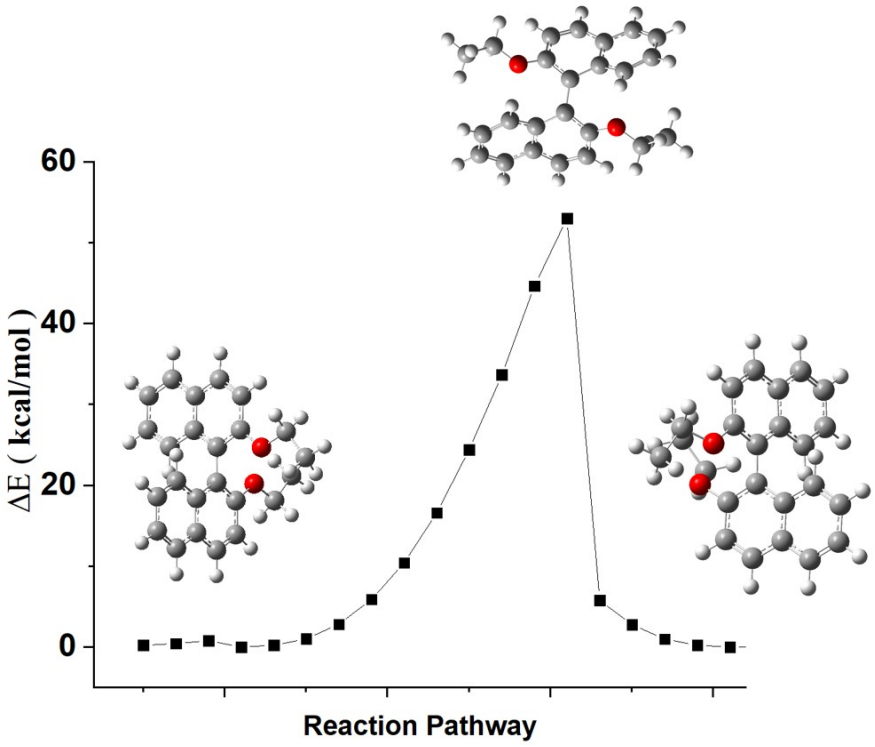


Figure S13. Energy barrier for the enantiomerization of 5-(from **5R** to **5S**).

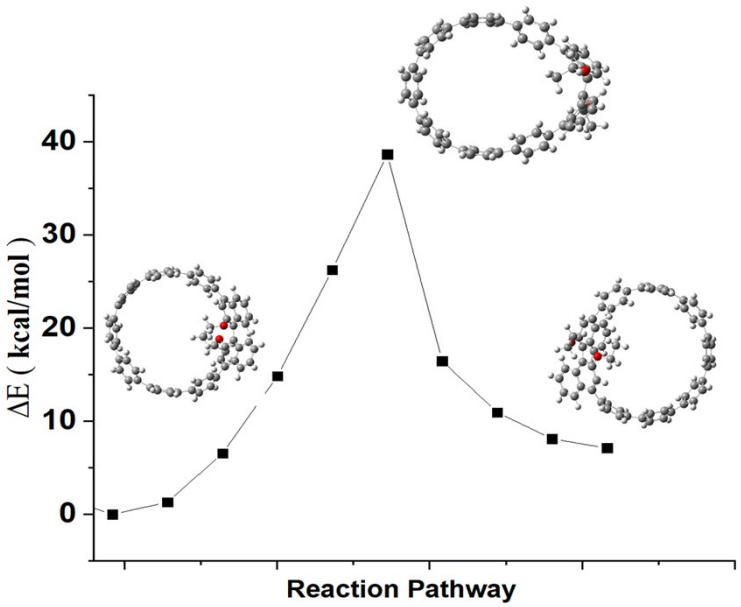


Figure S14. Energy barrier for the enantiomerization of **CR** (from **SCR** to **RCR**).

