Supporting Information

Absolute configuration retention of a configurationally labile ligand during dynamic processes of thiolate protected gold cluster

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Abstract: Monolayer protected metal clusters are dynamic nanoscale objects. For example, the chiral $Au_{38}(2\text{-PET})_{24}$ (2-PET: 2-phenylethylthiolate) racemizes at moderate temperature. In addition, ligands and metal atoms can easily exchange between clusters. Such processes are important for applications of monolayer protected metal clusters, however, the mechanistic study of such processes turns out to be challenging. Here we use a configurationally labile axial chiral ligand, biphenyl-2,2'-dithiol (R/S-BiDi), as a probe to study dynamic cluster processes. It is shown that the ligand exchange of free R/S-BiDi on a chiral $Au_{38}(2\text{-PET})_{24}$ cluster is diastereospecific. Using chiral chromatography, isolated single diastereomers of the type Anti-clock/Clock-$Au_{38}(2\text{-PET})_{22}(R/S\text{-BiDi})_1$ could be isolated. Upon heating the cluster framework racemizes, whereas the R/S-BiDi ligand does not. This finding demonstrates that during the dynamic cluster processes involved, cluster racemization and/or ligand exchange between clusters, the R/S-BiDi ligand is sufficiently confined thus preventing its racemization, and excludes the possibility that the ligand desorbs from the cluster surface.

Experimental Procedures

All chemicals were purchased from commercial suppliers and used as received without any further treatment. Biphenyl-2,2'-dithiol (BiDi) was synthesized from the biphenyl-2,2`-diol following the protocol for synthesis of BINAS reported before.[1] The synthesis and size selection of rac-$Au_{38}(2\text{-PET})_{24}$ was done according to previous work,[2] and the separation of the two enantiomers of $Au_{38}(2\text{-PET})_{24}$ was done using chiral HPLC.[3]

Ligand exchange reactions with free BiDi. Purified rac-$Au_{38}(2\text{-PET})_{24}$, A-$Au_{38}(2\text{-PET})_{24}$ and C-$Au_{38}(2\text{-PET})_{24}$, respectively were mixed with BiDi in toluene (cluster concentration 1mg/mL) at a molar ratio of cluster to free ligand of 1:50.[3, 4] Ligand exchange was performed at room temperature. After reaction, the solution was concentrated and immediately passed over a size-exclusion column to remove the free ligands. The collected product was then ready for use in the HPLC experiments.

Thermal treatment of Au_{38}. The collected Au_{38} clusters with one BiDi in its ligand shell was concentrated to 10 mg/mL, heated in an oil bath to 70°C, and injected to HPLC after various times.

HPL Chromatography. Chiral HPLC was performed on a JASCO 20XX HPLC system equipped with a semi-preparative Phenomenex Lux-5u-cellulose-1 column (5μm, 250 x 10 mm). The sample was injected in toluene and eluted with n-hexane/iso-propanol 75:25 at a flow rate of 2.5mL/min. A JASCO 2070 plus UV-vis detector was used for the detection.

UV-vis and CD Spectroscopy. UV-vis spectra were measured on a Varian Cary 50 spectrometer. A quartz cuvette of 2mm path length was used. CD spectra were recorded at the same conditions on a JASCO J-815 CD-spectrometer. For each CD spectrum ten scans were averaged at a scanning speed of 200nm/min with a data pitch of 1 nm. The anisotropy factors $g=\theta[\text{mdeg}]/(32980 \times A)^2$ were calculated from the UV-vis and CD spectra.

MALDI-TOF-MS. Mass spectra were recorded on a Bruker Autoflex mass spectrometer in positive linear mode with a nitrogen laser at near-threshold laser intensity. As matrix trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]-malononitrile was used. 3.5mg matrix was dissolved in 100 μl toluene. Matrix and sample were mixed at volume ratio 1:1, and 2μl of the mixture was applied to the MALDI plate and air-dried.

Density Functional Theory (DFT) Calculations. In this work, we applied the GPAW software package[5] to do all the calculations. PBE functional[6, 7] was used for the exchange-correlation energy, and the van der Waals interactions were described by the Tkatchenko-Scheffler model.[8] The clusters and ligand molecules were placed into a rectangle unit cell with a 8 Å vacuum extension in each dimension from the edge of the molecule or the cluster. Per atom, the electronic configuration of valence electrons is $H(1s_1)$, $C(2s_2\ 2p_2)$, $S(3s_2\ 3p_4)$ and $Ag(4d_{10}\ 5s_1)$. The remaining electrons were treated as a frozen core. The default PAW dataset package 0.9.20000 was used for all the atoms. The 2-PET ligands were replaced by HSCH3 in all the calculations.

The structure optimizations were done using the GPAW grid mode. The real-spacing was chosen as h=0.2 Å. For geometry optimizations, the geometry was considered to be converged when the maximum residual force was below 0.05 eV/Å. The racemization energy barrier of BiDi molecule was calculated by the nudged elastic band (NEB) method.[9] The barrier was computed by PBE+TS.[10, 11]

The CD spectra were simulated by the real-time-propagation time-dependent density functional theory (RT-TDDFT) method implemented in GPAW with localized basis sets (LCAO).[12] In the LCAO

mode, the default GPAW double-zeta polarized (dzp) basis sets were used for C, H, S, while the optimized double-zeta basis set (so-called "p-valence" basis set) was used for Ag atoms. The real-spacing h=0.3 and vacuum size 8 Å were chosen for the RT-TDDFT calculations. The XYZ coordinates of all the structures mentioned in this study are included in the supporting information.

Supporting figures

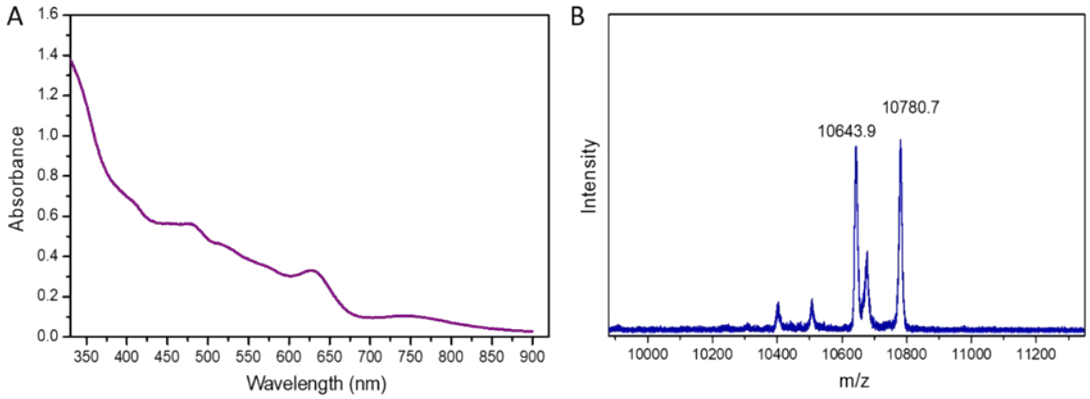


Figure S1. Characterization of rac-Au_{38}(2-PET)$_{24}$. (A) UV-vis spectrum of Rac-Au_{38}(2-PET)$_{24}$; (B) MALDI-TOF spectrum. The signal at 10780.7 corresponds to Au_{38}(2-PET)$_{24}$ (calculated mass 10778.4), the signal at 10643.9 corresponds to Au_{38}(2-PET)$_{23}$ (loss of one 2-PET ligand, calculated mass 10641.2).

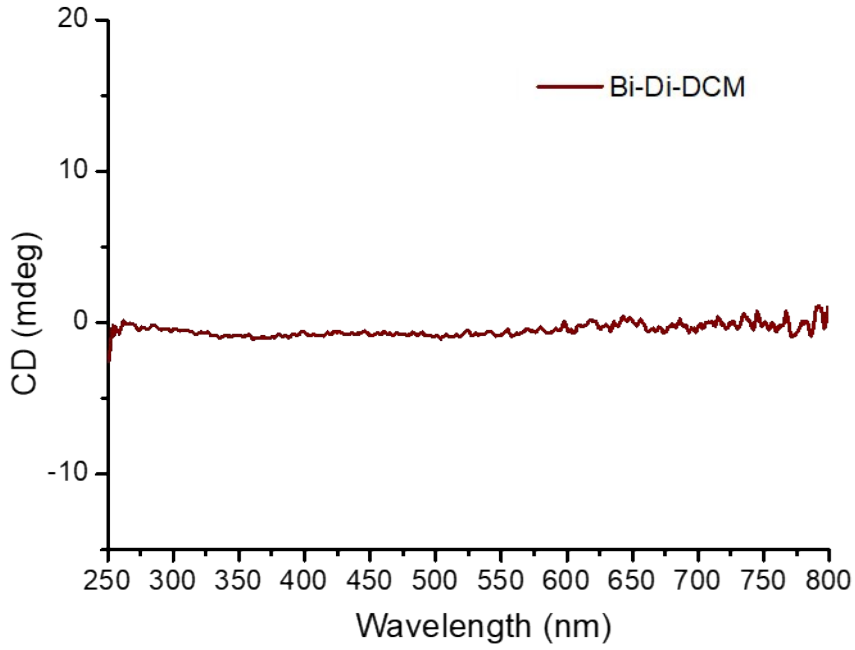


Figure S2. CD spectrum of BiDi dissolved in dichloromethane.

