Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Ligand exchange reactions on chiral Au_{38} cluster: CD modulation caused by the modification of ligand shell composition

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Synthesis of 2-thio[4]helicene (TH4) ligand

STEP 1: synthesis of 3-(benzo[c]phenanthren-2-ylthio)propanenitrile (1)

In a 100 mL three necked flask under argon were dissolved 2-bromo[4]helicene (1.02 g, 3.32 mmol, 1 eq) and 3-((tributylstannyl)thio)propanenitrile (1.87 g, 4.98 mmol, 1.5 eq) in degassed toluene (70 mL). Then, $Pd(PPh_3)_4$ (0.38 g, 0.33 mmol, 0.1 eq). The mixture was then stirred at reflux for 36 h. The orange solution was then allowed to reach the rt and after evaporation of toluene, the crude was purified by chromatography over silica gel column (petroleum ether/DCM, 1/1, Rf = 0.37). 0.72 g (69 % yield) of **1** were obtained as a yellow crystalline solid.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 9.21 (s, 1H), 9.03 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.0, 1.5 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.6 Hz, 1H), 7.89 – 7.81 (m, 3H), 7.75 (t, *J* = 8.5 Hz, 1H), 7.70 – 7.61 (m, 2H), 3.27 (d, *J* = 7.5 Hz, 2H), 2.64 (d, *J* = 7.1 Hz, 2H).

STEP 2: synthesis of 2-thio[4]helicene (2)

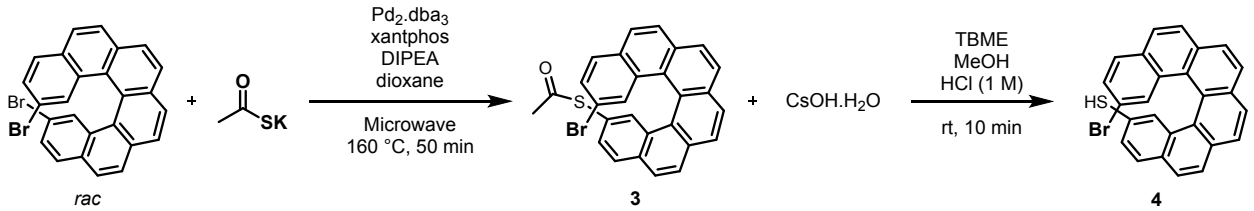
In a Schlenk flask under argon was dissolved **1** (0.23 g, 0.73 mmol, 1 eq) in dry THF (15 mL). Then a degassed solution of cesium hydroxide (165 mg, 1.1 mmol, 1.5 eq) in methanol (9 mL) was added and the mixture was stirred at rt for 2 h. After reaching to rt, the THF was evaporated under vacuum and then THF (15 mL) was added. Finally, HCl (6 M) was added dropwise until pH = 1 and the mixture became translucent. Then H_2O (30 mL) and DCM (30 mL) were added. The organic layer was extracted twice with DCM, washed with H_2O twice, dried over $MgSO_4$ and concentrated under vacuum. 0.19 g (100 %) of **2** were obtained as a yellow crystalline solid.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 9.22 (d, *J* = 1.7 Hz, 1H), 9.11 – 9.04 (m, 1H), 7.99 – 7.91 (m, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.81 – 7.72 (m, 3H), 7.64 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.51 (dt, *J* = 6.4, 3.5 Hz, 2H), 4.65 (s, 1H).

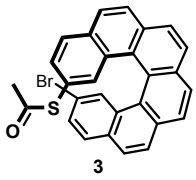
^{13}C NMR (76 MHz, Chloroform-*d*) δ 133.53, 132.54, 132.47, 131.42, 130.67, 130.16, 129.19, 128.58, 128.27, 127.94, 127.75, 127.27, 127.05, 126.75 (d, *J* = 2.3 Hz), 126.54, 126.04.

MALDI/TOF: 260.0664

Synthesis of 2-thio-15-bromo[6]helicene (TH6-Br) ligand



STEP 1: synthesis of (rac)-2-thioacetate-15-bromo[6]helicene (3)



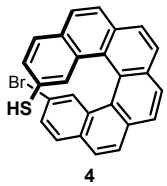
In a microwave flask under argon were dissolved (*rac*)-2,15-dibromo-[6]helicene (200 mg, 0.65 mmol, 1 eq), potassium thioacetate (111 mg, 0.98 mmol, 1.5 eq), Xantphos (19 mg, 33 µmol, 0.05 eq) and Pd_2dba_3 (15 mg, 16 µmol, 0.025 eq) in dioxane (3.5 mL) followed by the addition of Hunig's base (0.22 mL, 1.3 mmol, 2 eq). After degassing with argon the red solution was irradiated under microwave at 160 °C for 25 min. The organic layer was exctracted with ethyl acetate, washed with water, dried over Na_2SO_4 and concentrated under vacuum. The crude oil was purified by chromatography over silica gel column (petroleum ether/EtOAc, 8/2, Rf = 0.6 and 0.3). 30 mg of **3** were obtained as a yellow solid. The bis-substituted derivative was obtained as co-product.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.07 – 7.96 (m, 6H), 7.93 (d, *J* = 9.2 Hz, 3H), 7.71 – 7.67 (m, 2H), 7.63 (dd, *J* = 1.5, 0.8 Hz, 1H), 7.33 (ddd, *J* = 8.5, 6.1, 1.8 Hz, 2H), 2.15 (s, 3H).

^{13}C NMR (76 MHz, Chloroform-*d*) δ 194.43, 133.62, 133.40, 132.50, 132.00, 131.93, 131.51, 130.86, 130.58, 130.46, 129.91, 129.08, 129.01, 128.78, 127.91, 127.83, 127.81, 127.65, 127.61, 127.54, 127.11, 126.96, 126.61, 124.70, 123.84, 119.42, 30.01.

MS (ESI) m/z = 480.0174

STEP 2: synthesis of (rac)-2-thio-15-bromo[6]helicene (rac)-TH6-Br (4)



In a 100 mL flask under argon was dissolved **3** (30 mg, 0.062 mmol, 1 eq) in degassed MTBE (16 mL). Then a solution of $CsOH.H_2O$ (84 mg, 0.50 mmol, 8 eq) in degassed methanol (0.49 mL) was added dropwise and the mixture was stirred for 5 min at rt (it turns yellow). Finally, it was slowly added a solution of HCl (1.25 mL, 1.25 mmol, 1M, 20 eq) in H_2O (it becomes colorless). After extraction with MTBE, drying over Na_2SO_4 and concentration under vacuum, 9 mg (33 % yield) of **5** were obtained as a yellow solid.

Synthesized according to the following procedure: O. Stetsovych, P. Mutombo, M. Švec, M. Šámal, J. Nejedlý, I. Císařová, H. Vázquez, M. Moro-Lagares, J. Berger, J. Vacek, I. G. Stará, I. Starý, P. Jelínek, *J. Am. Chem. Soc.* **2018**, *140*, 940.

(*M*)-TH6-Br was synthesized following the same procedure as for the (*rac*)-TH6-Br starting from (*M*)-dibromo-[6]helicene.

MS (EI) m/z = 438.0074

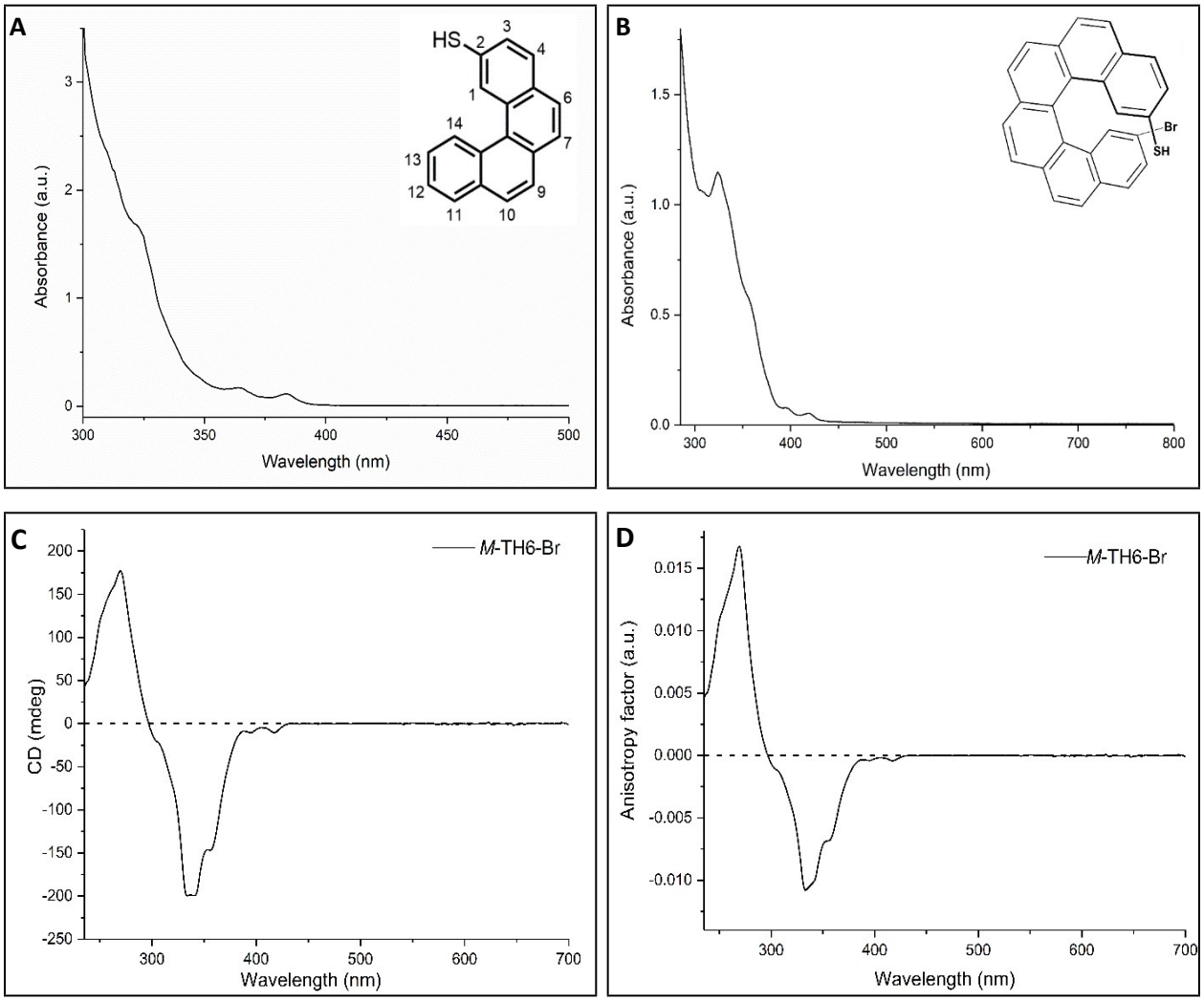


Fig. S1 UV-vis spectrum of **(A)** TH4 and **(B)** TH6-Br ligands in toluene. Insets: the structures and positional nomenclature of the ligands. **(C)** CD spectrum and **(D)** anisotropy factor *g* of *M*-TH6-Br ligand. The spectra were recorded in DCM and the solvent background was subtracted afterwards.

Table S1 Calculated masses for each exchange product in the mass spectrum.

$Au_{38}(2\text{-}PET)_{24-x}(TH4)_x$		
Number of exchanges	Formula	Theoretical masses/ Da
x=1	$Au_{38}(2\text{-}PET)_{23}(TH4)$	10901
x=2	$Au_{38}(2\text{-}PET)_{22}(TH4)_2$	11024
x=3	$Au_{38}(2\text{-}PET)_{21}(TH4)_3$	11147
x=4	$Au_{38}(2\text{-}PET)_{20}(TH4)_4$	11270
x=5	$Au_{38}(2\text{-}PET)_{19}(TH4)_5$	11393
x=6	$Au_{38}(2\text{-}PET)_{18}(TH4)_6$	11520
x=7	$Au_{38}(2\text{-}PET)_{17}(TH4)_7$	11643
x=8	$Au_{38}(2\text{-}PET)_{16}(TH4)_8$	11766
x=9	$Au_{38}(2\text{-}PET)_{15}(TH4)_9$	11889

$$\bar{x} = \frac{\sum I_x * x}{\sum I_x}$$

where $\bar{x}$ is an average exchange, I_x is an intensity of the peak and x is an exchange number.

