

Au₄₀(SR)₂₄ Cluster as a Chiral Dimer of 8-Electron Superatoms: Structure and Optical Properties

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1. GPAW computational details

We used the density-functional theory (DFT) as implemented in the real-space code package GPAW.^{1,2} The PAW setups for Au include scalar-relativistic effects. The 2-PET ligands were reduced to –SH groups in the initial sampling of a representative set (about 20) of potential structures. Structural relaxations were done using 0.2 Å grid spacing and convergence criterion of 0.05 eV/Å for the maximum forces acting on atoms. The most interesting structures were re-optimized using also methylthiolate SCH₃ ligand in order to check the effect of a sterically slightly more demanding ligand, particularly the SR *cis-trans* conformers within a given Au-S framework structure. Structural optimizations were done at the LDA level since this has been shown previously to reproduce the Au-Au distances well as compared to the existing crystal structures of Au₁₀₂(SR)₄₄, Au₂₅(SR)₁₈, and Au₃₈(SR)₂₄. Total energies were calculated with GGA-PBE (gradient-corrected functional of Perdew, Burke, and Ernzerhof).³ Linear optical absorption and circular dichroism (CD) spectra were calculated with the PBE level using linear-response (LR) time-dependent DFT (LR-TDDFT) formalism in GPAW.

For analysis of the electron states, projection of the Kohn-Sham states to spherical harmonics was done according to in Ref. 4. Projection analysis was done for the energetically best A1 structure in two parts including separately both of the two edge-connected 13 Au-atom icosahedra of the 26 atom cluster core.

2. Energetics and HOMO-LUMO gaps

	A1	A2	B1	B2	oblate	tetra
ΔE	0 / 0	0.07/0.32	0.10/0.42	0.22/1.05	1.57 / na	2.58 / na
E_g^{HL}	0.67/0.70	0.71/0.69	0.65/0.57	0.82/0.69	0.52 / na	0.23 / na

Table S1. Relative energies and HOMO-LUMO gaps (in eV) of structures **A1**, **A2**, **B1**, **B2**, and oblate and tetrahedral structures shown in Figure S4. In each entry, the first / second number refers to calculation with SH / SCH₃ ligand, respectively (oblate and tetrahedral clusters were calculated only with the SH ligand).