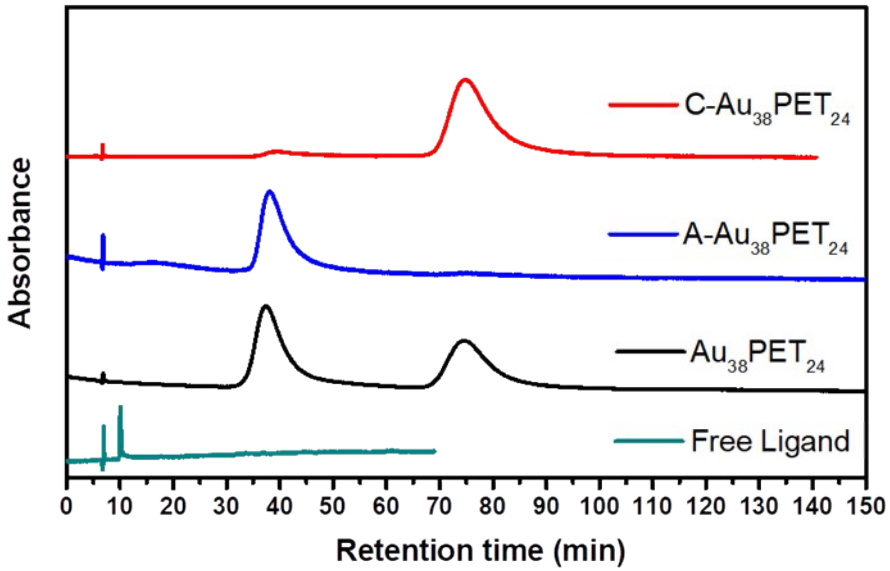


Figure S3. HPL Chromatogram of rac-$Au_{38}(2\text{-PET})_{24}$ (black), A-$Au_{38}(2\text{-PET})_{24}$ (blue), C-$Au_{38}(2\text{-PET})_{24}$ (red), and free ligand Bi-Di (green). The peak with retention time at 6.9min is the toluene injection peak.

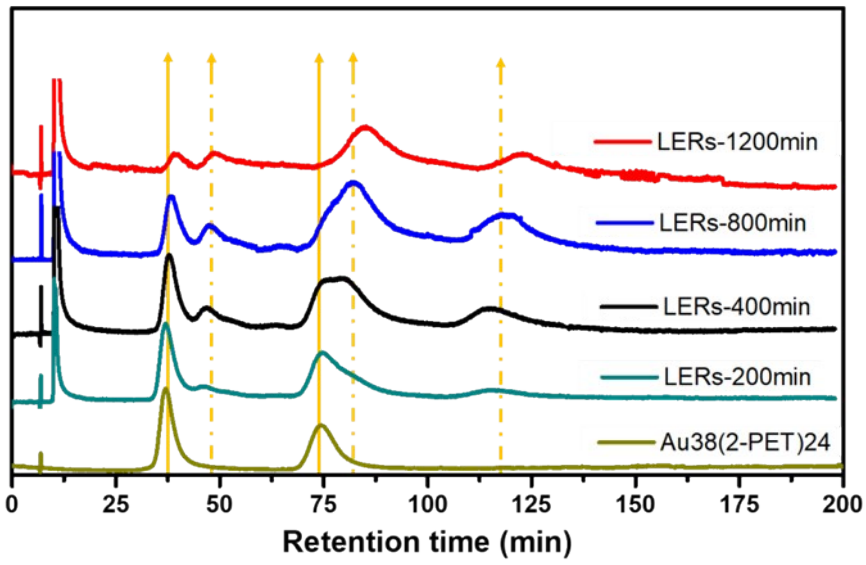


Figure S4. HPL Chromatograms during ligand exchange reaction between rac-$Au_{38}(2\text{-PET})_{24}$ and BiDi. The sample was put at room temperature and the chromatogram was recorded every 200 minutes. Solid arrows indicate the two enantiomers of $Au_{38}(2\text{-PET})_{24}$ and dashed arrows indicate the new peaks.

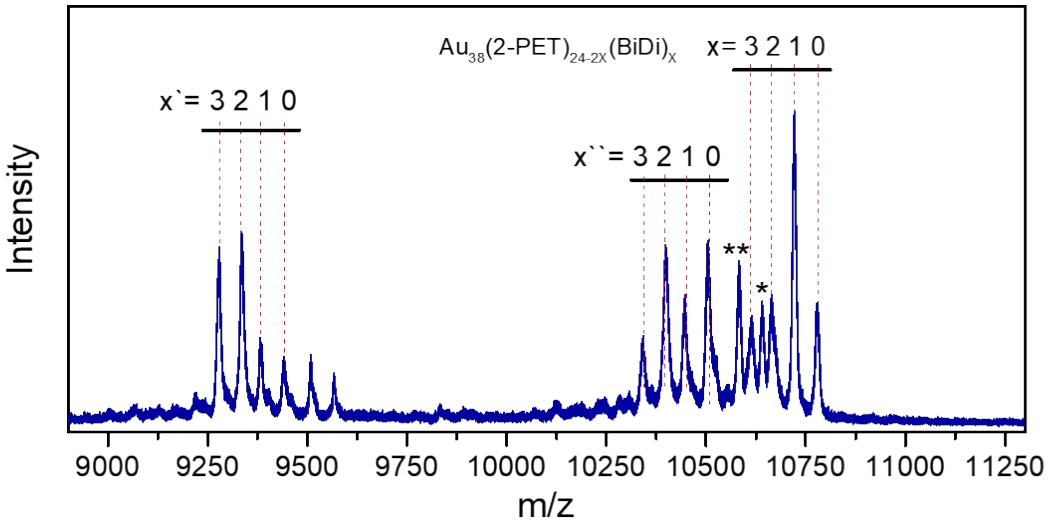
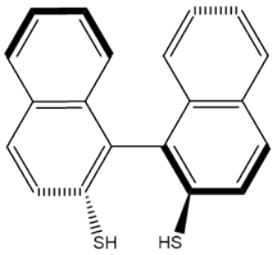
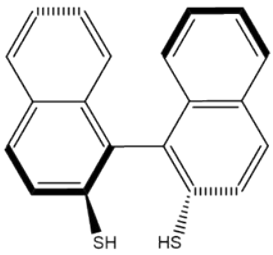


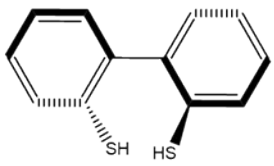
Figure S5. MALDI-TOF spectrum of reaction mixture of ligand exchange reaction between rac-Au_{38}(2-PET)$_{24}$ and BiDi at room temperature. The sample was collected after 18 hours. The Au_{38}(2-PET)$_{24-2x}$(BiDi)$_x$ species are marked with different values of x, and the related fragments Au_{34}(2-PET)$_{20-2x`}$(BiDi)$_{x`}$ after release of Au_4(2-PET)$_4$ are also visible, for example the signal at 9442.1 (x`=0) corresponds to Au_{34}(2-PET)$_{20}$ (calculated mass 9441.5). In addition, the fragment Au_{38}(2-PET)$_{22-2x``}$(BiDi)$_{x``}$ after release two 2-PET ligands are also marked, for example the signal at 10506.6 (x``=0) corresponds to Au_{38}(2-PET)$_{22}$ (calculated mass 10503.9). The signal at 10641.28 (*) corresponds to Au_{38}(2-PET)$_{23}$ (calculated mass 10641.15), the signal at 10583.26 (**) corresponds to Au_{37}(2-PET)$_{24}$ (calculated mass 10581.41).



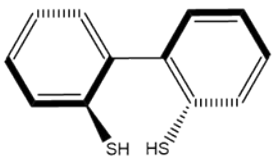
R-[1,1`-binaphthalene]-2,2`-dithiol



S-[1,1`-binaphthalene]-2,2`-dithiol



R-[1,1`-biphenyl]-2,2`-dithiol



S-[1,1`-biphenyl]-2,2`-dithiol

Figure S6. Two enantiomers of BiDi and BINAS.

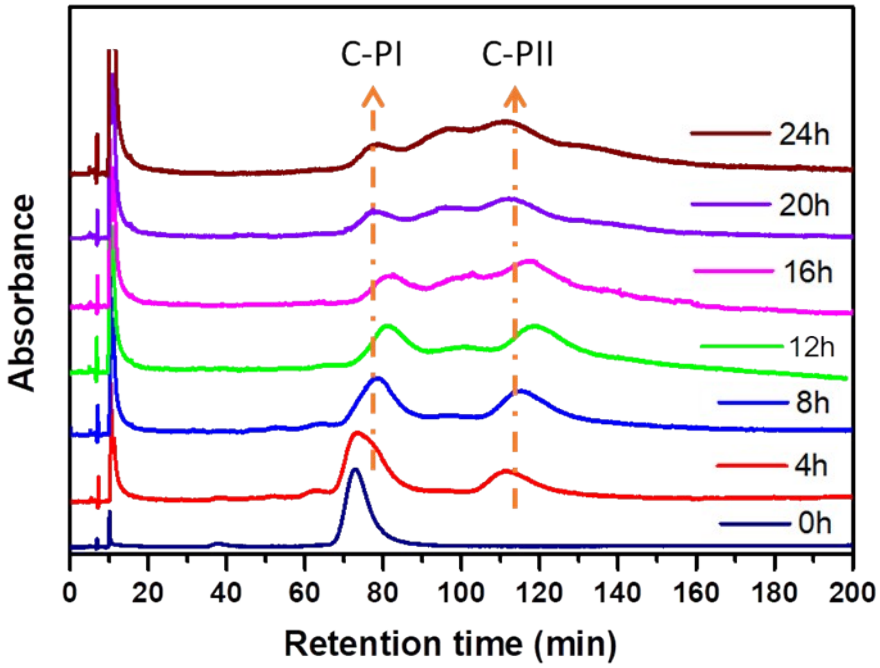


Figure S7. HPL Chromatograms of ligand exchange reaction between C-Au_{38}(2-PET)$_{24}$ and Bi-Di. The sample was put at room temperature and the chromatograms were recorded every 4 hours. Two main peaks are marked as C-PI (80min) and C-PII (112min).