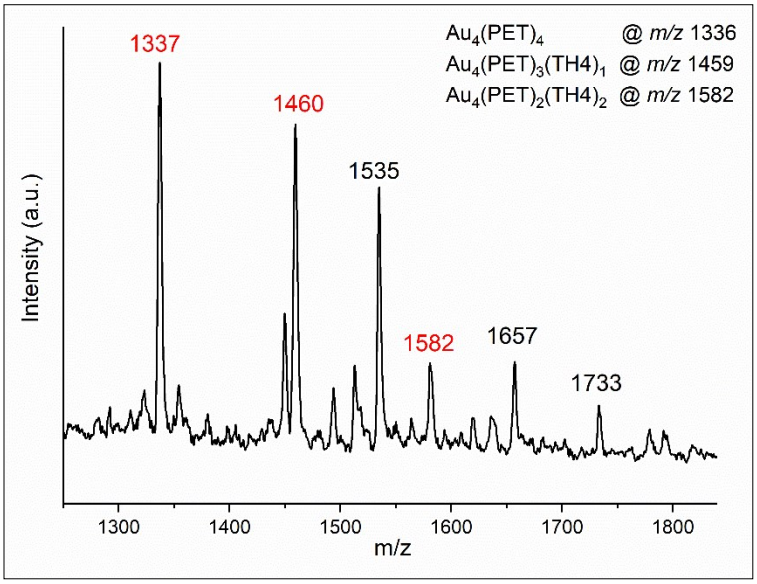


Fig. S2 MALDI analysis of the fragmentation pattern at lower *m/z* range when 1:100 cluster/ligand ratios were used for the reaction. The substituted $Au_4(2\text{-}PET)_{4-x}(TH4)_x$ cyclic species are marked in red.

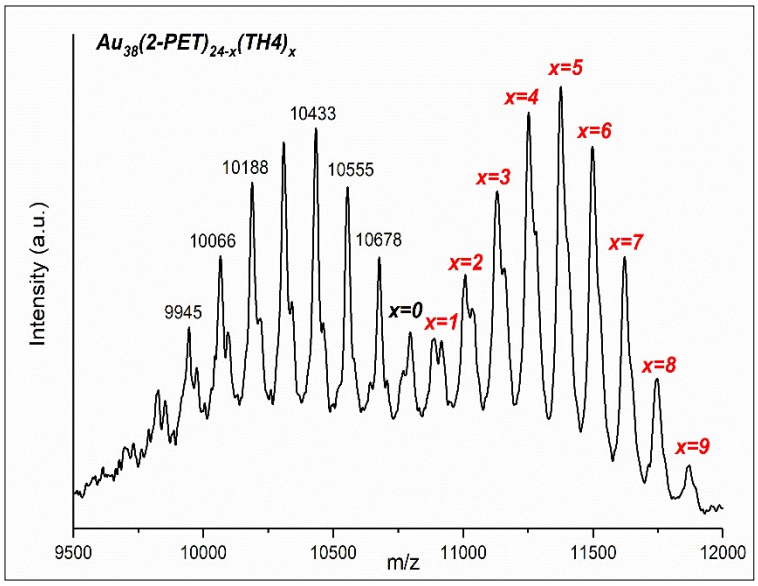


Fig. S3 MALDI analysis of the sample after ligand exchange reaction. The number of exchange species are marked in red.

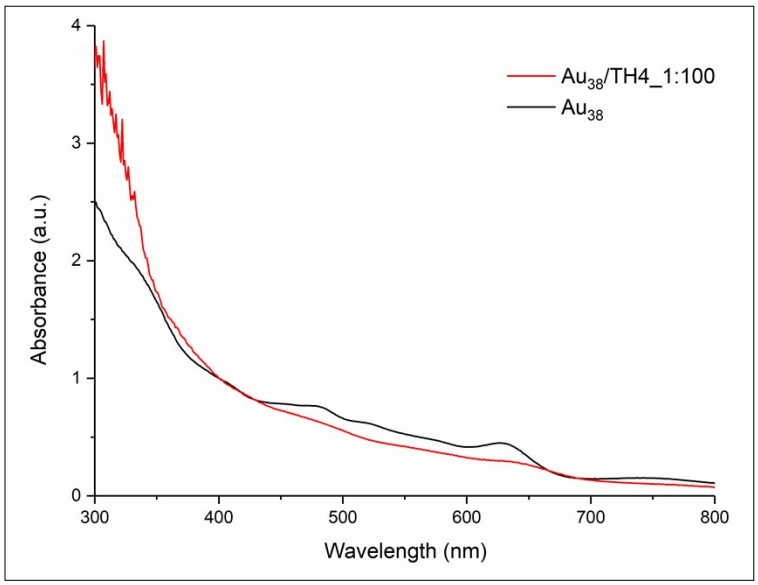


Fig. S4 UV-vis spectra of sample after ligand exchange reaction using 1:100 cluster/ligand ratio on a large-scale synthesis (5 mg of Au_{38}). The spectra are normalized and compared with Au_{38} before reaction.

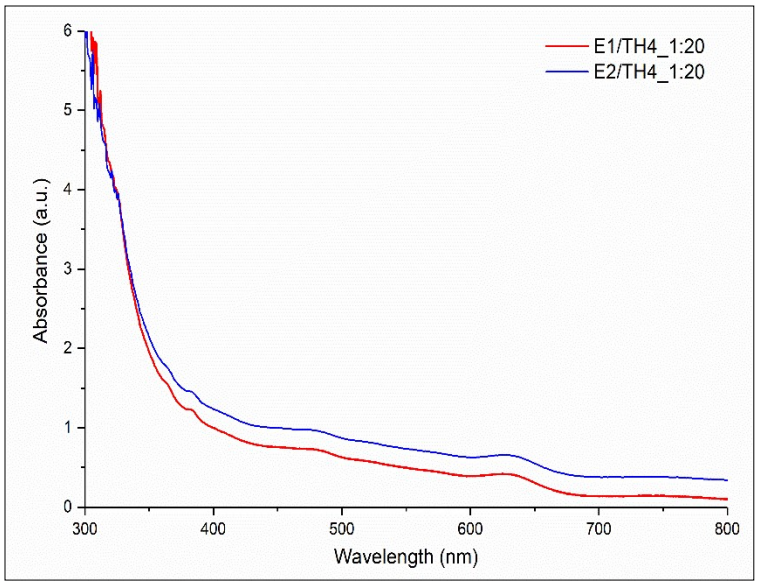


Fig. S5 UV-vis spectra of E1/ E2+TH4 using 1:20 cluster/ligand molar ratios. The spectra are normalized at 400 nm for better comparison.

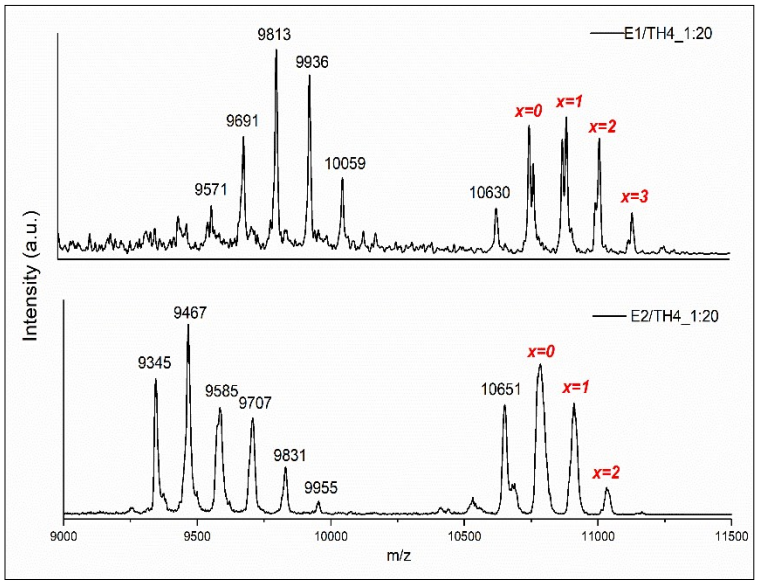


Fig. S6 MALDI mass spectra of E1/ E2+TH4 after ligand exchange reaction.

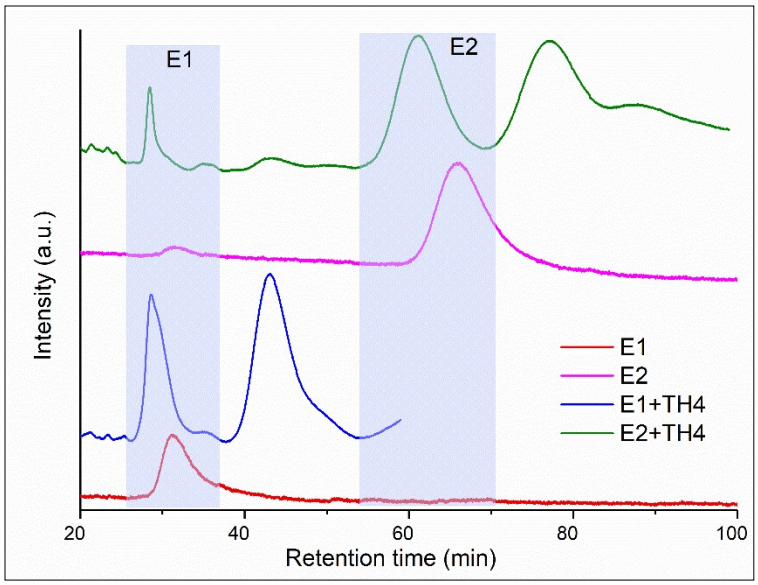


Fig. S7 HPLC separations of the exchanged species after ligand exchange reaction with enantiopure cluster. The chromatograms are compared with reference chromatogram of enantiopure cluster.

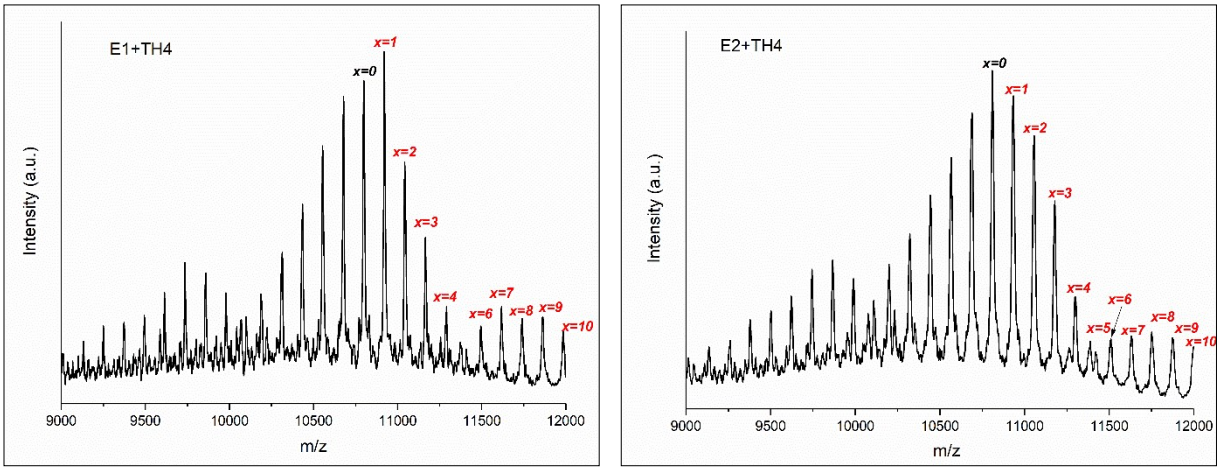


Fig. S8 MALDI mass spectra of E1/ E2+TH4 after ligand exchange reaction.

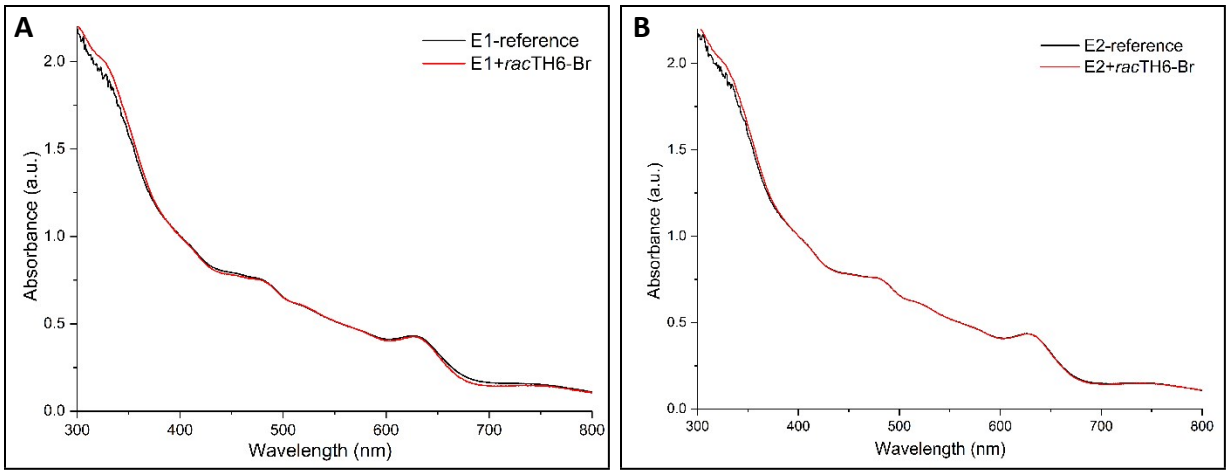


Fig. S9 UV-vis spectra of E1 **(A)** and E2 **(B)** enantiomers of Au_{38} after the ligand exchange reaction with *rac*TH6-Br (RT, 20 h). 1/20 cluster/ligand ratios were used in both cases. The spectra of the clusters before the reaction were recorded and used as references for further comparison. The spectra are normalized at 400 nm.