3. Analysis of electronic structure of A1

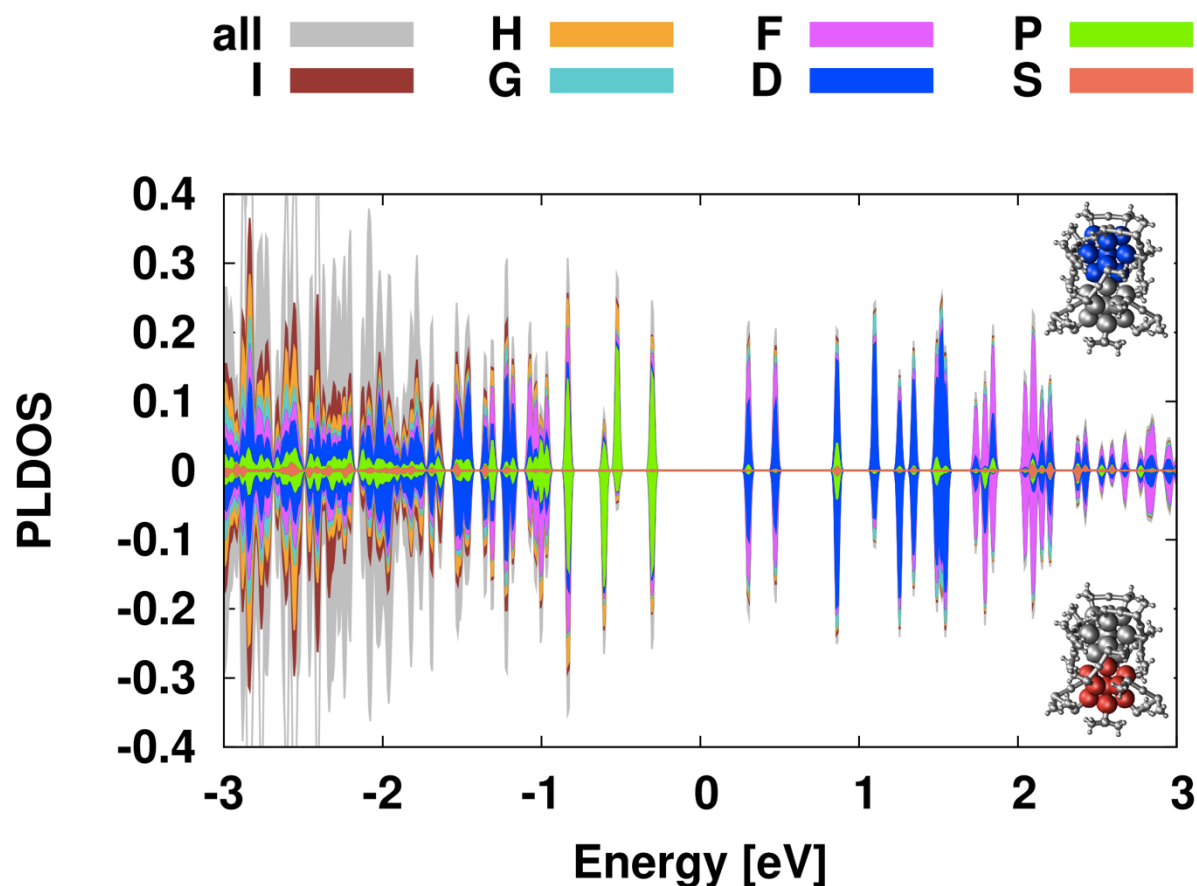


Figure S1. Projected local density of electron states (PLDOS) on the two Au_{13} icosahedral units (blue, upper panel; red, lower panel) of the core of structure A1. The details of the projection are discussed in ref. 4. The HOMO-LUMO gap of the cluster is centered around $E = 0$. The three P-like states just below the gap and opening of the D-like states just above the gap signify both icosahedral units having 8 shell electrons.

