Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Synthesis and Structural Features of Thiophene-fused Analogues of Warped Nanographene and Quintuple Helicene

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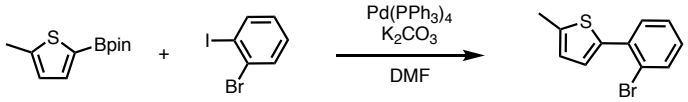
1. Experimental section

General procedure

Unless otherwise noted, all materials including dry solvent were obtained from commercial suppliers and used without further purification. Dichloromethane (CH_2Cl_2) was purified by passing through a solvent purification system (Glass Contour). All reactions were performed using standard vacuum-line and Schlenk techniques. Work-up and purification procedures were carried out with reagent-grade solvents under air. 1,3,5,7,9-Pentakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)corannulene (**3**)[1] and 3-bromo-5,5'-dimethyl-2,2'-bithiophene (**6**)[2] were synthesized according to the reported procedures. Analytical thin-layer chromatography (TLC) was performed using Wako silica gel 70 F_{254} coated plates (0.25 mm). The developed chromatogram was analyzed by UV lamp (254 nm and 365 nm). Flash column chromatography was performed with Kanto silica gel 60 N (spherical, neutral, 40–100 μm). High-resolution mass spectra (HRMS) were determined on a JEOL JMS-S3000 SpiralTOF (MALDI-TOF MS) or a JMS-T100TD instrument (DART). Melting points were measured on a MPA100 Optimelt automated melting point system. Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL ECA 500 spectrometer (^{1}H 500 MHz, ^{13}C 125 MHz) spectrometer. Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to $CHCl_3$ (δ 7.26 ppm), C_2HDCl_4 (δ 5.98 ppm), and $CHDCl_2$ (δ 5.32 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm), $C_2D_2Cl_4$ (δ 73.8 ppm), and CD_2Cl_2 (δ 53.8 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, td = triplet of doublets, m = multiplet), coupling constant (Hz), and integration.

Abbreviations: dba = (dibenzylidene)acetone; SPhos =2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl.

Synthesis of 2-(2-bromophenyl)-5-methylthiophene (4)

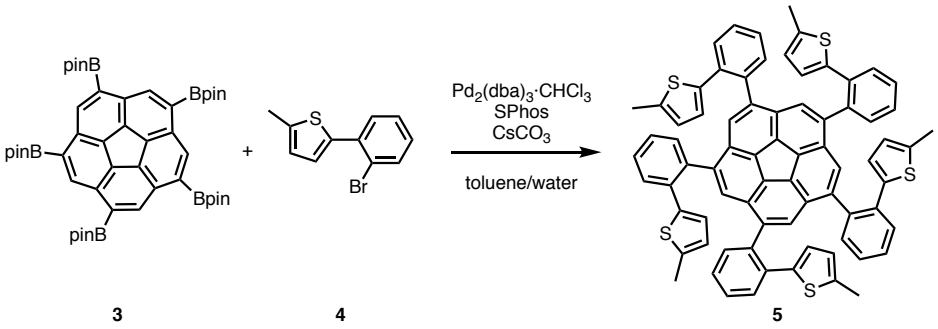


4

To a solution of $Pd(PPh_3)_4$ (520 mg, 447 μmol, 5.0 mol%) in DMF (40 mL) were added 4,4,5,5-tetramethyl-2-(5-methylthiophen-2-yl)-1,3,2-dioxaborolane (2.00 g, 8.93 mmol, 1.0 equiv), 1-bromo-2-iodobenzene (5.04 g, 17.9 mmol, 2.0 equiv), K_2CO_3 (1.23 g, 8.93 mmol, 1.0 equiv) and the resultant mixture was stirred at 100 °C for 24 h under argon atmosphere. After cooling the mixture to room temperature, the reaction mixture was extracted with EtOAc. The combined organic layer was dried over $MgSO_4$, and the solvent was removed under reduced pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane) to afford compound **4** (1.82 g, 81% yield) as colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (dd, J = 8.0, 1.0 Hz, 1H), 7.46 (dd, J = 8.0, 1.5 Hz, 1H), 7.31 (td, J = 8.5, 1.0 Hz, 1H), 7.15 (td, J = 7.5, 2.0 Hz, 1H), 7.10 (d, J = 3.5 Hz, 1H), 6.77–6.76 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.7 (4°), 139.2 (4°), 135.5 (CH), 133.6 (CH), 131.7 (CH), 128.6 (CH), 127.7 (CH), 125.2 (CH), 122.6 (4°), 15.3 (CH_3); HRMS (DART) *m/z* calcd for $C_{11}H_9BrS$ $[M+H]^+$: 251.9608, found 251.9600.

Synthesis of 5

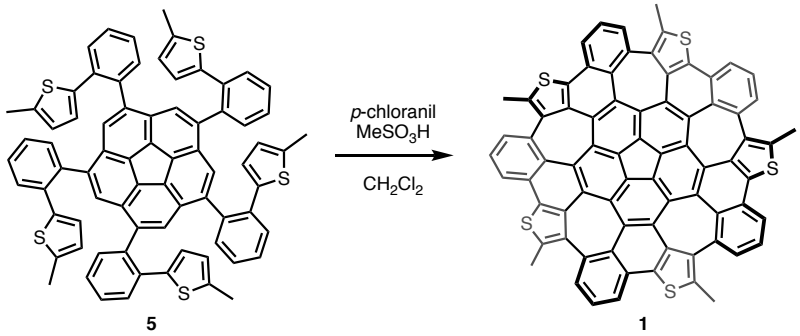


3 **4** **5**

To a solution of $Pd_2(dba)_3 \cdot CHCl_3$ (83.0 mg, 80.0 μmol, 20 mol%) and SPhos (66.0 mg, 160 μmol, 40 mol%) in toluene (8.0 mL) were added **3** (352 mg, 0.40 mmol, 1.0 equiv), compound **4** (1.12 g, 4.00 mmol, 10 equiv), and a solution of Cs_2CO_3 (1.30 g, 4.00 mmol, 10 equiv) in water (4.0 mL), and the resultant mixture was stirred at 80 °C for 48 h under argon atmosphere. After cooling the mixture to room temperature, the reaction mixture was extracted with CH_2Cl_2. The combined organic layers were dried over $MgSO_4$, and the solvent was removed under reduced pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane/$CHCl_3$ = 5:1 to 1:1) to afford compound **5** (400 mg, 90% yield) as a yellow solid.

^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.72–5.97 (m, 35H), 2.38–2.20 (m, 15H); ^{13}C NMR (125 MHz, CD_2Cl_2) δ 142.21 (4°), 142.11 (4°), 141.91 (4°), 141.76 (4°), 141.60 (4°), 141.21 (4°), 140.98 (4°), 139.98 (4°), 138.32 (4°), 137.65 (4°), 135.71 (4°), 135.50 (4°), 135.28 (4°), 135.00 (4°), 134.57 (4°), 134.52 (4°), 133.50 (4°), 132.02 (4°), 131.57 (CH), 131.24 (4°), 130.62 (4°), 130.40 (4°), 130.06 (CH), 129.96 (CH), 129.35 (CH), 128.53 (CH), 128.28 (CH), 127.66 (CH), 127.06 (CH), 126.87 (CH), 126.64 (CH), 126.48 (CH), 125.68 (CH), 15.51 (CH_3); HRMS (MALDI-TOF) *m/z* calcd for $C_{75}H_{50}S_5$ $[M]^+$: 1110.2510, found: 1110.2504; Mp: >300 °C.

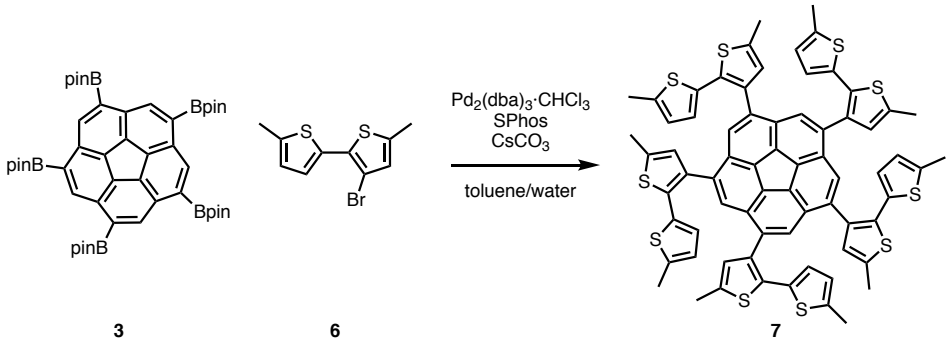
Synthesis of 1



To a solution of compound **5** (400 mg, 360 μmol, 1.0 equiv) in dry CH_2Cl_2 (73 mL) was added *p*-chloranil (818 mg, 3.60 mmol, 10 equiv) at 0 °C. After stirring the mixture for 10 min, methanesulfonic acid (7.3 mL) was added to the mixture. The mixture was further stirred for 90 min at 0 ℃. The reaction mixture was neutralized with sat. $NaHCO_3$ aq., and then extracted with $CHCl_3$. The combined organic phase was dried over $MgSO_4$ and the organic solvent was removed under reduced pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane/$CHCl_3$ = 5:1 to 1:1) to afford compound **1** (155 mg, 40% yield) as an orange solid.

^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 100 °C) δ 7.95 (d, J = 7.5 Hz, 5H), 7.54 (t, J = 7.5 Hz, 5H), 7.33 (d, J = 7.5 Hz, 5H), 2.65 (s, 15H); Due to poor solubility and precipitation of **1** during NMR measurements, ^{13}C NMR of **1** could not be recorded. HRMS (MALDI-TOF) *m/z* calcd for $C_{75}H_{30}S_5$ $[M]^+$: 1090.0946, found: 1090.0951.

Synthesis of 7

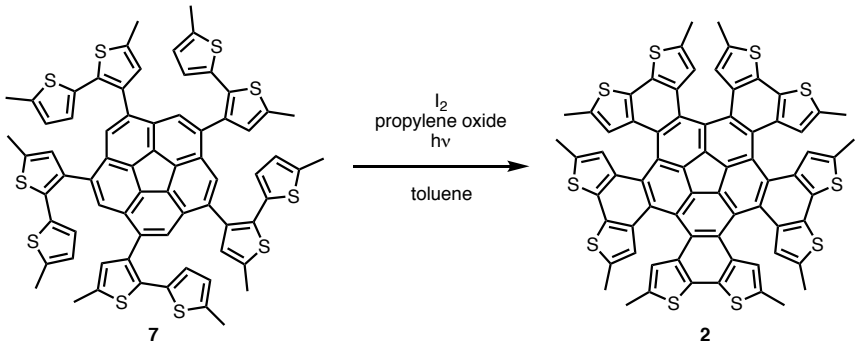


3 **6** **7**

To a solution of $Pd_2(dba)_3 \cdot CHCl_3$ (124 mg, 120 μmol, 20 mol%) and SPhos (99.0 mg, 240 μmol, 40 mol%) in toluene (12 mL) were added **3** (582 mg, 0.600 mmol, 1.0 equiv), compound **6** (1.31 g, 4.80 mmol, 8 equiv) and a solution of Cs_2CO_3 (2.00 g, 6.00 mmol, 10 equiv) in water (6 mL), and the resultant mixture was stirred at 80 °C for 48 h under argon atmosphere. After cooling the mixture to room temperature, the reaction mixture was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$, and the solvent was removed under reduced pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane/$CHCl_3$ = 4:1 to 2:1) to afford compound **7** (540 mg, 74% yield) as a yellow solid.

^{1}H NMR (500 MHz, CD_2Cl_2) δ 6.69 (d, J = 3.5 Hz, 5H), 6.61 (s, 5H), 6.64 (dd, J = 3.5, 1.0 Hz, 5H), 2.46 (s, 15H), 2.26 (s, 15H); ^{13}C NMR (125 MHz, CD_2Cl_2) δ 140.27 (4°), 138.08 (4°), 136.28 (4°), 135.73 (4°), 135.63 (4°), 134.19 (4°), 132.11 (4°), 130.67 (4°), 130.39 (CH), 127.80 (CH), 126.53 (CH), 125.62 (CH), 15.40 (CH_3); HRMS (MALDI-TOF) *m/z* calcd for $C_{70}H_{50}S_{10}$ $[M]^+$: 1210.1114, found: 1210.1108; Mp: >300 °C.

Synthesis of 2



To a solution of **7** (108 mg, 149 μmol, 1.0 equiv) in toluene (75.0 mL), I_2 (187 mg, 744 μmol, 5.0 equiv) were added followed by propylene oxide (846 mg, 100 equiv). The reaction mixture was irradiated for 48 h under an argon atmosphere using a photochemical reactor fitted with a 100-watt mercury lamps. After completion, the reaction mixture was extracted with $Na_2S_2O_3$ and water, and dried over $MgSO_4$. The organic layer was concentrated to dryness under reduced pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane/$CHCl_3$ = 4:1 to 2:1) to give compound **2** (36.0 mg, 20% yield) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 2H), 7.76 (s, 2H), 7.73 (s, 2H), 7.55 (s, 2H), 6.75 (s, 2H), 2.59 (s, 6H), 2.54 (s, 6H), 2.52 (s, 6H), 2.51 (s, 6H), 2.34 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.08 (4°), 136.71 (4°), 136.49 (4°), 136.42 (4°), 136.39 (4°), 135.51 (4°), 135.25 (4°), 135.14 (4°), 135.06 (4°), 134.79 (4°), 134.07 (4°), 133.86 (4°), 133.72 (4°), 133.16 (4°), 132.88 (4°), 131.60 (4°), 129.74 (4°), 129.17 (4°), 129.15 (4°), 129.02 (4°), 128.78 (4°), 127.79 (4°), 127.71 (CH), 127.33 (CH), 127.18 (CH), 127.05 (CH), 127.00 (CH), 126.77 (4°), 126.24 (4°), 124.74 (4°), 16.18 (CH_3), 16.10 (CH_3), 16.08 (CH_3), 15.97 (CH_3); HRMS (MALDI-TOF) *m/z* calcd for $C_{70}H_{40}O_{10}$ $[M]^+$: 1200.0331, found: 1200.0352; Mp: >300 °C.