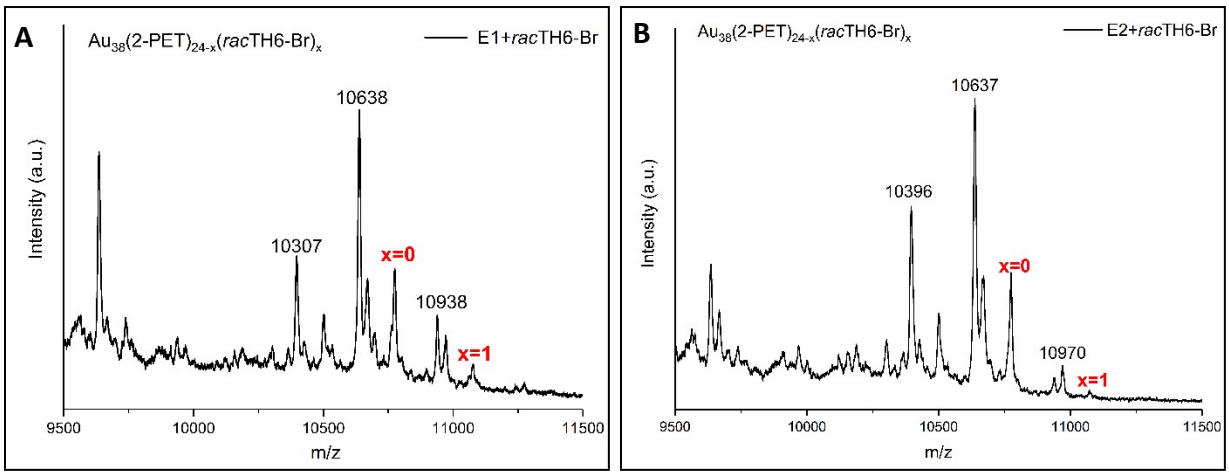


Fig. S10 MALDI mass spectra of E1 **(A)** and E2 **(B)** enantiomers of Au_{38} after the ligand exchange reaction with *rac*TH6-Br (RT, 20 h). 1/20 cluster/ligand ratios were used in both cases. Maximum one exchange species was detected with average exchange numbers ($\bar{x}$) of 0.23 and 0.1 for E1 and E2 enantiomers, respectively.

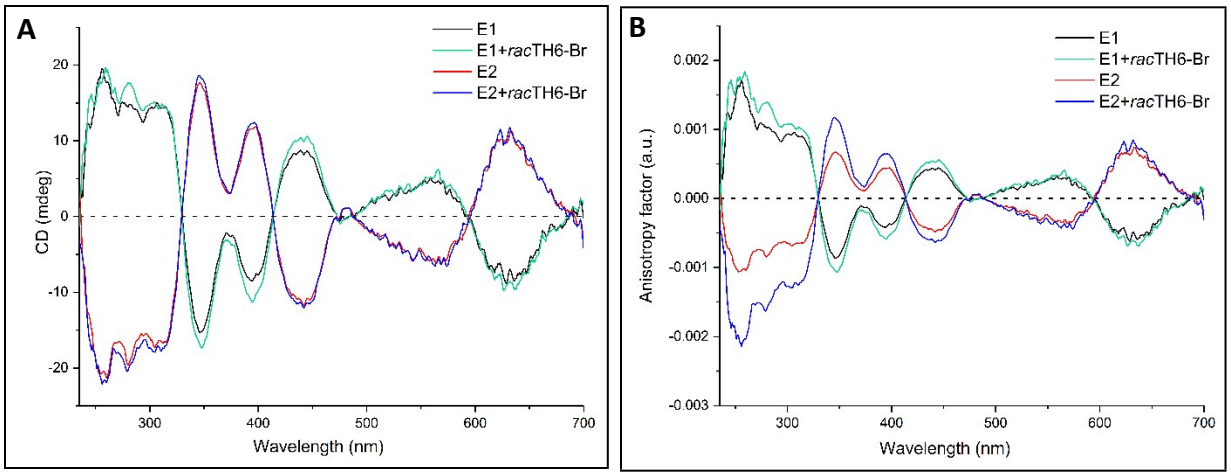


Fig. S11 CD spectra **(A)** and anisotropy factors *g* **(B)** of the E1/E2 enantiomers of Au_{38} after the ligand exchange reaction with *rac*TH6-Br (RT, 20 h). 1/20 cluster/ligand ratios were used in both cases. The spectra were recorded in DCM and the solvent background was subtracted afterwards.

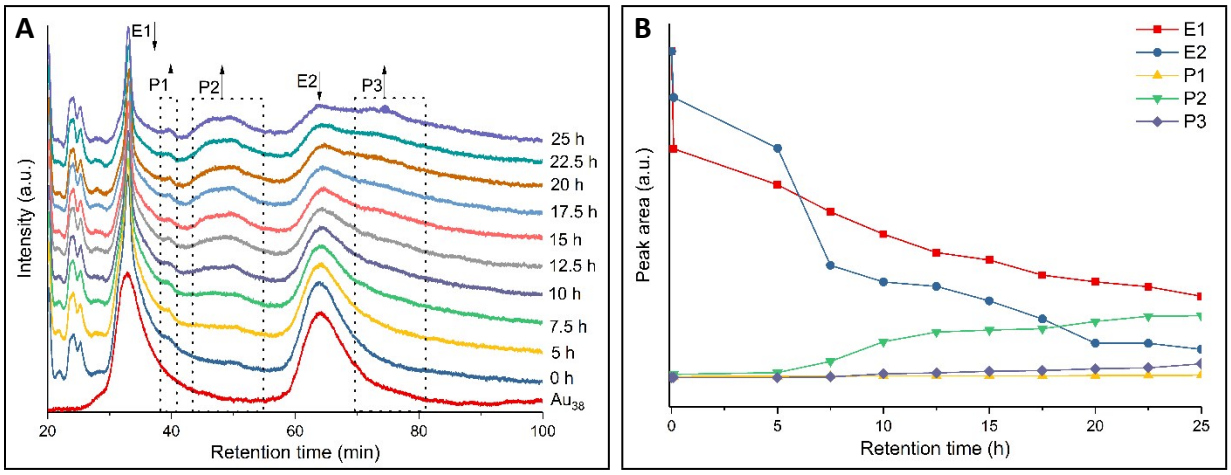


Fig. S12 (A) *In situ* HPLC monitoring of the ligand exchange reaction between racemic Au_{38} cluster and enantiopure (*M*-form) TH6-Br ligand (RT, 25 h, 1/20 cluster/ligand ratios). The chromatograms were recorded every 150 min upon injecting 5 µL sample (note the chromatograms are plotted up to 100 min). The chromatogram of pure Au_{38} cluster before the reaction was recorded and used as a reference for further comparison. The ascending and descending arrows indicate the increase and decrease of the peaks' intensity during the course of reaction, respectively. **(B)** The evolution of the peaks' area during ligand exchange reaction.

The percentage of the exchange sample in the reaction mixture after 25 h is calculated according to the following equation:

$$Exchange\ species\ in\ the\ sample\ \% = \frac{A(P1) + A(P2) + A(P3)}{A(E1) + A(E2) + A(P1) + A(P2) + A(P3)}$$

where ***A*** is the area of each peak in the HPLC chromatogram.

Based on the equation, the calculated contents of the exchange species and unreacted Au_{38} cluster in the crude mixture are 41 and 59 %, respectively.

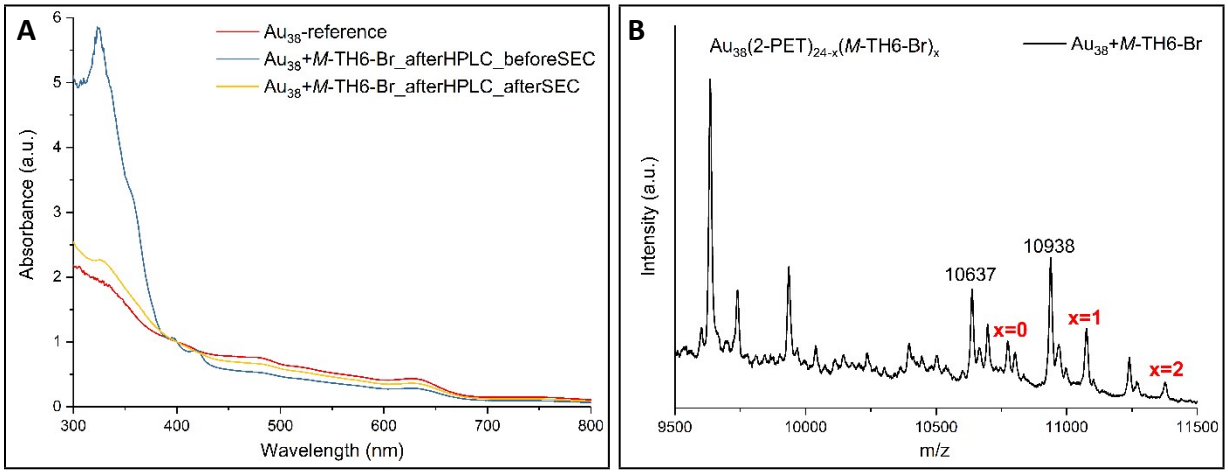


Fig. S13 UV-vis spectra **(A)** and MALDI mass spectrum **(B)** of Au_{38} after the ligand exchange reaction with *M*-TH6-Br (RT, 25 h). 1/20 cluster/ligand ratios were used in both cases. The UV-vis spectra of Au_{38} cluster before the reaction was recorded and used as a reference for further comparison. The spectra are normalized at 400 nm. Maximum two exchanges were detected on MALDI with an average exchange number ($\bar{x}$) of 0.66.

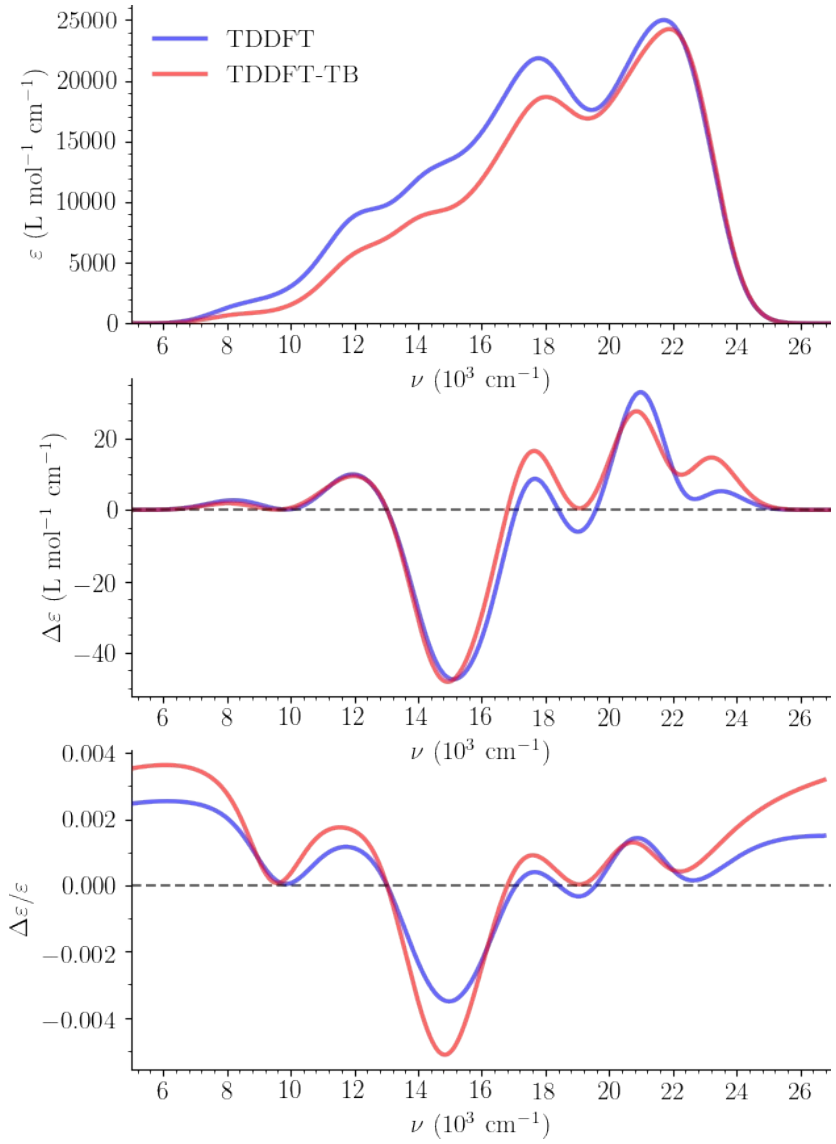


Fig. S14 Simulated absorption and CD spectra of [$Au_{38}(SCH_3)_{24}$] obtained by convoluting the calculated oscillator and rotatory strengths with Gaussians having a FWHM of 2000 cm^{-1}: they are plotted along with the anisotropy factor as functions of the transition energy (TDDFT and TDDFT-TB results for the 300 lowest-lying dipole-allowed transitions).