Table S1 Energy level (unit: eV) of frontier molecular orbitals for **5** and **CR** under the theoretical level of B3LYP-D3BJ/def2TZVP

Molecule	5R	5S	RCR	SCR
LUMO+3	-0.28436	-0.28436	-1.21118	-1.20492
LUMO+2	-0.41007	-0.41007	-1.5282	-1.50942
LUMO+1	-1.19186	-1.19186	-1.76331	-1.68847
LUMO	-1.35078	-1.35078	-2.07461	-1.99461
HOMO	-5.66055	-5.66055	-5.39497	-5.28803
HOMO-1	-5.88015	-5.88015	-5.58218	-5.61293
HOMO-2	-6.5403	-6.5403	-5.65184	-5.62817
HOMO-3	-6.57105	-6.57105	-6.00097	-5.9743
GAP	4.30977	4.30977	3.32035	3.29341

Table S2 Energy (Ha.) for strain energy calculations of **RCR** and **SCR** under the theoretical level of B3LYP-D3BJ/def2TZVP

Biphenyl	-463.5204245

Triphenyl	-694.6848842
Fragment	-1002.305718
RCR	-2695.622544
SCR	-2695.624642
RCR strain energy (kcal/mol)	62.29
SCR strain energy (kcal/mol)	60.97

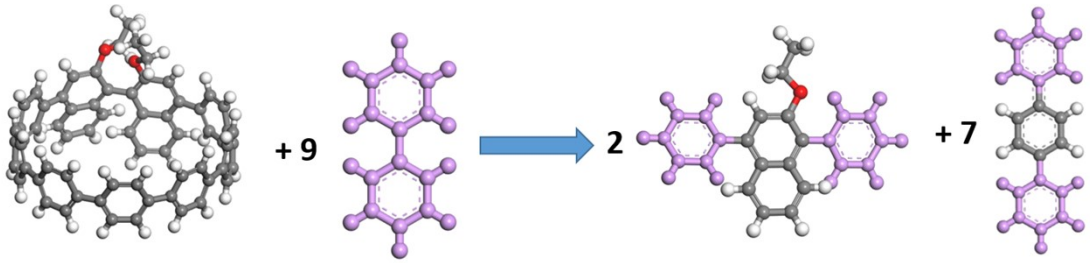


Figure S14. The calculation scheme of strain energy in **RCR** and **SCR**

Table S3 relaxed structure of **CR**, **5** and their transition state using theoretical level of D3-B3lYP/DEF2TZVP.

RCR							
C	7.391083	-0.113515	1.112928	C	6.365254	4.291315	-0.861422
C	7.369181	-0.726331	-0.146271	C	7.280626	1.260181	1.247333
C	7.450095	0.124308	-1.256318	C	7.113982	2.090624	0.130699
C	7.099124	-3.085668	0.745481	C	7.312478	1.494097	-1.122125
C	6.971391	-2.142858	-0.284320	C	-1.446606	-1.194973	3.146730
C	5.429170	-3.669616	-1.369319	C	-2.026997	0.073895	2.565385
C	6.185644	-2.514207	-1.381872	O	-3.092845	-0.304938	1.699809
C	6.339364	-4.245891	0.758269	O	-5.781086	-2.025106	1.873697
C	4.265958	-5.437367	-0.090438	C	-7.804419	-1.396916	2.946472
C	5.413600	-4.520834	-0.257975	C	-6.779375	-1.000587	1.907333
C	3.510520	-5.875837	-1.185711	H	7.377104	-0.723456	2.006162
C	2.390821	-6.036467	1.328550	H	7.527069	-0.294284	-2.250689
C	3.708752	-5.639960	1.178810	H	7.756413	-2.882984	1.581173
C	1.561002	-6.224839	0.215845	H	4.736746	-3.837497	-2.181753
C	2.185712	-6.249034	-1.037479	H	6.054728	-1.826262	-2.204747
C	-0.413182	-5.194063	1.283023	H	6.423448	-4.916102	1.604042
C	0.094023	-6.055864	0.303605	H	3.928362	-5.825020	-2.182239
C	-2.044947	-5.874688	-0.838492	H	1.974826	-6.095604	2.325472
C	-0.793961	-6.464197	-0.700572	H	4.271264	-5.364914	2.060919
C	-1.658924	-4.612350	1.147081	H	1.597018	-6.438805	-1.924958