2. X-ray crystallography

Details of the crystal data and a summary of the intensity data collection parameters are listed in Table S1. In each case, a suitable crystal was mounted with mineral oil on a MiTeGen Micromounts and transferred to the goniometer of a Rigaku PILATUS diffractometer. Graphite-monochromated Mo Kα radiation was used. The structures were solved by direct methods with (SIR-97)[3] and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/7)[4] with Yadokari-XG program.[5,6] The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions. CCDC 1865257–1865259 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data and structure refinement details

	5	**1**	**2**
CCDC	1865257	1865258	1865259
formula	$C_{77}H_{51.5}Cl_6S_5$	$C_{77}H_{32}Cl_4S_5$	$C_{73.5}H_{47}S_{11}$
fw	1349.68	1259.12	1282.77
T (K)	123(2)	123(2)	123(2)
λ (Å)	0.71073	0.71073	0.71073
cryst syst	Monoclinic	Triclinic	Triclinic
space group	*C*2/*c*	*P*-1	*P*-1
a (Å)	21.7713(6)	11.7912(14)	14.8387(10)
b (Å)	21.4590(6)	15.1661(13)	15.0351(11)
c (Å)	27.4874(7)	17.2181(19)	15.9054(11)
α (deg)	90	66.531(7)	113.736(7)
β (deg)	92.893(3)	86.454(10)	99.059(6)
γ (deg)	90	69.296(8)	103.599(6)
V (Å^3)	12825.5(6)	2630.7(5)	3027.9(4)
Z	8	2	2
D_{calc} (g / cm^3)	1.398	1.590	1.407
μ (mm^{-1})	0.477	0.477	0.444
F(000)	5564	1284	1328
cryst size (mm)	0.20 × 0.10 × 0.05	0.20 × 0.05 × 0.03	0.03 × 0.02 × 0.02
θ range (deg)	1.959–24.999	3.018–25.000	2.086–24.999
reflns collected	57659	24536	37421
indep reflns/R_{int}	11307/0.0853	9106/0.0417	10586/0.1942
params	821	780	812
GOF on F^2	1.033	1.026	1.004
R_1, wR_2 [I>2σ(I)]	0.0899, 0.2491	0.0595, 0.1560	0.0926, 0.1941
R_1, wR_2 (all data)	0.1146, 0.2702	0.0774, 0.1679	0.2633, 0.2747

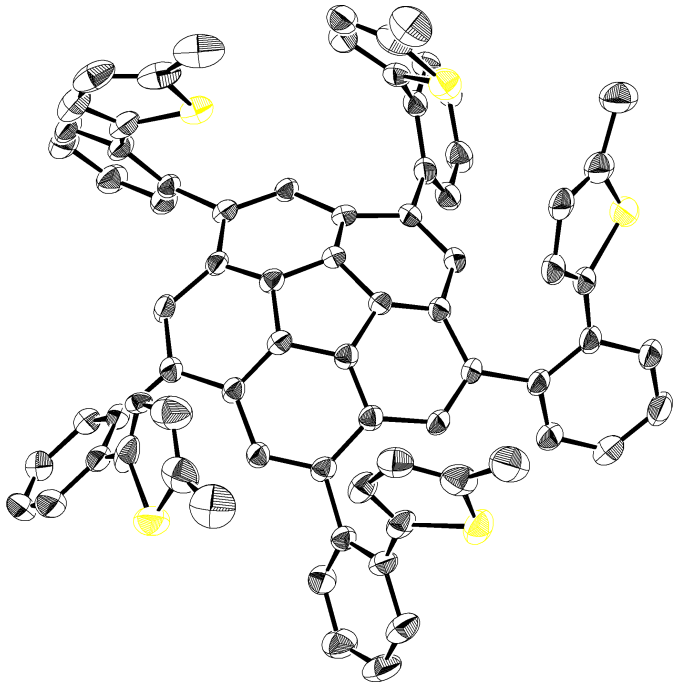


Figure S1. ORTEP drawing of **5** with 50% thermal probability. All hydrogen atoms and solvent molecules (chloroform) are omitted for clarity.

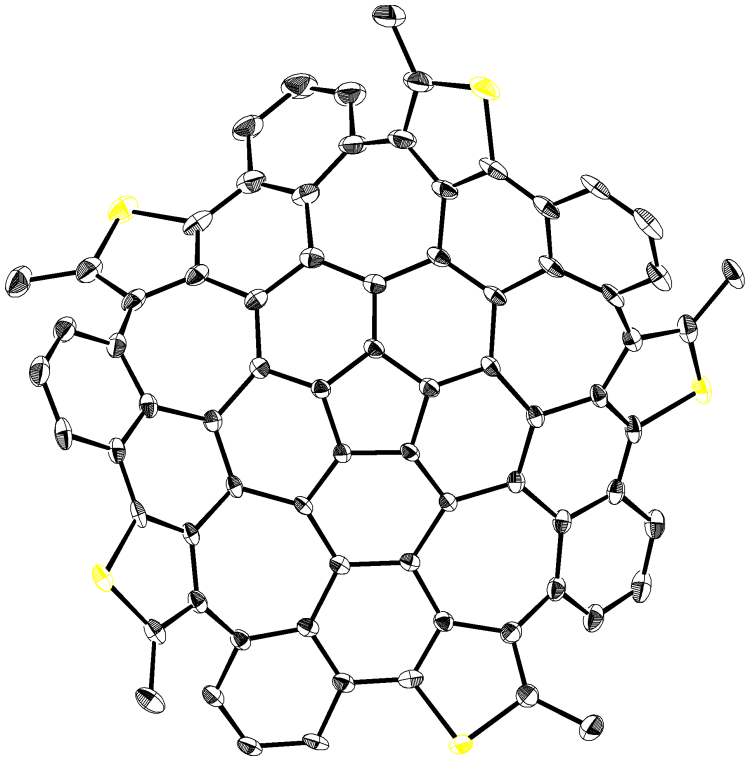


Figure S2. ORTEP drawing of **1** with 50% thermal probability. All hydrogen atoms and solvent molecules (1,1,2,2-tetrachloroethane) are omitted for clarity.

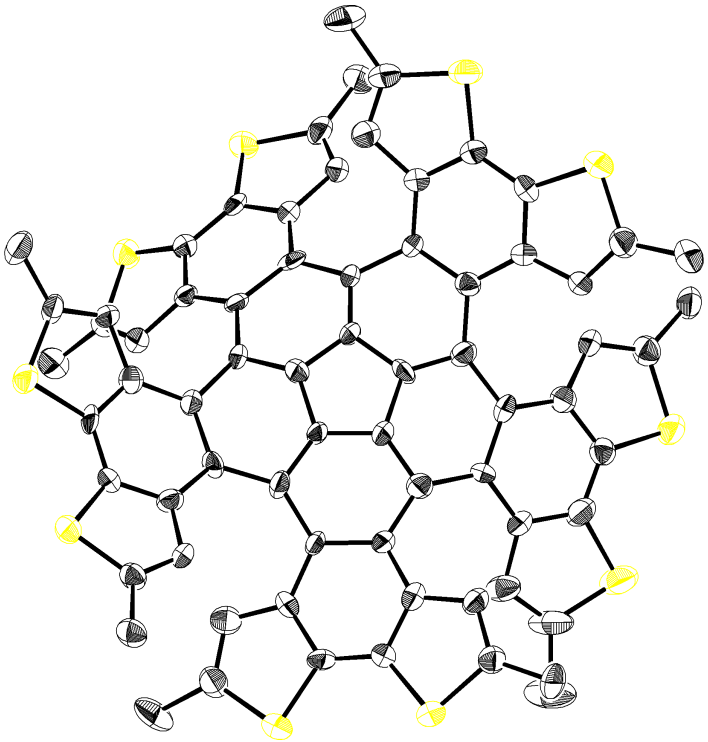


Figure S3. ORTEP drawing of **2** with 50% thermal probability. All hydrogen atoms and solvent molecules (CS_2 and pentane) are omitted for clarity.

3. Photophysical properties

Absorption and fluorescence properties

Dilute solutions in degassed spectral-grade dichloromethane in a 1 cm square quartz cell were used for all measurements. The UV-vis absorption spectra were recorded on a Shimadzu UV-3510 spectrometer with a resolution of 0.5 nm. The emission spectra were measured using an F-4500 Hitachi spectrometer or Shimadzu RF-6000 with a resolution of 0.4 nm. The absolute fluorescence quantum yields (Φ_F) were determined using a Shimadzu RF-6000 with calibrated integrating sphere system (207-21460-41).

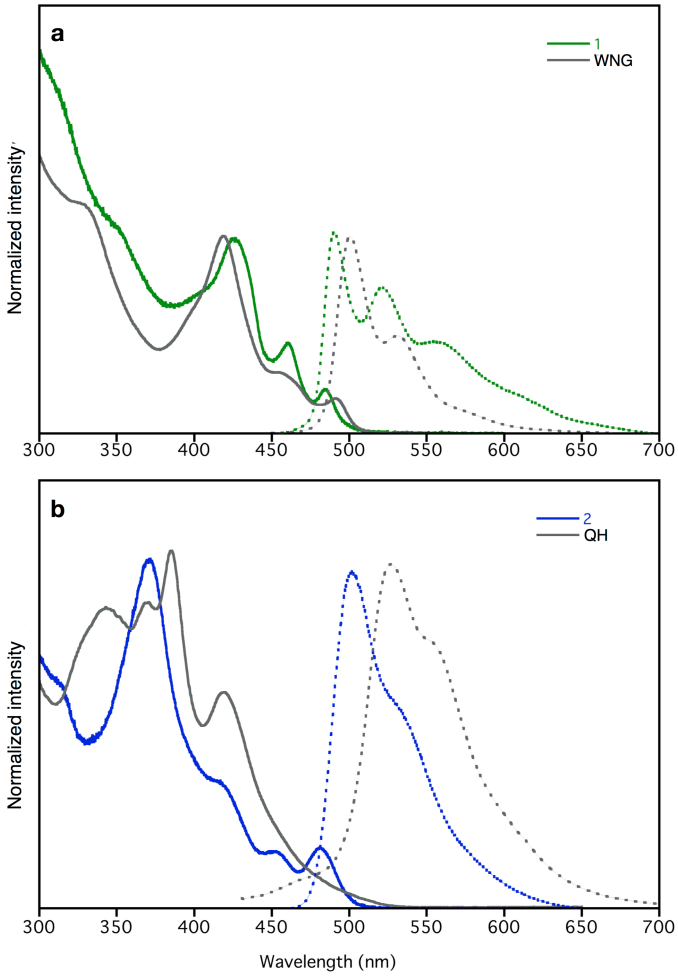


Figure S4. UV/Vis absorption spectra (solid line) and fluorescence spectra (broken line) of a) **1** (green) and WNG (gray) in CH_2Cl_2, and b) **2** (blue) and QH (gray) in CH_2Cl_2. Fluorescence spectra were recorded upon excitation at 445 nm (**1**) and 380 nm (**2**).

3. Theoretical study

The Gaussian 16 program[7] running on a NEC LX 110Rh-1 system was used for optimization (B3LYP/6-31G(d)).[8] Structures were optimized without any symmetry assumptions. Visualization of the results was performed by use of GaussView 5.0.9 software.

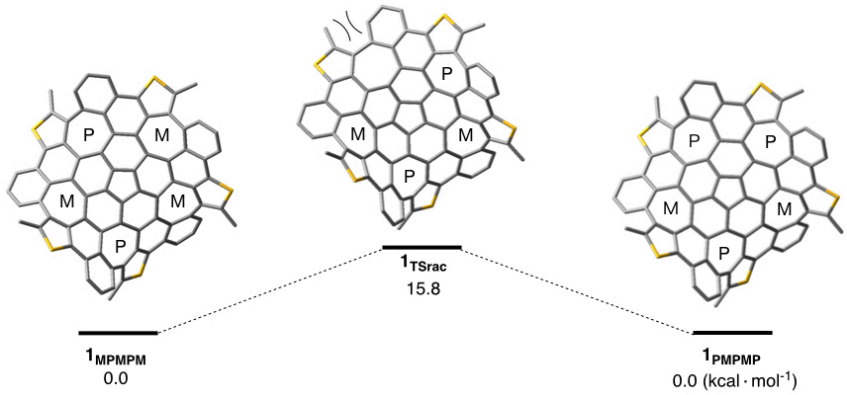


Figure S5. The dynamic conformational behavior of **1**. The racemization pathways of **1** (**1**$_{MPMPM}$ ⇔ **1**$_{TSrac}$ ⇔ **1**$_{PMPMP}$) determined by DFT calculation. Values (kcal·mol^{-1}) are relative Gibbs free energies at 298.15 K and 1 atm calculated at the B3LYP/6-31G(d) level of theory.

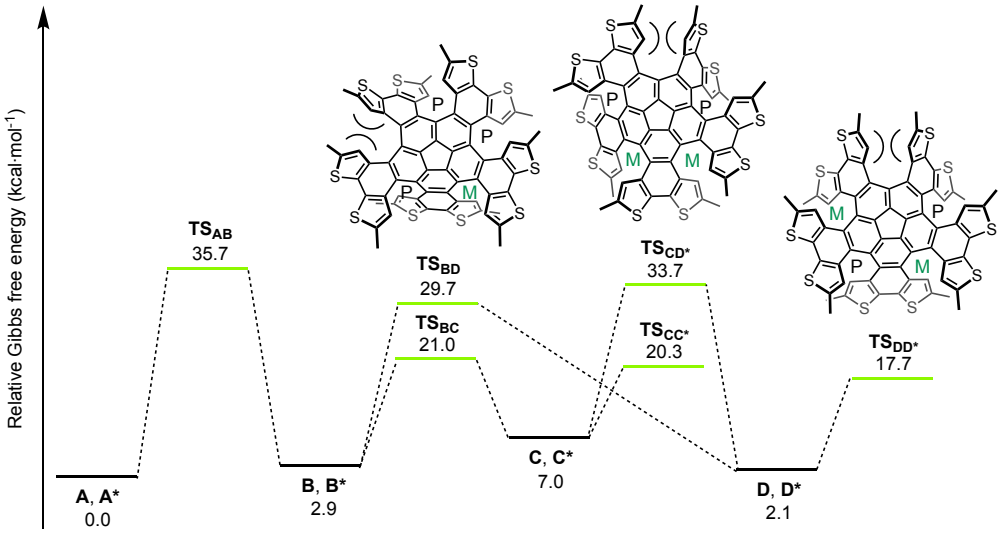
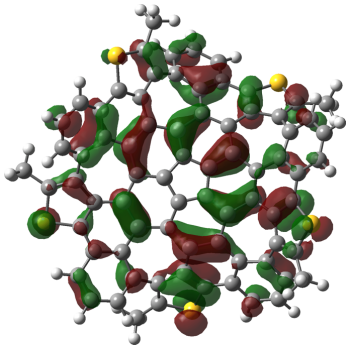
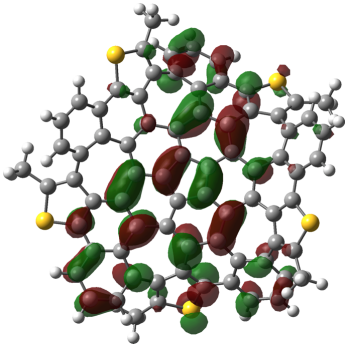


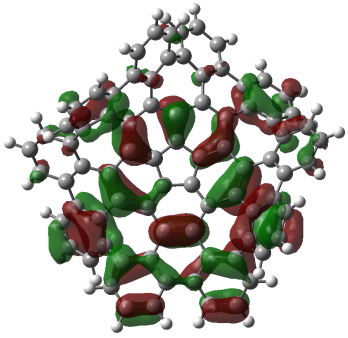
Figure S6. Interconversion pathway among enantiomeric structure of each ground or transition state. Values (kcal·mol^{-1}) are relative Gibbs free energies at 298.15 K and 1 atm calculated at the B3LYP/6-31G(d) level of theory.