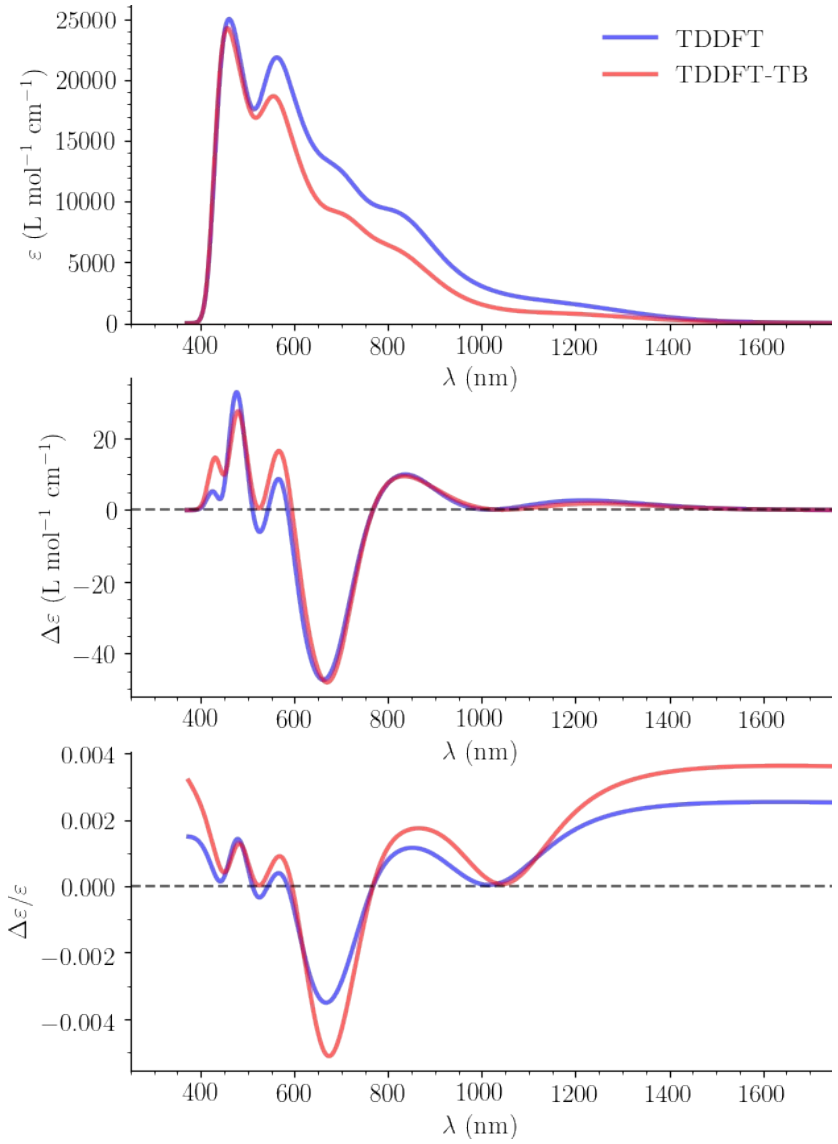


Fig. S15 Simulated absorption and CD spectra of $[Au_{38}(SCH_3)_{24}]$ obtained by convoluting the calculated oscillator and rotatory strengths with Gaussians having a FWHM of 2000 cm^{-1}: they are plotted along with the anisotropy factor as functions of the transition wavelength (TDDFT and TDDFT-TB results for the 300 lowest-lying dipole-allowed transitions).

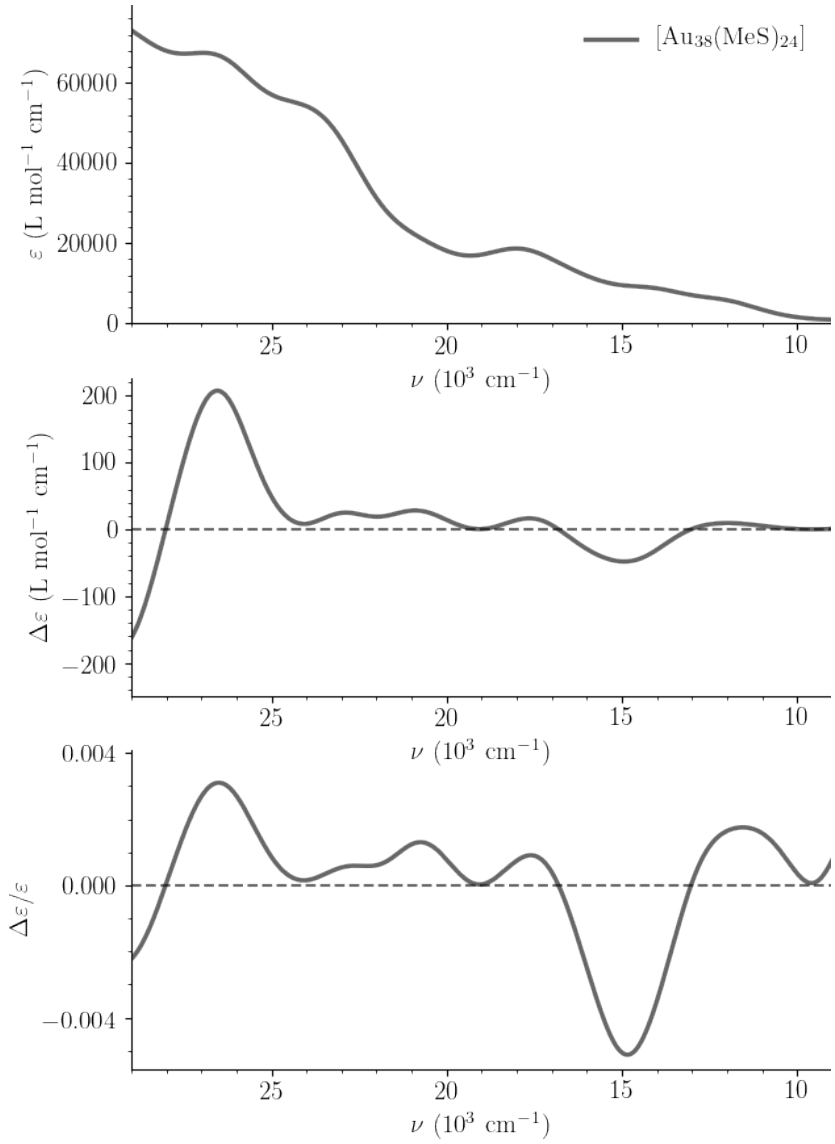


Fig. S16 Simulated absorption and CD spectra of $[Au_{38}(SCH_3)_{24}]$ obtained by convoluting the calculated oscillator and rotatory strengths with Gaussians having a FWHM of 2000 cm^{-1}: they are plotted along with the anisotropy factor as functions of the transition energy (TDDFT-TB results for the 1500 lowest-lying dipole-allowed transitions).

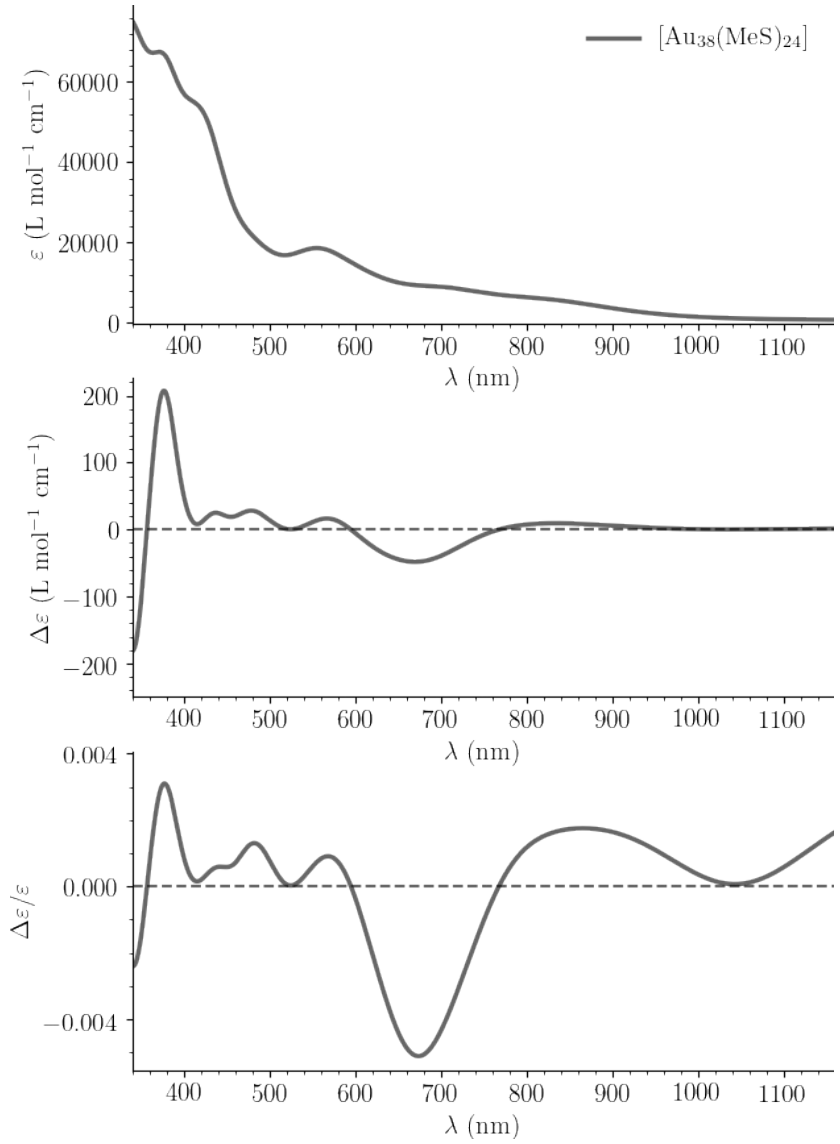


Fig. S17 Simulated absorption and CD spectra of $[Au_{38}(SCH_3)_{24}]$ obtained by convoluting the calculated oscillator and rotatory strengths with Gaussians having a FWHM of 2000 cm^{-1}: they are plotted along with the anisotropy factor as functions of the transition wavelength (TDDFT-TB results for the 1500 lowest-lying dipole-allowed transitions).

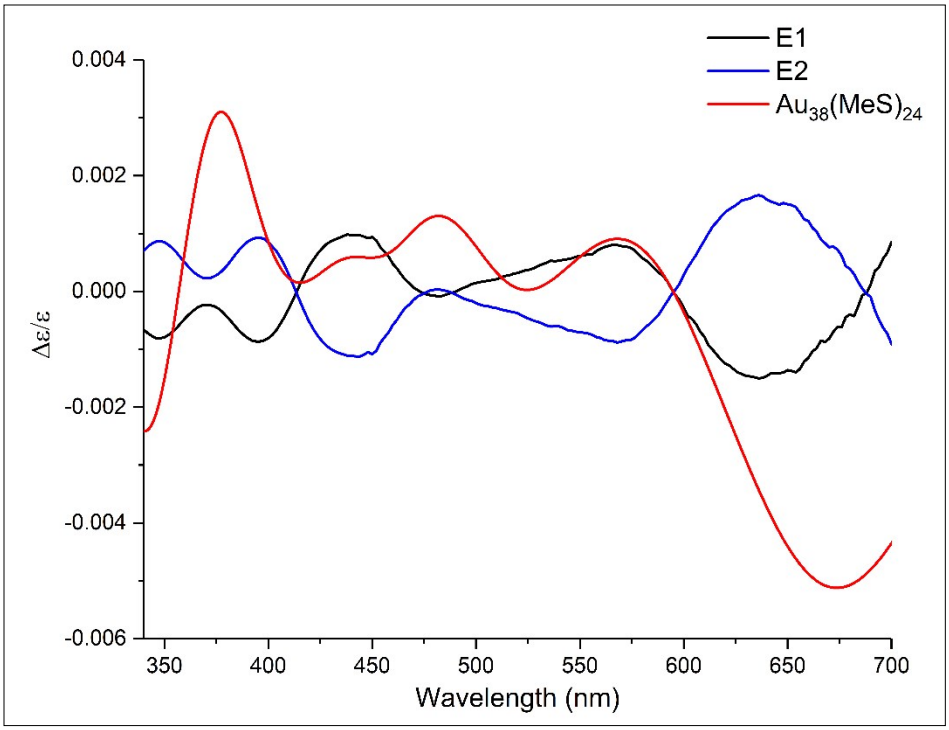


Fig. S18 Comparison between simulated (red curve) and measured (black and blue curves) anisotropy factors. The red curve represents a model [$Au_{38}(MeS)_{24}$] obtained by convoluting the calculated oscillator and rotatory strengths with Gaussians having a FWHM of 2000 cm^{-1} (TDDFT-TB results for the 1500 lowest-lying dipole-allowed transitions). The black and blue curves represent the E1 and E2 enantiomers of $Au_{38}(2\text{-PET})_{24}$ clusters (E1: left-handed enantiomer and E2: right-handed enantiomer). The calculated curve fits well with E1 enantiomer of the cluster.