4. Derivative optical spectra

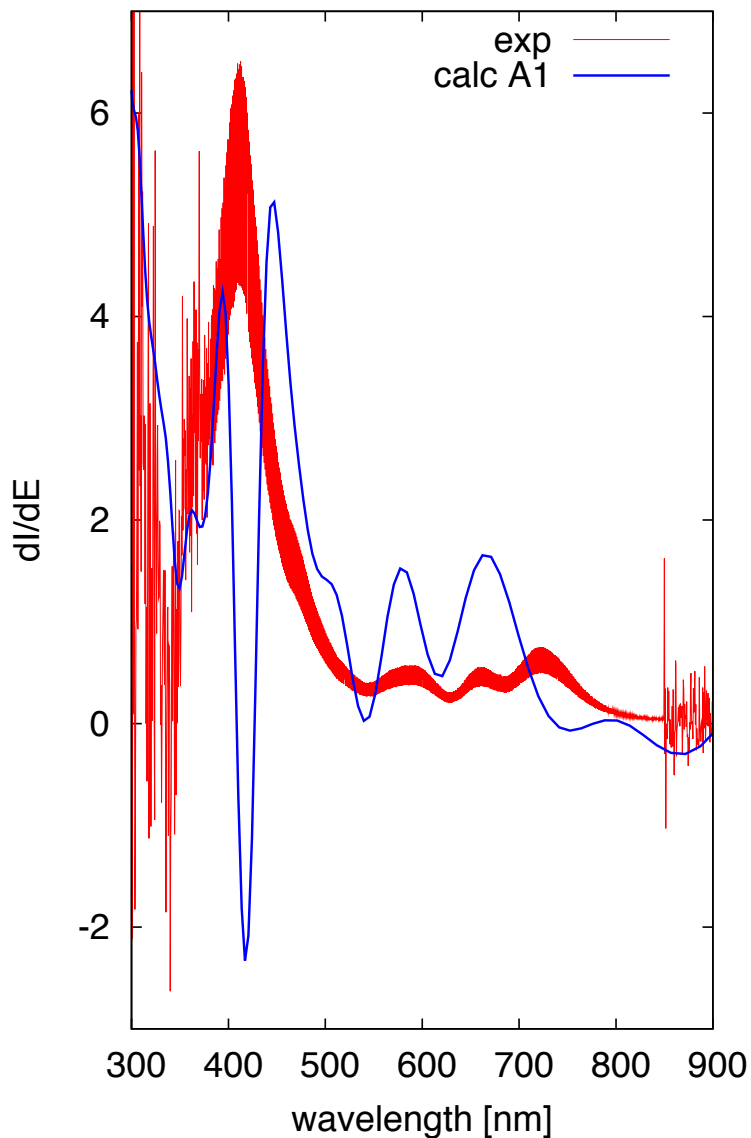


Figure S2. Derivative of the optical absorption spectrum (red, from ref. 22 of the main text) and of the calculated LR-TDDFT spectrum for structure A1 (blue). In the theoretical spectrum the single transitions have been folded by 0.1 eV Gaussians. The maxima in the data correspond to the most rapid changes in the slope of the corresponding spectra. These changes are seen to agree quite well in the range of 400 – 700 nm. The experimental data becomes noisy for the range above 850 nm where the theoretical spectrum has weak features.

5. $\text{Au}_{38}(\text{SR})_{24}$ CD spectra

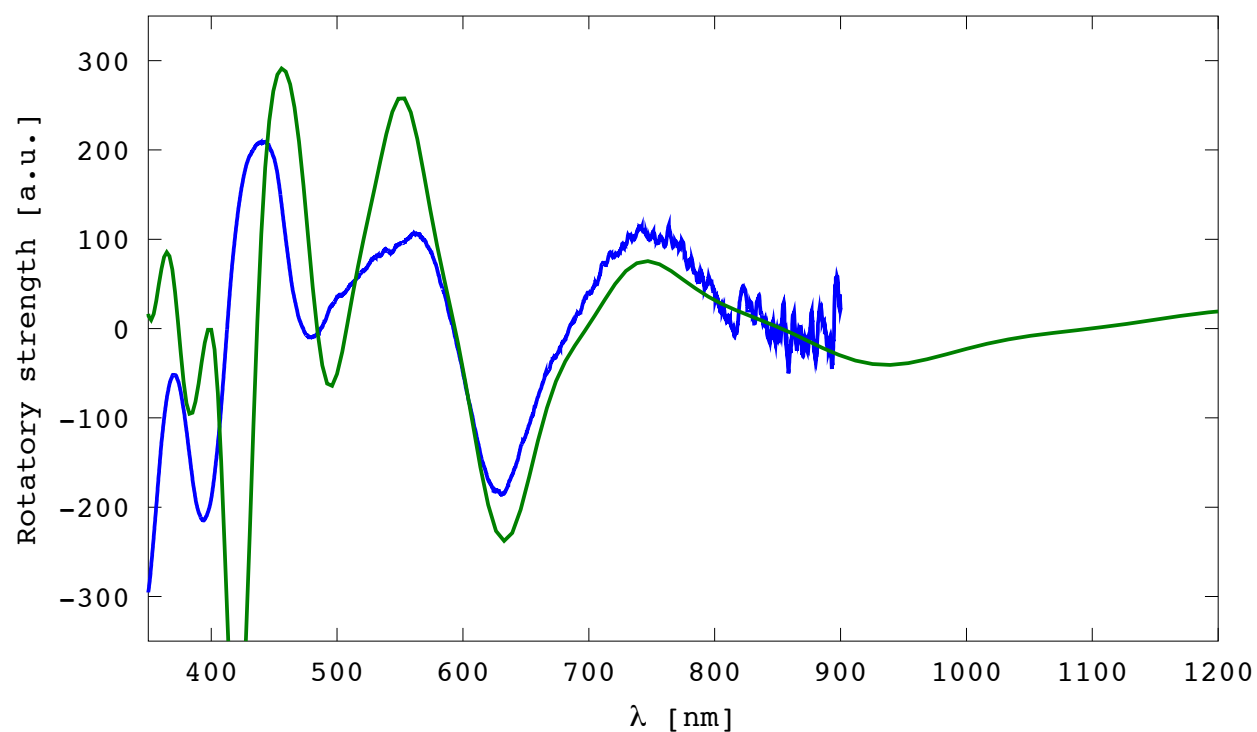


Figure S3. Calculated CD spectrum of $\text{Au}_{38}(\text{SCH}_3)_{24}$ (green) from LR-TDDFT by using GPAW as compared to the recently measured CD signal (blue) from an enantiopure solution of $\text{Au}_{38}(\text{2-PET})_{24}$ (ref. 30 of the main text). The structure of $\text{Au}_{38}(\text{SCH}_3)_{24}$ was taken from ref. 13 of the main text.