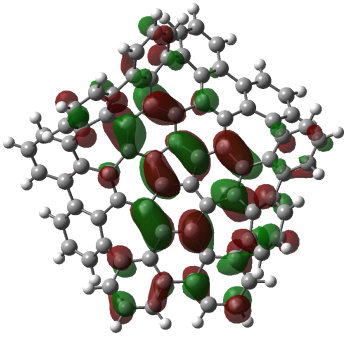
HOMO of **1** (–5.09 eV)



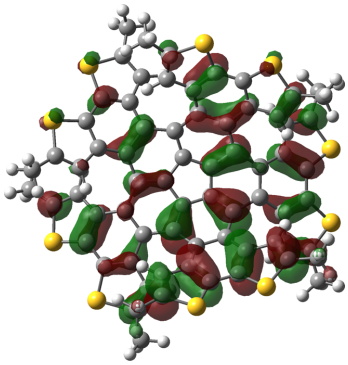
LUMO of **1** (–1.98 eV)



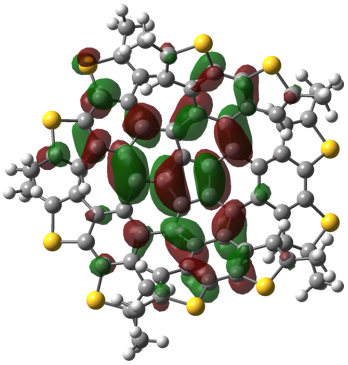
HOMO of **WNG** (–5.11 eV)



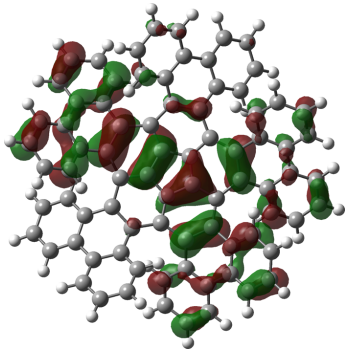
LUMO of **WNG** (–2.09 eV)



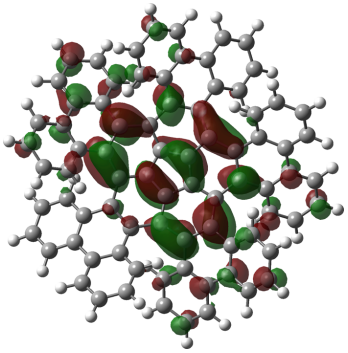
HOMO of **2** (–4.97 eV)



LUMO of **2** (–1.85 eV)



HOMO of **QH** (–5.28 eV)



LUMO of **QH** (–2.17 eV)

Figure S7. Frontier molecular orbitals of **1**, **2**, **WNG**, and **QH** calculated at B3LYP/6-31G(d) level of theory (isovalue = 0.02).

Table S2. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).[a]

	E	*E* + *ZPE*	*H*	*G*
1	-4867.13496846	-4866.335595	-4866.280710	-4866.417394
1_{TSrac}	-4867.11294847	-4866.312795	-4866.259087	-4866.392261
A	-6673.51421332	-6672.637858	-6672.568245	-6672.741092
B	-6673.51067675	-6672.633927	-6672.564454	-6672.736513
C	-6673.50288702	-6672.626474	-6672.556894	-6672.729943
D	-6673.51274930	-6672.635487	-6672.566210	-6672.737677
TS_{AB}	-6673.45931716	-6672.583230	-6672.514586	-6672.684166
TS_{BC}	-6673.48360008	-6672.607188	-6672.538614	-6672.707695
TS_{BD}	-6673.46930176	-6672.592784	-6672.524207	-6672.693796
TS_{CC*}	-6673.48473584	-6672.608304	-6672.539727	-6672.708785
TS_{CD}	-6673.46218285	-6672.585896	-6672.517228	-6672.687340
TS_{DD*}	-6673.48863003	-6672.611987	-6672.543398	-6672.712876

a) *E*: electronic energy; *ZPE*: zero-point energy; *H* (= $E + ZPE + E_{vib} + E_{rot} + E_{trans} + RT$): sum of electronic and thermal enthalpies; *G* (= $H - TS$): sum of electronic and thermal free energies.

Table S3. Cartesian coordinates of optimized structures.

1

C	0.519423	-1.110756	0.260247	C	4.756489	-3.526028	0.090360	H	5.486357	-6.831411	0.518572
C	1.221349	0.114902	0.247284	C	5.388304	-2.264853	0.115913	H	6.591908	-4.596814	0.481130
C	0.270115	1.150727	0.144669	C	4.697130	-1.077898	0.299532	H	6.995999	0.925947	2.518205
C	-1.004880	0.584001	0.241535	C	-3.795767	-4.096566	0.233351	H	6.993855	3.166055	3.571685
C	-0.853760	-0.810226	0.325531	C	-4.726877	-4.989794	-0.303103	H	5.366779	4.867270	2.756224
C	-1.886649	-1.699633	0.326642	C	-4.384890	-5.945125	-1.266735	H	1.677769	6.741585	-2.497288
C	1.052467	-2.358395	0.065842	C	-3.073722	-6.040451	-1.668745	H	-0.145627	7.163166	-4.129440
C	2.577989	0.262318	0.261856	C	1.544217	-6.123530	-2.080578	H	-2.346642	6.064121	-3.782680
C	0.546492	2.456166	-0.143796	C	1.576640	-5.146045	-1.105059	H	-6.301271	3.959948	1.119791
C	-2.182110	1.265987	0.133792	C	2.815489	-4.865760	-0.367800	H	-7.485845	2.759619	2.937177
C	-1.448497	-3.073507	0.061542	C	3.575991	-5.998629	-0.073036	H	-6.988515	0.359436	3.330347
C	-3.178146	-1.016646	0.555620	C	4.926909	-5.929275	0.289017	C	1.675910	7.866479	0.011473
C	-3.345224	0.414118	0.449044	C	5.529993	-4.697501	0.278586	H	2.313117	8.437671	-0.676308
C	-1.976844	2.643698	-0.317721	C	6.929760	-0.320769	0.287169	H	0.657094	7.889521	-0.381610
C	1.981571	2.734987	0.020277	C	5.617440	0.019045	0.548729	H	1.683970	8.393675	0.972568
C	-0.660669	3.229448	-0.507733	C	5.318233	1.280525	1.244688	C	-6.843816	3.704467	-1.562653
C	3.261974	-1.050368	0.229739	C	6.247556	1.650902	2.221602	H	-7.251803	2.843721	-1.027992
C	2.968095	1.707035	0.328668	C	6.256114	2.918387	2.814050	H	-7.324126	4.606961	-1.162379
C	2.545092	-2.328179	0.024168	C	5.344624	3.849395	2.377421	H	-7.136665	3.622804	-2.615986
C	-0.029184	-3.364851	-0.144432	C	2.147056	6.450243	0.183085	C	-5.552262	-4.984780	2.731756
C	-2.450185	-4.095746	-0.255499	C	1.654190	5.273801	-0.338315	H	-6.565069	-5.290002	2.437681
C	-2.105401	-5.149864	-1.155273	C	0.611030	5.264857	-1.381608	H	-4.849013	-5.715124	2.325167
C	-0.731125	-5.315013	-1.457780	C	0.746322	6.191701	-2.414906	H	-5.503945	-5.037959	3.826081
C	0.274976	-4.595404	-0.824729	C	-0.287644	6.445441	-3.326617	C	2.653348	-6.838938	-2.800634
C	-4.581190	1.013564	0.943651	C	-1.500647	5.820184	-3.145983	H	3.606954	-6.328306	-2.652406
C	-5.384854	0.288918	1.882415	C	-5.348108	3.748332	-1.431693	H	2.773416	-7.876719	-2.463522
C	-5.150249	-1.109180	1.992492	C	-4.509601	3.080511	-0.566287	H	2.446032	-6.871507	-3.876984
C	-4.217134	-1.763037	1.202162	C	-5.015307	2.332171	0.605148	C	8.169319	0.526899	0.210590
C	-0.562095	4.451817	-1.303751	C	-6.029544	2.935135	1.349177	H	7.915176	1.588556	0.195508
C	-1.662477	4.852846	-2.129151	C	-6.708865	2.255080	2.369987	H	8.852470	0.356290	1.052702
C	-2.936370	4.295672	-1.832255	C	-6.417672	0.929521	2.602456	H	8.725715	0.295560	-0.706230
C	-3.116570	3.340924	-0.844679	C	-5.209045	-3.603636	2.253726	S	3.524245	6.173015	1.228869
C	4.215006	2.142413	0.956844	C	-4.324166	-3.197569	1.281264	S	-4.458310	4.771680	-2.542951
C	4.340734	3.483741	1.453850	H	-5.755247	-4.925366	0.034035	S	-6.018669	-2.238288	3.005429
C	3.433756	4.451813	0.958021	H	-5.141386	-6.614634	-1.665914	S	-0.091923	-6.503537	-2.559734
C	2.357649	4.114168	0.157139	H	-2.766185	-6.814078	-2.366466	S	7.107605	-2.025641	-0.046015
C	3.336699	-3.555472	-0.082528	H	3.104133	-6.969129	-0.175405				

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C	-0.486705	-1.121538	-0.577666	C	-4.367676	-3.877297	-0.291807	H	-4.818496	-7.212820	0.266326
C	-1.270832	0.055669	-0.623186	C	-5.033934	-2.762041	-0.853865	H	-5.985647	-5.254231	-0.708444
C	-0.380987	1.156100	-0.589890	C	-4.582143	-1.445908	-0.806008	H	-7.299429	1.016395	-2.532727
C	0.921593	0.661740	-0.751420	C	4.005858	-3.754467	0.070689	H	-7.762206	3.349384	-2.479575
C	0.858152	-0.751015	-0.724684	C	4.983390	-4.490689	0.746426	H	-6.213915	4.862889	-1.239799
C	1.938870	-1.551521	-0.482586	C	4.702287	-5.245068	1.890582	H	-1.787199	5.906352	3.368844
C	-0.920890	-2.318323	-0.061411	C	3.408733	-5.294164	2.355698	H	0.277411	6.351555	4.674483
C	-2.624325	0.109952	-0.469194	C	-1.195573	-5.412575	2.977794	H	2.472380	5.727205	3.678747
C	-0.714131	2.377932	-0.057755	C	-1.290312	-4.728736	1.785330	H	5.849531	4.231579	-2.145748
C	2.058578	1.395632	-0.576861	C	-2.500756	-4.779729	0.950524	H	7.049102	2.877002	-3.842484
C	1.601029	-2.854939	0.072325	C	-3.125741	-6.027680	0.903116	H	6.815262	0.406835	-3.814844
C	3.200434	-0.834544	-0.750958	C	-4.361314	-6.227725	0.279221	C	-2.424260	7.513760	1.333911
C	3.278044	0.593044	-0.821504	C	-4.995063	-5.144290	-0.277182	H	-2.930585	7.802208	2.264257
C	1.805477	2.724002	-0.045783	C	-6.594483	-1.218967	-2.011847	H	-1.349272	7.621183	1.493432
C	-2.184502	2.539694	0.019539	C	-5.530586	-0.509337	-1.438895	H	-2.730153	8.232220	0.564233
C	0.473373	3.182986	0.336276	C	-5.483900	0.989037	-1.410228	C	6.685778	4.302886	0.469521
C	-3.219402	-1.232217	-0.371998	C	-6.584106	1.609914	-2.012419	H	7.120870	3.446382	-0.050766
C	-3.134203	1.493693	-0.381442	C	-6.870784	2.972802	-1.986292	H	6.980084	5.208723	-0.076606
C	-2.403182	-2.390453	0.008992	C	-6.019927	3.797641	-1.310922	H	7.138532	4.364695	1.465609
C	0.207515	-3.179995	0.359129	C	-2.764265	6.114035	0.903670	C	5.859785	-4.918278	-2.263980
C	2.668202	-3.720563	0.584256	C	-2.038888	4.943843	0.978220	H	6.887632	-5.097786	-1.922143
C	2.390837	-4.564393	1.704758	C	-0.807778	4.873463	1.777901	H	5.204390	-5.622579	-1.746251
C	1.032402	-4.701951	2.095575	C	-0.831427	5.556286	2.995475	H	5.830418	-5.150696	-3.335272
C	-0.020890	-4.212733	1.334819	C	0.331950	5.825919	3.725595	C	-2.268526	-5.982863	3.861125
C	4.450124	1.199792	-1.433005	C	1.542534	5.464173	3.182428	H	-3.252596	-5.621769	3.554356
C	5.288291	0.407265	-2.283003	C	5.193493	4.160219	0.574850	H	-2.290602	-7.080325	3.841335
C	5.181497	-1.006955	-2.156188	C	4.311305	3.389519	-0.153789	H	-2.104889	-5.682409	4.903137
C	4.293216	-1.597275	-1.269947	C	4.766865	2.587855	-1.310340	C	-7.827269	-0.912624	-2.841337
C	0.403891	4.264018	1.323260	C	5.666299	3.163777	-2.204563	H	-8.584402	-0.343939	-2.288251
C	1.594352	4.708953	1.989813	C	6.361600	2.395501	-3.152916	H	-7.591683	-0.369231	-3.763125
C	2.842233	4.388267	1.393863	C	6.216183	1.025303	-3.151864	H	-8.304126	-1.849765	-3.147941
C	2.955325	3.493451	0.345963	C	5.412105	-3.507121	-2.015269	S	-4.312363	5.871443	0.134990
C	-4.492649	1.864080	-0.792196	C	4.489502	-3.016280	-1.120223	S	4.387474	5.058555	1.842542
C	-4.847424	3.263257	-0.739872	H	6.002669	-4.452111	0.379397	S	6.135252	-2.222703	-2.976022
C	-3.970311	4.174818	-0.107931	H	5.494765	-5.795681	2.389368	S	0.468158	-5.580874	3.493531
C	-2.702147	3.838484	0.322465	H	3.153526	-5.914552	3.210102	S	-6.510391	-2.924541	-1.720878
C	-3.065057	-3.670931	0.242317	H	-2.629982	-6.868231	1.374563				