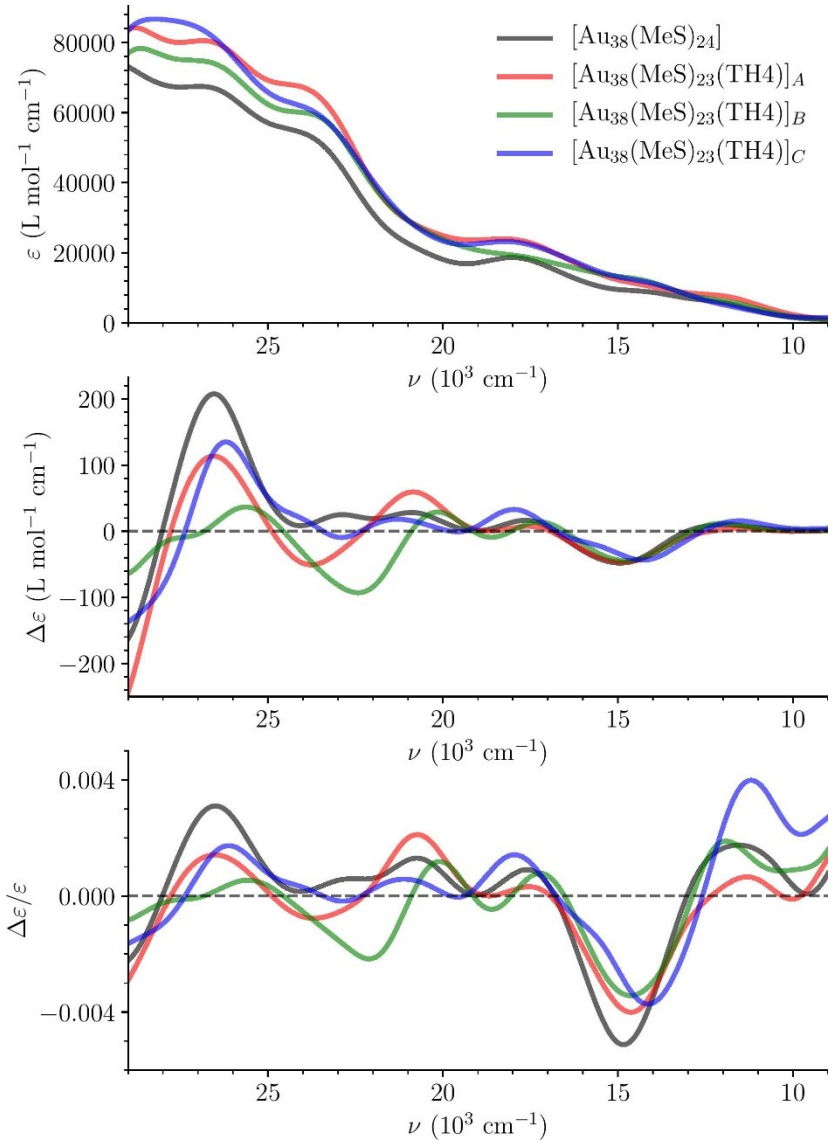


Fig. S19 Simulated absorption and CD spectra of the $[Au_{38}(SCH_3)_{24}]$ and $[Au_{38}(SCH_3)_{23}(TH4)]$ clusters obtained by convoluting the calculated oscillator and rotatory strengths with Gaussians having a FWHM of 2000 cm^{-1}: they are plotted along with the anisotropy factor as functions of the transition energy (TDDFT-TB results for the 1500 lowest-lying dipole-allowed transitions).

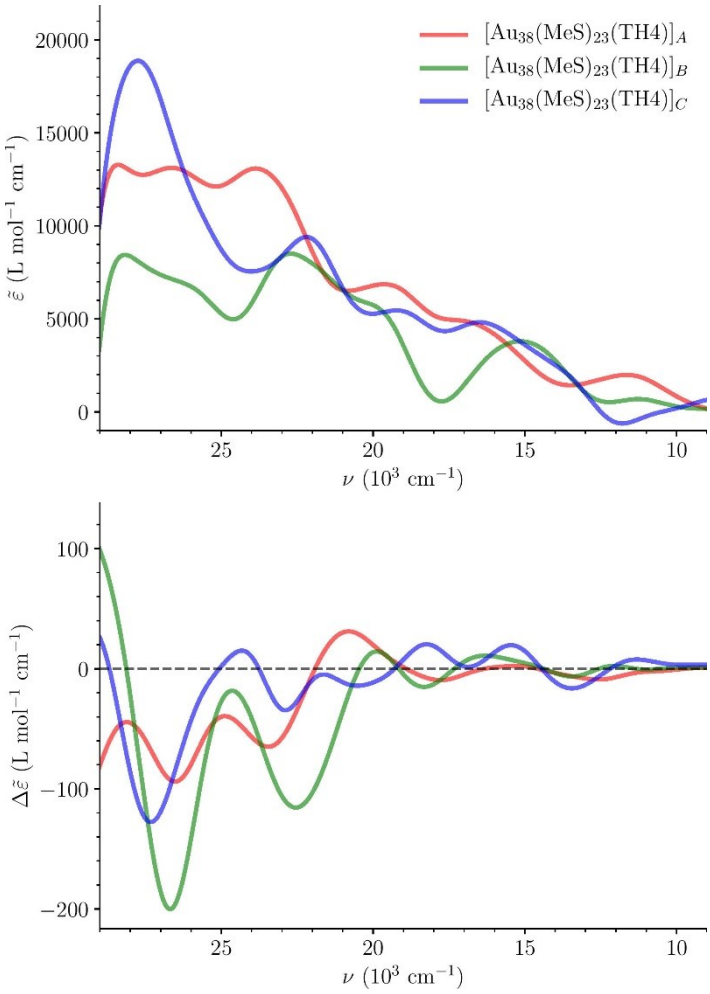


Fig. S20 Differences between the simulated absorption (Top) and CD (Bottom) spectra of the $[Au_{38}(SCH_3)_{23}(TH4)]$ regioisomers and those of $[Au_{38}(SCH_3)_{24}]$ taken as references: they are plotted as functions of the transition energy (TDDFT-TB results for the 1500 lowest-lying dipole-allowed transitions).

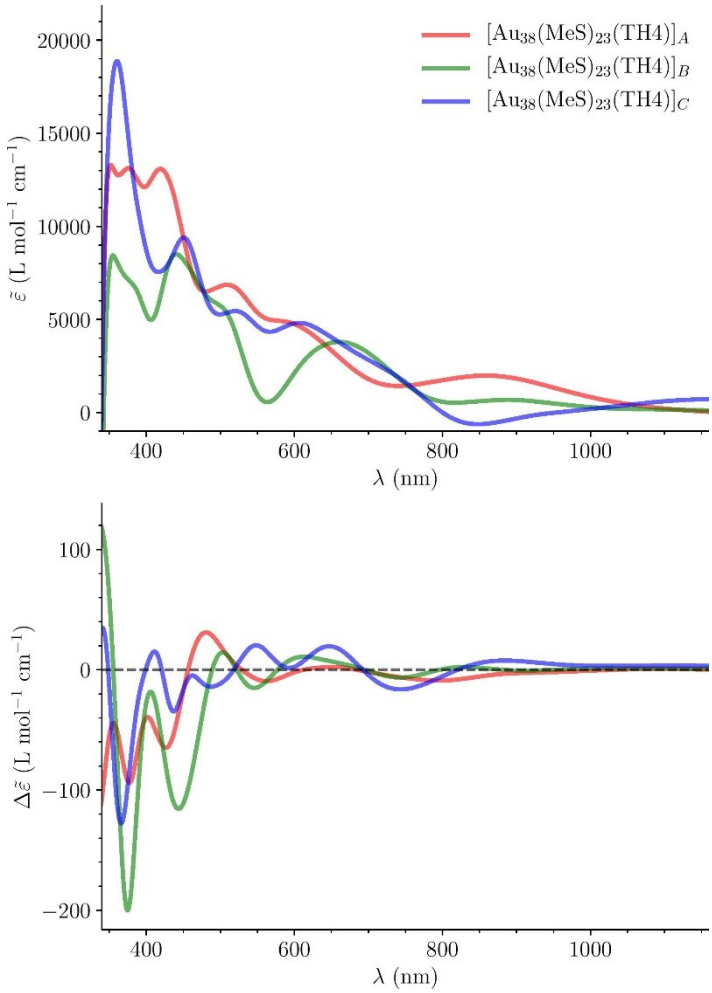
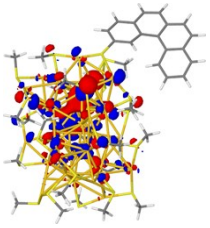
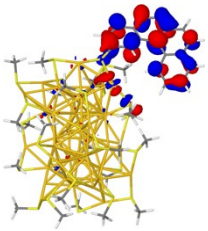
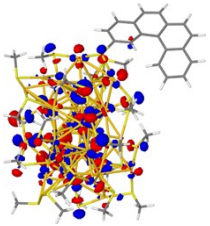
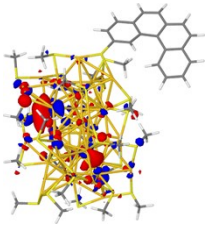
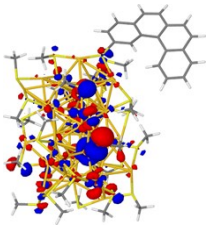
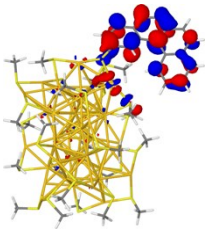
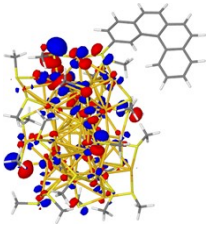
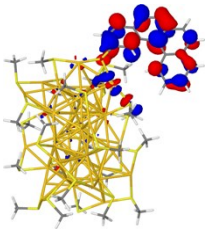


Fig. S21 Differences between the simulated absorption (Top) and CD (Bottom) spectra of the $[Au_{38}(SCH_3)_{23}(TH4)]$ regioisomers and those of $[Au_{38}(SCH_3)_{24}]$ taken as references: they are plotted as functions of the transition wavelength (TDDFT-TB results for the 1500 lowest-lying dipole-allowed transitions).

Table S2. Selected features of the five transitions in $[Au_{38}(SCH_3)_{23}(TH4)]_A$ having the CT numbers (see Text): energy E (in cm^{-1}), wavelength λ (in nm), oscillator strength f, rotatory strength R (in 10^{-40} esu^2 cm^2), and CT character; the transitions between NTOs having weights greater than 10% are also depicted (TDDFT-TB results)

#	E	λ	f	R	CT
76	15937	628	0.002	2.095	0.450
	(71%)		→		
	(15%)		→		
144	18767	533	0.019	-21.647	0.513
	(83%)		→		
200	20206	495	0.006	0.943	0.461
	(78%)		→		
786	28530	351	0.002	2.142	0.460

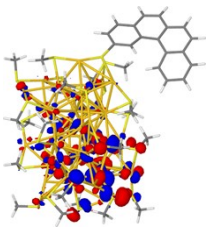
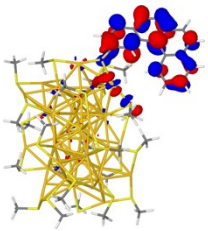
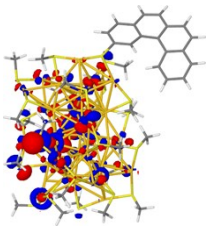
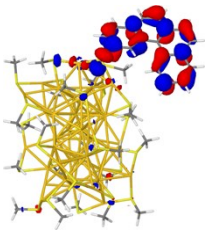
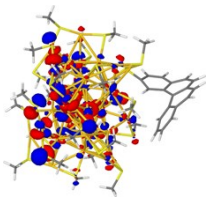
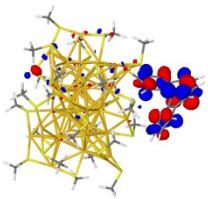
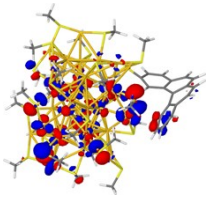
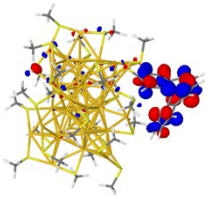
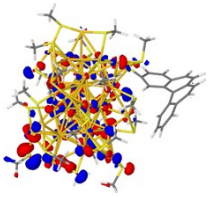
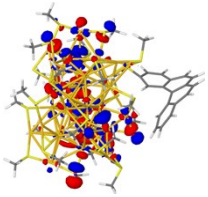
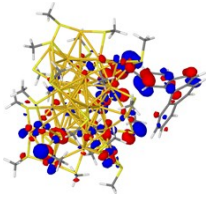
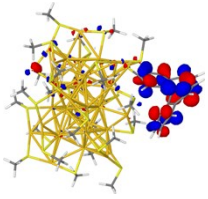
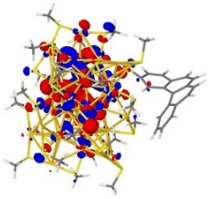
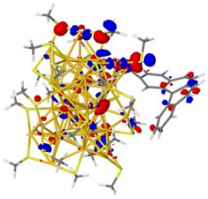
		(79%)		→		
1205	31539	317		0.001	0.991	0.443
		(68%)		→		