6. Synthesis and characterization of Au₄₀(2-PET)₂₄

Au₄₀(2-PET)₂₄ clusters were prepared as described earlier.⁵ Briefly, *L*-glutathionate-protected gold clusters were prepared in water and methanol by reduction of Au(III) with sodium borohydride in the presence of *L*-glutathione. The resulting clusters precipitated from the reaction mixture and were collected by centrifugation. The clusters were re-dissolved in water and mixed with neat 2-PET and acetone (the latter is to facilitate the phase transfer). The mixture was heated to 80 °C for 3 h, during which the clusters were transferred into the organic phase. After this, excess thiol was removed by extensive washing with methanol. The reaction mixture contains Au₃₈(2-PET)₂₄, Au₄₀(2-PET)₂₄ and clusters of higher mass. Au₄₀ cluster was isolated by Size-Exclusion Chromatography.⁶ The purity of the sample was confirmed with MALDI mass spectrometry (performed by Amal Dass, Univ. of Mississippi, USA) as reported earlier.⁶

All chemical were delivered from standard suppliers and used without further purification. Nanopure water (> 18 MΩ) was used.

Near Infrared-Visible spectra were measured on a JASCO J-670 spectrometer using chloroform as solvent. Quartz cuvettes with a path-length of 1 mm were used.

7. HAADF-STEM imaging and analysis

The monolayer-protected clusters were imaged with an aberration-corrected STEM after drop casting onto grids. The microscope employed was a JEM2100F STEM (JEOL) which is equipped with a high-angle annular dark field (HAADF) detector and a spherical aberration(*C_s*) probe corrector (CEOS). The electron beam energy was 200kV. The HAADF detector was used to collect signal scattered between an inner angle 62 mrad and outer angle 164 mrad(camera length of 10cm). The experiment is similar to the previous conducted study of monolayer-protected Au₃₈ clusters.^{7,8}

In the main text, Figure 2(a) is a plot of the measured HAADF intensities of each cluster as a function of the measured aspect ratios. The aspect ratio was obtained from a “Fit Ellipse” module in the software package ImageJ.⁹ Figure 2(b) is a histogram of the HAADF intensities. It shows a major peak, which we assign to monolayer-protected Au₄₀ monomers and a much weaker peak at higher intensity that corresponds to dimers. By making a Gaussian fit to the main peak we can exclude anomalies from the aspect ratio all the particles outside two standard deviations from the mean intensity (as shown by the dotted lines in Figure 2(a)). The aspect ratios of the clearly monomeric nanoparticles are then plotted in Figure 2(c) divided into bins of size 0.01.

The range of the aspect ratios may be interpreted in terms of different orientation of an ellipsoidal on the support. Thus, on this model the maximum measured aspect ratio of 1.8-2.1 corresponds to the actual aspect ratio of the monolayer-protected Au₄₀ clusters. This should be compared to a value of about 1.5 obtained previously for Au₃₈.⁸

8. Full reference 23 of the main text

J. Enkovaara, C. Rostgaard, J. J. Mortensen, J. Chen, M. Dulak, L. Ferrighi, J. Gavnholt, C. Glinsvad, V. Haikola, H. Hansen, H. Kristoffersen, M. Kuisma, A. Larsen, L. Lehtovaara, M. Ljungberg, O. Lopez- Acevedo, P. Moses, J. Ojanen, T. Olsen, V. Petzold, N. Romero, J. Stausholm-Moller, M. Strange, G. Tritsarlis, M. Vanin, M. Walter, B. Hammer, H. Hakkinen, G. Madsen, R. Nieminen, J. Norskov, M. Puska, T. Rantala, J. Schiotz, K. Thygesen and K. W. Jacobsen, *J.Phys.:Condens.Matter* **2010** 22 253202.

