Core Packing-Dependent Metallic Transition in Thiolate-Protected Gold Nanoclusters: Twinned-FCC vs. Pure-FCC Configurations

Youqiong Fang[†] and Lin Xiong*[,†]

[†] School of Food and Chemical Engineering, Shaoyang University, Shaoyang 422000, People's Republic of China

*Corresponding author: linxiong@hnsyu.edu.cn

Contents

I. Computational methods and details

The geometric optimizations of $Au_{191}(SR)_{66}$, $Au_{212}(SR)_{60}$ and $Au_{224}(SR)_{72}$ clusters are implemented in CP2K Code[1] based on the level of PBE[2, 3](D3BJ)[4, 5]/DZVP-MOLOPT-SR-GTH. To ensure the rationality of structural optimization, the sizes of cells of these clusters are set by Multiwfn software (version 3.8_dev)[6, 7]. The convergence threshold of density matrix of inner SCF is 1.0E-06. The maximum geometry change, RMS geometry change, Maximum force and RMS force is set to 3E-3, 1.5E-3, 4.5E-4 and 3E-4, respectively. The single-point energy calculations of all clusters are implemented using the ORCA 5.0.4 program system[8, 9] at theoretical level of PBE (D3BJ)/Def2-TZVP. All electronic excitation calculations were performed using the sTDA approach implemented in the ORCA 5.0.4 program system software at the PBE(D3BJ)/Def2-SVP[10] level. The convergence criteria were maintained at their default settings throughout the computational procedures. Note that the Def2 basis set family incorporates relativistic pseudopotentials for elements beyond the fourth period, thereby effectively accounting for scalar relativistic effects in these heavy metal-containing systems.

It is noted that the energy threshold is set to 4 eV in sTDA calculations, which is sufficient to ensure that the computed spectra cover the wavelength range of interest. Additionally, the parameters of PThresh and PTLimit are set to 1.0×10^{-4} and 30, respectively, to control the range of configuration functions, with negligible sacrifice in accuracy. All R ligands were simplified to H in sTDA calculations.

E_{ave} can be calculated by Equation (1). Where R denotes methyl groups, while $E_{Aun(SR)m}$, E_{HSR}, $E_{[SR]^-}$, $E_{[H]^-}$, and $E_{Au(I)SR}$ correspond to the electron energies associated with $Au_n(SR)_m$ clusters, $HSCH_3$, $[SCH_3]^-$, H^-, and $AuSCH_3$, respectively.

$$E_{ave} = \frac{1}{n} \times \left[E_{Au_n(SR)_m} + \frac{n-m}{2} \times \left(E_{HSR} + E_{[SR]^-} - E_{[H]^-} \right) - n \times E_{Au^{(I)}SR} \right] \quad \cdots\cdots(1)$$

The average atomization energy can be calculated using Equation (2). Where the $E_{cluster}$ and ΣE_{atoms} represent the total electronic energy of the cluster and the sum of energies of all isolated atoms constituting the cluster, respectively; N denotes the total number of atoms in the cluster.

$$E_{atomization} = \frac{1}{N} \left(E_{cluster} - \sum E_{atoms} \right) \cdots(2)$$

Furthermore, we simulated the powder X-ray diffraction (XRD) curves of three large-sized face-centered cubic (FCC) configured gold clusters using the Debye formula, as shown in equation (3), the scattering contributions from atomic clusters are

rigorously accounted for through a double summation term. The diffraction vector modulus s is related to the Bragg angle θ by the fundamental equation $s = (4\pi\sin\theta)/\lambda$, where λ represents the incident X-ray wavelength (Mo $K\alpha$ radiation, $\lambda = 0.1051967$ nm in this study). To accurately model lattice thermal vibrations, the Debye-Waller factor ($B = 0.03$) is incorporated to account for the attenuation of scattering amplitude caused by atomic thermal motion. Furthermore, a peak broadening coefficient ($\alpha = 1.01$) was introduced to optimize the full width at half maximum (FWHM) of diffraction peaks. The atomic scattering factors for all constituent elements (Au, S, and H) were explicitly included in the simulations. This computational approach has been successfully employed for comparative analysis between theoretical and experimental XRD patterns.

$$I(s) = \sum_i \sum_{j \neq i} \frac{\cos\theta}{\left(1 + \alpha \cos(2\theta)\right)} \exp\left(\frac{-Bs^2}{2}\right) f_i f_j \frac{\sin(2\pi d_{ij})}{2\pi d_{ij}} \quad \ldots\ldots\ldots(3)$$

As depicted in Fig. S6, $Au_{212}(SR)_{60}$, $Au_{224}(SR)_{72}$, and FCC-structured $Au_{279}(SR)_{84}$ exhibit nearly identical peak profiles and positions. Notably, $Au_{279}(SR)_{84}$ displays a characteristic fingerprint peak at approximately 4.8 nm^{-1}, which originates from the octahedral geometry of its inner gold core. Additionally, two distinct peaks appear in the 6-9 nm^{-1} region, corresponding to the FCC-type core structure. The remarkable replication of these fingerprint peaks and FCC-derived characteristic peaks by both $Au_{212}(SR)_{60}$ and $Au_{224}(SR)_{72}$ provides compelling evidence that these clusters share the same well-defined FCC configuration as $Au_{279}(SR)_{84}$.