A

C	-3.097370	1.383334	0.015039	C	1.238770	5.667066	0.340477	H	-1.351604	-4.855956	1.543640
C	-2.244658	2.555372	-0.211301	C	-5.302274	0.793110	1.250175	H	4.202734	-2.786614	1.540354
C	-2.560965	0.019816	-0.160039	C	-6.477861	1.364009	1.627582	H	3.949872	3.135158	1.540632
C	-0.772651	2.441731	-0.160317	S	-6.601094	3.026399	1.050812	H	-1.762639	4.721901	1.541227
C	-0.358254	1.142530	-0.276298	C	-5.007350	2.929861	0.335262	H	-5.036744	-0.214476	1.541906
C	-1.197293	0.012221	-0.276070	C	-4.291934	3.944897	-0.313351	H	-7.323096	-0.269170	2.708049
C	0.976048	0.693912	-0.275943	C	-7.583760	0.758163	2.436428	H	-7.769493	1.318346	3.361349
C	-0.381596	-1.134996	-0.275700	C	2.425747	5.301180	-0.307567	H	-8.527418	0.728241	1.877358
C	-3.123872	-1.345053	-0.209888	S	-4.886934	5.480917	-0.903108	H	-1.363635	4.966376	-1.629933
C	0.961581	-0.713703	-0.275736	C	-3.295510	5.885991	-1.550289	H	4.301534	2.833769	-1.628517
C	-2.272633	-2.518130	0.016851	C	-2.388729	4.907165	-1.286987	H	5.768627	4.523167	2.707202
C	0.358270	3.373101	0.016062	C	-2.919660	3.776231	-0.565623	H	7.064645	3.501947	3.358012
C	-0.810128	-2.429532	-0.158921	S	3.703494	6.342410	-0.894483	H	7.327398	4.424275	1.873041
C	1.736673	2.924543	-0.209878	C	4.580358	4.955042	-1.544015	H	6.084554	-4.085852	2.707253
C	2.083696	1.489447	-0.159752	C	3.929057	3.789888	-1.283460	H	5.516127	-5.634801	3.358246
C	0.313906	-3.386744	-0.209235	C	2.689245	3.944378	-0.562164	H	6.473378	-5.598300	1.872509
C	1.692753	-2.939765	0.016467	C	5.790986	-0.669488	-0.311964	H	-2.005495	-7.046424	2.712031
C	3.319068	0.701494	0.015862	C	6.582953	3.845369	2.433977	H	-3.652612	-6.979590	3.366779
C	2.060330	-1.521403	-0.159555	C	5.692586	-5.070217	2.434191	H	-3.327346	-7.883454	1.882859
C	3.317948	-0.748066	-0.210461	C	1.152810	-5.714571	-0.309521	H	-1.815941	-4.819466	-1.627359
C	2.611222	-3.944604	0.492071	C	-3.063337	-6.976607	2.441273	H	-5.144026	0.236131	-1.630843
C	4.558708	1.263968	0.491521	C	-5.078360	-2.862546	-0.309567	H	4.021583	-3.214958	-1.631594
C	0.205563	4.725295	0.493091	S	0.730761	-7.307273	-0.898207	H	-1.241664	-8.050620	-3.173888
C	-4.430947	1.656522	0.490676	C	-0.794441	-6.699417	-1.546108	H	-2.062110	-8.445279	-1.658572
C	-2.944561	-3.701640	0.493543	C	-0.952305	-5.374337	-1.283597	H	-2.602912	-7.058768	-2.618272
C	-2.392230	-4.796784	1.253193	C	0.142009	-4.771432	-0.562316	H	7.274253	-3.666704	-3.177520
C	-3.298284	-5.738022	1.632005	S	-6.723093	-2.954164	-0.899177	H	7.391811	-4.570860	-1.662979
S	-4.917815	-5.341558	1.056490	C	-6.616244	-1.316270	-1.548466	H	5.908029	-4.653944	-2.625989

C	-4.333874	-3.856119	0.339523	C	-5.404997	-0.756276	-1.285894	H	-2.523042	6.878476	2.708848
C	3.824433	-3.757940	1.250236	C	-4.493711	-1.609967	-0.563352	H	-1.152004	7.792125	3.365842
C	4.440221	-4.910621	1.627774	S	7.175003	-1.562695	-0.901918	H	-1.944433	8.332963	1.881090
S	3.561920	-6.328235	1.053025	C	6.125218	-2.824614	-1.550687	H	5.738229	5.789276	-3.168521
C	2.328719	-5.313648	0.338012	C	4.816342	-2.565560	-1.287249	H	6.632726	5.620668	-1.653087
C	4.756622	2.475295	1.249926	C	4.581503	-1.339120	-0.564812	H	6.254610	4.184462	-2.617542
C	6.043393	2.704549	1.626793	C	-1.719966	-7.614262	-2.288095	H	-3.726425	7.241743	-3.178814
S	7.119670	1.430869	1.051610	C	6.709234	-3.987178	-2.293322	H	-3.298744	8.043271	-1.662339
C	5.773298	0.572103	0.336767	C	-1.625828	7.443832	2.439560	H	-2.043260	7.241529	-2.619934
C	-0.885915	5.286159	1.251808	C	5.867472	5.152199	-2.284669	H	-8.040096	-1.309522	-3.175902
C	-0.706746	6.580125	1.631136	C	-3.084639	7.170404	-2.291781	H	-8.668239	-0.650562	-1.660513
S	0.836987	7.211797	1.057353	C	-7.772542	-0.719336	-2.290534	H	-7.517423	0.291988	-2.621220

B

C	-2.597748	2.040854	0.149470	C	2.750962	4.970901	0.430585	H	3.623307	-3.626597	1.075274
C	-1.481763	2.974815	-0.031244	C	5.394592	0.947230	0.679299	H	-2.395473	-4.663987	-1.302620
C	-2.475818	0.640121	-0.264583	C	6.730029	0.788864	0.885982	H	-4.803602	0.732556	1.566553
C	-0.099835	2.477624	-0.183822	S	7.316222	-0.718352	0.184585	H	-0.274767	4.713139	1.885992
C	-0.063163	1.143856	-0.509822	C	5.700308	-1.139949	-0.339238	H	4.854485	1.797822	1.072714
C	-1.184607	0.289918	-0.550123	C	5.279924	-2.336727	-0.934514	H	2.682741	-4.323054	-1.761904
C	1.098963	0.344869	-0.570810	C	-0.599564	-5.383327	1.552089	H	-3.440116	-3.606702	1.275413
C	-0.709368	-1.044028	-0.531811	C	-5.572443	-1.330058	-1.402091	H	-4.893539	1.961664	-1.233274
C	-3.407351	-0.495216	-0.529627	C	-3.074130	4.834797	0.349294	H	-0.139370	5.278885	-1.245372
C	0.691531	-1.004973	-0.522172	C	3.734037	4.380520	-0.375128	H	4.744524	1.650769	-2.073676
C	-2.902855	-1.867158	-0.551297	S	6.251163	-3.624703	-1.613341	H	6.773775	4.270774	-3.558876
C	1.250352	3.044795	0.000636	C	4.802740	-4.561827	-1.997354	H	7.729170	3.726132	-2.174983
C	-1.469116	-2.146366	-0.272231	C	3.673869	-3.914604	-1.602816	H	6.889298	2.540603	-3.187583
C	2.436151	2.273611	-0.383249	C	3.908085	-2.632493	-0.985690	H	-0.310190	6.840543	3.321465
C	2.385352	0.797884	-0.443047	S	-1.601465	-6.499836	2.456311	H	1.311837	7.257198	3.906071
C	-0.679796	-3.267021	0.268250	C	-3.007853	-5.462614	2.227591	H	0.585465	8.178279	2.584019
C	0.796052	-3.252693	0.223662	C	-2.702738	-4.368327	1.481681	H	-1.951560	8.301670	-2.124282
C	3.363736	-0.305705	-0.350541	C	-1.328820	-4.299733	1.035704	H	-1.150020	8.709054	-0.602298
C	1.514789	-2.077460	-0.323151	S	-7.121491	-0.789796	-2.016433	H	-0.281226	7.780710	-1.834844
C	2.928371	-1.694033	-0.522219	C	-6.623251	0.894347	-1.867001	H	-6.953834	1.048923	2.950772
C	4.763050	-0.132569	-0.038897	C	-5.369950	1.000005	-1.353017	H	-6.908368	2.535952	3.915449
C	1.515003	4.324407	0.614359	C	-4.734323	-0.258063	-1.029669	H	-7.876699	2.470975	2.437844
C	-3.762956	2.556310	0.820646	S	-3.287860	6.546288	0.054401	H	-3.365002	-6.828009	-2.276379
C	-3.744920	-2.898274	-1.083437	C	-1.727829	6.633803	-0.766501	H	-5.071344	-7.038904	-1.850031
C	1.495304	-4.300075	0.932434	C	-1.098506	5.428066	-0.765665	H	-4.630339	-6.513628	-3.479166
C	2.892658	-4.387385	1.296916	C	-1.834334	4.367787	-0.121800	H	-7.820996	1.916509	-3.347346
C	3.238187	-5.495006	2.004929	S	5.186886	5.104548	-1.027777	H	-8.473776	1.996886	-1.706722
S	1.844838	-6.526189	2.307786	C	5.592647	3.608556	-1.873308	H	-7.055108	2.965542	-2.138563
C	0.795235	-5.387483	1.491591	C	4.678247	2.633315	-1.623046	H	5.319280	-5.100125	2.259205
C	-3.388287	-4.255006	-1.432521	C	3.597573	3.035177	-0.756253	H	4.600170	-6.010319	3.601924
C	-4.400049	-4.989090	-1.964530	C	6.809934	3.537483	-2.743594	H	4.942704	-6.820078	2.068510
S	-5.887447	-4.047082	-2.090550	C	0.684885	7.171884	3.009670	H	-4.707338	-6.781752	2.421880
C	-5.081702	-2.635388	-1.435114	C	-1.257529	7.925192	-1.362496	H	-4.268296	-5.945268	3.915882
C	-4.794425	1.813459	1.501242	C	-6.933914	2.141363	2.892060	H	-5.068143	-5.057558	2.604595
C	-5.747157	2.583990	2.092169	C	-4.368774	-6.416295	-2.418145	H	5.401040	-5.793974	-3.670011
S	-5.438611	4.302335	1.831763	C	-7.543702	1.998144	-2.288995	H	5.515332	-6.598499	-2.099976
C	-3.978680	3.939421	0.937674	C	4.594024	-5.879122	2.512727	H	3.927844	-6.318014	-2.834345
C	0.692410	5.057880	1.545163	C	-4.329712	-5.834030	2.826153	H	7.120320	2.572335	1.988922
C	1.254035	6.202987	2.018830	C	4.922391	-5.886180	-2.687075	H	8.151892	1.208440	2.460221
S	2.853793	6.469749	1.327166	C	7.668859	1.705028	1.609469	H	8.465604	2.073809	0.951216

C

C	2.700197	-1.991131	-0.597422	C	1.084211	4.804364	1.978600	H	3.161838	-4.236583	0.639227
C	3.311864	-0.707826	-0.236896	C	5.518190	-1.833295	-0.371962	H	-3.315073	-3.916627	-1.733439
C	1.255128	-2.222921	-0.392592	S	7.162745	-1.723612	0.216660	H	-4.926329	1.661003	-1.402549
C	2.490984	0.521224	-0.193097	C	6.762549	-0.291718	1.164438	H	0.030807	4.588122	2.109350
C	1.154893	0.245382	-0.347095	C	5.465286	0.077335	0.983815	H	5.029548	0.914353	1.513438
C	0.576933	-1.038953	-0.378376	C	4.264979	3.863964	0.426422	H	1.582582	6.732322	4.590762
C	0.106890	1.184694	-0.316774	C	1.113030	6.800825	3.601502	H	1.227379	7.835849	3.256068
C	-0.819139	-0.895435	-0.338345	C	4.951802	-2.848780	-1.155151	H	0.043428	6.602914	3.720016
C	0.392839	-3.376895	-0.034344	C	7.795682	0.353155	2.036753	H	8.185311	-0.340861	2.791909
C	-1.117669	0.481098	-0.356046	C	-1.227199	-5.543478	0.913684	H	8.651926	0.715676	1.454066
C	-1.071672	-3.214245	0.079834	C	3.872116	-6.842582	1.527923	H	7.357988	1.210297	2.557195
C	2.726877	1.964318	0.014639	C	-5.809506	-5.197254	-2.400926	H	3.874433	-7.197691	2.566029
C	-1.722557	-1.914803	-0.226340	C	-5.761364	-0.623162	0.378911	H	4.099097	-7.704565	0.887764

C	1.613816	2.854837	0.363777	C	-2.252528	5.337642	-0.746980	H	4.683740	-6.117857	1.413401
C	0.231262	2.508663	0.004006	C	-6.962706	3.448987	-2.296613	H	-6.360786	-5.916412	-1.782343
C	-3.107543	-1.404524	-0.260449	C	-4.702720	0.285500	0.552372	H	-6.431782	-4.974531	-3.276682
C	-3.390315	0.004992	0.030606	C	-5.117290	1.416857	1.343748	H	-4.895733	-5.687004	-2.750759
C	-1.048424	3.244520	-0.187274	C	-6.417425	1.379894	1.742376	H	-7.746207	3.893782	-1.670127
C	-2.353541	1.032083	-0.159786	S	-7.234488	-0.065224	1.142013	H	-7.050579	3.895364	-3.294960
C	-2.318250	2.513613	-0.298461	C	-1.046992	4.648051	-0.507738	H	-7.170653	2.378225	-2.382528
C	4.716059	-0.773564	0.092487	C	0.075623	5.525034	-0.759895	H	-4.447614	2.219385	1.627706
C	1.952140	4.022480	1.133779	C	-0.253531	6.803344	-1.081630	H	1.106210	5.205796	-0.736809
C	-3.471823	3.234117	-0.766345	S	-2.000460	7.028946	-1.126920	H	5.098117	1.277869	-1.565991
C	-4.234680	-2.212281	-0.634562	C	4.005409	2.608240	-0.151480	H	2.124229	-4.317024	-2.261572
C	0.969031	-4.619409	0.422738	C	5.108613	2.188097	-0.979707	H	-3.758006	-3.378927	1.333991
C	0.149929	-5.711703	0.767513	C	6.154604	3.057434	-1.012734	H	-6.493567	3.198823	2.853879
S	1.063965	-7.113901	1.281261	S	5.853897	4.465359	0.007236	H	-8.021412	2.792162	2.055977
C	2.567309	-6.206280	1.158995	C	3.553592	-2.955127	-1.230431	H	-7.531550	1.921906	3.514779
C	2.349126	-4.940383	0.715327	C	3.159005	-4.071928	-2.052506	H	-5.479159	-4.837457	2.517394
C	-5.548096	-1.809727	-0.338263	C	4.197121	-4.778968	-2.573876	H	-5.430782	-6.506492	1.928570
S	-6.731781	-2.948327	-0.943037	S	5.752063	-4.114811	-2.060086	H	-4.728659	-6.109406	3.501296
C	-5.458507	-3.958572	-1.635101	C	-1.818371	-4.286171	0.692033	H	3.106391	-6.236632	-3.685161
C	-4.224892	-3.445915	-1.380168	C	-3.142836	-4.262760	1.273957	H	4.635869	-5.764177	-4.447404
C	-3.450086	4.636977	-0.887020	C	-3.556674	-5.439281	1.813422	H	4.643624	-6.839961	-3.044609
S	-4.959392	5.284716	-1.497320	S	-2.321641	-6.685971	1.665061	H	7.434624	2.009179	-2.359039
C	-5.599594	3.656383	-1.711335	C	-7.157955	2.371636	2.586334	H	7.568165	3.773102	-2.484409
C	-4.713598	2.714138	-1.295695	C	-4.865126	-5.742166	2.476527	H	8.308524	2.926007	-1.121220
C	3.272329	4.498448	1.187764	C	4.147801	-5.966407	-3.485814	H	1.706641	7.608457	-1.327910
S	3.421947	5.896625	2.229136	C	7.433779	2.939753	-1.783525	H	0.493159	8.358773	-2.383231
C	1.704624	5.822779	2.633205	C	0.667239	7.945974	-1.381725	H	0.543049	8.766917	-0.664190