C	-3.496008	-3.825115	-0.247445	H	0.224824	-4.863103	2.090207
C	-2.457560	-4.854854	0.024784	H	-2.677325	-6.165386	-1.667173
C	-3.342987	-2.949315	-1.377152	H	-0.478607	-7.198849	-1.430389
C	-2.517595	-3.260984	-2.482830	H	-1.970581	-3.855543	1.852753
C	-2.928972	-1.112072	-3.467233	H	-2.019746	-4.215965	-2.514254
C	-2.324462	-2.377250	-3.513431	H	-2.773480	-0.405562	-4.272692
C	-5.023487	-2.215910	0.762985	H	-1.695460	-2.651127	-4.350567
C	-4.393374	-3.482087	0.727481	H	-4.542508	-4.124147	1.585710
C	-4.727367	-1.254406	-0.182797	H	-6.821206	-0.245638	-1.506358
C	-3.959483	-1.659521	-1.328669	H	-4.149427	0.221978	-2.367707
C	-6.593438	0.807424	-1.406349	H	-8.157133	1.432487	-2.706112
C	-3.707704	-0.760929	-2.394994	H	-5.756868	4.568824	-1.055829
C	-7.332689	1.744677	-2.077878	H	-7.632028	3.850506	-2.470719
C	-3.782915	0.643984	1.016445	H	-2.599008	2.296706	1.694588
C	-4.750252	0.206032	0.121525	H	-3.443866	4.401160	-1.895212
C	-5.192055	2.577816	-0.460431	H	-1.105868	5.903603	2.166318
C	-5.514748	1.183617	-0.567471	H	-3.072088	4.493950	2.364242
C	-5.982807	3.516601	-1.164017	H	-1.535316	5.888100	-2.096430
C	-7.031634	3.115896	-1.950232	H	0.564616	7.199717	1.855084
C	-3.457375	2.005320	1.112248	H	2.951784	5.362968	-2.036142
C	-3.357921	4.255590	0.248582	H	0.544497	5.556763	-2.102356
C	-4.079939	2.964497	0.340159	H	2.985873	6.965009	1.930677
C	-2.963000	4.761190	-0.995720	H	5.282771	5.869267	-1.806417
C	-1.630345	5.617595	1.265250	H	5.750011	3.109773	2.239155
C	-2.742468	4.802434	1.380397	H	4.068772	4.839532	2.164251
C	-1.091824	5.939399	0.012216	H	7.003638	4.155346	-1.723840
C	-1.859335	5.592214	-1.107873	H	7.226568	1.675946	2.243938
C	1.076058	6.793247	0.992682	H	7.249248	2.091967	-2.020409
C	0.335005	6.317999	-0.099431	H	-1.033751	-1.820826	2.355835
C	2.442270	5.806394	-1.191119	H	-2.214941	-1.760741	3.674701
C	1.063799	5.919137	-1.226760	H	-0.647452	-0.951840	3.848814
C	2.455076	6.665329	1.035837	H	-2.407390	0.730772	3.354958
C	4.485984	5.446836	0.147180	H	-1.265982	0.622794	2.001593
C	3.159595	6.074901	-0.020750	H	-8.572983	-0.625443	3.021873
C	5.388920	5.273231	-0.908779	H	-7.335116	-1.511364	3.924524
C	5.698085	3.733099	1.358332	H	-8.282593	-2.340555	2.681274
C	4.734013	4.724303	1.318900	H	-6.321151	-0.042561	2.157301
C	6.472780	3.420870	0.233829	H	-7.231544	-0.906519	0.917178
				SCR			
C	6.835536	-1.626986	1.190238	C	6.464192	2.265315	-1.343129
C	6.932923	-2.415931	0.038561	C	7.063940	-0.262121	1.145959
C	7.464942	-1.807948	-1.106503	C	7.397896	0.376650	-0.053102
C	5.996824	-4.494272	1.130177	C	7.691210	-0.442238	-1.151727
C	6.215216	-3.707161	-0.008321	C	-6.814406	2.150249	3.642878