9. Additional structures for $\text{Au}_{40}(\text{SH})_{24}$ with alternative core shapes

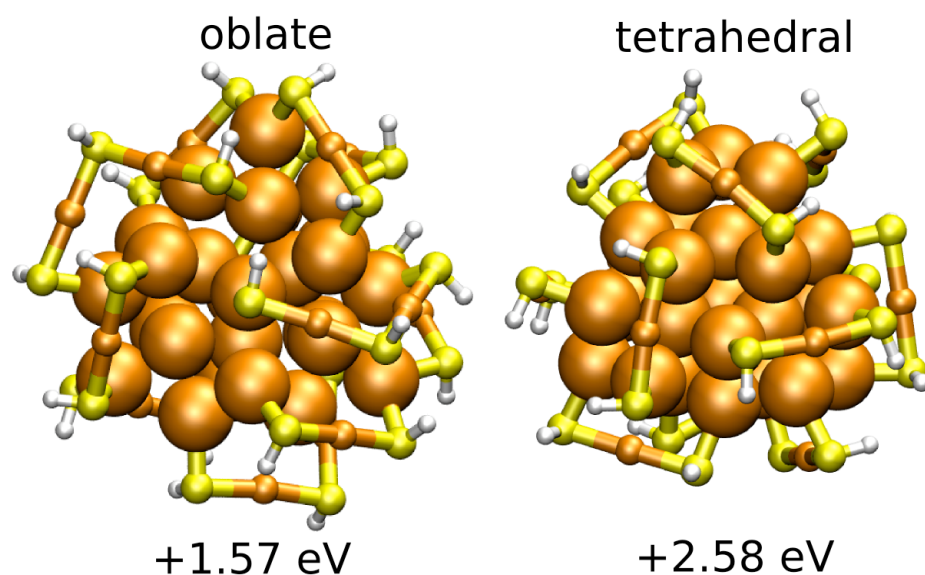


Figure S4. The relative total energies are with respect to **A1**.

9. References

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Coordinates of A1 with methylthiolate ligands (GGA-PBE optimized)

Au	12.515956338379183	21.065280110431843	16.585076870062526
Au	12.726062347482992	20.993801513133459	11.885696665021568
Au	12.781901620741237	18.080845691069165	16.694480955536136
Au	12.720389500191883	17.986391102392108	11.870877558247431
Au	14.319772571052443	21.809801813729031	14.294311669087470
Au	14.387876071006129	17.103137319463155	14.294908826441763
Au	10.917860483559929	21.777119075274008	14.140292815526145
Au	11.262408367526028	17.007326281273539	14.276872749875112
Au	15.096579010591814	19.505567565850409	15.798600473835803
Au	10.305215317033063	19.406400803594561	15.672111803014232
Au	15.096502963641417	19.503487317787133	12.803862890461946
Au	10.305401651233515	19.381554757397371	12.700662834725190
Au	12.698223827284055	19.510662288088319	14.241849583880819
Au	10.517427073860896	14.199497537237960	14.120164005608164
Au	15.306669936811209	14.398548659621691	14.523194942681009
Au	10.700237204096702	11.193174426649412	14.318303681245602
Au	15.412356313534511	11.461911461892203	14.492603740966592
Au	12.801448164840048	15.289066771215060	15.904828637225592
Au	12.997621186821691	10.527569351036647	16.099802069354102
Au	12.921063743869569	15.204133296508232	12.720957038645533
Au	13.207542177743919	10.484224183430754	12.721146103198876
Au	11.379762726572306	12.814934792731902	16.627625032270526
Au	11.596374995472583	12.710868347477462	11.890688223013903
Au	14.306939674350916	13.002709244197312	16.889304907482401
Au	14.592055984629404	12.887689479959661	12.080227941871369
Au	12.987398820567273	12.810182170577797	14.372798679081177
S	17.219292129399484	18.965367968274890	11.872882681184702
S	17.603492467704751	15.058889103572296	14.399806913042426