D

C	1.716245	-2.703201	0.397282	C	-5.318172	-0.647081	-1.687714	H	3.793337	-3.668088	-1.168336
C	0.305636	-3.128735	0.490929	C	0.974524	-4.838034	2.158173	H	4.636987	2.189898	0.692144
C	2.081931	-1.505541	-0.364658	S	0.323755	-5.999913	3.294790	H	-1.276240	5.003807	-1.531974
C	-0.750474	-2.390803	-0.213893	C	-1.320069	-5.504560	2.901511	H	-5.116973	0.413920	-1.721782
C	-0.333226	-1.177830	-0.694619	C	-1.332748	-4.538860	1.944790	H	-2.257952	-4.093399	1.610620
C	1.001131	-0.757456	-0.743687	C	-4.065503	-4.035696	-1.182208	H	-7.813426	-0.749949	-3.829644
C	-1.169773	-0.029199	-0.781779	C	-7.626211	-0.432665	-2.796236	H	-8.552779	-0.596312	-2.231627
C	1.011588	0.664158	-0.800782	C	2.314342	-4.454140	2.047758	H	-7.422273	0.642290	-2.801960
C	3.335804	-0.798640	-0.759482	C	-2.489041	-6.131425	3.597484	H	-2.543265	-7.211148	3.409590
C	-0.320181	1.103086	-0.731826	C	5.545726	0.515161	-2.001541	H	-2.440724	-5.991068	4.684506
C	3.345525	0.650450	-0.876542	C	6.132222	-4.765849	-2.415384	H	-3.419316	-5.681452	3.237812
C	-2.206753	-2.570446	-0.463620	C	6.354851	4.009061	2.060852	H	6.285392	-4.908093	-3.492369
C	2.113037	1.431693	-0.556873	C	1.212651	5.169098	1.418551	H	7.073837	-5.023839	-1.914724
C	-3.073656	-1.409482	-0.626231	C	-4.935608	2.827267	0.246817	H	5.369419	-5.477013	-2.084392
C	-2.507605	-0.034011	-0.494067	C	-2.981802	7.286259	-1.978081	H	6.949882	4.802789	1.591651
C	1.796090	2.738078	0.033362	C	0.148462	4.367480	0.962951	H	6.470339	4.113247	3.146875
C	0.396626	3.198645	0.147306	C	-1.091105	4.841315	1.539396	H	6.784948	3.047811	1.763851
C	-3.032488	1.304621	-0.200713	C	-0.985568	5.963551	2.298939	H	-3.615986	7.453562	-2.857548
C	-0.713841	2.366897	-0.371212	S	0.678971	6.525794	2.387713	H	-3.196677	8.089215	-1.261995
C	-2.187643	2.486258	-0.374462	C	-4.355507	1.547738	0.316962	H	-1.937622	7.384865	-2.289793
C	-0.029034	-4.146243	1.458372	C	-5.221569	0.627726	1.011263	H	-2.037273	4.335832	1.436505
C	-4.389363	-1.622112	-1.161026	C	-6.397100	1.167461	1.432975	H	-4.953610	-0.401272	1.215222
C	-2.859659	3.727841	-0.624247	S	-6.525452	2.867644	0.978353	H	-0.933321	-5.203377	-0.758433
C	2.825512	3.500777	0.698047	C	-2.718320	-3.863422	-0.811074	H	4.541331	-2.129746	1.077793
C	4.433852	-1.534826	-1.310817	C	-1.995337	-5.108242	-0.940377	H	3.808228	3.397285	-1.790248
C	5.544570	-0.874236	-1.873675	C	-2.752597	-6.166764	-1.330031	H	-3.032631	6.188909	2.855834
S	6.723426	-1.997519	-2.522017	S	-4.435469	-5.700211	-1.587145	H	-1.893586	6.746249	4.097622
C	5.696960	-3.368824	-2.094780	C	2.681145	-3.357132	1.248817	H	-2.179591	7.727684	2.655862
C	4.552295	-2.964545	-1.484511	C	4.052545	-2.986325	1.516870	H	5.380314	5.006890	-3.029862
C	2.536276	4.744859	1.282239	C	4.698630	-3.785552	2.407063	H	7.084515	4.586089	-2.789301
S	3.937526	5.484483	2.026798	S	3.645032	-5.061840	3.009078	H	6.288438	4.193039	-4.317776
C	4.917430	4.071959	1.644137	C	4.441286	1.270256	-1.558504	H	6.599833	-2.817579	2.419902
C	4.198970	3.136951	0.967744	C	4.562981	2.646038	-1.983138	H	6.170354	-3.558030	3.973351
C	-4.228007	3.883734	-0.344187	C	5.703344	2.930060	-2.664811	H	6.698163	-4.574024	2.626708
S	-4.805586	5.476960	-0.781397	S	6.722941	1.500254	-2.848000	H	-1.247493	-7.678344	-1.354022
C	-3.205510	5.932151	-1.377912	C	-2.076871	6.696574	3.016984	H	-2.842546	-8.274086	-0.865156
C	-2.310092	4.921467	-1.217361	C	6.140023	4.245843	-3.232071	H	-2.518318	-7.923317	-2.567056
C	-4.890450	-2.925395	-1.361847	C	6.114608	-3.681230	2.884620	H	-7.242404	-0.542952	2.386650
S	-6.495290	-2.924518	-2.065370	C	-2.321373	-7.585453	-1.542060	H	-7.677802	0.989367	3.165801
C	-6.469550	-1.165614	-2.189005	C	-7.500580	0.503482	2.198191	H	-8.447779	0.521645	1.644818

TS_{AB}

C	-0.674613	3.169669	-0.295622	C	0.562070	5.236303	1.188034	H	-2.831956	3.841449	1.448341
C	0.732174	3.045928	0.048147	S	1.329536	6.216997	2.416844	H	-4.962170	-1.199175	0.695022
C	-1.445480	1.969720	-0.649769	C	2.533709	4.962028	2.714564	H	-0.744899	-3.787956	1.901471
C	1.522042	1.940899	-0.498435	C	2.352375	3.894580	1.890622	H	2.983710	3.016279	1.938913
C	0.770897	0.936188	-1.057579	C	5.256384	2.617920	-0.512268	H	7.622571	-2.308923	-2.793113
C	-0.648320	0.928019	-1.086332	C	8.087862	-1.444197	-2.310720	H	8.785273	-1.820632	-1.551369
C	1.252725	-0.404512	-1.151691	C	-0.581832	5.529921	0.428755	H	8.681592	-0.913732	-3.065401
C	-1.067972	-0.421423	-1.175457	C	3.572706	5.146384	3.778005	H	4.222941	4.267249	3.815771
C	-2.864351	1.611472	-0.499724	C	-5.623503	1.103930	-1.003528	H	3.123943	5.280138	4.770239
C	0.100383	-1.226349	-1.130499	C	-5.172182	5.169732	2.422693	H	4.203747	6.022509	3.583407
C	-3.303262	0.276434	-0.873218	C	-7.077759	-2.824980	1.710833	H	-4.209043	5.509207	2.815435
C	2.969602	1.682356	-0.581206	C	-2.670021	-5.099444	-0.241223	H	-5.788656	4.840462	3.268529
C	-2.345280	-0.839918	-0.884937	C	3.744018	-4.012562	0.904067	H	-5.673589	6.034969	1.970997
C	3.498939	0.336177	-0.813875	C	-0.191708	-5.233600	4.310553	H	-7.205796	-1.740786	1.782943
C	2.547173	-0.837082	-0.888894	C	-1.423091	-4.514731	-0.511887	H	-7.927016	-3.226152	1.143570
C	-2.462640	-2.258871	-0.508688	C	-0.431720	-5.520571	-0.804789	H	-7.134704	-3.243628	2.723424
C	-1.272854	-3.089873	-0.525134	C	-0.895944	-6.797465	-0.754008	H	-1.237442	-4.978222	4.114276
C	2.577976	-2.262439	-0.431683	S	-2.609600	-6.845574	-0.327214	H	-0.129669	-6.321630	4.437503
C	0.064836	-2.488850	-0.598805	C	3.726723	-3.154062	-0.207967	H	0.096013	-4.775545	5.265159
C	1.328368	-2.890564	-0.008774	C	5.622646	-4.512993	-0.660620	H	0.592846	-5.289094	-1.068408
C	1.232255	4.016787	0.991812	S	5.148991	-5.057095	0.938212	H	2.578948	4.585945	-1.005517
C	4.925437	0.256770	-1.003457	C	3.869800	2.806504	-0.601204	H	-2.933969	4.390055	-1.701113
C	1.367487	-3.730181	1.173611	C	3.571443	4.205554	-0.812030	H	-4.651435	-1.781094	-2.453241
C	-3.662229	-2.880131	0.009689	C	4.652434	5.028287	-0.795955	H	0.891252	-7.840288	-1.271354
C	-3.898644	2.456978	0.062926	S	6.146147	4.127048	-0.532394	H	-0.148878	-8.731298	-0.148309
C	-5.256495	2.199276	-0.208354	C	-1.214971	4.502039	-0.289578	H	-0.584532	-8.629157	-1.858885
S	-6.323980	3.306025	0.626878	C	-2.332181	5.008656	-1.046077	H	-6.854889	-2.516652	-3.582540
C	-4.954577	4.071510	1.427129	C	-2.548692	6.343994	-0.903197	H	-8.283298	-2.024035	-2.658422
C	-3.774821	3.524984	1.024955	S	-1.383780	7.069379	0.208821	H	-7.819421	-1.124874	-4.108122
C	-3.750252	-4.283924	0.115350	C	-4.666473	0.118970	-1.289729	H	-4.219101	6.569108	-2.209950
S	-5.268944	-4.808784	0.808447	C	-5.228508	-0.937005	-2.094372	H	-3.158790	7.989787	-2.166460
C	-5.770799	-3.138170	1.048949	C	-6.543262	-0.769640	-2.399376	H	-4.256518	7.664977	-0.819495
C	-4.836670	-2.265842	0.583309	S	-7.185524	0.715325	-1.688163	H	3.675173	6.888940	-1.160346
C	2.588990	-4.175694	1.688944	C	-0.149547	-8.068173	-1.022282	H	5.326470	6.816131	-1.807002
S	2.408525	-5.023042	3.203017	C	-7.424365	-1.651267	-3.230291	H	5.063617	7.020381	-0.070614
C	0.666514	-4.755504	3.179316	C	-3.597881	7.189865	-1.557285	H	7.740993	-4.881996	-0.881910
C	0.284937	-4.074280	2.064286	C	4.685656	6.515679	-0.968659	H	6.836665	-4.769772	-2.398950
C	5.779751	1.338943	-0.695763	C	6.789162	-5.133363	-1.367325	H	6.717384	-6.227412	-1.398516
S	7.468564	0.975481	-0.980437	C	4.779394	-3.543636	-1.115251	H	4.820106	-3.231777	-2.148212
C	7.034795	-0.565884	-1.709028	C	5.692273	-0.768295	-1.652383	H	5.227286	-1.587780	-2.157661

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C	-1.163565	3.183637	-0.518902	C	-0.065676	5.811620	-0.636548	H	-2.917223	3.612421	1.584959
C	0.270386	3.372173	-0.416286	S	0.801943	7.326922	-0.774285	H	-4.471717	-1.967105	1.281598
C	-1.724376	1.809570	-0.538350	C	2.346051	6.476162	-0.752965	H	0.035443	-4.360784	1.460298
C	1.166102	2.192783	-0.454291	C	2.175114	5.134065	-0.625603	H	3.018085	4.458562	-0.622856
C	0.586118	1.089965	-1.033936	C	4.479944	2.599975	1.378003	H	7.915477	0.595586	-3.070592
C	-0.828409	0.887802	-1.032021	C	8.176440	1.091617	-2.130058	H	8.960912	0.496989	-1.644737
C	1.226922	-0.168740	-1.128784	C	-1.437907	5.622301	-0.805731	H	8.611479	2.068566	-2.374224
C	-1.057880	-0.509120	-1.073698	C	3.631242	7.237094	-0.867319	H	4.475945	6.541792	-0.854558
C	-3.016911	1.246587	-0.163408	C	-5.718146	0.363798	-0.125494	H	3.762186	7.940918	-0.035759
C	0.207660	-1.148608	-1.128697	C	-5.187861	4.684101	2.982141	H	3.680693	7.817174	-1.797235
C	-3.324333	-0.142320	-0.477482	C	-6.213553	-3.954746	2.373289	H	-4.229296	5.188466	3.137177
C	2.523991	1.951534	0.004841	C	-1.993182	-5.408278	-0.544982	H	-5.558970	4.351499	3.959604
C	-2.236520	-1.109417	-0.679662	C	4.398953	-3.615720	0.186240	H	-5.898882	5.425898	2.597474
C	3.297171	0.827598	-0.515759	C	1.013189	-6.286548	3.330581	H	-6.434495	-2.911892	2.619813
C	2.576804	-0.411281	-0.922626	C	-0.862481	-4.644335	-0.872688	H	-7.103840	-4.382011	1.894921
C	-2.120688	-2.556727	-0.422138	C	0.171840	-5.466881	-1.449047	H	-6.053620	-4.500728	3.311488
C	-0.855466	-3.225113	-0.674314	C	-0.151929	-6.783406	-1.553348	H	-0.069217	-6.129716	3.299200
C	2.864648	-1.860765	-0.679147	S	-1.772691	-7.101309	-0.925231	H	1.203455	-7.351470	3.147368
C	0.392754	-2.453132	-0.758914	C	4.174686	-2.477465	-0.612054	H	1.360603	-6.062082	4.346833
C	1.757502	-2.754781	-0.335744	C	6.414604	-3.015718	-1.161061	H	1.119954	-5.074428	-1.796144
C	0.798999	4.704310	-0.519212	S	6.038511	-4.210016	0.072356	H	1.377443	3.732734	2.036931
C	4.730674	1.056519	-0.485776	C	3.113480	2.705894	1.086650	H	-3.956010	3.472942	-1.423401
C	2.028288	-3.825477	0.599027	C	2.442998	3.541136	2.051460	H	-4.681982	-2.309992	-1.897605
C	-3.151426	-3.381907	0.170551	C	3.256699	4.046417	3.018662	H	1.634718	-7.513299	-2.461272
C	-4.029081	1.966083	0.574970	S	4.926686	3.525419	2.790613	H	0.860321	-8.683766	-1.380851