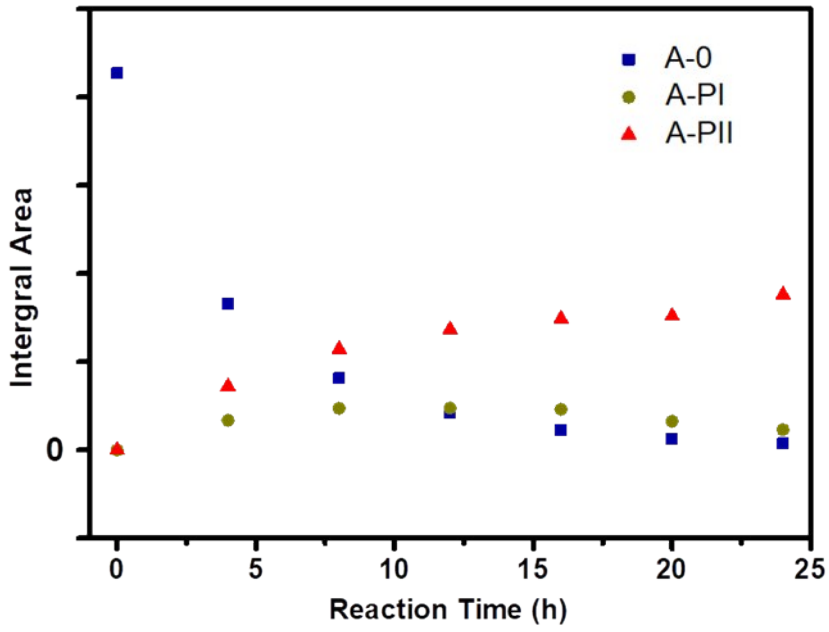


Figure S8. Integrated peak areas (arbitrary units) for peaks A-PI and A-PII at different reaction time. A-0 is the peak of A-Au_{38}(2-PET)$_{24}$. Data extracted from Figure 3.

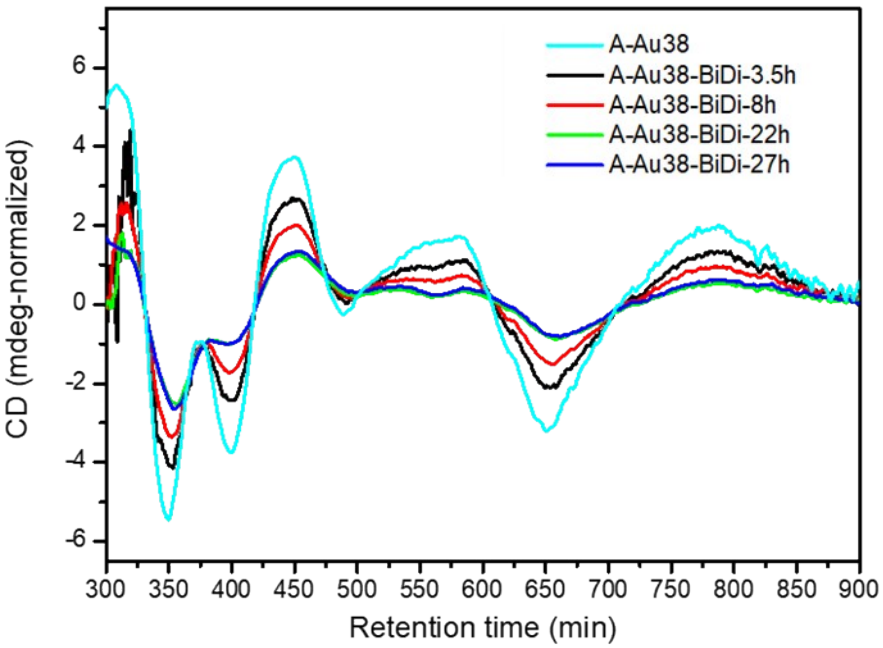


Figure S9. CD spectra of ligand exchange reaction between A-Au_{38}(2-PET)$_{24}$ and BiDi. The sample was at room temperature and the spectrum was recorded over time. Spectra have been normalized to -1 at 375nm.

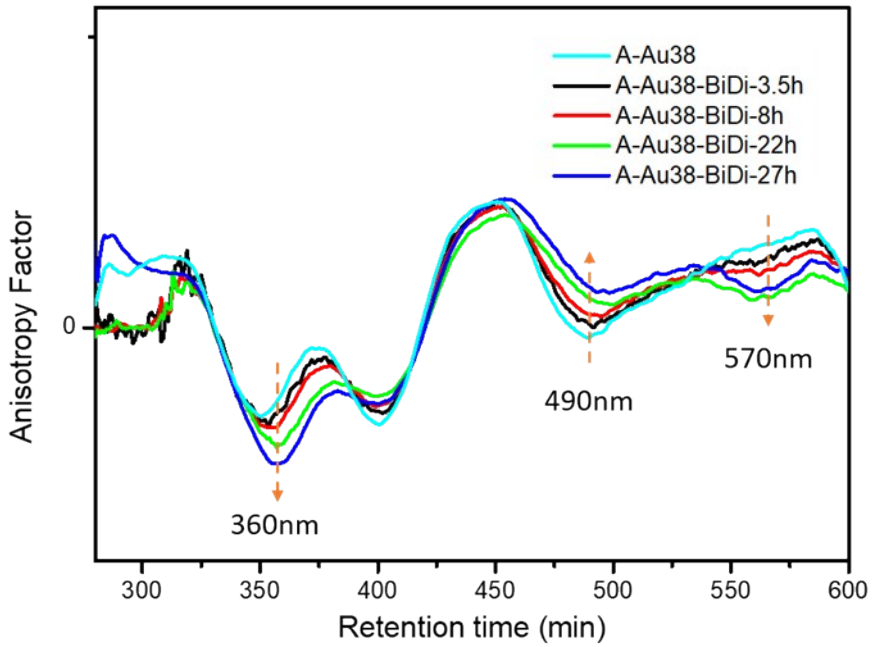


Figure S10. Anisotropy factors of A-Au_{38}(2-PET)$_{24}$ during ligand exchange with BiDi. The sample was at room temperature.

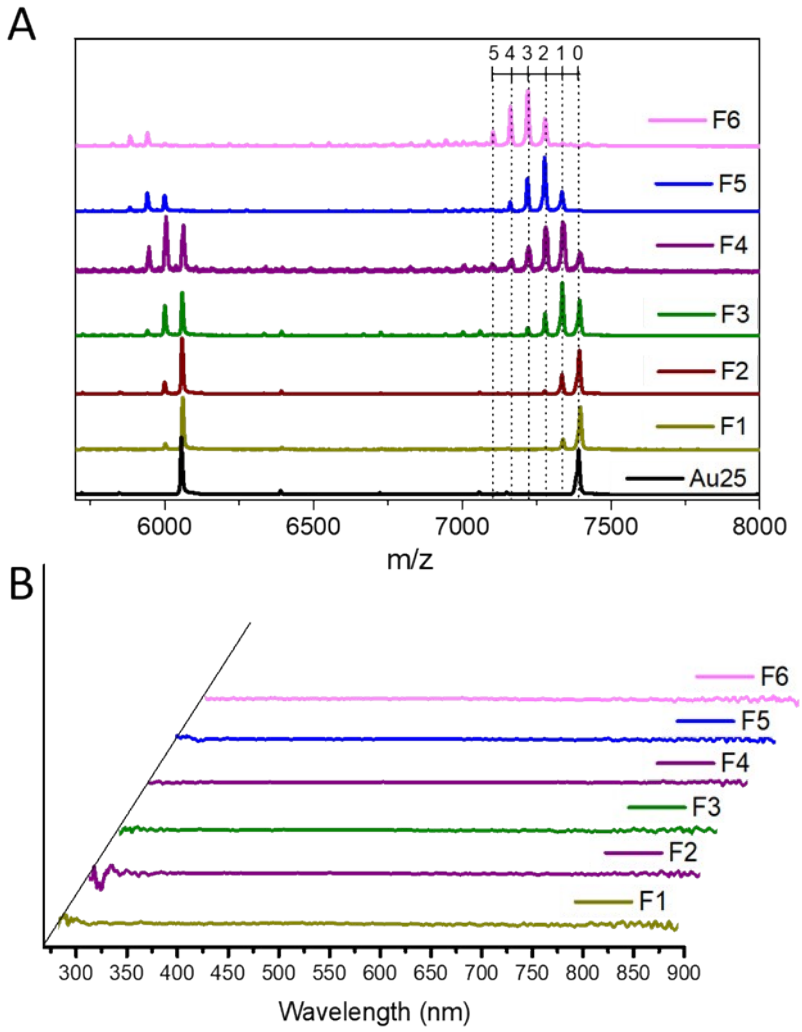


Figure S11. FMALDI-TOF (A) and CD spectra (B) of a sample prepared by ligand exchange of Au_{25}(2-PET)$_{18}$ cluster with BIDI. After ligand exchange the sample was passed over a size exclusion column and six fractions were collected. The labels in panel A corresponds to the number of BiDi ligands of the cluster.