Au	17.209030845182475	17.013452142286290	13.201642942166542
S	12.953352837575117	17.193165862491611	9.622534881415023
S	15.708020603594786	13.445196710869851	10.042284749511159
Au	14.277347038000872	15.314391406405617	9.998842568157924
S	8.201569951747514	18.801345598707883	16.607790273383028
S	8.199786185809257	14.745756516155994	14.301987427550591
Au	8.393699034018669	16.797523399140214	15.388570344146050
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Au	11.405955232773531	15.397992946595799	18.608852537870892
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S	10.298684667169793	24.093260628684014	13.906403465788308
S	14.910614626096677	24.111858268783930	14.597501986352331
Au	12.599728508413882	24.301316676418097	14.281624658340963
S	17.285273661777406	9.987338248780850	14.539075501503524
S	15.255649797185793	13.351509726611464	19.055375393795718
S	19.538276308084441	11.695808964301433	18.240585130025096
Au	18.412645575107476	10.798109769071445	16.393816715481478
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S	10.434231948741665	12.722609088962530	9.796778460516988
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Au	7.821647177169219	9.617850113494288	12.609204947899050
S	12.221826564172060	22.569091251782542	18.419460198454267
S	17.060659336348259	19.156208892282098	17.110427720699445
S	15.799572078589147	21.247128561317098	21.089684219283551

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C	9.492755279665168	24.552748590484740	15.492758410837910
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H	20.075337715244054	10.741758625131487	20.391981667411191
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C	7.863813273393104	10.371574085021143	15.860812043153516
H	7.025662442524033	9.693515034490199	16.059531153891864
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H	7.110294256961288	8.322842153697263	8.577755575020236
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C	10.729701340651349	21.906737240051317	19.262082411400190
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H	18.033117640047916	21.248927126927828	16.251661915243858
H	18.575227497255892	19.793159961734936	15.356739915321702

C	16.919552322761422	22.688839134659641	21.305573941753117
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H	16.482845578349089	23.338157281437930	22.072125738772904
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C	7.018972976472154	19.834702305354952	12.098768933352806
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H	6.830801556741804	19.461556494643105	13.111977050359330
C	14.442970650118244	22.139643117140857	9.244975550030942
H	15.257556223374118	22.447805595956645	9.910474530243743
H	14.493288547115988	22.707394360254355	8.309620206481599
H	14.520943013526193	21.069127727548555	9.039136187410310
C	8.345481899950146	22.103361487107819	6.937313539179951
H	7.505281598292134	21.650102344490517	6.398643746591925
H	8.844092723940296	22.836806725765790	6.293912261351507
H	7.986444736294789	22.589670354818537	7.849101266396261

Coordinates of B1 with methylthiolate ligands (GGA-PBE optimized)

Au	12.883318650410153	14.411718348346106	15.060649359059081
Au	12.996952488588546	14.606814898454719	10.215480056415419
Au	12.795467151132360	11.214617192061317	15.008928092612024
Au	12.910732787923431	11.197666798093211	10.133795003679820
Au	14.496720056642408	15.199952123110704	12.722759567161624
Au	14.213155711190874	10.392990125874142	12.594377170243718
Au	11.506822724891805	15.302620067127155	12.607513078313449
Au	11.283556118627484	10.516414986747163	12.591746329453168
Au	15.279083398135164	12.605509443336892	14.099565648769822
Au	10.411797643441181	13.007964641223262	13.995183161860346
Au	15.192432389386884	12.879216058078915	11.115063651464837
Au	10.675362453276652	12.891131008557808	10.996549554914001
Au	12.885253853581231	12.861679546205691	12.637779351646666
Au	10.996583867611315	12.992598192978811	21.605031980372104
Au	11.209193667672013	12.801782267345747	16.800509904791220
Au	14.582903199314387	12.914072325601220	21.691412520981110
Au	14.405083742855773	12.881502032194392	16.879073154156966
Au	10.402350440471167	14.390256622593748	19.193944261741414
Au	15.197933657582917	14.402193138809301	19.212178270482834
Au	10.396617293713140	11.391523591440565	19.199592525264627
Au	15.193835655175855	11.399023933925836	19.377495190799472
Au	12.811277252395858	15.191529312028706	20.797932959199219
Au	12.715886980632327	10.675723908444985	20.820923083457785
Au	12.706340693239234	15.310192592472092	17.800300927503130
Au	12.909255697751691	10.484719857589171	17.813501062450637
Au	12.799128554335793	12.910055731514777	19.248184703515879
S	17.239717529318117	15.510657758589511	18.556797677013876
S	17.542006005382721	12.640309769377579	14.887277405505035