C	-5.358961	1.512559	0.596892	C	-1.982641	4.323521	-0.815698	H	0.173921	-8.374084	-2.980599
S	-6.383100	2.524270	1.591491	C	-3.354861	4.358008	-1.268453	H	-6.945225	-3.302945	-2.639013
C	-5.010165	3.539666	2.031855	C	-3.837961	5.601065	-1.527256	H	-8.214668	-3.053322	-1.429760
C	-3.868771	3.124381	1.418070	S	-2.617991	6.842953	-1.239217	H	-8.171952	-2.045747	-2.881697
C	-3.080148	-4.787165	0.083486	C	-4.713847	-0.473598	-0.637242	H	-5.813551	5.082506	-2.143106
S	-4.401261	-5.574740	0.919013	C	-5.281775	-1.567305	-1.385359	H	-5.171277	6.522058	-2.957203
C	-5.015496	-4.020703	1.476225	C	-6.641115	-1.572665	-1.429756	H	-5.722731	6.627004	-1.281087
C	-4.265382	-2.990028	1.001049	S	-7.319785	-0.217625	-0.522631	H	1.814959	5.136112	4.151742
C	3.345084	-4.206018	0.890908	C	0.668258	-7.899598	-2.123671	H	3.426028	5.872052	4.162246
S	3.433100	-5.441448	2.123398	C	-7.543866	-2.541034	-2.130752	H	3.107997	4.434173	5.140668
C	1.680476	-5.419150	2.307470	C	-5.206315	5.981819	-2.002961	H	8.562389	-2.792727	-1.114654
C	1.101560	-4.535675	1.450427	C	2.886634	4.916819	4.180563	H	7.781716	-2.230954	-2.600798
C	5.305220	1.891043	0.488820	C	7.755919	-3.005364	-1.827958	H	7.986490	-3.966555	-2.304152
S	7.026181	2.104460	0.252293	C	5.346827	-2.206289	-1.399967	H	5.359561	-1.493372	-2.203342
C	6.958877	1.218090	-1.266068	C	5.702622	0.748752	-1.502656	H	5.435129	0.307043	-2.452545

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C	0.877595	-2.896406	0.320696	C	-0.449805	-4.452919	2.323992	H	2.663454	-4.544258	-1.138507
C	-0.589177	-2.905775	0.396228	S	-1.400903	-5.183096	3.599501	H	4.856276	1.023737	0.799229
C	1.552000	-1.953212	-0.565807	C	-2.824818	-4.282130	3.088191	H	0.407464	3.528643	2.057910
C	-1.381462	-2.044927	-0.483476	C	-2.562115	-3.514883	1.997244	H	-3.316001	-2.865310	1.579003
C	-0.669081	-1.059879	-1.116703	C	-4.991973	-3.048090	-1.028353	H	-7.533561	1.814891	-3.341017
C	0.732537	-1.005575	-1.134956	C	-7.950790	0.850903	-3.034844	H	-8.794105	1.050077	-2.361449
C	-1.206243	0.253873	-1.302903	C	0.943524	-4.499350	2.209396	H	-8.355140	0.357538	-3.927471
C	1.118950	0.367074	-1.263001	C	-4.115660	-4.411711	3.837043	H	-4.870638	-3.758639	3.389168
C	2.972888	-1.643009	-0.870115	C	5.563623	-1.034428	-1.877220	H	-4.005705	-4.132222	4.892242
C	-0.085009	1.122926	-1.222993	C	4.730636	-6.299525	-2.093600	H	-4.500844	-5.438813	3.809213
C	3.375938	-0.265317	-1.018722	C	6.877399	2.552876	2.139892	H	3.773966	-6.761826	-1.832262
C	-2.827283	-1.900588	-0.736581	C	2.505518	4.964223	0.243765	H	5.510640	-6.768683	-1.480935
C	2.356692	0.808791	-0.857896	C	-3.968977	3.718718	0.635854	H	4.949378	-6.539842	-3.141418
C	-3.420289	-0.610917	-1.079882	C	-0.403122	4.885566	4.445383	H	7.040498	1.473402	2.066851
C	-2.526555	0.621408	-1.099572	C	1.301945	4.395717	-0.205867	H	7.734440	3.054703	1.673536
C	2.389240	2.173810	-0.342607	C	0.324955	5.415926	-0.495764	H	6.877547	2.825702	3.202573
C	1.179225	2.976771	-0.371749	C	0.754699	6.686174	-0.271187	H	0.660027	4.645961	4.347602
C	-2.639721	2.031927	-0.621589	S	2.415404	6.709130	0.329667	H	-0.490504	5.967900	4.602429
C	-0.129223	2.350652	-0.601636	C	-3.832372	2.873475	-0.477260	H	-0.780509	4.391799	5.349577
C	-1.446925	2.683287	-0.084512	C	-5.748397	4.146136	-1.063897	H	-0.663132	5.200861	-0.883352
C	-1.208834	-3.610222	1.496415	S	-5.414649	4.703763	0.566374	H	-2.108801	-4.755915	-0.719950
C	-4.811156	-0.649495	-1.453109	C	-3.605929	-3.100901	-0.831536	H	3.759823	-3.071486	1.064191
C	-1.618695	3.477853	1.117402	C	-3.148693	-4.472311	-0.809713	H	4.658605	2.212550	-1.951248
C	3.535648	2.754755	0.314990	C	-4.134764	-5.398506	-0.931891	H	-0.992700	7.756481	-0.862868
C	3.872360	-2.675460	-1.281799	S	-5.721248	-4.639519	-1.095632	H	-0.093938	8.537318	0.448281
C	5.171161	-2.366146	-1.729836	C	1.617379	-3.672519	1.293582	H	0.517644	8.619446	-1.208728
S	6.056915	-3.799068	-2.215217	C	3.035133	-3.682218	1.578417	H	6.726650	3.273560	-3.035821
C	4.659021	-4.820888	-1.864841	C	3.413877	-4.509202	2.589443	H	8.219682	2.432088	-2.586812
C	3.612525	-4.091459	-1.397032	S	2.030509	-5.333461	3.297708	H	7.511761	2.174997	-4.185849
C	3.577640	4.133736	0.595749	C	4.665227	0.011752	-1.579731	H	5.515032	-4.140176	2.561305
S	5.043615	4.593303	1.434045	C	5.198476	1.278130	-2.025962	H	5.094860	-5.806888	2.988134
C	5.588119	2.916985	1.469530	C	6.438409	1.209926	-2.577706	H	4.882591	-4.515153	4.175652
C	4.701849	2.092958	0.847956	S	7.046513	-0.446589	-2.603277	H	-2.955163	-7.174267	-0.852935
C	-2.892853	3.891131	1.523641	C	0.011583	7.969209	-0.484275	H	-4.404351	-7.329524	-1.864231
S	-2.875362	4.691440	3.073866	C	7.270126	2.328279	-3.126752	H	-4.549810	-7.348850	-0.102461
C	-1.136953	4.440423	3.217302	C	4.796759	-4.757725	3.109096	H	-7.859473	4.429981	-1.428011
C	-0.636463	3.801950	2.124283	C	-4.008442	-6.890900	-0.939812	H	-6.852350	4.345645	-2.881097
C	-5.589000	-1.824984	-1.318356	C	-6.888264	4.716494	-1.851517	H	-6.857614	5.812339	-1.886702
S	-7.249429	-1.610194	-1.827692	C	-4.831851	3.217710	-1.458643	H	-4.780077	2.908160	-2.492827
C	-6.893887	0.023891	-2.369803	C	-5.600059	0.350928	-2.116219	H	-5.184642	1.274110	-2.456038

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C	0.095471	1.686714	2.771747	C	-0.379313	1.096574	5.518524	H	-1.926963	-1.002063	-3.908736
C	0.289871	0.332531	3.267222	S	-0.329066	0.628475	7.203348	H	1.212749	-1.831820	5.013884
C	0.607499	2.063168	1.456025	C	0.508736	-0.872243	6.796516	H	3.659302	-7.573041	1.440304
C	0.603832	-0.759224	2.336281	C	0.700817	-0.985497	5.455148	H	2.298307	-8.683786	1.659611
C	1.126541	-0.336847	1.136247	C	-0.833357	-4.140669	3.394509	H	3.179964	-8.082022	3.068600
C	1.107316	1.016126	0.715039	C	2.799774	-7.801952	2.078381	H	1.431710	-2.685250	7.436383
C	1.250130	-1.172906	-0.000000	C	-0.928065	2.256926	4.954126	H	0.058779	-2.196573	8.442516
C	1.107316	1.016126	-0.715039	C	0.921935	-1.823399	7.877424	H	1.606022	-1.354661	8.595805
C	0.717188	3.350629	0.724952	C	1.266075	5.761071	-0.697865	H	2.106466	5.732197	5.227427
C	1.126541	-0.336847	-1.136247	C	2.125159	6.544146	4.494255	H	1.430526	7.321879	4.835958

C	0.717188	3.350629	-0.724952	C	-2.988949	5.558023	-4.158364	H	3.131306	6.981457	4.495317
C	0.292488	-2.188869	2.362359	C	-0.379313	1.096574	-5.518524	H	-2.975764	5.967866	-3.143922
C	0.607499	2.063168	-1.456025	C	0.102324	-4.981221	-2.777260	H	-2.634851	6.340476	-4.841160
C	0.860610	-3.089252	1.361600	C	-3.852760	-2.516505	-5.388635	H	-4.030966	5.339684	-4.423567
C	1.153388	-2.550598	-0.000000	C	0.198588	0.124841	-4.684777	H	-3.972221	-1.428867	-5.386793
C	0.095471	1.686714	-2.771747	C	0.700817	-0.985497	-5.455148	H	-3.779595	-2.844170	-6.433192
C	0.289871	0.332531	-3.267222	C	0.508736	-0.872243	-6.796516	H	-4.764840	-2.959840	-4.969841
C	0.860610	-3.089252	-1.361600	S	-0.329066	0.628475	-7.203348	H	1.212749	-1.831820	-5.013884
C	0.603832	-0.759224	-2.336281	C	0.961630	-4.469135	-1.788722	H	-1.926963	-1.002063	3.908736
C	0.292488	-2.188869	-2.362359	C	1.882080	-6.619505	-2.142015	H	-1.420127	4.149112	2.210363
C	0.198588	0.124841	4.684777	S	0.468195	-6.640645	-3.188732	H	1.385258	3.951719	-3.535817
C	0.961630	-4.469135	1.788722	C	-0.709812	-2.751680	3.242112	H	1.431710	-2.685250	-7.436383
C	-0.709812	-2.751680	-3.242112	C	-1.776114	-2.071999	3.939021	H	0.058779	-2.196573	-8.442516
C	-0.697320	2.563219	-3.600815	C	-2.635414	-2.893425	4.600829	H	1.606022	-1.354661	-8.595805
C	1.071279	4.561140	1.410148	S	-2.180251	-4.585920	4.414283	H	2.106466	5.732197	-5.227427
C	1.266075	5.761071	0.697865	C	-0.697320	2.563219	3.600815	H	1.430526	7.321879	-4.835958
S	1.726650	7.089793	1.743422	C	-1.413687	3.755179	3.218149	H	3.131306	6.981457	-4.495317
C	1.747498	6.017291	3.143896	C	-2.127308	4.334155	4.221333	H	-2.975764	5.967866	3.143922
C	1.394283	4.749507	2.806425	S	-1.953120	3.442868	5.733038	H	-2.634851	6.340476	4.841160
C	-0.928065	2.256926	-4.954126	C	1.071279	4.561140	-1.410148	H	-4.030966	5.339684	4.423567
S	-1.953120	3.442868	-5.733038	C	1.394283	4.749507	-2.806425	H	-3.972221	-1.428867	5.386793
C	-2.127308	4.334155	-4.221333	C	1.747498	6.017291	-3.143896	H	-3.779595	-2.844170	6.433192
C	-1.413687	3.755179	-3.218149	S	1.726650	7.089793	-1.743422	H	-4.764840	-2.959840	4.969841
C	-0.833357	-4.140669	-3.394509	C	0.921935	-1.823399	-7.877424	H	2.298307	-8.683786	-1.659611
S	-2.180251	-4.585920	-4.414283	C	2.125159	6.544146	-4.494255	H	3.659302	-7.573041	-1.440304
C	-2.635414	-2.893425	-4.600829	C	-2.988949	5.558023	4.158364	H	3.179964	-8.082022	-3.068600
C	-1.776114	-2.071999	-3.939021	C	-3.852760	-2.516505	5.388635	C	1.995202	-5.426670	-1.495698
C	0.102324	-4.981221	2.777260	C	2.799774	-7.801952	-2.078381	C	1.995202	-5.426670	1.495698
S	0.468195	-6.640645	3.188732	H	1.385258	3.951719	3.535817	H	2.871295	-5.183824	-0.916238
C	1.882080	-6.619505	2.142015	H	-1.420127	4.149112	-2.210363	H	2.871295	-5.183824	0.916238