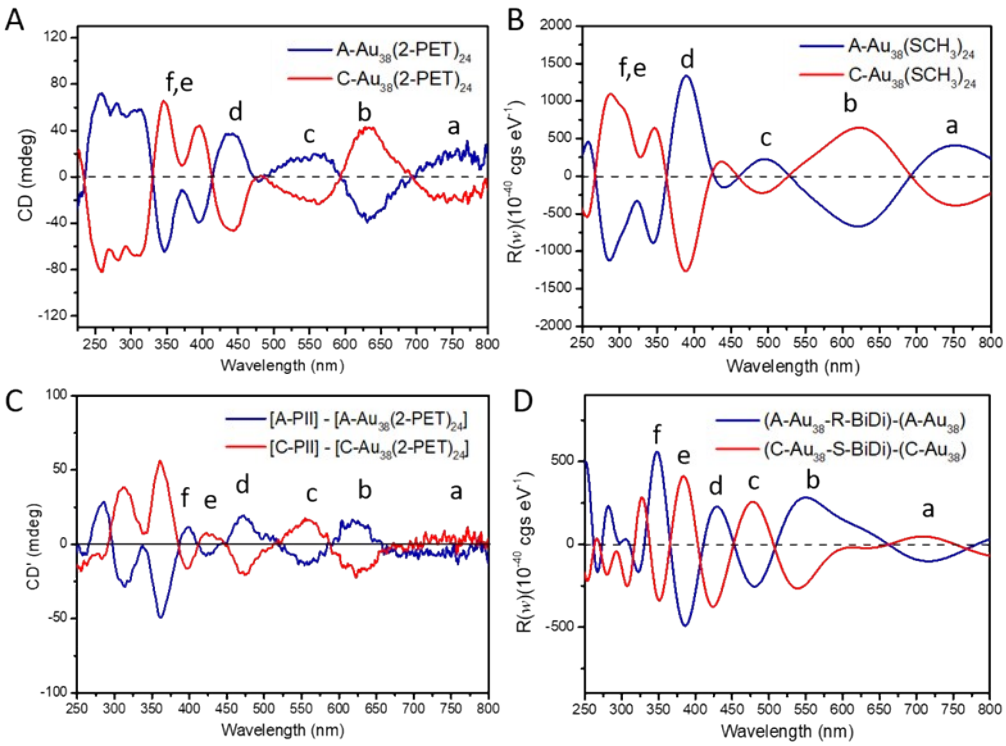


Figure S12. Experimental and calculated CD spectra of $Au_{38}(SR)_{24}$ clusters. (A) Experimental CD spectra of enantiopure A/C-$Au_{38}(2\text{-PET})_{24}$; (B) Calculated CD spectra of enantiopure A/C-$Au_{38}(SCH_3)_{24}$; (C) and (D) Experimental and calculated signal after subtracting the CD spectra of enantiopure $Au_{38}(SR)_{24}$ from the corresponding cluster with one BiDi in its ligand shell. Calculatione were performed with real-time Density Functional Theory Method in GPAW code. For the experimental spectra the clusters were dissolved in dichloromethane and the spectra were recorded at the same concentration for the two enantiomers.

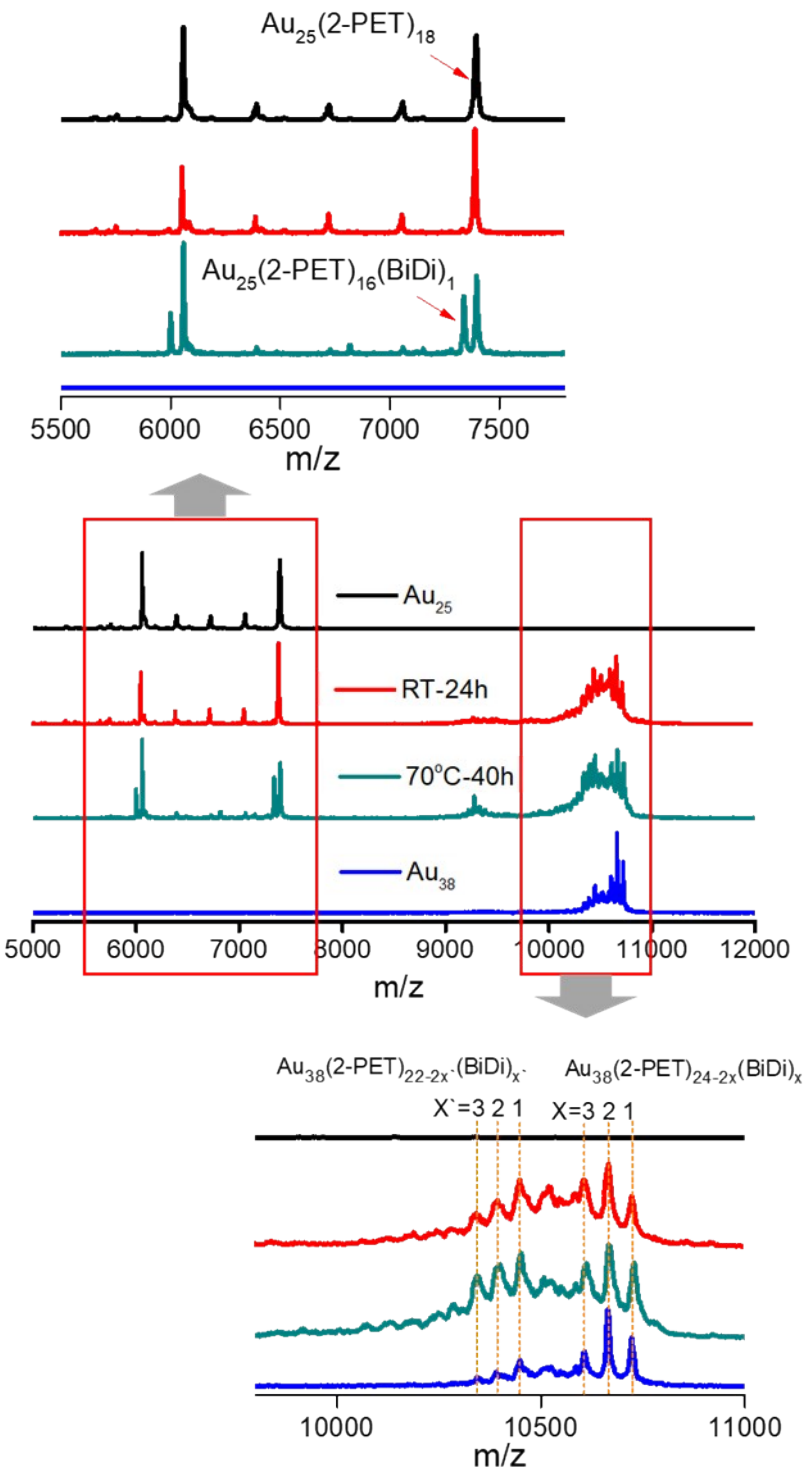


Figure S13. MALDI mass spectra of $Au_{25}(2\text{-PET})_{18}$ (black) and $Au_{38}(2\text{-PET})_{24\text{-}2x}(BiDi)_x$ (blue). After mixing the two samples at room temperature (red) and at 70°C (green) for 24h separately (in the absence of free ligand) the MALDI spectra were measured. Top and bottom frames are zoom areas of the spectra (the number of exchanged BiDi ligands (x and x`) are given at the bottom for Au_{38}).

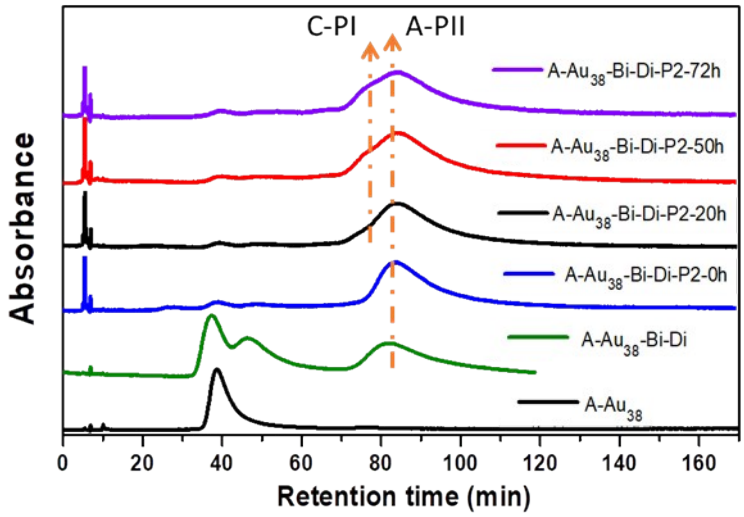


Figure S14. HPL Chromatograms of A-Au_{38}(2-PET)$_{22}$(R-BiDi)$_1$ sample at 70°C as a function of time. A-PII corresponds to A-Au_{38}-(2-PET)$_{22}$(R-BiDi)$_1$, and C-PI corresponds to C-Au_{38}-(2-PET)$_{22}$-(R-BiDi)$_1$.

XYZ coordinates of the clusters mentioned in this study

Structure of A-Au38-R-BiDi

170

Au	13.336658	13.096391	12.438500
Au	14.304091	15.708951	13.176746
Au	14.384316	15.598974	16.015118
Au	16.203770	17.483927	14.322754
Au	18.872854	13.603538	13.098044
Au	12.014196	14.498425	14.507483
Au	16.592180	14.603559	14.581001
Au	14.373238	12.860871	15.107463
Au	12.010795	11.399128	14.399240
Au	11.914796	15.501066	11.625075
Au	16.993603	15.792366	12.013716
Au	16.210705	13.002405	12.209796
Au	17.075285	11.804329	14.708597
Au	18.812782	13.721231	16.093855
Au	14.602532	14.699323	10.485415
Au	14.610904	11.695498	10.270217
Au	17.101557	16.285021	16.789730
Au	10.503679	12.921025	12.586986
Au	18.902473	16.194405	14.278910
Au	14.706076	10.722558	13.204808
Au	9.273796	14.972038	10.125485
Au	16.205364	13.417717	17.198893
Au	15.107701	18.606041	17.119291
Au	12.306677	10.603903	11.513763
Au	12.218235	16.105158	8.507763
Au	9.293850	12.620541	15.498675