C	4.446296	-4.949341	-1.108453	C	-5.890024	2.865275	2.683636
C	5.478605	-4.028562	-1.153931	O	-5.843287	2.098136	1.485099
C	4.963311	-5.415840	1.175835	O	-3.515373	0.337504	1.875287
C	2.739783	-6.149663	0.227735	C	-1.989919	1.108728	3.507191
C	4.101060	-5.592248	0.085280	C	-2.563863	-0.116069	2.830718
C	2.014579	-6.668672	-0.853038	H	6.439671	-2.058434	2.099616
C	0.646828	-5.962207	1.436419	H	7.638197	-2.400433	-1.995645
C	2.028299	-5.894849	1.405146	H	6.601567	-4.336660	2.014033
C	-0.091697	-6.290320	0.293463	H	3.812765	-5.063759	-1.977551
C	0.630969	-6.739675	-0.820097	H	5.620349	-3.451693	-2.057657
C	-2.301471	-5.699741	1.355311	H	4.781823	-5.958718	2.094588
C	-1.506032	-5.865940	0.213838	H	2.535027	-6.958178	-1.756991
C	-3.089975	-4.479778	-0.995724	H	0.132601	-5.618934	2.323454
C	-1.990108	-5.321228	-0.981902	H	2.549167	-5.502181	2.267846
C	-3.393002	-4.845817	1.346583	H	0.101942	-7.084608	-1.699081
C	-4.444419	-2.830469	0.259316	H	-2.017122	-6.180177	2.282535
C	-3.742029	-4.134318	0.192843	H	-3.352082	-3.968245	-1.912038
C	-5.369528	-2.357879	-0.711998	H	-1.417756	-5.438349	-1.892077
C	-6.064951	-3.228643	-1.583911	H	-3.932127	-4.660626	2.267237
C	-7.136644	-1.353198	-2.649499	H	-5.913544	-4.294861	-1.480019
C	-6.931919	-2.743282	-2.527757	H	-7.825515	-0.975962	-3.394477
C	-4.136323	-0.551935	1.054047	H	-7.466301	-3.425347	-3.176177
C	-3.933324	-1.935885	1.177324	H	-3.220893	-2.299768	1.900409
C	-4.863257	-0.035513	-0.011089	H	-3.875107	-0.248431	-2.386955
C	-5.581260	-0.944973	-0.830975	H	-6.631742	0.586520	-1.917765
C	-3.386368	0.711160	-2.414953	H	-2.271345	0.211426	-4.153124
C	-6.476237	-0.480318	-1.826745	H	-1.526368	4.081636	-2.525001
C	-2.481090	0.968802	-3.408487	H	-1.088653	2.403764	-4.233246
C	-4.920893	2.397883	0.534497	H	-4.378679	4.338877	1.309150
C	-4.606241	1.389216	-0.355696	H	-2.308707	6.151855	-1.839647
C	-3.023165	2.937315	-1.472347	H	0.464214	4.815968	2.002881
C	-3.709007	1.680042	-1.428070	H	-1.758859	3.876749	1.731770
C	-2.070561	3.151845	-2.499909	H	-0.084441	7.124413	-1.563080
C	-1.814732	2.205585	-3.455452	H	2.244380	5.994372	2.263321
C	-4.223317	3.624073	0.514746	H	4.290570	5.605631	-2.193252
C	-2.173017	4.872352	-0.117575	H	1.977966	6.295694	-1.998487
C	-3.235565	3.872499	-0.409700	H	4.515514	5.183706	2.062922
C	-1.707851	5.863095	-0.986882	H	5.151481	3.681775	-2.215507
C	-0.146402	5.158133	1.179460	H	7.784425	2.458186	1.755576
C	-1.408176	4.616375	1.024625	H	6.569850	4.566547	1.729359
C	0.409697	5.990124	0.200367	H	6.377281	1.604156	-2.194578
C	-0.441382	6.413450	-0.829033	H	6.839617	0.332906	2.021066
C	2.680170	5.907627	1.276929	H	8.034440	0.005484	-2.075609
C	1.883052	6.109851	0.143287	H	-6.436065	1.151561	3.862579