Au	17.207039283076039	14.073553245660197	16.701091262688170
S	12.786017665956646	17.615065406769702	17.120877226312015
S	15.622459416421522	17.211111064299946	13.441608104315259
Au	14.185779469776271	17.276277203527378	15.287838358921846
S	8.390361927086055	10.238058602811178	18.499188630569392
S	8.125514105510881	12.970524435555102	14.725751385416308
Au	8.408469589020370	11.612285438973331	16.600359519611153
S	12.825490779776766	8.183690809879671	17.122856179000486
S	10.188373665011255	8.487476503139836	13.275704358626772
Au	11.531542648800979	8.486952371079305	15.201910295700801
S	13.304074724482899	10.701503726142207	7.772290576089060
S	12.699045856438895	15.296201164611153	7.891615755281665
Au	12.998726914367552	13.002475430536242	7.608189587352656
S	10.420771649125840	13.306950706511277	23.956234099757726
S	14.995192757018890	12.570007282747161	24.073170781232601
Au	12.701505135933729	12.916463175250085	24.191156226344528
S	14.746838900504203	8.116831850426941	12.043122850380755
S	9.060514793067004	12.364369143150659	9.296697104411964
S	10.747964441125044	7.976847913638813	9.566398415978734
Au	12.799650770801431	8.126006660949418	10.711680748209508
Au	9.994583591727690	10.198363744443075	9.416258886416115
S	16.886404470051058	13.556181912957834	9.563429325580081
S	11.046870291511329	17.619665011032009	12.195777407472505
S	15.181814176419868	17.925859900685378	9.973733211444964
Au	15.928167721739989	15.704886800823580	9.802781901602033
Au	13.079416633784145	17.688826051253109	10.997679907150054
S	17.492699004089541	10.795888824721493	19.761979177076455
S	13.568760484833129	16.789267922441564	22.407576031153170
S	17.868416617180223	14.891495356859236	22.042224633276220

Au	17.599070119250886	12.802143121395867	20.998470375025221
Au	15.680476533210438	15.738222398980412	22.190391035310142
S	11.994236860500598	9.101272569447119	22.481268008122491
S	8.089281162538061	14.899259147497558	19.503943236172155
S	7.667375459176120	10.899801355158717	21.966131244471487
Au	9.869636918243899	10.091674858650380	22.192257146326732
Au	7.937360712634099	12.928923852277563	20.802596610172202
C	16.784929442726657	17.188610645022564	17.982043880143461
H	17.666449751641245	17.639572304591319	17.509846605107164
H	16.506584078996461	17.773628318194898	18.865811617916339
H	15.949095847542340	17.166069069882898	17.271532259992743
C	17.887614723861478	11.002454320410743	15.638474348946080
H	18.869369988556514	11.052075206269521	16.123037460312467
H	17.908493668434634	10.264589950582023	14.827745642432586
H	17.124799042893692	10.731521545598650	16.373569497629305
C	11.153792732695699	18.050884693554330	16.405046545953951
H	10.845724658858266	17.323323575561503	15.649034209345478
H	11.238833894413192	19.045429075078314	15.951779195298878
H	10.429686293720627	18.073137530039855	17.227631932601287
C	17.277778906940039	16.747149555727084	14.070508841186822
H	17.240591822453055	15.879604930812469	14.742160416374356
H	17.693991661937854	17.611864392305016	14.600699788877273
H	17.903813746881049	16.515635001229430	13.200086634599483
C	8.849711230609019	8.550888446918504	17.949808328897316
H	9.087248479346826	7.962645050472859	18.844945600666847
H	9.707644843539615	8.554965376299782	17.264694375715564
H	7.975694322935260	8.117600848562088	17.449719881623508
C	7.750156200855512	14.639527432820699	15.394853810779010
H	7.531022812508714	15.286284833106395	14.536124479674504