Au	18.503668	19.085472	16.000479
Au	12.075327	13.218148	9.922781
Au	12.587687	10.323657	8.287164
Au	13.404417	11.399717	17.600740
Au	18.398279	14.576180	19.206104
Au	18.395849	11.205535	17.801586
Au	20.383921	15.899199	11.328193
Au	14.518664	8.497993	10.611238
Au	9.495878	9.815851	13.311835
Au	21.669193	14.398895	14.312833
Au	18.091208	11.715908	10.212542
S	14.558817	16.083719	8.501697
S	9.904935	16.402029	8.392594
S	15.391244	8.449601	12.785271
S	17.880230	9.875427	15.946284
S	13.225245	17.247889	17.366640
S	14.937634	12.447393	19.021551
S	20.239481	18.124144	14.768485
S	10.198707	14.698485	16.098293
S	22.399706	15.105541	12.205159
S	8.198184	10.596150	15.094125
S	8.352643	13.530778	11.723766
S	11.821548	10.118546	16.452099
S	10.642246	8.872113	11.513959
S	19.104918	12.395923	19.694315
S	17.821184	16.833961	19.040276
S	16.816763	20.223543	17.137884
S	13.822567	8.343585	8.385752
S	19.992434	12.155772	11.509020
S	11.216622	12.189042	7.941851
S	16.386251	11.153782	8.710220

S	18.432295	16.645041	10.273578
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H	13.688235	14.558851	19.093084
H	14.842948	14.365705	20.446192
C	9.543936	11.573794	8.376578
H	9.182350	10.958577	7.543874
H	8.893850	12.448311	8.508172
C	9.391132	15.517475	6.868672
H	9.833389	14.516442	6.828290
H	9.731435	16.107327	6.009548
C	23.435495	16.573919	12.583476
H	22.922232	17.268894	13.255335
H	23.683485	17.070164	11.638679
S	21.194517	13.700914	16.490747
C	20.286556	19.101309	13.215854
H	19.286127	19.243587	12.798867
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C	18.021877	11.823689	21.054813
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H	14.475554	18.084970	9.920807

H	14.711178	18.467714	8.179563
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C	10.892427	14.401640	17.767241
H	11.468737	15.289565	18.052059
H	11.547236	13.521979	17.767525
C	6.594103	11.060350	14.330221
H	6.739809	11.677900	13.438154
H	6.009316	11.607202	15.079108
C	21.749681	11.951682	16.546741
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H	21.297039	11.360367	15.744759
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H	16.042643	8.363555	15.615412
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H	18.332462	14.468660	9.148579
H	19.111870	15.738165	8.144138
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H	12.141844	6.975192	7.338173
H	11.699865	7.295873	9.043726
C	11.958528	18.062096	16.320351
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H	11.675607	19.005384	16.802025
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H	17.299822	12.452343	6.890761
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H	6.073366	10.135268	14.057131
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H	16.706768	8.243112	17.277973
H	17.328560	15.715728	8.346337
H	12.979245	6.097075	8.656564
H	11.092324	17.392227	16.263680
H	15.518462	12.268710	6.773557
H	21.249205	10.825699	13.048339
H	20.565275	9.818369	11.731787
H	19.525372	10.343102	13.101034
H	17.252954	20.472389	12.336152
C	16.337500	19.988398	11.975554
H	15.772168	20.692862	11.354768
H	16.595549	19.098597	11.392821
S	15.331425	19.572212	13.452844
Au	13.391796	18.583298	12.601669
S	11.358500	17.874706	11.679604
H	10.073647	19.141640	13.291607
C	10.098526	18.087830	12.993470
H	10.305957	17.455019	13.861891
H	9.134233	17.809618	12.551806

C	18.127060	19.851789	19.673489
C	19.322279	19.138401	19.128353
C	17.057163	20.368418	18.916113
C	19.345795	17.751898	18.851622
C	18.118607	20.084930	21.062593
C	20.524725	19.858875	19.024187
C	16.045813	21.111609	19.549030
C	20.547991	17.134987	18.474937
C	17.101807	20.799839	21.689249
C	21.714851	19.243048	18.645821
C	16.060640	21.325918	20.921055
C	21.722694	17.873566	18.373013
H	18.940699	19.680025	21.655893
H	20.506287	20.924873	19.253735
H	15.236857	21.515160	18.941339
H	20.552271	16.064833	18.267088
H	17.124868	20.948589	22.768576
H	22.630518	19.829594	18.567671
H	15.261496	21.902874	21.386082
H	22.645203	17.368975	18.082762

Structure of A-Au38-S-BiDi

170

Au	12.754828	12.776919	16.831259
Au	11.077629	14.015638	14.890660
Au	12.686800	16.197653	13.880052
Au	10.394115	14.881140	12.281201
Au	13.264165	10.932828	11.588334
Au	12.597780	15.602730	16.807619
Au	12.906498	13.585973	12.725175
Au	14.476693	14.238646	15.054079
Au	15.107731	14.114363	17.823471
Au	10.212361	13.987872	17.601284
Au	10.614445	11.911380	12.918249
Au	13.004289	11.211077	14.403245
Au	15.393473	12.295304	13.129130
Au	14.669373	13.393425	10.497440
Au	10.479338	11.393877	15.892897
Au	12.811769	9.913694	16.907021
Au	12.701729	15.786341	10.925062
Au	8.296764	15.296796	15.009220
Au	12.692449	14.084073	19.375305
Au	11.609358	12.885602	10.320806
Au	15.284431	11.685693	16.179806
Au	9.507385	13.611021	20.677715
Au	15.205968	15.303299	12.516505
Au	10.742039	18.113214	11.818629
Au	14.190282	11.484714	18.899651
Au	7.993611	11.598022	18.202974
Au	14.290817	16.736069	19.562456

Au	9.994111	15.689471	9.295308
Au	11.094060	11.536036	18.783924
Au	12.685350	8.797109	19.716776
Au	16.892153	16.002064	15.497664
Au	15.796879	16.311407	9.673480
Au	17.705463	13.684467	11.186707
Au	10.520213	9.820723	10.276544
Au	15.894524	8.986975	18.119102
Au	15.392339	13.615190	21.005018
Au	13.378751	10.993890	8.417338
Au	13.389312	8.294225	13.888911
S	8.260393	10.479111	16.169474
S	7.415638	12.686161	20.193062
S	17.116318	10.148225	16.502237
S	8.174631	15.270189	17.347637
S	17.748734	11.926819	12.729875
S	11.897228	18.488964	13.818443
S	16.877724	16.862238	13.323571
S	8.075905	15.446684	12.688536
S	10.158916	13.487411	8.513557
S	13.024987	17.744226	17.867550
S	11.819433	9.246484	8.417101
S	15.650167	15.922873	21.281176
S	11.473103	14.675836	21.362913
S	17.212551	15.311885	17.709364
S	15.212054	11.286254	21.101282
S	17.899538	15.301892	9.504267
S	13.747327	17.427626	9.523774
S	9.679755	17.967005	9.744525
S	14.681950	7.555338	19.519936
S	13.862041	8.582218	11.613509

S	10.697020	9.816781	20.413475
S	12.913450	7.642952	16.087530
S	9.106229	10.205229	12.096213
C	16.041498	18.493195	13.382543
C	11.168599	10.526348	22.043684
C	7.197331	11.330643	21.411346
C	13.221236	17.137329	7.790735
C	10.725897	9.557136	6.974749
S	14.961598	12.691320	8.219096
C	11.170430	13.644978	6.992104
C	18.575584	14.086885	17.637400
C	7.124234	11.389945	15.057182
C	17.109577	8.999384	15.071601
C	14.255815	18.643965	16.847584
C	16.576296	11.828792	8.092184
C	18.647837	12.651023	14.153436
C	7.888091	18.134312	10.084509
C	9.353890	8.701843	13.113306
C	8.536548	16.979763	17.898634
C	10.576244	18.609112	15.083898
C	11.174358	7.060212	16.084333
C	15.689287	8.523980	11.467976
C	7.087250	13.988693	12.181234
C	14.751078	16.280537	22.840614
C	11.064808	16.453506	21.163286
C	19.094238	16.531214	10.150260
H	15.923232	18.832651	12.346384
H	16.680199	19.194370	13.932252
H	15.057959	18.428190	13.856200
H	10.444378	11.313493	22.293694
H	12.175220	10.952879	22.022154

H	11.122973	9.721844	22.787495
H	6.277393	10.795030	21.149702
H	7.098792	11.776591	22.407743
H	8.045410	10.638563	21.386141
H	12.142904	17.322647	7.729508
H	13.445461	16.115265	7.475080
H	13.758215	17.849417	7.151695
H	9.973369	8.760013	6.949090
H	11.338070	9.519345	6.066802
H	10.227668	10.527967	7.055457
H	10.543432	14.098654	6.215925
H	11.482125	12.639241	6.685018
H	12.060536	14.255688	7.160817
H	18.867229	13.874416	18.672291
H	19.425364	14.532463	17.108301
H	18.262651	13.161366	17.144432
H	6.095500	11.142817	15.341873
H	7.318533	11.057150	14.031069
H	7.286668	12.470522	15.128215
H	17.535786	9.530893	14.211986
H	16.089495	8.677393	14.833667
H	17.730488	8.131412	15.320485
H	13.735920	19.041677	15.966264
H	15.063124	17.976267	16.522306
H	14.665322	19.464182	17.447565
H	16.590607	11.278584	7.144472
H	16.729675	11.143184	8.930275
H	17.360682	12.594193	8.092951
H	18.553198	11.953027	14.995232
H	18.228853	13.623334	14.439231
H	19.700480	12.758500	13.871489