C	3.853394	5.679518	-1.206761	H	-7.811971	2.052623	3.213532
C	2.538175	6.097655	-1.094500	H	-6.891968	2.709861	4.576706
C	3.986128	5.464417	1.162783	H	-6.256801	3.875006	2.469700
C	5.690298	4.271613	-0.216830	H	-4.881755	2.950021	3.101317
C	4.568006	5.227030	-0.089813	H	-1.257579	0.813171	4.260047
C	5.762918	3.456852	-1.353527	H	-2.777117	1.682809	3.997574
C	7.215144	2.725903	0.874459	H	-1.496680	1.749796	2.776258
C	6.520358	3.925177	0.859264	H	-3.049285	-0.773835	3.559731
C	7.123422	1.821863	-0.191780	H	-1.775180	-0.686357	2.329471
				5R			
C	-3.312350	-0.496728	1.485796	C	2.373941	-1.757387	2.522250
C	-3.192352	0.408418	0.406762	C	1.035919	-1.067986	2.655949
C	-4.306322	1.124211	-0.092277	H	-5.269927	0.976919	0.380615
C	-2.918307	2.157224	-1.764370	H	-2.822265	2.830798	-2.606344
C	-4.176382	1.982349	-1.151765	H	-5.036344	2.523962	-1.523968
C	-0.958781	-0.991501	1.349553	H	-2.298800	-1.885517	2.763709
C	-2.221731	-1.182420	1.944955	H	-0.096507	2.227164	1.125905
C	-0.786656	-0.118940	0.294078	H	-0.858159	1.619907	-1.780156
C	-1.914455	0.594562	-0.203365	H	1.307515	4.196046	1.502632
C	0.890254	2.277952	0.688048	H	4.430898	2.478713	-0.873043
C	-1.818525	1.481639	-1.304016	H	3.576270	4.340008	0.500984
C	1.677898	3.378994	0.896639	H	2.747452	-1.732273	-2.245185
C	1.067290	-1.003201	-1.088919	H	-1.154406	-4.074334	-2.207454
C	0.557035	0.031773	-0.322498	H	-0.556102	-4.467116	-0.589580
C	2.655606	1.275831	-0.668655	H	0.100789	-5.308174	-2.006549
C	1.346175	1.191855	-0.103732	H	1.690162	-3.557291	-1.185828
C	3.441017	2.429816	-0.435171	H	1.104270	-3.175168	-2.816854
C	2.967242	3.462247	0.328868	H	3.100808	-1.300753	3.196686
C	2.362895	-0.920065	-1.646838	H	2.744290	-1.668448	1.500437
C	3.131468	0.193569	-1.437487	H	2.288685	-2.815976	2.772295
C	-0.268751	-4.350977	-1.634630	H	1.110622	-0.021402	2.357481
C	0.802947	-3.293211	-1.770185	H	0.671608	-1.101041	3.689109
O	0.256852	-2.072316	-1.279765	H	-4.283530	-0.641678	1.942984
O	0.089210	-1.745826	1.814266	H	4.123729	0.252667	-1.867831
				5S			
C	-3.131454	0.193457	-1.437506	C	0.268860	-4.351025	-1.634441
C	-2.655636	1.275736	-0.668672	C	-0.802840	-3.293275	-1.770103
C	-3.441086	2.429696	-0.435198	H	-4.430967	2.478555	-0.873073
C	-1.678002	3.378943	0.896607	H	-1.307647	4.196014	1.502591
C	-2.967347	3.462149	0.328831	H	-3.576405	4.339891	0.500938
C	-1.067245	-1.003251	-1.088900	H	-2.747364	-1.732375	-2.245192
C	-2.362844	-0.920155	-1.646840	H	0.858130	1.619887	-1.780181
C	-0.557026	0.031751	-0.322493	H	0.096441	2.227174	1.125887
C	-1.346204	1.191808	-0.103745	H	2.822212	2.830794	-2.606401