TS_{CD}

C	0.211550	-3.126892	0.091959	C	-1.544080	-4.777506	1.653521	H	1.997874	-4.698025	-1.784217
C	-1.235634	-2.876792	0.102774	S	-2.720342	-5.563549	2.685273	H	5.039336	0.664830	-2.134640
C	1.107660	-2.177227	-0.595780	C	-3.906830	-4.312519	2.325409	H	1.381386	3.230687	2.167333
C	-1.805004	-1.735243	-0.619044	C	-3.414859	-3.398052	1.448462	H	-3.998922	-2.539212	1.155045
C	-0.896031	-0.816977	-1.054538	C	-5.477927	-1.946432	-1.480447	H	-7.164673	3.703490	-2.367264
C	0.492693	-1.025469	-1.028473	C	-7.729650	2.766968	-2.342151	H	-8.550078	2.890133	-1.623847
C	-1.170720	0.582956	-1.125601	C	-0.173886	-5.047479	1.614920	H	-8.181179	2.617177	-3.330837
C	1.135631	0.232042	-1.127386	C	-5.260880	-4.342906	2.965209	H	-5.841290	-3.472443	2.644986
C	2.574315	-2.063938	-0.674989	C	5.361416	-1.961187	-0.213077	H	-5.195940	-4.325794	4.060272
C	0.094041	1.216393	-1.062556	C	4.018875	-6.674590	-2.370368	H	-5.823029	-5.242650	2.684934
C	3.211952	-0.765618	-0.516362	C	7.366901	2.099141	-3.002655	H	2.985211	-6.944655	-2.606745
C	-3.179351	-1.278765	-0.889387	C	3.344101	4.690707	-0.659770	H	4.414538	-7.429189	-1.679244
C	2.445710	0.455126	-0.776585	C	-3.078567	4.141307	1.497107	H	4.605838	-6.737654	-3.295113
C	-3.515269	0.141166	-0.974110	C	1.120767	4.340244	4.806569	H	7.333152	1.029309	-3.229477
C	-2.395711	1.171590	-0.819768	C	2.036518	4.245158	-0.374350	H	7.476960	2.644847	-3.948015
C	2.768538	1.903282	-0.738125	C	1.159429	5.371690	-0.153146	H	8.269983	2.288920	-2.408989
C	1.720965	2.845377	-0.409579	C	1.766738	6.586144	-0.215841	H	2.119647	4.009114	4.506507
C	-2.206924	2.494970	-0.159150	S	3.485285	6.434502	-0.580889	H	1.189485	5.395445	5.099086
C	0.313250	2.388515	-0.375642	C	-3.201288	3.500370	0.252926	H	0.829833	3.771367	5.698456
C	-0.867979	2.864922	0.306262	C	-4.880268	5.175676	0.111132	H	0.101188	5.279715	0.045995
C	-2.063106	-3.650206	0.999680	S	-4.316351	5.352377	1.762066	H	-2.937293	-4.152379	-1.473967
C	-4.888647	0.422322	-1.316441	C	-4.136199	-2.277990	-1.262921	H	2.931221	-3.894347	1.092770
C	-0.757705	3.512061	1.597347	C	-3.909166	-3.680783	-1.530356	H	4.900888	1.176673	0.922665
C	4.024335	2.416148	-1.195647	C	-5.021565	-4.373814	-1.886923	H	0.082872	7.832271	0.187830
C	3.415657	-3.180534	-0.981540	S	-6.449570	-3.334145	-1.925852	H	1.605022	8.465368	0.836619
C	4.805583	-3.110769	-0.793671	C	0.716001	-4.181207	0.949795	H	1.273399	8.576785	-0.896154
S	5.602996	-4.587438	-1.289482	C	2.069160	-4.476614	1.369297	H	7.182515	1.645890	2.002600
C	4.059766	-5.300421	-1.775486	C	2.199690	-5.536061	2.211233	H	7.908219	0.174514	2.676583
C	3.025305	-4.448473	-1.544938	S	0.639745	-6.253281	2.587437	H	8.509973	0.838895	1.153110
C	4.314083	3.792171	-1.107337	C	4.583882	-0.797209	-0.062852	H	4.316234	-5.496269	2.476156
S	5.883229	4.181827	-1.783051	C	5.321623	0.219206	0.645462	H	3.632133	-7.129658	2.485233
C	6.125061	2.501292	-2.267995	C	6.588846	-0.136222	0.991679	H	3.433922	-6.086578	3.898248
C	5.079281	1.718878	-1.894107	S	6.971868	-1.767719	0.445259	H	-4.153872	-6.301942	-2.170359
C	-1.890102	4.017409	2.242420	C	1.153318	7.937551	-0.012653	H	-5.532606	-5.980356	-3.239309
S	-1.535856	4.590251	3.851834	C	7.602542	0.668688	1.745921	H	-5.805439	-6.354811	-1.533177
C	0.159473	4.136861	3.675500	C	3.458784	-6.093136	2.801384	H	-6.927947	5.860649	0.028742
C	0.401857	3.594140	2.450481	C	-5.138374	-5.827802	-2.226873	H	-6.058748	5.907596	-1.512328

C	-5.851198	-0.607083	-1.469695	C	-5.954255	6.066805	-0.434085	H	-5.732266	7.128230	-0.269946
S	-7.442943	-0.008888	-1.879578	C	-4.188487	4.195132	-0.536673	H	-4.273032	4.089329	-1.609224
C	-6.826409	1.633669	-1.963486	C	-5.502747	1.672843	-1.661388	H	-4.952396	2.583687	-1.713566

TS_{DD^*}

C	-1.750204	-0.791394	2.914885	C	-1.147032	-1.385340	5.630170	H	0.477030	1.574174	-4.218749
C	-0.380583	-0.751352	3.366930	S	-0.557095	-1.774022	7.233141	H	2.127183	-1.058968	4.894371
C	-2.047823	-0.602886	1.470445	C	1.112058	-1.566759	6.701870	H	8.400872	-1.764127	3.025405
C	0.712695	-0.651913	2.366087	C	1.179443	-1.211224	5.391780	H	7.971842	-2.337757	1.404523
C	0.344668	-1.144617	1.140477	C	3.750780	1.341289	3.469932	H	8.801078	-0.786927	1.607764
C	-1.018526	-1.092602	0.700492	C	8.038931	-1.448412	2.039117	H	2.190372	-1.086214	8.510602
C	1.185458	-1.143743	-0.000000	C	-2.461143	-1.492687	5.171128	H	2.244210	-2.797425	8.070543
C	-1.018526	-1.092602	-0.700492	C	2.242355	-1.779361	7.661662	H	3.196753	-1.615977	7.152183
C	-3.088162	0.108868	0.736432	C	-5.009139	1.673996	-0.699658	H	-5.308864	3.948268	4.454954
C	0.344668	-1.144617	-1.140477	C	-5.354895	2.852176	4.469643	H	-6.358302	2.572213	4.814502
C	-3.088162	0.108868	-0.736432	C	-6.285782	-2.435756	-4.643440	H	-4.634205	2.491216	5.209647
C	2.057585	-0.110485	2.397267	C	-1.147032	-1.385340	-5.630170	H	-6.868267	-1.817150	-5.337607
C	-2.047823	-0.602886	-1.470445	C	4.752215	0.639851	-2.782997	H	-6.394186	-3.478879	-4.965587
C	3.030275	-0.455611	1.361561	C	1.582578	3.672009	-5.839583	H	-6.733974	-2.339365	-3.649905
C	2.539983	-0.824885	-0.000000	C	-0.100710	-1.068087	-4.737987	H	1.760180	4.701260	-5.503707
C	-1.750204	-0.791394	-2.914885	C	1.179443	-1.211224	-5.391780	H	1.993189	3.582906	-6.853111
C	-0.380583	-0.751352	-3.366930	C	1.112058	-1.566759	-6.701870	H	0.500886	3.518524	-5.900733
C	3.030275	-0.455611	-1.361561	S	-0.557095	-1.774022	-7.233141	H	2.127183	-1.058968	-4.894371
C	0.712695	-0.651913	-2.366087	C	4.409538	-0.289448	-1.782886	H	0.477030	1.574174	4.218749
C	2.057585	-0.110485	-2.397267	C	6.701719	-0.777703	-2.118889	H	-4.572962	-1.479385	2.540147
C	-0.100710	-1.068087	4.737987	S	6.456559	0.606875	-3.174572	H	-3.341602	1.061709	-3.548864
C	4.409538	-0.289448	1.782886	C	2.422702	0.913727	3.348215	H	3.196753	-1.615977	-7.152183
C	2.422702	0.913727	-3.348215	C	1.550943	1.703044	4.183770	H	2.244210	-2.797425	-8.070543
C	-2.762412	-1.238692	-3.819605	C	2.184522	2.667668	4.905014	H	2.190372	-1.086214	-8.510602
C	-4.017297	0.986688	1.417817	S	3.922304	2.660433	4.602388	H	-4.634205	2.491216	-5.209647
C	-5.009139	1.673996	0.699658	C	-2.762412	-1.238692	3.819605	H	-6.358302	2.572213	-4.814502
S	-6.011062	2.682122	1.720396	C	-4.137877	-1.567663	3.527723	H	-5.308864	3.948268	-4.454954
C	-5.043672	2.262218	3.128325	C	-4.849280	-2.014038	4.595672	H	-6.733974	-2.339365	3.649905
C	-4.052832	1.388066	2.806746	S	-3.859527	-2.066955	6.058433	H	-6.394186	-3.478879	4.965587
C	-2.461143	-1.492687	-5.171128	C	-4.017297	0.986688	-1.417817	H	-6.868267	-1.817150	5.337607
S	-3.859527	-2.066955	-6.058433	C	-4.052832	1.388066	-2.806746	H	0.500886	3.518524	5.900733
C	-4.849280	-2.014038	-4.595672	C	-5.043672	2.262218	-3.128325	H	1.993189	3.582906	6.853111
C	-4.137877	-1.567663	-3.527723	S	-6.011062	2.682122	-1.720396	H	1.760180	4.701260	5.503707
C	3.750780	1.341289	-3.469932	C	2.242355	-1.779361	-7.661662	H	7.971842	-2.337757	-1.404523
S	3.922304	2.660433	-4.602388	C	-5.354895	2.852176	-4.469643	H	8.400872	-1.764127	-3.025405
C	2.184522	2.667668	-4.905014	C	-6.285782	-2.435756	4.643440	H	8.801078	-0.786927	-1.607764
C	1.550943	1.703044	-4.183770	C	1.582578	3.672009	5.839583	C	5.547795	-1.116026	-1.480604
C	4.752215	0.639851	2.782997	C	8.038931	-1.448412	-2.039117	C	5.547795	-1.116026	1.480604
S	6.456559	0.606875	3.174572	H	-3.341602	1.061709	3.548864	H	5.472950	-2.022726	-0.903414
C	6.701719	-0.777703	2.118889	H	-4.572962	-1.479385	-2.540147	H	5.472950	-2.022726	0.903414

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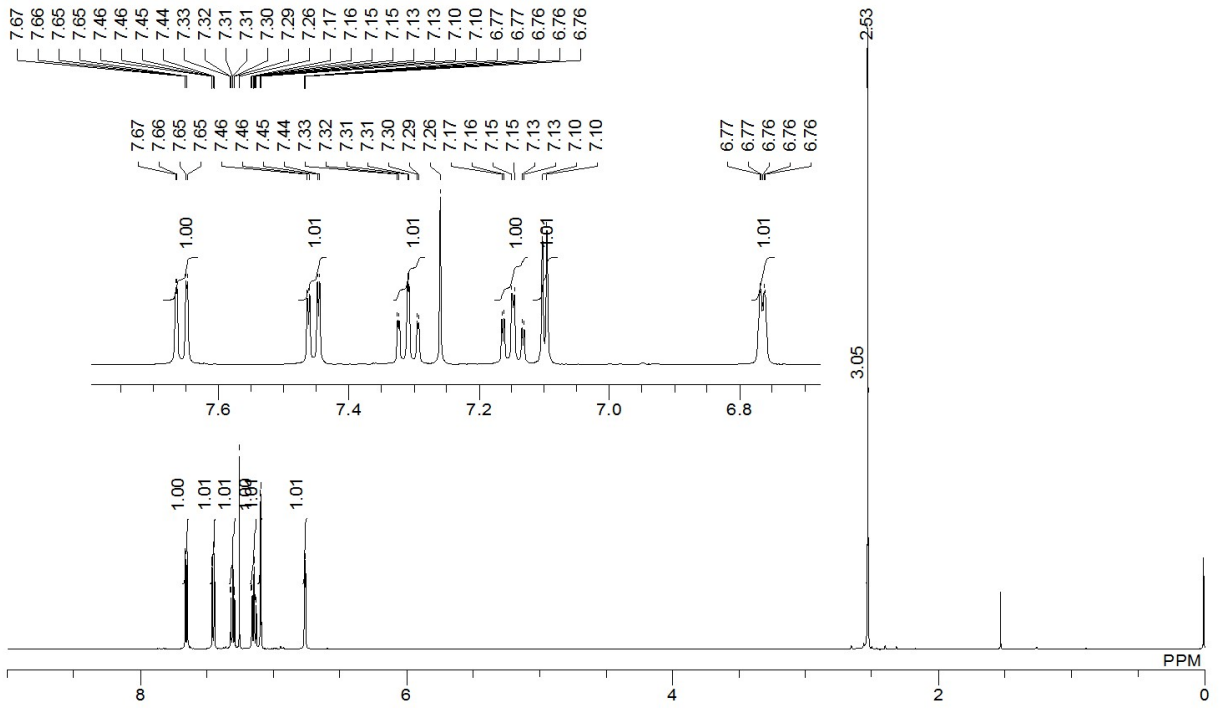
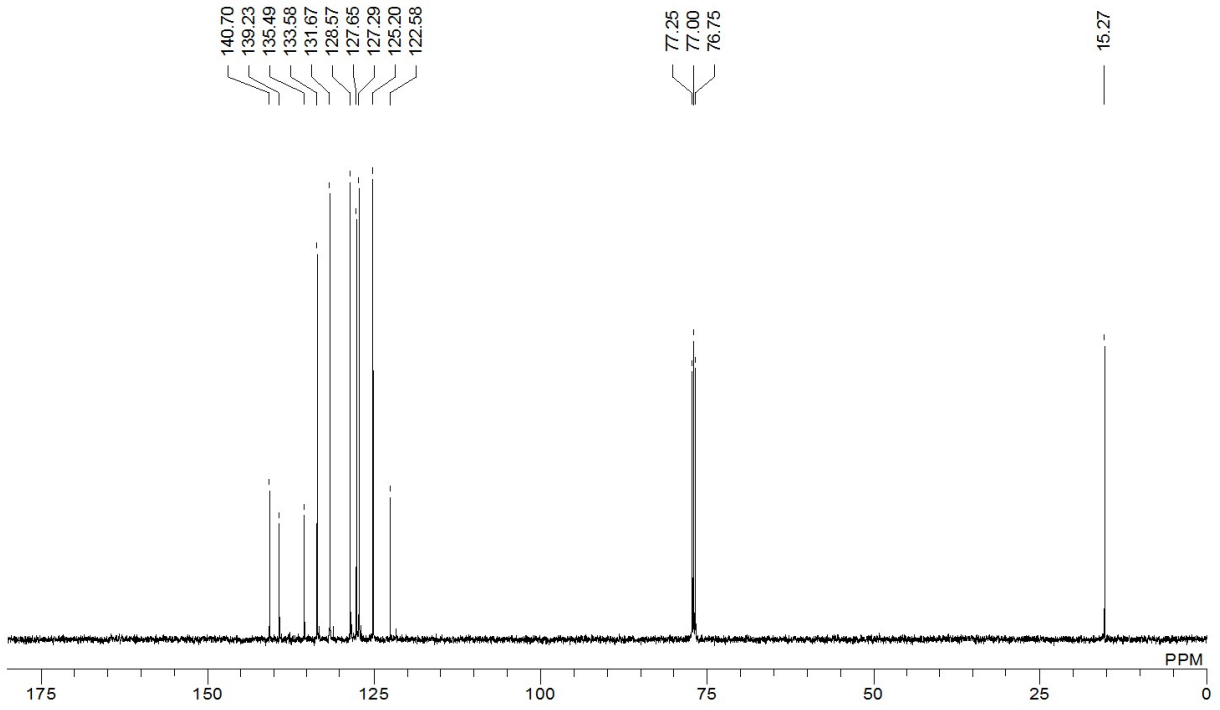
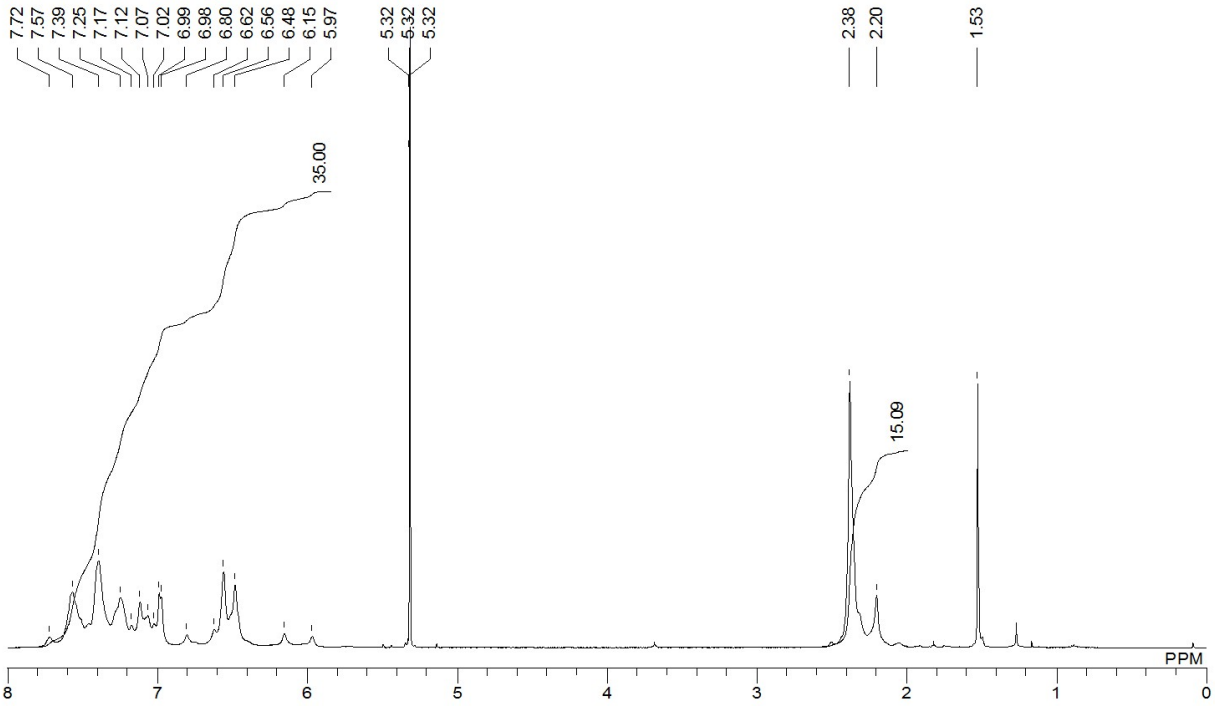
6. ^{1}H and ^{13}C NMR spectra of new compounds