H	7.349874	17.934551	9.151037
H	7.706850	19.166222	10.405123
H	7.565849	17.438786	10.867208
H	8.851346	8.856176	14.075728
H	10.419872	8.512791	13.282559
H	8.900885	7.857637	12.581462
H	7.759671	17.647118	17.508638
H	9.523625	17.310234	17.560600
H	8.500354	16.974686	18.994593
H	9.999092	19.520758	14.892134
H	11.061635	18.670538	16.065372
H	9.920485	17.731102	15.052274
H	10.928839	6.795941	17.119747
H	11.102926	6.170841	15.447011
H	10.489554	7.838916	15.733988
H	15.931859	8.710654	10.415645
H	16.036161	7.524362	11.752421
H	16.167320	9.283364	12.093610
H	6.093488	14.066442	12.635457
H	7.569722	13.056299	12.485131
H	7.002755	14.018521	11.089035
H	14.687621	17.368649	22.945950
H	15.335683	15.862247	23.667873
H	13.748131	15.840804	22.839680
H	10.314440	16.719061	21.916769
H	10.686178	16.663006	20.159239
H	11.982296	17.033943	21.325409
H	19.105635	17.379486	9.456591
H	20.082815	16.060287	10.175756
H	18.806919	16.867662	11.151860
C	16.119480	8.403375	21.859274

C	17.087425	9.258460	21.110085
C	15.105890	7.620886	21.271254
C	16.833487	10.604032	20.765322
C	16.296154	8.319868	23.253401
C	18.360762	8.727905	20.844244
C	14.325440	6.771324	22.078808
C	17.847599	11.373001	20.174976
C	15.505900	7.495768	24.049110
C	19.360296	9.495197	20.250679
C	14.517948	6.708166	23.453608
C	19.100958	10.826761	19.920258
H	17.078310	8.928580	23.708797
H	18.553558	7.689084	21.114840
H	13.554568	6.160687	21.606440
H	17.628851	12.408641	19.916784
H	15.669198	7.460493	25.127043
H	20.336388	9.054699	20.049816
H	13.899731	6.044352	24.057997
H	19.873594	11.443005	19.460150

Structure of C-Au38-R-BiDi

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Au	13.624841	12.790284	16.813309
Au	15.327804	14.019903	14.891575
Au	13.705708	16.190603	13.882850
Au	16.003706	14.880984	12.281412
Au	13.137221	10.931563	11.592511
Au	13.799547	15.606243	16.808073
Au	13.493976	13.582560	12.728683
Au	11.906162	14.256024	15.039951
Au	11.286672	14.115024	17.817417
Au	16.184578	13.992438	17.598942
Au	15.785237	11.911990	12.917592
Au	13.393899	11.208926	14.403289
Au	11.004150	12.293613	13.130656
Au	11.728429	13.395503	10.508164
Au	15.911984	11.395486	15.892312
Au	13.584302	9.912731	16.907454
Au	13.695785	15.784081	10.927306
Au	18.099508	15.301672	15.008290
Au	13.695707	14.086837	19.373985
Au	14.791792	12.886777	10.321363
Au	11.114058	11.684651	16.178143
Au	16.876673	13.668754	20.617443
Au	11.190121	15.307571	12.509572
Au	15.603430	18.100868	11.869200
Au	12.206918	11.486654	18.902481
Au	18.401020	11.595079	18.190928
Au	12.082841	16.772371	19.523237

Au	16.398077	15.690583	9.300428
Au	15.296019	11.555726	18.763800
Au	13.709998	8.801931	19.718203
Au	9.509311	16.005093	15.494197
Au	10.600884	16.308733	9.672316
Au	8.689757	13.684763	11.185634
Au	15.904209	9.812819	10.283846
Au	10.504979	8.989304	18.114405
Au	11.000854	13.615045	20.998072
Au	13.080784	10.995753	8.480082
Au	13.015837	8.286608	13.898279
S	18.136473	10.492235	16.149042
S	18.953667	12.693807	20.173725
S	9.285236	10.148520	16.493093
S	18.226923	15.273758	17.346336
S	8.648979	11.926929	12.728750
S	14.466534	18.477312	13.875232
S	9.533043	16.878191	13.323040
S	18.321716	15.444331	12.687683
S	16.242191	13.492581	8.511014
S	13.372165	17.768597	17.847851
S	14.614897	9.230466	8.430266
S	10.731168	15.929448	21.246059
S	14.913842	14.707294	21.351954
S	9.178667	15.309528	17.703791
S	11.163218	11.281954	21.102499
S	8.498163	15.303036	9.506733
S	12.650700	17.424610	9.516723
S	16.676094	17.962852	9.788796
S	11.717113	7.556532	19.516520
S	12.541373	8.579119	11.622416

S	15.684782	9.849697	20.412500
S	13.499154	7.634764	16.098129
S	17.297659	10.200472	12.108546
C	10.380527	18.501921	13.373932
C	15.196053	10.570207	22.028185
C	19.146997	11.347236	21.405312
C	13.192555	17.110243	7.792499
C	15.693739	9.561275	6.981214
S	11.474244	12.680389	8.238100
C	15.231194	13.646060	6.987117
C	7.824644	14.073857	17.626474
C	19.255686	11.430048	15.037942
C	9.292384	8.997779	15.065394
C	12.134544	18.649527	16.819881
C	9.865141	11.813352	8.090552
C	7.747118	12.647985	14.152164
C	18.473640	18.136034	10.107224
C	17.021990	8.700711	13.128481
C	17.867315	16.980198	17.909914
C	15.814703	18.578259	15.112668
C	15.243358	7.067268	16.103086
C	10.714294	8.535076	11.481921
C	19.298475	13.974166	12.190258
C	11.636751	16.292566	22.802319
C	15.295266	16.487646	21.140490
C	7.302356	16.535467	10.150219
H	10.476832	18.845301	12.336746
H	9.761314	19.205147	13.942576
H	11.375484	18.421804	13.821809
H	15.933591	11.339623	22.291515
H	14.200190	11.020345	21.980814

H	15.208388	9.765107	22.772661
H	20.073898	10.815830	21.159470
H	19.231588	11.798512	22.400623
H	18.303473	10.650323	21.368059
H	14.265233	17.330492	7.737544
H	13.008603	16.072973	7.500282
H	12.637065	17.785257	7.131731
H	16.444750	8.763027	6.938248
H	15.069929	9.531948	6.080622
H	16.193844	10.530854	7.064689
H	15.856122	14.099677	6.209331
H	14.922584	12.638304	6.683564
H	14.338228	14.254728	7.153386
H	7.520508	13.870708	18.659824
H	6.978216	14.505339	17.080137
H	8.149952	13.145301	17.147137
H	20.289055	11.240890	15.347922
H	19.097742	11.062628	14.017583
H	19.042778	12.504085	15.079483
H	8.868185	9.529813	14.205323
H	10.310584	8.670162	14.827273
H	8.667941	8.133169	15.317187
H	12.653650	19.050751	15.940863
H	11.337158	17.969641	16.495756
H	11.714144	19.467766	17.415211
H	9.861092	11.262533	7.143268
H	9.696479	11.129171	8.927078
H	9.081194	12.578861	8.080706
H	7.844666	11.951035	14.993261
H	8.162304	13.622932	14.435999
H	6.693479	12.752573	13.871162

H	18.997921	17.948399	9.162622
H	18.658596	19.163572	10.440522
H	18.804941	17.428658	10.875917
H	17.522049	8.851589	14.092431
H	15.952429	8.526484	13.292285
H	17.466993	7.848052	12.603415
H	18.639696	17.650887	17.516338
H	16.876320	17.313427	17.586939
H	17.916681	16.966930	19.005259
H	16.389214	19.490696	14.918395
H	15.351369	18.631943	16.104559
H	16.469198	17.700909	15.056043
H	15.473205	6.762578	17.131355
H	15.337750	6.206564	15.432856
H	15.926728	7.865301	15.798191
H	10.470094	8.714478	10.428655
H	10.360760	7.540790	11.777171
H	10.245812	9.304787	12.102052
H	20.294235	14.054424	12.639440
H	18.814201	13.045730	12.505399
H	19.376484	13.990801	11.097385
H	11.694297	17.380898	22.913670
H	11.063191	15.865767	23.633659
H	12.642037	15.858297	22.785946
H	16.054548	16.761827	21.881552
H	15.659158	16.694662	20.130823
H	14.372573	17.056755	21.311476
H	7.286086	17.380713	9.452600
H	6.314656	16.061571	10.180439
H	7.588684	16.878971	11.149958
C	10.258470	8.396691	21.847084

C	9.292465	9.253059	21.096699
C	11.279570	7.619178	21.265095
C	9.543931	10.600500	20.754616
C	10.072550	8.308913	23.240517
C	8.019292	8.724875	20.829063
C	12.058614	6.773162	22.077814
C	8.531989	11.370070	20.163193
C	10.861679	7.489631	24.042274
C	7.020234	9.493092	20.235624
C	11.859316	6.710471	23.452026
C	7.280153	10.824034	19.905443
H	9.282558	8.913269	23.688675
H	7.825091	7.687419	21.101460
H	12.838481	6.168004	21.612396
H	8.750487	12.406933	19.908354
H	10.695200	7.455025	25.119234
H	6.041783	9.054363	20.038130
H	12.483933	6.054738	24.059099
H	6.508931	11.441097	19.444939

Structure of C-Au38-S-BiDi

170

Au	17.001957	13.004756	12.417734
Au	16.009703	15.603657	13.193195
Au	15.998242	15.404037	16.027449
Au	14.101460	17.314337	14.410216
Au	11.508481	13.395503	13.101201
Au	18.306965	14.394538	14.511312
Au	13.796241	14.406089	14.586923
Au	16.015543	12.673023	15.097550
Au	18.379805	11.281010	14.315960
Au	18.407213	15.474965	11.712550
Au	13.387062	15.679846	12.069175
Au	14.119156	12.874108	12.196698
Au	13.320572	11.604955	14.691096
Au	11.595187	13.504217	16.108383
Au	15.712471	14.606901	10.488927
Au	15.716708	11.682683	10.193416
Au	13.207810	16.007109	16.812151
Au	19.873484	12.919252	12.575191
Au	11.467902	15.995063	14.277061
Au	15.675043	10.598134	13.122968
Au	21.093195	14.995470	10.123128
Au	14.199455	13.209336	17.203365
Au	15.201227	18.392965	17.198502
Au	18.025969	10.582402	11.407080
Au	18.086765	16.112539	8.592605
Au	21.103304	12.524328	15.394590
Au	11.800053	18.807007	16.004988