C	1.818500	1.481646	-1.304041	H	5.269916	0.977023	0.380589
C	-0.890322	2.277926	0.688029	H	5.036300	2.524021	-1.524027
C	2.918269	2.157240	-1.764414	H	2.298847	-1.885405	2.763762
C	0.958810	-0.991446	1.349589	H	-2.288827	-2.815825	2.772016
C	0.786665	-0.118916	0.294094	H	-2.744231	-1.668166	1.500204
C	3.192352	0.408488	0.406755	H	-3.100888	-1.300582	3.196449
C	1.914449	0.594597	-0.203369	H	-1.110523	-0.021310	2.357517
C	4.306307	1.124288	-0.092303	H	-0.671743	-1.101054	3.689135
C	4.176348	1.982401	-1.151810	H	-0.100636	-5.308232	-2.006378
C	2.221765	-1.182330	1.944991	H	0.556124	-4.467143	-0.589365
C	3.312369	-0.496631	1.485810	H	1.154561	-4.074379	-2.207193
C	-2.373988	-1.757211	2.522046	H	-1.690088	-3.557345	-1.185792
C	-1.035930	-1.067916	2.655935	H	-1.104100	-3.175267	-2.816795
O	-0.089164	-1.745777	1.814330	H	-4.123712	0.252521	-1.867862
O	-0.256784	-2.072355	-1.279698	H	4.283555	-0.641553	1.942996

TS(RCR-SCR)

C	-7.680200	0.447500	0.986200	C	-6.547900	-4.142900	-0.533900
C	-7.536000	0.988100	-0.305000	C	-7.579800	-0.918200	1.213700
C	-7.516000	0.068100	-1.369700	C	-7.296600	-1.811000	0.164800
C	-7.164100	3.338900	0.566700	C	-7.381500	-1.296300	-1.140500
C	-7.101700	2.397100	-0.478900	C	2.560200	1.571100	3.077300
C	-5.502900	3.866900	-1.585300	C	2.686200	0.276500	2.268300
C	-6.326800	2.749700	-1.598400	O	4.047800	-0.188900	2.367300
C	-6.324300	4.447500	0.590300	O	3.521300	0.159600	-1.855400
C	-4.164500	5.471600	-0.260400	C	2.392000	-1.033100	-3.538100
C	-5.402600	4.679700	-0.444700	C	2.553000	0.327500	-2.884300
C	-3.494700	6.106700	-1.319900	H	-7.753900	1.106500	1.843900
C	-2.103300	5.601800	1.023000	H	-7.498900	0.424200	-2.394100
C	-3.460800	5.322100	0.945700	H	-7.819100	3.164900	1.413900
C	-1.385100	6.059100	-0.096000	H	-4.816300	4.023800	-2.410900
C	-2.138500	6.404700	-1.234200	H	-6.252000	2.071000	-2.439800
C	0.846100	5.660900	1.023700	H	-6.333000	5.102900	1.456200
C	0.087800	5.883500	-0.139900	H	-4.026700	6.308700	-2.244900
C	1.982800	5.043500	-1.421600	H	-1.575000	5.328600	1.929000
C	0.734900	5.650000	-1.367200	H	-3.948200	4.842000	1.788000
C	2.084200	5.029000	0.972400	H	-1.646400	6.847900	-2.093900
C	3.622800	3.505300	-0.308300	H	0.428900	5.901100	1.995700
C	2.635400	4.613000	-0.253100	H	2.416400	4.808700	-2.388800
C	4.691300	3.315100	0.623100	H	0.213000	5.841800	-2.298100
C	5.173600	4.362600	1.452400	H	2.577000	4.760000	1.899800
C	6.718100	2.844500	2.526300	H	4.760600	5.357300	1.326100
C	6.162400	4.137800	2.381800	H	7.494000	2.671100	3.265600
C	3.923700	1.211900	-1.092500	H	6.524000	4.954000	2.999400
C	3.319200	2.477500	-1.189800	H	2.484100	2.604000	-1.864700