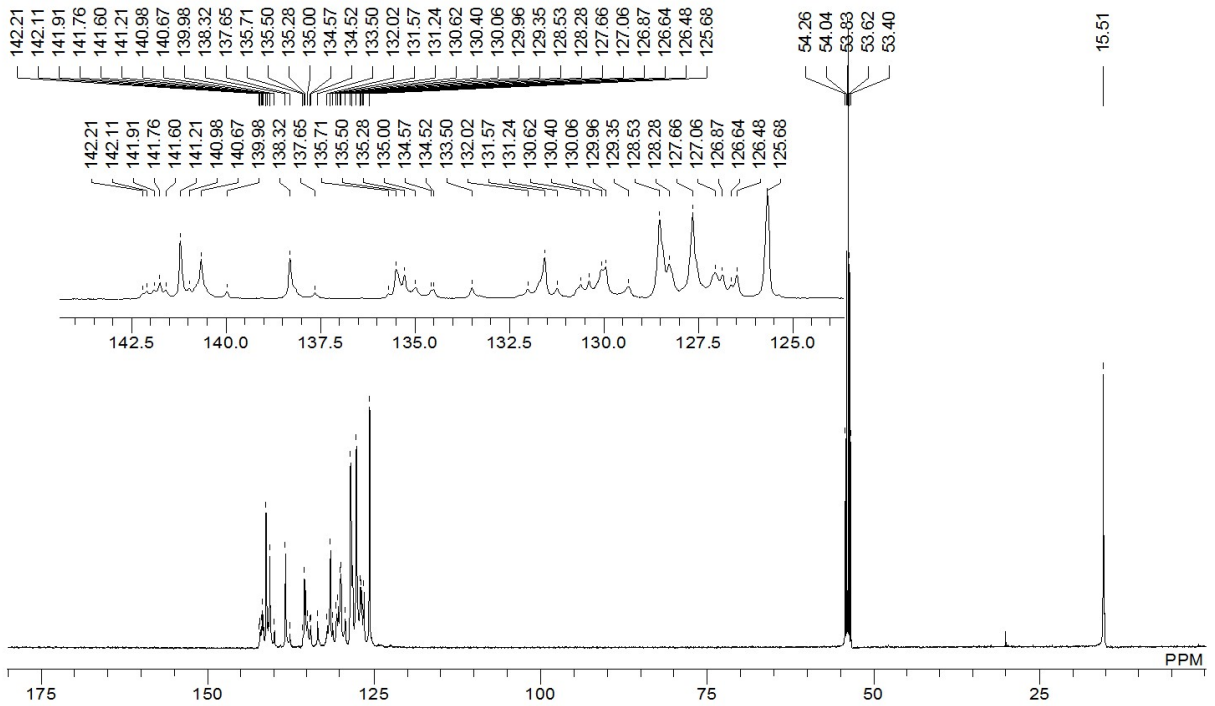
Compound **4** ($CDCl_3$)



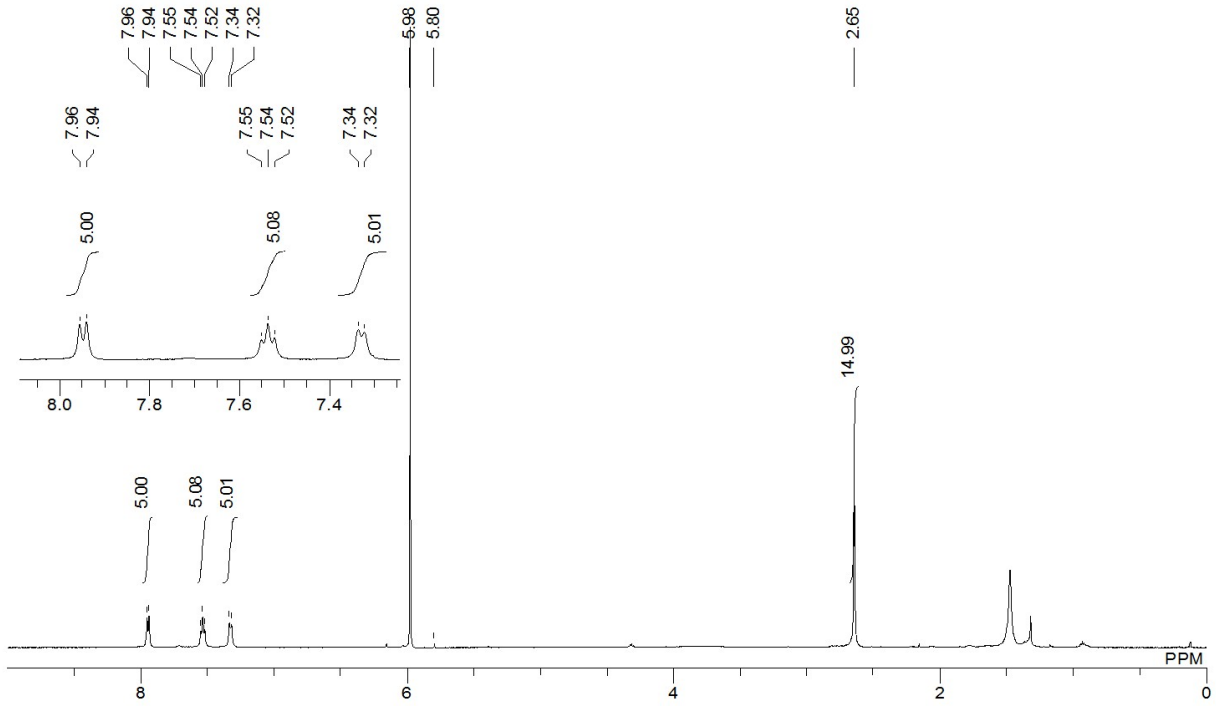


Compound **5** (CD_2Cl_2)

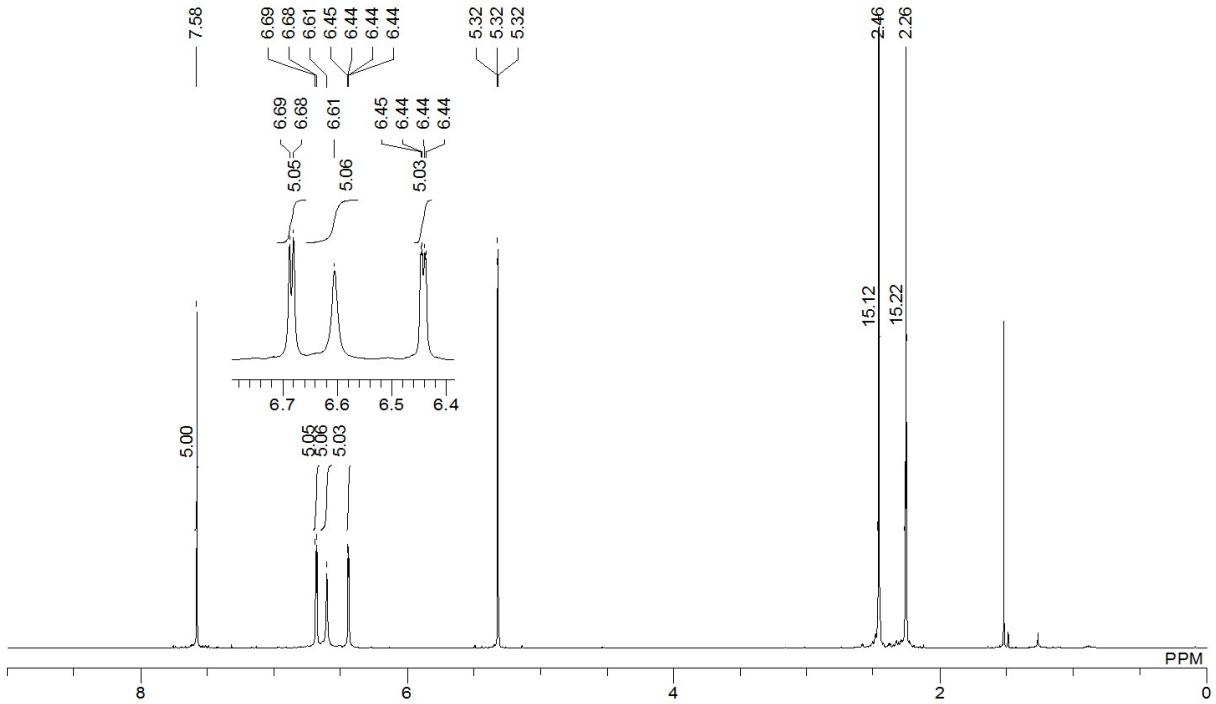


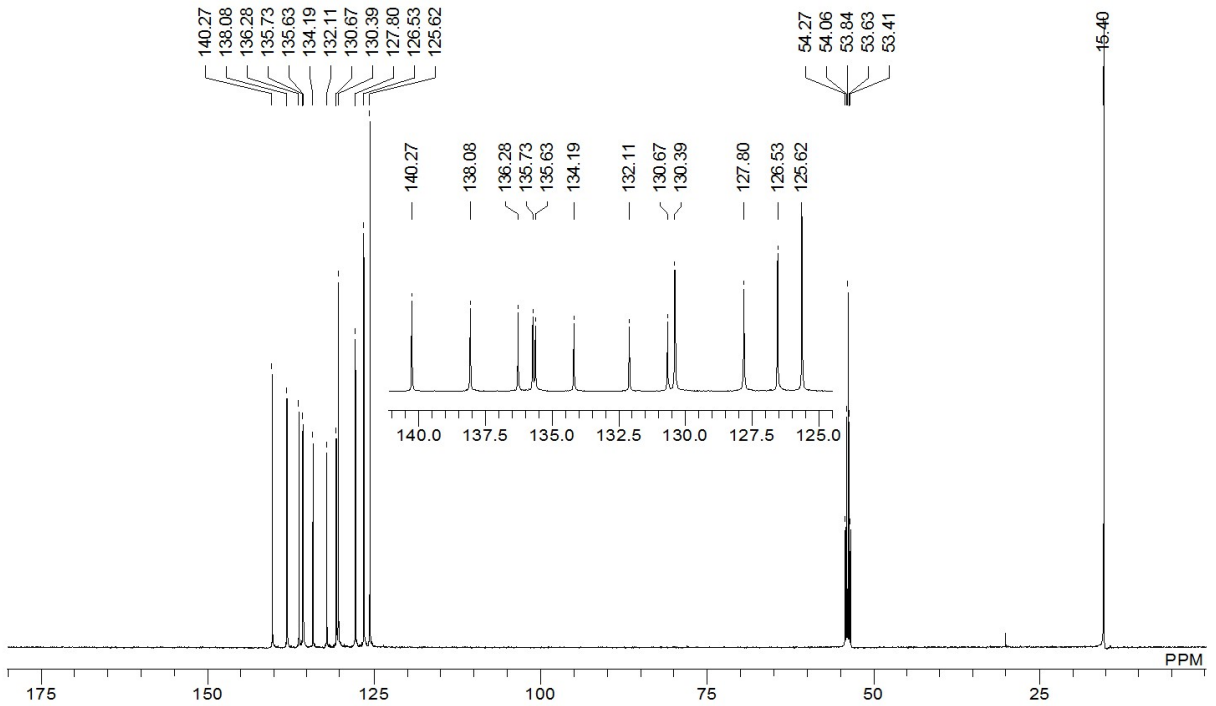


Compound **1** ($C_2D_2Cl_4$, 100 °C)



Compound **7** (CD_2Cl_2)





Compound **2** ($CDCl_3$)