H	8.595186963455928	15.043753793810755	15.959217754041170
H	6.870101269115836	14.565257016846301	16.043400348253090
C	14.508643911525985	7.751434451220858	16.527777403775271
H	15.167073143678735	7.739453582233581	17.403773305221193
H	14.867821328649246	8.481718579490700	15.797120471329443
H	14.469607501125015	6.754654405784930	16.074967673407027
C	8.500950167902019	8.938864221988748	13.825809721459143
H	8.074284498910972	8.081312510754541	14.358790129447836
H	7.907296078989486	9.142435425645999	12.927045506926012
H	8.504993740218191	9.821724298557912	14.477523064868695
C	15.098541702815012	10.413553043600647	7.524924599417719
H	15.307140135041141	9.374448518822085	7.811663473565554
H	15.702942848973800	11.101478171604027	8.124311985527473
H	15.322169144789683	10.551452006728285	6.460899039239794
C	10.924328619933682	15.634911864146748	7.577262629167929
H	10.752122507526066	15.587510612185740	6.495612842956008
H	10.716501531149433	16.650459970312223	7.935381524275043
H	10.277004253365950	14.913484590853328	8.085804483429289
C	10.190345364384671	15.101822180756669	24.262849702469662
H	9.184102158773982	15.367934022522023	23.916989089849082
H	10.941815468675138	15.700737797387792	23.739133439388379
H	10.262786321979798	15.273172729549882	25.343347269645864
C	15.243946427074976	10.774507014384197	24.361789310206280
H	16.273492116782137	10.533346628565804	24.072568272656277
H	14.534225932787590	10.173699170951977	23.783697667339631
H	15.110155992725126	10.580814840426495	25.433065124115370
C	16.167956136340639	8.214709494602559	10.886039388117226
H	17.073399226415763	8.347537955067851	11.488480704678043
H	16.062412964594447	9.052963766591075	10.191689681790772

H	16.232620785944164	7.270439093735175	10.332831558958846
C	7.427799455419636	12.249938168224057	10.132273369753092
H	6.756118451016018	11.644855921973390	9.511423012857863
H	7.030353058571208	13.268524312363224	10.220335417507831
H	7.520559519407577	11.808620492351380	11.128144311580913
C	11.168645297758800	7.484253271498500	7.852257361654738
H	11.569602849753643	6.465160323581507	7.886489919338995
H	11.900015146192667	8.168811624287253	7.412368950994803
H	10.243979582163345	7.497428212609126	7.264408687892673
C	18.475356235175475	13.615970310374509	10.482898170254929
H	18.332313355848395	13.970132024474402	11.507706966007053
H	19.161255808351207	14.279430356288580	9.943338824268773
H	18.884915287983251	12.599126656792427	10.501681809852018
C	9.710984135646727	17.681050949856559	10.936974844381817
H	9.849077337106996	16.915481722917558	10.168715598135806
H	9.711319841859593	18.677107309591285	10.479796131540057
H	8.759465281439804	17.515558064614229	11.456406769698752
C	14.850976089185172	18.452064940909164	8.249530357612127
H	15.813602669849990	18.495552965511841	7.725864218766883
H	14.406665508785192	19.454306471879047	8.283871970934097
H	14.178060521410481	17.753001114220318	7.741096897320322
C	17.474977748662045	9.439063565770697	20.998200701479586
H	18.465376524115914	9.378110377666948	21.465988592482379
H	17.265080192713430	8.505503477339877	20.462881028855378
H	16.708175941715172	9.604637127704638	21.760095424727865
C	13.716456844881430	18.394530430342588	21.528096441587948
H	14.107238278928120	18.260493600785388	20.516093221363807
H	14.376504171208781	19.050471183805620	22.108038236755498
H	12.714483783680830	18.837664281583724	21.475719199399446

C	18.352202344597863	14.510402528165180	23.769369959116673
H	18.454705578211289	15.461015658460580	24.305112265728393
H	19.320197265087586	13.997950360381992	23.738250359182441
H	17.603238371709740	13.880690132554502	24.261512286344114
C	11.898637292796588	7.462836253344145	21.662280134504677
H	12.912609247684523	7.045670506425445	21.644454202978359
H	11.519499396222805	7.545157675991591	20.639442417017154
H	11.245409216178516	6.813991303010069	22.256600026547559
C	8.062772582812771	16.288570049739327	20.703348205086943
H	7.062983494159566	16.345207756103211	21.148257250402356
H	8.270034486784667	17.209423306092482	20.144277254026054
H	8.818576754218302	16.154479834534367	21.483158613300869
C	7.140688227357979	11.385061939629107	23.653096518139144
H	7.069401409122671	10.474313762909100	24.259280911596026
H	6.152162083540519	11.853099055600996	23.570102926936510
H	7.855762843773464	12.078966964165829	24.107229437772901