Au	18.335665	13.268135	9.959240
Au	17.798330	10.400605	8.207101
Au	17.015200	11.193342	17.573986
Au	12.000141	14.286093	19.280277
Au	12.092158	10.929261	17.803635
Au	10.075272	15.702971	11.401507
Au	15.811570	8.484702	10.499365
Au	20.884071	9.803979	13.102931
Au	8.797537	14.115512	14.317325
Au	12.282149	11.606233	10.131102
S	15.749973	16.076124	8.572693
S	20.395485	16.439470	8.420771
S	14.956161	8.328015	12.672505
S	12.593856	9.641111	15.914802
S	17.080379	17.031843	17.457531
S	15.487618	12.213359	19.006346
S	10.046819	17.871088	14.778508
S	20.175026	14.573654	16.056034
S	8.059833	14.821558	12.213109
S	22.194609	10.509889	14.903137
S	22.028296	13.554743	11.714238
S	18.647451	10.009477	16.379997
S	19.716717	8.858513	11.315423
S	11.349985	12.082065	19.710108
S	12.507731	16.566801	19.080000
S	13.465951	19.971294	17.153494
S	16.543726	8.424153	8.275740
S	10.381409	12.015841	11.444896
S	19.157639	12.279621	7.929216
S	13.984790	11.114128	8.599256
S	11.965412	16.557695	10.324224

C	16.373966	13.615616	19.788153
H	16.728006	14.331591	19.041142
H	15.661851	14.111878	20.457840
C	20.830217	11.651011	8.349758
H	21.163460	10.998753	7.534201
H	21.497663	12.517228	8.438136
C	20.880320	15.557192	6.885480
H	20.461143	14.545639	6.862032
H	20.501093	16.134043	6.034534
C	6.978889	16.251650	12.604155
H	7.467494	16.946743	13.294606
H	6.730785	16.758429	11.664933
S	9.227644	13.443705	16.510122
C	9.963238	18.882364	13.249460
H	10.954203	19.045261	12.818779
H	9.342854	18.343649	12.521582
C	12.406832	11.513500	21.092382
H	13.469488	11.620699	20.847801
H	12.153638	12.118783	21.970121
C	17.908741	8.359720	16.065405
H	16.994419	8.439703	15.468924
H	18.657103	7.769510	15.522439
C	22.761557	14.679439	12.965678
H	23.651270	15.143329	12.524291
H	22.051796	15.448853	13.281261
C	18.937956	7.378598	12.070169
H	18.407797	7.643312	12.988906
H	18.222218	6.967692	11.347605
C	15.301921	17.758764	9.148813
H	15.838155	18.019773	10.068250
H	15.546906	18.470514	8.352277

C	13.143521	8.341084	12.394769
C	19.533348	14.223827	17.736824
H	18.942490	15.088560	18.059607
H	18.900236	13.328952	17.736156
C	23.794846	10.997853	14.150313
H	23.646814	11.647226	13.281060
H	24.382530	11.515948	14.916521
C	8.715270	11.683628	16.554770
H	7.622281	11.652390	16.485405
H	9.161928	11.114331	15.734439
C	14.115678	8.732956	16.385368
H	14.465135	8.188422	15.500100
H	14.895426	9.424494	16.726152
C	12.120371	15.469162	8.856604
H	12.090385	14.414393	9.149170
H	11.295988	15.694751	8.170289
C	17.827396	7.111624	8.219864
H	18.229160	7.083139	7.200374
H	18.639280	7.312800	8.926747
C	18.388744	17.883808	16.497290
H	18.042965	18.116310	15.484151
H	18.655458	18.806662	17.025763
C	13.989127	12.483806	7.378638
H	13.035242	12.478380	6.840352
H	14.146325	13.452379	7.861878
C	9.949980	10.459110	12.308299
H	17.219051	13.223721	20.364830
H	20.829556	11.098480	9.293952
H	21.974302	15.517821	6.850911
H	6.065226	15.860331	13.065938
H	9.500299	19.843372	13.503362

H	12.166032	10.462104	21.284431
H	17.694674	7.884108	17.029139
H	23.044888	14.077897	13.839199
H	19.725706	6.646636	12.280767
H	14.222840	17.767763	9.340555
H	12.855118	9.164119	11.731405
H	12.863015	7.380318	11.947339
H	12.654117	8.462481	13.367772
H	20.388983	14.079488	18.405664
H	24.312050	10.081625	13.843808
H	9.043672	11.264793	17.513214
H	13.863731	8.025445	17.182898
H	13.079471	15.687669	8.372393
H	17.345913	6.155541	8.454977
H	19.259237	17.218088	16.448606
H	14.812773	12.284404	6.683016
H	9.063786	10.670941	12.918380
H	9.708394	9.697145	11.558702
H	10.765105	10.115372	12.951440
H	13.012357	20.343927	12.515286
C	13.944298	19.896957	12.150470
H	14.497243	20.637569	11.561162
H	13.718246	19.018909	11.538353
S	14.937002	19.457273	13.629275
Au	16.898508	18.487030	12.795664
S	18.934950	17.832813	11.852277
H	20.256252	19.030798	13.489329
C	20.200092	17.983854	13.169500
H	19.972351	17.337027	14.022707
H	21.156462	17.686272	12.723145
C	12.108799	19.618462	19.672132

C	10.947705	18.848488	19.126797
C	13.176605	20.150185	18.921120
C	10.963415	17.455765	18.876135
C	12.072123	19.912439	21.050730
C	9.725852	19.532642	18.997713
C	14.147770	20.949747	19.550955
C	9.779730	16.804691	18.495470
C	13.041863	20.694353	21.671003
C	8.556888	18.881424	18.615044
C	14.087460	21.222763	20.911198
C	8.587422	17.508101	18.363798
H	11.248911	19.505571	21.639244
H	9.711551	20.602774	19.209778
H	14.957489	21.356020	18.944523
H	9.804688	15.731730	18.301641
H	12.973372	20.896095	22.739164
H	7.630216	19.446390	18.517773
H	14.853768	21.848452	21.369478
H	7.684263	16.974714	18.063261

Structure of A-Au38

158

Au	13.896201	16.760048	12.510293
Au	14.527935	15.120511	14.806778
Au	13.395752	12.590680	14.186202
Au	15.860490	12.919143	16.028131
Au	18.578419	13.841458	12.156336
Au	11.891512	15.102355	13.616372
Au	15.976066	13.220635	13.172285
Au	13.683771	14.009797	11.667631
Au	11.886733	15.923414	10.608655
Au	12.921713	17.410587	15.126875
Au	17.404009	15.088950	14.721616
Au	16.540491	15.806527	12.078251
Au	16.211512	13.501942	10.337954
Au	17.307997	11.194383	11.721824
Au	15.903077	17.606663	14.276655
Au	15.925708	18.486185	11.415132
Au	15.613773	10.687118	14.323850
Au	14.178988	15.405711	17.787268
Au	11.289327	17.801062	12.681654
Au	18.280167	12.213279	14.486676
Au	14.704036	16.014603	9.881038
Au	11.197754	19.999409	15.206813
Au	14.441350	11.321787	11.660566
Au	13.681725	10.609889	16.891397
Au	13.297928	18.596436	10.476954
Au	14.599727	19.925810	16.309317
Au	9.060175	15.699148	11.993657

Au	17.282656	10.388785	17.105040
Au	13.807019	19.476130	13.322475
Au	14.889784	21.397249	10.869521
Au	11.875745	12.591028	9.718369
Au	15.592006	8.474508	11.879834
Au	16.197226	10.486835	8.916617
Au	20.611578	14.320571	14.526153
Au	15.597313	18.915867	8.311616
Au	10.078263	18.306742	9.786657
Au	20.525623	11.401417	12.497498
Au	19.084564	17.083017	11.003439
S	16.730639	19.021805	16.050474
S	12.556345	20.917709	16.875257
S	15.511027	16.658550	7.695649
S	12.654580	17.170792	17.528044
S	16.411772	12.653862	8.078879
S	11.876045	11.568752	15.758739
S	12.635453	10.454879	10.311502
S	15.626540	13.652781	18.323889
S	19.372702	10.982689	16.246458
S	9.627406	14.271044	13.750077
S	22.090538	12.895943	13.397765
S	8.213774	16.954126	10.207838
S	9.644439	19.276260	13.621071
S	10.844554	14.530951	8.916759
S	11.754436	19.769148	9.072299
S	16.091034	8.247646	9.600121
S	15.181970	8.341188	14.178293
S	15.352660	9.484953	18.078783
S	15.912480	21.197374	8.763591
S	20.276646	15.067685	10.942764

S	13.783792	21.842371	12.879328
S	18.178579	19.235634	10.942410
S	19.427044	15.939820	15.720341
C	11.457980	9.724259	11.510018
C	12.057615	22.202600	12.362792
C	12.731709	22.680027	16.404743
C	16.638205	7.421804	14.811735
C	22.934862	11.967685	14.736857
S	19.197357	9.704705	11.597009
C	20.010096	9.418800	15.528393
C	14.570029	7.567911	8.836704
C	11.664061	15.003548	7.345815
C	8.517974	18.186935	14.577097
C	12.113851	19.209778	7.361629
C	16.924238	17.972460	17.540632
C	17.285866	16.207184	7.633087
C	9.618353	12.611034	12.968724
C	6.945709	18.082676	10.903670
C	19.722965	9.543772	9.847651
C	14.814633	12.997481	7.243305
C	15.294907	10.153446	19.785191
C	19.858786	17.491188	14.844226
C	14.767110	22.120953	7.664610
C	10.969239	16.497347	17.768280
C	11.305280	12.925347	16.852386
C	18.689005	20.105354	12.472023
C	20.181854	14.411790	9.231456
C	17.259502	14.365855	18.750195
H	10.484401	9.598491	11.023802
H	11.868252	8.746428	11.790359
H	11.357161	10.344384	12.405404