Table S3. Selected features of the five transitions in $[Au_{38}(SCH_3)_{23}(TH4)]_B$ having the highest CT numbers (see Text): energy E (in cm^{-1}), wavelength λ (in nm), oscillator strength f, rotatory strength R (in 10^{-40} esu^2 cm^2), and CT character; the transitions between NTOs having weights greater than 10% are also depicted (TDDFT-TB results)

#	E	λ	f	R	CT
160	19118	523	0.000	0.760	0.421
	(74%)		→		
189	19848	503	0.003	0.263	0.371
	(57%)		→		
	(16%)		→		
219	20540	487	0.001	-12.633	0.355
	(37%)		→		
	(14%)		→		
287	21906	457	0.001	-9.469	0.370

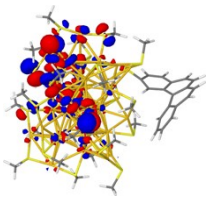
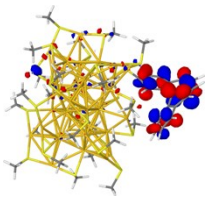
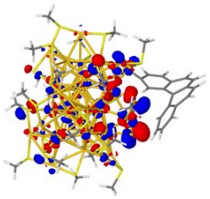
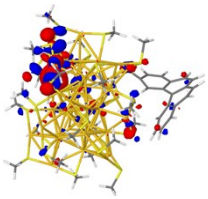
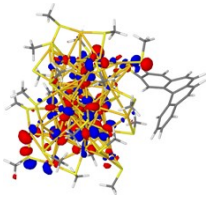
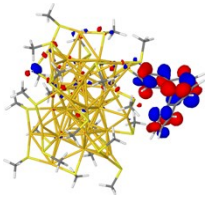
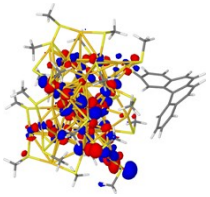
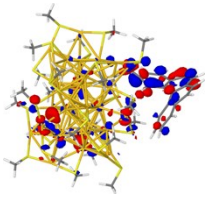
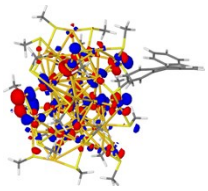
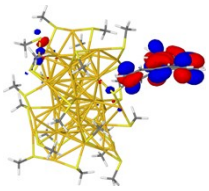
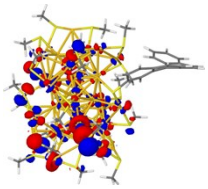
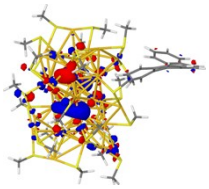
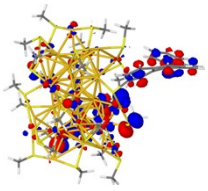
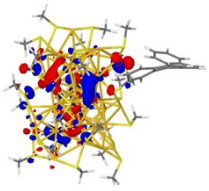
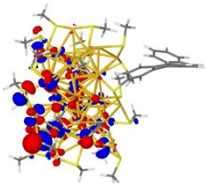
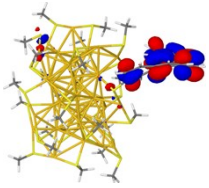
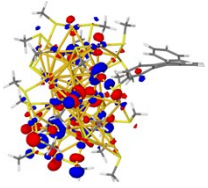
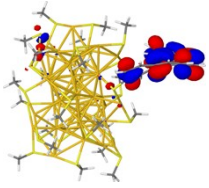
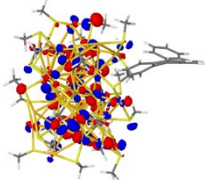
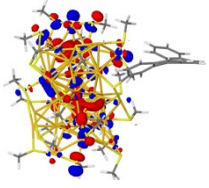
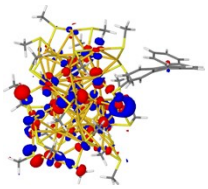
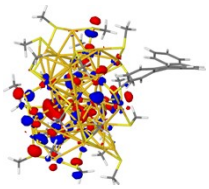
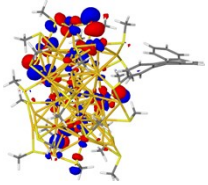
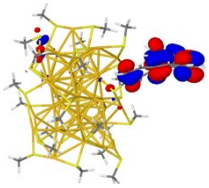
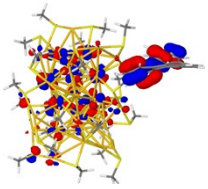
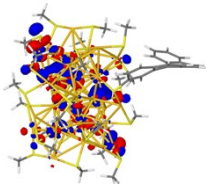
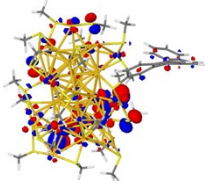
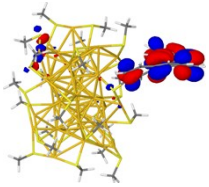
	(63%)		→			
	(10%)		→			
1192	31405	318	0.003	29.198	0.338	
	(43%)		→			
	(12%)		→			

Table S4. Selected features of the five transitions in $[Au_{38}(SCH_3)_{23}(TH4)]_C$ having the highest CT numbers (see Text): energy E (in cm^{-1}), wavelength λ (in nm), oscillator strength f, rotatory strength R (in 10^{-40} esu^2 cm^2), and CT character; the transitions between NTOs having weights greater than 10% are also depicted (TDDFT-TB results)

#	E	λ	f	R	CT
224	20857	480	0.004	-26.931	0.464
	(56%)		→		
	(12%)		→		
	(11%)		→		
247	21282	470	0.000	-0.283	0.535
	(66%)		→		
264	21666	462	0.006	2.891	0.470
	(55%)		→		
	(11%)		→		

	(10%)		→			
400	24110	415	0.012	26.098	0.458	
	(39%)		→			
	(38%)		→			
463	25042	399	0.002	27.461	0.461	
	(54%)		→			

Optimized geometries

$[Au_{38}(SCH_3)_{24}$

Au	1.996965	0.014444	0.006727
Au	0.014363	-0.995218	1.561730
Au	-1.474546	1.227327	2.370605
Au	-2.549868	-1.473270	2.167107
Au	-2.458659	-1.168304	-2.427533
Au	1.418971	1.199074	2.434032
Au	-1.917738	-0.004688	-0.021119
Au	0.023018	1.837247	0.155059
Au	2.510472	2.765685	0.015915
Au	2.574455	-1.319995	2.339057
Au	-1.379572	-2.695855	-0.169820
Au	0.064945	-0.813740	-1.617479
Au	-1.381201	1.487277	-2.243567
Au	-4.001317	0.991964	-1.341059
Au	1.440605	-2.626569	-0.063883
Au	2.607308	-1.463665	-2.351181
Au	-4.104214	0.629708	1.492575
Au	-0.309576	-2.403529	4.023232
Au	4.053162	1.004342	1.377700
Au	-4.055481	-1.648641	-0.237312
Au	1.446279	1.493933	-2.194639
Au	5.531944	-1.287312	2.719031
Au	-2.545464	2.666349	0.189424
Au	-3.516881	0.258191	4.420963
Au	4.059047	0.667369	-1.609518
Au	3.599133	-4.050298	1.804689
Au	3.540393	3.747012	2.543471
Au	-5.467752	-1.999823	2.478671
Au	4.146766	-1.648255	0.114162
Au	5.530058	-1.718549	-2.655627
Au	-0.382794	4.679695	0.121468
Au	-5.367204	3.394327	0.237966
Au	-3.206754	3.941483	-2.319624
Au	-3.578583	-4.012594	-1.934527
Au	3.447664	0.337961	-4.540363
Au	5.375051	3.112999	-0.320730
Au	-5.397295	-1.177938	-2.939735
Au	-0.152115	-2.769799	-3.645865
S	5.102428	4.950077	1.197730
S	6.101582	1.871872	-2.214688
S	2.029295	2.874049	4.141945
S	6.212411	0.992433	2.537851
S	5.223486	-3.535218	3.483363
S	2.022565	-4.985750	0.290179
S	5.236067	-1.185733	-4.972303
S	6.206600	-2.750253	-0.619154
S	1.708151	1.953334	-4.603547
S	-2.079569	-5.053431	-0.440321
S	-5.167780	-3.457521	-3.637959

S	-5.993821	1.140346	-2.744211
S	-5.944726	-3.099100	0.421468
S	-5.330303	-1.270410	4.747542
S	-1.864477	1.918532	4.704950
S	-5.893462	2.132069	2.184907
S	-5.494000	4.486689	-1.883793
S	-0.994992	3.762886	-3.169980
S	-2.668353	5.072349	0.888279
S	1.916368	5.137656	-0.318705
S	-2.315013	-2.410287	-4.594685
S	2.019127	-3.708980	-3.192336
S	-2.613771	-3.102988	4.041745
S	2.041341	-2.410793	4.478069
C	-6.720443	-0.073398	4.882407
H	-7.671559	-0.618293	4.775818
H	-6.666144	0.402914	5.874496
H	-6.615144	0.691759	4.103163
C	-7.227978	1.175529	1.323114
H	-7.280765	0.180089	1.790814
H	-8.183683	1.713191	1.426064
H	-6.964314	1.071864	0.259350
C	-7.271466	-1.989189	-0.217642
H	-7.504271	-2.284653	-1.251741
H	-8.172356	-2.086156	0.408435
H	-6.912442	-0.955210	-0.225715
C	-0.518978	0.908651	5.452123
H	0.373899	1.546356	5.507252
H	-0.818313	0.573835	6.456589
H	-0.293033	0.044849	4.805237
C	-2.678493	-4.470454	2.793629
H	-2.836563	-5.428410	3.313897
H	-3.492187	-4.268716	2.077461
H	-1.736963	-4.470892	2.243794
C	-6.672818	-4.295806	-2.989404
H	-7.567691	-3.836289	-3.437920
H	-6.607930	-5.355737	-3.284289
H	-6.700982	-4.229421	-1.894357
C	-0.807070	-5.663712	-1.631233
H	0.165375	-5.237884	-1.357734
H	-0.777740	-6.763446	-1.562741
H	-1.050368	-5.366809	-2.658310
C	-5.065480	1.693703	-4.253029
H	-5.559346	1.282022	-5.147055
H	-5.103302	2.793079	-4.277616
H	-4.015966	1.364125	-4.200718
C	-1.481694	3.578083	-4.941226
H	-1.986045	4.498023	-5.273440
H	-0.567830	3.427397	-5.537146
H	-2.161727	2.720462	-5.032965
C	-5.298465	6.270838	-1.462268
H	-5.040148	6.815742	-2.383420
H	-6.256216	6.635243	-1.057945
H	-4.501929	6.390704	-0.715984
C	-2.474729	-0.814636	-5.493591

H	-2.056539	-0.881071	-6.509919
H	-3.561102	-0.645231	-5.511171
H	-2.022871	0.002805	-4.921137
C	0.396728	0.748341	-5.089671
H	-0.551845	1.279465	-4.960287
H	0.530930	0.460538	-6.143949
H	0.383075	-0.140156	-4.436074
C	2.297322	5.176796	-2.120373
H	1.940782	6.130388	-2.540876
H	3.396825	5.129720	-2.145474
H	1.881261	4.332571	-2.690537
C	5.303539	2.985459	-3.468613
H	5.843212	3.945393	-3.488162
H	5.373840	2.500657	-4.456241
H	4.239688	3.144146	-3.232239
C	6.673459	-0.060837	-5.207968
H	7.575011	-0.689583	-5.279485
H	6.531512	0.505796	-6.141285
H	6.769303	0.614301	-4.347391
C	6.658833	4.724828	2.161082
H	7.499876	5.067343	1.537629
H	6.595687	5.328172	3.080180
H	6.792896	3.661965	2.404047
C	5.443184	-4.389940	-1.033866
H	6.071441	-4.882208	-1.792858
H	5.415234	-5.001042	-0.117106
H	4.415801	-4.261095	-1.411699
C	6.745929	-4.288747	2.767046
H	7.609257	-3.952465	3.362714
H	6.650734	-5.384722	2.820218
H	6.867724	-3.962498	1.725067
C	0.641086	4.006335	3.707832
H	-0.233065	3.661377	4.271818
H	0.898072	5.040198	3.983463
H	0.426134	3.926636	2.628715
C	5.521750	1.500129	4.183563
H	6.137066	1.054985	4.981234
H	5.559005	2.599592	4.252285
H	4.473222	1.176668	4.279292
C	2.555361	-0.953691	5.478950
H	2.254225	-1.093266	6.528871
H	3.651473	-0.950270	5.379545
H	2.163730	-0.009268	5.076897
C	-2.749770	4.539336	2.656655
H	-2.941868	5.422892	3.286430
H	-3.540642	3.783307	2.786113
H	-1.790960	4.087456	2.904998
C	0.724324	-5.233655	1.581793
H	-0.197943	-5.523753	1.063105
H	1.034831	-6.023719	2.281629
H	0.548157	-4.283264	2.112250
C	2.775951	-3.562485	-4.864269
H	3.859829	-3.687916	-4.722111
H	2.374298	-4.346286	-5.525607