C	4.849800	0.933900	-0.083300	H	6.595500	0.052300	-1.906100
C	5.285000	2.009800	0.743100	H	6.721600	0.821600	1.824400
C	6.317000	-0.995600	-1.861400	H	7.344000	-1.520200	-3.660800
C	6.291700	1.812200	1.725700	H	5.308100	-4.737500	-1.667400
C	6.728500	-1.872900	-2.838700	H	6.701000	-3.926800	-3.536500
C	4.448900	-1.028700	1.354800	H	3.431300	-2.685600	2.243600
C	5.059400	-0.509100	0.221500	H	2.887100	-3.943300	-1.803300
C	5.142200	-2.811400	-0.706000	H	1.523800	-6.484500	2.207800
C	5.527800	-1.432400	-0.767900	H	3.601800	-5.191000	2.238900
C	5.583500	-3.689900	-1.728900	H	0.786900	-5.163000	-1.818400
C	6.361400	-3.235900	-2.770900	H	-0.564600	-6.180400	2.481900
C	4.070800	-2.386200	1.420000	H	-3.290700	-5.980700	-1.626100
C	3.377900	-4.413000	0.241300	H	-0.899800	-6.377700	-1.799500
C	4.291200	-3.249500	0.361600	H	-2.972800	-5.937900	2.657800
C	2.609100	-4.524200	-0.930700	H	-5.504500	-5.878100	-1.228800
C	1.806900	-5.926900	1.320900	H	-5.819400	-2.444000	2.303400
C	2.995400	-5.202100	1.338000	H	-4.123500	-4.156100	2.458700
C	0.935500	-5.875900	0.216700	H	-7.219500	-4.143400	-1.387100
C	1.414000	-5.228600	-0.936900	H	-7.621600	-1.283000	2.234800
C	-1.152400	-6.182900	1.570700	H	-7.216400	-1.953200	-1.988300
C	-0.507200	-6.205800	0.320800	H	2.282000	2.412100	2.438400
C	-2.709800	-6.069300	-0.713900	H	3.528300	1.801000	3.528100
C	-1.337800	-6.268300	-0.813200	H	1.818100	1.485600	3.875500
C	-2.527300	-6.018400	1.671800	H	2.013700	-0.506900	2.642400
C	-4.627100	-5.131400	0.600400	H	2.445300	0.443500	1.213500
C	-3.324600	-5.834000	0.528100	H	1.675100	-0.979800	-4.362500
C	-5.570300	-5.130800	-0.443900	H	2.032500	-1.761500	-2.806000
C	-5.799500	-3.219200	1.546300	H	3.353900	-1.382100	-3.922900
C	-4.826400	-4.201200	1.635100	H	1.600900	0.675100	-2.460000
C	-6.629700	-3.109600	0.417300	H	2.896500	1.080600	-3.606900

TS(5R-5S)

C	2.572900	2.402000	-0.398300	C	-2.795800	2.470800	-2.284200
C	2.832100	1.354700	0.519000	C	-1.315300	2.694900	-2.038200
C	4.047900	1.285800	1.249100	H	4.795300	2.057700	1.085300
C	3.287900	-0.723300	2.351100	H	3.470500	-1.521300	3.064600
C	4.276400	0.269400	2.145600	H	5.209400	0.225900	2.698900
C	0.406300	1.458300	-0.901900	H	1.211900	3.260400	-1.803100
C	1.389300	2.460000	-1.094600	H	-1.156400	1.763800	1.292200
C	0.609800	0.411800	-0.010300	H	1.349700	-1.450900	1.820100
C	1.835100	0.343800	0.716100	H	-3.333200	2.336800	2.292300
C	-1.952300	1.028500	1.322800	H	-4.782100	-1.629800	1.487100
C	2.101400	-0.687800	1.657200	H	-5.161000	0.644600	2.387800
C	-3.168900	1.344100	1.883600	H	-1.137200	-3.857300	-0.622000
C	-0.289500	-1.887900	-0.328500	H	2.996900	-3.307700	-2.049200

C	-0.465200	-0.603900	0.160900	H	2.724600	-1.689300	-2.716400
C	-2.754700	-1.236200	0.853500	H	2.407400	-3.127500	-3.715700
C	-1.707300	-0.262400	0.782700	H	0.261700	-2.139000	-2.834800
C	-3.996500	-0.880300	1.441600	H	0.530800	-3.773700	-2.196300
C	-4.206300	0.383300	1.942100	H	-3.263400	3.388600	-2.653800
C	-1.318200	-2.858600	-0.239900	H	-3.288000	2.167900	-1.356500
C	-2.523600	-2.534600	0.330600	H	-2.943900	1.681600	-3.026300
C	2.350500	-2.716200	-2.703300	H	-1.157000	3.466100	-1.272900
C	0.920200	-2.746200	-2.200000	H	-0.807300	3.021800	-2.956500
O	0.928400	-2.206200	-0.873800	H	3.329600	3.166800	-0.549400
O	-0.773400	1.452300	-1.590000	H	-3.316200	-3.274900	0.394400

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