H	12.034210	23.198631	11.904104
H	11.678771	21.454161	11.659711
H	11.442023	22.192106	13.272486
H	11.749464	23.156820	16.505207
H	13.445263	23.139711	17.099173
H	13.104399	22.779884	15.378672
H	16.463818	6.355054	14.632979
H	17.553688	7.736343	14.304492
H	16.719326	7.615489	15.886812
H	23.461082	11.117162	14.287451
H	23.657850	12.651233	15.198618
H	22.224915	11.619905	15.494813
H	20.899105	9.661759	14.934644
H	20.278023	8.746000	16.350702
H	19.272625	8.943248	14.877812
H	14.715730	7.541451	7.750532
H	14.438058	6.548503	9.217961
H	13.701386	8.187893	9.084876
H	11.548571	14.185772	6.626096
H	11.140215	15.893786	6.976544
H	12.722852	15.236199	7.493389
H	7.896073	17.634409	13.861456
H	9.077652	17.473555	15.189267
H	7.890421	18.823181	15.210633
H	11.308390	19.563984	6.708800
H	13.072498	19.648663	7.058848
H	12.194148	18.121674	7.306543
H	17.879274	17.441704	17.450312
H	16.932467	18.617046	18.427309
H	16.108566	17.241474	17.618994
H	17.747681	16.737272	6.792496

H	17.792078	16.470207	8.570272
H	17.348223	15.123786	7.474868
H	8.591962	12.368463	12.670788
H	10.280445	12.586143	12.094984
H	9.969726	11.897452	13.723009
H	6.564076	18.702381	10.083030
H	6.134772	17.464590	11.305788
H	7.360358	18.724737	11.687938
H	19.053022	8.825354	9.360135
H	19.668938	10.505332	9.330435
H	20.750816	9.164331	9.840076
H	14.727406	12.337228	6.373259
H	13.965796	12.844038	7.921144
H	14.840170	14.044436	6.919387
H	14.355701	9.820287	20.242262
H	16.144812	9.733521	20.335257
H	15.346789	11.247616	19.782923
H	20.917786	17.703419	15.024140
H	19.669645	17.399385	13.767487
H	19.238855	18.293354	15.261027
H	15.042214	21.900801	6.626841
H	13.722132	21.850473	7.847605
H	14.909153	23.188862	7.864682
H	10.281267	17.343533	17.654467
H	10.732783	15.725690	17.028862
H	10.887836	16.089134	18.781630
H	10.549994	13.493029	16.296391
H	10.856167	12.483825	17.748520
H	12.134987	13.585854	17.130737
H	19.776773	20.230318	12.460499
H	18.201458	21.086523	12.455522

H	18.375320	19.559816	13.365387
H	20.699444	15.103038	8.556350
H	20.698656	13.444787	9.242920
H	19.146935	14.269998	8.909254
H	17.940315	13.519779	18.901934
H	17.647108	15.001952	17.949488
H	17.158089	14.938174	19.678890

Structure of C-Au38

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Au	15.717066	16.298286	12.561109
Au	15.069592	14.695439	14.819645
Au	16.203915	12.181561	14.176603
Au	13.801299	12.478841	16.067631
Au	11.004689	13.394348	12.189775
Au	17.761198	14.704721	13.678841
Au	13.619209	12.800105	13.198214
Au	15.926339	13.598167	11.684287
Au	17.714300	15.522355	10.621639
Au	16.614798	16.998865	15.200663
Au	12.196293	14.673882	14.734169
Au	13.034390	15.355974	12.086716
Au	13.391812	13.022861	10.398724
Au	12.297378	10.706644	11.802957
Au	13.687166	17.193920	14.301905
Au	13.696830	18.012667	11.482630
Au	13.992695	10.261060	14.330131
Au	15.421410	15.002873	17.794857
Au	18.310436	17.394571	12.695635
Au	11.323526	11.811616	14.517097
Au	14.890777	15.607999	9.906794
Au	18.401049	19.597013	15.208895
Au	15.110078	10.898528	11.608747
Au	15.952741	10.150238	16.865934
Au	16.309124	18.183992	10.499048
Au	14.992638	19.528688	16.321121
Au	20.602770	15.297212	12.079543

Au	12.393610	9.906867	17.096859
Au	15.801447	19.011112	13.390335
Au	14.784106	20.913658	10.874840
Au	17.723326	12.198436	9.713302
Au	13.998534	8.001250	11.797649
Au	13.399558	10.075426	8.913113
Au	8.986010	13.919508	14.529517
Au	14.006680	18.512444	8.318183
Au	19.528671	17.882689	9.795937
Au	9.066974	10.999199	12.516710
Au	10.587942	16.606281	11.000860
S	12.854364	18.619164	16.073498
S	17.044420	20.509907	16.881973
S	14.105596	16.253948	7.715558
S	16.949291	16.775536	17.585865
S	13.167746	12.260759	8.119165
S	17.729254	11.149148	15.731627
S	16.960457	10.066274	10.303316
S	14.010416	13.223580	18.351452
S	10.295570	10.549282	16.282780
S	20.023952	13.874630	13.838449
S	7.501055	12.494018	13.415130
S	21.381573	16.527927	10.250989
S	19.964043	18.864799	13.636225
S	18.765566	14.143429	8.926497
S	17.865602	19.354338	9.084668
S	13.516262	7.809413	9.509746
S	14.400581	7.903694	14.099049
S	14.310898	9.002236	18.083181
S	13.706630	20.790171	8.795017
S	9.347739	14.621712	10.918513

S	15.847452	21.370243	12.897446
S	11.471244	18.775753	10.939040
S	10.172434	15.535556	15.724485
C	18.142921	9.357429	11.509487
C	17.573814	21.731890	12.388767
C	16.881977	22.278528	16.428530
C	12.963891	6.968370	14.751930
C	6.699419	11.566690	14.783481
S	10.381868	9.278008	11.649663
C	9.623321	9.004782	15.552958
C	15.072800	7.204575	8.748679
C	17.938671	14.639996	7.367594
C	21.077276	17.790159	14.621752
C	17.493740	18.812872	7.370879
C	12.668625	17.574144	17.568932
C	12.333881	15.794193	7.627167
C	20.043112	12.230283	13.025909
C	22.655449	17.673126	10.907499
C	9.907063	9.118697	9.885964
C	14.753672	12.607559	7.268133
C	14.361657	9.716061	19.769129
C	9.735103	17.079350	14.842023
C	14.834157	21.717245	7.682367
C	18.634697	16.085958	17.796883
C	18.247362	12.503382	16.853231
C	10.940376	19.673038	12.444804
C	9.459245	13.949457	9.218265
C	12.363466	13.921852	18.748878
H	19.105400	9.202399	11.008668
H	17.727747	8.394962	11.832993
H	18.266609	10.009091	12.378957

H	17.586828	22.712454	11.900069
H	17.960651	20.967199	11.707827
H	18.186749	21.756582	13.298805
H	17.871344	22.741627	16.510378
H	16.192604	22.741856	17.143820
H	16.492661	22.391762	15.410667
H	13.131226	5.907540	14.533709
H	12.030038	7.298707	14.289468
H	12.919174	7.122591	15.836826
H	6.187228	10.695221	14.359200
H	5.967436	12.235345	15.253450
H	7.433805	11.250707	15.530816
H	8.703213	9.262236	15.014990
H	9.401031	8.306012	16.367104
H	10.326738	8.551625	14.850958
H	14.936940	7.189032	7.661332
H	15.253614	6.187898	9.116364
H	15.911014	7.858758	9.013508
H	18.054115	13.841867	6.625941
H	18.453411	15.542621	7.016443
H	16.879721	14.859319	7.529274
H	21.722820	17.243135	13.922457
H	20.514936	17.069965	15.222402
H	21.681614	18.436932	15.267378
H	18.294437	19.174965	6.715758
H	16.532942	19.256197	7.081137
H	17.413746	17.725094	7.306605
H	11.724103	17.026218	17.473307
H	12.639608	18.227650	18.448895
H	13.496177	16.858625	17.658745
H	11.880485	16.330076	6.785820

H	11.812903	16.046572	8.559147
H	12.277998	14.712059	7.459634
H	21.078026	11.987969	12.757108
H	19.413671	12.232809	12.128049
H	19.658842	11.500706	13.748500
H	23.028032	18.273060	10.069671
H	23.470385	17.066044	11.317200
H	22.246246	18.332401	11.680658
H	10.576437	8.377228	9.435019
H	10.000747	10.071114	9.354814
H	8.872607	8.760465	9.848273
H	14.837852	11.945366	6.398485
H	15.608552	12.458162	7.939870
H	14.724825	13.653533	6.941660
H	15.287111	9.373569	20.246424
H	13.495776	9.333885	20.321447
H	14.334952	10.810143	19.732260
H	8.676568	17.291536	15.026917
H	9.916484	16.981050	13.764544
H	10.355607	17.886396	15.249576
H	14.543633	21.497278	6.649324
H	15.882701	21.450073	7.847672
H	14.692690	22.784079	7.887065
H	19.330866	16.926762	17.686817
H	18.860472	15.319583	17.049437
H	18.723028	15.668221	18.805698
H	18.992931	13.099708	16.314917
H	18.693777	12.059178	17.749784
H	17.395861	13.138528	17.127947
H	9.854177	19.809502	12.413950
H	11.444394	20.646971	12.415992

H	11.234100	19.138445	13.352164
H	8.970104	14.645035	8.526507
H	8.920844	12.994163	9.228649
H	10.497952	13.782204	8.921472
H	11.687114	13.072530	18.902937
H	11.984620	14.540579	17.930901
H	12.443911	14.510780	19.668934

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