H	2.570414	-2.566330	-5.278057

$[Au_{38}(SCH_3)_{23}$(TH4), regioisomer a

Au	1.979073	0.050117	0.191716
Au	-0.042866	-0.860985	1.749490
Au	-1.537014	1.382267	2.315705
Au	-2.622751	-1.381109	2.252712
Au	-2.352371	-1.363686	-2.338315
Au	1.354173	1.386688	2.493926
Au	-1.904255	-0.029507	0.006547
Au	0.020614	1.874381	0.120823
Au	2.528796	2.774224	0.014357
Au	2.484017	-1.158438	2.608021
Au	-1.336525	-2.710954	0.056244
Au	0.144902	-0.912207	-1.505174
Au	-1.284281	1.321876	-2.295043
Au	-3.932740	0.851581	-1.475699
Au	1.447821	-2.587069	0.241985
Au	2.719590	-1.582421	-2.064540
Au	-4.135056	0.681319	1.377774
Au	-0.432714	-2.185114	4.243251
Au	4.015933	1.112728	1.563909
Au	-4.011043	-1.702119	-0.188479
Au	1.535947	1.340905	-2.139663
Au	5.403930	-1.132421	3.062523
Au	-2.558628	2.648578	-0.002140
Au	-3.652320	0.502371	4.339390
Au	4.111953	0.605051	-1.385541
Au	3.508396	-3.812536	2.194716
Au	3.460333	3.905679	2.537199
Au	-5.537617	-1.882528	2.483264
Au	4.140163	-1.582755	0.429175
Au	5.658813	-1.814434	-2.263189
Au	-0.394224	4.697236	-0.104987
Au	-5.380169	3.339211	-0.090813
Au	-3.119430	3.751694	-2.601961
Au	-3.456288	-4.175164	-1.692438
Au	3.628096	0.074592	-4.331719
Au	5.408984	3.102800	-0.217252
Au	-5.257394	-1.440899	-2.977220
Au	0.030949	-3.026492	-3.366194
S	5.089721	5.016066	1.188858
S	6.184296	1.755623	-2.015869
S	1.881406	3.154409	4.132801
S	6.110733	1.140932	2.831378
S	2.029717	-4.925582	0.700787
S	5.426247	-1.469293	-4.621355
S	6.316393	-2.574468	-0.112579
S	1.888561	1.676209	-4.555527
S	-1.993187	-5.094422	-0.090736

S	-4.980524	-3.762699	-3.491747
S	-5.875877	0.879209	-2.952865
S	-5.935541	-3.106167	0.478091
S	-5.464880	-1.018689	4.707451
S	-2.028841	2.198089	4.587760
S	-5.955900	2.207613	1.921766
S	-5.430627	4.279779	-2.286486
S	-0.874422	3.542424	-3.349036
S	-2.709410	5.096943	0.539382
S	1.928678	5.114440	-0.473289
S	-2.098959	-2.741727	-4.409534
S	2.201709	-3.888003	-2.768598
S	-2.732958	-2.897801	4.217045
S	1.894712	-2.113584	4.799946
C	-6.863041	0.175991	4.735484
H	-7.808887	-0.380290	4.641317
H	-6.833966	0.713436	5.696731
H	-6.743826	0.891806	3.912446
C	-7.262430	1.190234	1.088658
H	-7.322581	0.225184	1.615499
H	-8.222673	1.727568	1.132776
H	-6.968790	1.023144	0.041126
C	-7.229928	-2.035440	-0.281573
H	-7.430094	-2.400092	-1.300379
H	-8.151804	-2.082769	0.318780
H	-6.860370	-1.007326	-0.346444
C	-0.706690	1.240789	5.440070
H	0.179740	1.887684	5.491242
H	-1.041786	0.962847	6.450651
H	-0.453368	0.342744	4.853088
C	-2.761499	-4.340183	3.055178
H	-2.951356	-5.260931	3.629520
H	-3.545499	-4.179369	2.296604
H	-1.799677	-4.386471	2.543007
C	-6.503870	-4.564169	-2.839724
H	-7.382052	-4.160333	-3.367494
H	-6.413073	-5.644865	-3.035843
H	-6.583005	-4.401435	-1.757340
C	-0.689754	-5.776933	-1.202669
H	0.262441	-5.298455	-0.948364
H	-0.631358	-6.864789	-1.033430
H	-0.920632	-5.584891	-2.257389
C	-4.894417	1.349279	-4.456626
H	-5.343641	0.870839	-5.340978
H	-4.948656	2.443585	-4.554888
H	-3.842881	1.042203	-4.340231
C	-1.297644	3.245021	-5.121965
H	-1.801844	4.135922	-5.525863
H	-0.362600	3.071626	-5.677660
H	-1.963291	2.373363	-5.184245
C	-5.280146	6.091101	-1.979044
H	-4.990888	6.577866	-2.923235
H	-6.259383	6.465420	-1.640573
H	-4.518058	6.273773	-1.209894

C	-2.227670	-1.205387	-5.411399
H	-1.771913	-1.333026	-6.405481
H	-3.313047	-1.042862	-5.479272
H	-1.799806	-0.352112	-4.873630
C	0.603334	0.435924	-5.025970
H	-0.352689	0.965323	-4.958501
H	0.777715	0.095305	-6.058372
H	0.569327	-0.418268	-4.328111
C	2.374817	5.048846	-2.259447
H	2.029781	5.972194	-2.750574
H	3.474703	5.007456	-2.239141
H	1.984307	4.167458	-2.790163
C	5.423941	2.791001	-3.356296
H	5.962719	3.749719	-3.417981
H	5.524700	2.247471	-4.310110
H	4.353153	2.960706	-3.163500
C	6.861626	-0.350293	-4.900991
H	7.769051	-0.974531	-4.909045
H	6.736548	0.149213	-5.874198
H	6.933883	0.384151	-4.087894
C	6.599734	4.819757	2.229227
H	7.472173	5.118368	1.626852
H	6.506892	5.469749	3.113593
H	6.704593	3.768619	2.530874
C	5.701728	-4.299583	-0.392862
H	6.394469	-4.814057	-1.076391
H	5.702398	-4.809076	0.579166
H	4.680735	-4.281768	-0.809635
C	0.512934	4.253890	3.568380
H	-0.386486	3.933540	4.106668
H	0.752806	5.302839	3.798539
H	0.350811	4.114126	2.486207
C	5.345324	1.726146	4.416458
H	5.904726	1.295398	5.261914
H	5.407872	2.826110	4.445753
H	4.285116	1.432581	4.464021
C	2.369500	-0.581460	5.702832
H	2.053458	-0.650924	6.755288
H	3.466490	-0.574433	5.616792
H	1.975617	0.327096	5.227658
C	-2.846340	4.677610	2.335213
H	-3.064026	5.597861	2.900841
H	-3.638060	3.926283	2.484656
H	-1.894043	4.248775	2.643365
C	0.732954	-5.153733	2.002471
H	-0.155290	-5.585222	1.522030
H	1.112600	-5.816385	2.795261
H	0.468138	-4.171214	2.426732
C	3.006038	-3.856407	-4.424246
H	4.086019	-3.966248	-4.244661
H	2.626564	-4.688296	-5.037854
H	2.806803	-2.893564	-4.913212
S	5.079340	-3.346501	3.976599
C	6.430904	-4.276326	3.226994

C	7.636497	-3.654282	2.848197
C	6.232094	-5.631440	2.990639
C	8.626156	-4.413633	2.259719
H	7.790188	-2.590662	3.055567
C	7.177400	-6.400560	2.278267
H	5.323377	-6.099338	3.375586
C	8.436684	-5.783614	1.974561
H	9.586903	-3.951832	2.007811
C	6.951794	-7.774769	1.885275
C	9.498922	-6.576904	1.456521
C	5.647233	-8.395524	1.805639
C	8.082934	-8.553815	1.531500
C	9.345536	-7.925929	1.313082
H	10.456760	-6.096011	1.230092
C	5.563331	-9.824128	1.705843
C	4.432560	-7.672617	1.700202
C	7.958492	-9.966547	1.380852
H	10.187821	-8.548430	0.991555
C	4.297528	-10.454420	1.685624
C	6.753394	-10.588242	1.536461
C	3.208754	-8.311545	1.636793
H	4.442758	-6.588284	1.593839
H	8.859364	-10.548610	1.157133
C	3.131878	-9.716248	1.675025
H	4.260335	-11.548738	1.639078
H	6.675261	-11.678703	1.465275
H	2.301785	-7.712727	1.516856
H	2.158998	-10.217720	1.645377

$[Au_{38}(SCH_3)_{23}$(TH4), regioisomer b

Au	2.008930	-0.110022	-0.116540
Au	-0.005804	-1.054597	1.319231
Au	-1.429414	1.023118	2.394716
Au	-2.532296	-1.707449	1.934015
Au	-2.526284	-0.942904	-2.590510
Au	1.499615	0.977827	2.367219
Au	-1.970306	-0.018617	-0.109427
Au	0.027141	1.745286	0.171228
Au	2.555234	2.615758	0.189798
Au	2.490859	-1.627398	2.094560
Au	-1.435465	-2.720517	-0.497089
Au	0.029536	-0.741176	-1.771799
Au	-1.409563	1.633225	-2.210243
Au	-4.060747	1.095092	-1.296126
Au	1.287382	-2.780797	-0.279501
Au	2.573361	-1.390034	-2.488029
Au	-4.104407	0.452194	1.510900
Au	-0.308641	-2.766864	3.395957
Au	4.113582	0.690142	1.339808
Au	-4.072819	-1.646149	-0.444122
Au	1.467428	1.579926	-2.156445

Au	5.434951	-1.790159	2.518146
Au	-2.543578	2.605126	0.383835
Au	-3.411772	-0.193702	4.328828
Au	4.084178	0.697348	-1.611496
Au	3.427628	-4.354969	1.238060
Au	3.559886	3.278526	2.869926
Au	-5.459535	-2.239010	2.228755
Au	4.073473	-1.838106	-0.125796
Au	5.549039	-1.556943	-2.843887
Au	-0.349494	4.542925	0.612600
Au	-5.359077	3.328011	0.517656
Au	-3.180288	4.120277	-1.964329
Au	-3.583641	-3.906344	-2.245564
Au	3.400330	0.667099	-4.516191
Au	5.416608	3.026909	-0.073207
Au	-5.456389	-0.947323	-3.066023
Au	-0.196094	-2.370760	-4.065827
S	5.141277	4.624075	1.689204
S	6.095170	1.999007	-2.104171
S	1.985838	2.323049	4.371817
S	6.241123	0.462851	2.515363
S	5.005560	-4.100455	3.010902
S	5.213782	-0.786847	-5.081996
S	6.156040	-2.846149	-0.935172
S	1.695416	2.334775	-4.489080
S	-1.888918	-5.089098	-1.060416
S	-5.192395	-3.186938	-3.875644
S	-6.058312	1.349721	-2.674299
S	-6.002405	-3.114335	0.089033
S	-5.242517	-1.718699	4.549842
S	-1.625046	1.268405	4.855486
S	-5.868900	1.905399	2.355546
S	-5.465876	4.630539	-1.481435
S	-0.960251	4.001564	-2.807113
S	-2.632606	4.892693	1.418106
S	1.952158	5.003431	0.187493
S	-2.403265	-1.949826	-4.861494
S	1.931578	-3.428578	-3.664711
S	-2.687804	-3.632445	3.415962
S	2.043000	-2.894443	4.104910
C	-6.605049	-0.525709	4.862400
H	-7.568317	-1.044203	4.734486
H	-6.507813	-0.154769	5.895226
H	-6.514305	0.313566	4.160865
C	-7.238202	1.048806	1.445513
H	-7.288023	0.011773	1.811308
H	-8.183542	1.581663	1.633967
H	-7.008892	1.054548	0.369131
C	-7.298241	-1.908757	-0.424158
H	-7.553449	-2.098034	-1.478483
H	-8.193545	-2.035341	0.204625
H	-6.902591	-0.891571	-0.338338
C	-0.353400	0.021543	5.344138
H	0.433291	0.562821	5.889586

H	-0.783121	-0.775039	5.968973
H	0.078882	-0.431426	4.441221
C	-2.785181	-4.838099	2.021886
H	-3.156526	-5.790884	2.434005
H	-3.484553	-4.473893	1.249167
H	-1.787391	-4.980349	1.591610
C	-6.692122	-4.078370	-3.298155
H	-7.586065	-3.613049	-3.742315
H	-6.602355	-5.122164	-3.640352
H	-6.740066	-4.062817	-2.201702
C	-0.827999	-5.419471	-2.520385
H	0.223116	-5.386530	-2.206865
H	-1.089894	-6.410060	-2.923975
H	-0.977177	-4.654408	-3.293077
C	-5.139084	2.065442	-4.119053
H	-5.617487	1.725374	-5.050726
H	-5.212354	3.160056	-4.039754
H	-4.078036	1.769128	-4.095132
C	-1.436242	4.059217	-4.591162
H	-1.910230	5.028912	-4.806448
H	-0.521451	3.959444	-5.196610
H	-2.140002	3.240478	-4.797952
C	-5.234060	6.356562	-0.875727
H	-4.963664	6.987764	-1.736277
H	-6.182528	6.698777	-0.432249
H	-4.433285	6.378240	-0.124048
C	-2.586416	-0.292937	-5.632941
H	-2.198564	-0.287921	-6.663260
H	-3.671954	-0.119947	-5.608425
H	-2.111802	0.480176	-5.018185
C	0.365351	1.209673	-5.100079
H	-0.578134	1.744588	-4.944263
H	0.514519	1.006126	-6.171929
H	0.324011	0.269774	-4.523211
C	2.304266	5.266931	-1.601320
H	1.933200	6.259588	-1.900923
H	3.404036	5.232720	-1.638331
H	1.892523	4.489167	-2.262157
C	5.260405	3.226330	-3.219822
H	5.794495	4.187285	-3.153528
H	5.312285	2.844168	-4.252396
H	4.201327	3.351749	-2.945808
C	6.628071	0.377695	-5.243974
H	7.535797	-0.227655	-5.396749
H	6.454843	1.027294	-6.115775
H	6.737680	0.969758	-4.325842
C	6.696873	4.257464	2.610027
H	7.536167	4.702487	2.052351
H	6.627167	4.704384	3.614281
H	6.837774	3.170258	2.677163
C	5.395068	-4.408549	-1.587194
H	6.073613	-4.836766	-2.341999
H	5.271690	-5.113201	-0.748700
H	4.406753	-4.204199	-2.031246

C	6.512208	-4.852526	2.261837
H	7.368604	-4.646318	2.923677
H	6.348164	-5.938208	2.175074
H	6.694497	-4.410307	1.272693
C	0.702752	3.615601	4.080280
H	-0.183925	3.323532	4.654912
H	1.076057	4.593169	4.419854
H	0.457016	3.647246	3.006430
C	5.555703	0.872114	4.190982
H	6.147655	0.344461	4.955543
H	5.629780	1.960384	4.346941
H	4.496524	0.579119	4.252620
C	2.574584	-1.553398	5.237259
H	2.173876	-1.738202	6.245012
H	3.672678	-1.633784	5.222069
H	2.301291	-0.553018	4.875681
C	-2.779638	4.159551	3.111127
H	-3.035319	4.971226	3.811447
H	-3.555763	3.377942	3.127232
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C	2.799399	-3.138466	-5.255319
H	3.868644	-3.296487	-5.049617
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H	2.635073	-2.104284	-5.583473
S	1.907598	-5.123626	-0.463584
C	0.925550	-6.168124	0.626748
C	0.590965	-7.420393	0.060997
C	0.875491	-6.008320	2.012432
C	0.497698	-8.532223	0.868723
H	0.545636	-7.532954	-1.026081
C	0.851050	-7.147608	2.861640
H	1.077314	-5.022197	2.440443
C	0.789431	-8.441640	2.248502
H	0.350195	-9.520464	0.419084
C	1.219575	-7.079790	4.261052
C	1.231526	-9.588184	2.967009
C	0.934074	-5.981133	5.145323
C	1.948222	-8.166936	4.800387
C	1.897311	-9.435637	4.152407
H	1.152186	-10.573000	2.493689
C	1.748810	-5.778805	6.303578
C	-0.251058	-5.227494	5.030398
C	2.717313	-7.970466	5.988270
H	2.381125	-10.292359	4.634503
C	1.481281	-4.677979	7.147665
C	2.704631	-6.776164	6.653974
C	-0.559902	-4.227214	5.945490
H	-0.963012	-5.498408	4.248488
H	3.346305	-8.795363	6.341188
C	0.351321	-3.900457	6.964623
H	2.144829	-4.496734	8.000639
H	3.344868	-6.617741	7.528663
H	-1.517569	-3.702516	5.886975
H	0.123112	-3.085802	7.659135

$[Au_{38}(SCH_3)_{23}(TH4)$, regioisomer c

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Au	-0.012374	-0.822341	1.654372
Au	-1.500909	1.389830	2.329995
Au	-2.568892	-1.383664	2.276959
Au	-2.454432	-1.287280	-2.336818
Au	1.365902	1.437505	2.403295
Au	-1.931492	-0.002658	0.027801
Au	0.016786	1.875930	0.078749
Au	2.542315	2.765901	-0.071023
Au	2.556706	-1.075461	2.538137
Au	-1.383735	-2.689438	0.001130
Au	0.070219	-0.900755	-1.542524
Au	-1.361690	1.354871	-2.293030
Au	-3.988452	0.921492	-1.383305
Au	1.413150	-2.594521	0.218257
Au	2.618938	-1.604378	-2.121980
Au	-4.119461	0.690919	1.466658
Au	-0.319601	-2.176675	4.147875
Au	4.073652	1.109657	1.413328
Au	-4.052356	-1.658279	-0.148515
Au	1.476767	1.341829	-2.223798
Au	5.537003	-1.298588	2.951417
Au	-2.558604	2.691397	0.055778
Au	-3.619635	0.489154	4.395468
Au	4.078568	0.564015	-1.515764
Au	3.325359	-3.699579	2.076690
Au	3.480199	3.839646	2.498097
Au	-5.493360	-1.899232	2.542016
Au	4.117421	-1.599567	0.358617
Au	5.540573	-1.892328	-2.411513
Au	-0.339224	4.706688	-0.008939
Au	-5.369768	3.410542	0.077634
Au	-3.151107	3.852072	-2.493255
Au	-3.603071	-4.070125	-1.795430
Au	3.500577	0.073475	-4.419091
Au	5.435602	3.104229	-0.316990
Au	-5.381858	-1.283328	-2.911969
Au	-0.179603	-2.942418	-3.464720
S	5.116656	4.958420	1.161430
S	6.130547	1.741372	-2.132468
S	1.979463	3.032111	4.156958
S	6.063828	1.018241	2.820019
S	5.145821	-3.521119	3.685375
S	1.849536	-4.967507	0.623403
S	5.296915	-1.464390	-4.752457
S	6.094608	-2.886354	-0.324720
S	1.789397	1.710950	-4.636923
S	-2.166272	-5.027703	-0.196845
S	-5.168044	-3.584254	-3.540965

S	-5.971931	1.041743	-2.803034
S	-5.955303	-3.085568	0.525092
S	-5.373803	-1.090027	4.782771
S	-1.984295	2.180978	4.616457
S	-5.925409	2.221458	2.063161
S	-5.437942	4.418100	-2.088101
S	-0.922122	3.601061	-3.271776
S	-2.633517	5.122865	0.674950
S	1.967921	5.115052	-0.490607
S	-2.307284	-2.583019	-4.488021
S	1.956415	-3.864397	-2.870757
S	-2.584629	-2.953276	4.209609
C	-6.799361	0.072799	4.853044
H	-7.734625	-0.502293	4.767639
H	-6.763756	0.597047	5.821305
H	-6.710005	0.802810	4.038484
C	-7.243449	1.225819	1.222200
H	-7.297781	0.249656	1.728416
H	-8.203132	1.761713	1.291252
H	-6.966062	1.080018	0.166755
C	-7.269268	-1.997056	-0.173661
H	-7.490452	-2.331807	-1.198000
H	-8.178068	-2.064797	0.444601
H	-6.905194	-0.965938	-0.217708
C	-0.697669	1.159314	5.442585
H	0.273128	1.671537	5.386012
H	-0.979636	0.968124	6.488951
H	-0.615896	0.214935	4.888669
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H	-2.913266	-5.298261	3.615523
H	-3.578472	-4.182811	2.345633
H	-1.832551	-4.438982	2.450128
C	-6.685430	-4.390480	-2.877796
H	-7.573379	-3.933235	-3.342065
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H	-6.718628	-4.296960	-1.784948
C	-0.872460	-5.738170	-1.304899
H	0.079532	-5.247003	-1.073880
H	-0.806318	-6.819687	-1.100968
H	-1.119986	-5.580550	-2.361314
C	-5.034765	1.541194	-4.325024
H	-5.509398	1.079354	-5.204929
H	-5.092911	2.637014	-4.402134
H	-3.980439	1.233114	-4.245306
C	-1.359292	3.356238	-5.048166
H	-1.836608	4.271250	-5.430504
H	-0.430525	3.167875	-5.609284
H	-2.051304	2.506672	-5.128951
C	-5.239079	6.215102	-1.730933
H	-4.970599	6.725257	-2.668911
H	-6.198597	6.598267	-1.348577
H	-4.448645	6.357498	-0.982089
C	-2.439124	-1.001977	-5.416799
H	-2.006883	-1.091904	-6.425387

H	-3.523173	-0.822211	-5.454116
H	-1.987364	-0.177593	-4.854352
C	0.479329	0.488991	-5.086798
H	-0.469296	1.026053	-4.987203
H	0.623803	0.158521	-6.127140
H	0.458884	-0.372874	-4.397619
C	2.339287	5.078807	-2.294977
H	1.967175	6.005216	-2.759955
H	3.439798	5.048162	-2.314602
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C	5.348635	2.786114	-3.453963
H	5.898106	3.737763	-3.528464
H	5.418602	2.241200	-4.409416
H	4.284682	2.968243	-3.235288
C	6.730252	-0.340640	-5.018565
H	7.635738	-0.966256	-5.062796
H	6.591526	0.192403	-5.971851
H	6.816484	0.364401	-4.181287
C	6.606423	4.714930	2.222702
H	7.495264	5.007769	1.641847
H	6.508121	5.353418	3.114865
H	6.685224	3.658223	2.514364
C	5.208166	-4.480681	-0.691015
H	5.852840	-5.088069	-1.346318
H	5.020438	-5.016711	0.255621
H	4.241267	-4.285909	-1.181361
C	6.370428	-4.563572	2.799717
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H	5.937458	-5.573092	2.712682
H	6.593813	-4.145700	1.809675
C	0.619381	4.210291	3.744197
H	-0.268407	3.889644	4.303199
H	0.909331	5.232708	4.029902
H	0.404095	4.150804	2.664669
C	5.206329	1.439392	4.413177
H	5.847087	1.108143	5.245523
H	5.071852	2.531986	4.452765
H	4.221751	0.946505	4.469030
C	-2.762728	4.678225	2.463922
H	-2.986854	5.590966	3.039144
H	-3.549596	3.920526	2.608918
H	-1.806695	4.253852	2.767927
C	0.525595	-5.173878	1.890699
H	-0.339971	-5.634332	1.397020
H	0.886183	-5.814823	2.708153
H	0.239912	-4.180987	2.275959
C	2.801198	-3.798793	-4.504662
H	3.875772	-3.900925	-4.291231
H	2.445810	-4.620204	-5.146417
H	2.609163	-2.826217	-4.977612
S	1.763285	-1.162997	4.826569
C	2.778821	-2.426007	5.574958
C	3.836674	-1.907296	6.355457
C	2.534970	-3.793686	5.550458

C	4.431198	-2.709515	7.301685
H	4.101381	-0.851714	6.256477
C	3.219026	-4.658072	6.441403
H	1.768740	-4.193900	4.879402
C	4.058319	-4.066250	7.439653
H	5.166727	-2.287772	7.995535
C	3.026274	-6.091835	6.488170
C	4.423501	-4.824419	8.588101
C	2.755093	-6.913512	5.335737
C	3.222649	-6.750257	7.726304
C	3.921567	-6.083170	8.775491
H	5.044813	-4.351712	9.356567
C	2.347422	-8.274495	5.509548
C	3.096961	-6.497019	4.031470
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H	4.108928	-6.624735	9.709293
C	2.154023	-9.088709	4.368695
C	2.284224	-8.813728	6.828070
C	3.002044	-7.340029	2.942275
H	3.526673	-5.505883	3.894723
H	2.850476	-8.557292	8.875614
C	2.475026	-8.635414	3.101690
H	1.805970	-10.117940	4.512394
H	1.932666	-9.841932	6.967648
H	3.345737	-6.980925	1.965981
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