II. Supporting figures and tables

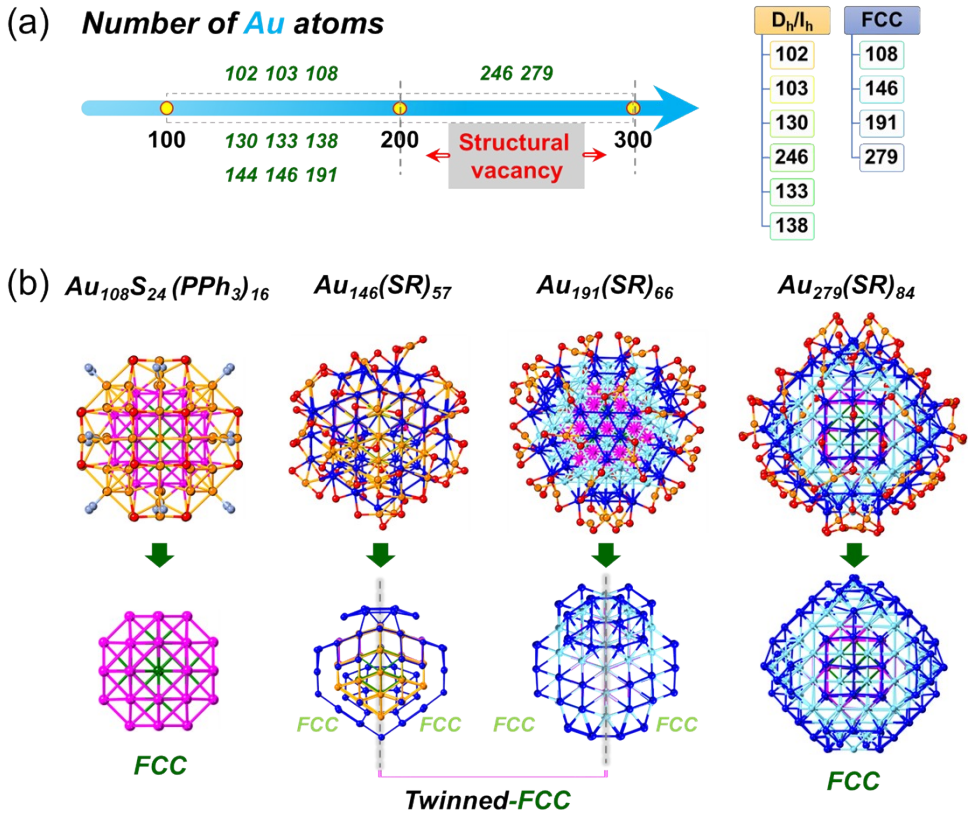

Fig. S1. (a) Currently experimentally determined large-sized RS-AuNCs and their structural configuration characteristics. (b) Large-sized RS-AuNCs with FCC structural features.

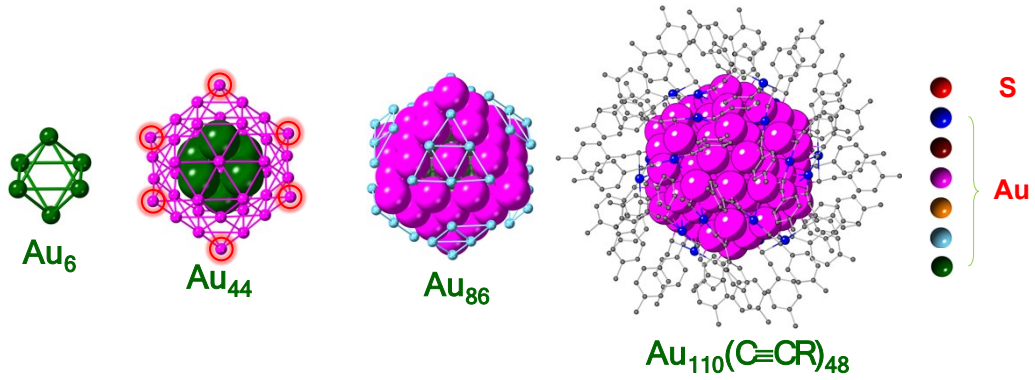

Fig. S2. Structural analysis of $[Au_{110}(C{\equiv}CR)_{48}]^{2+}$.

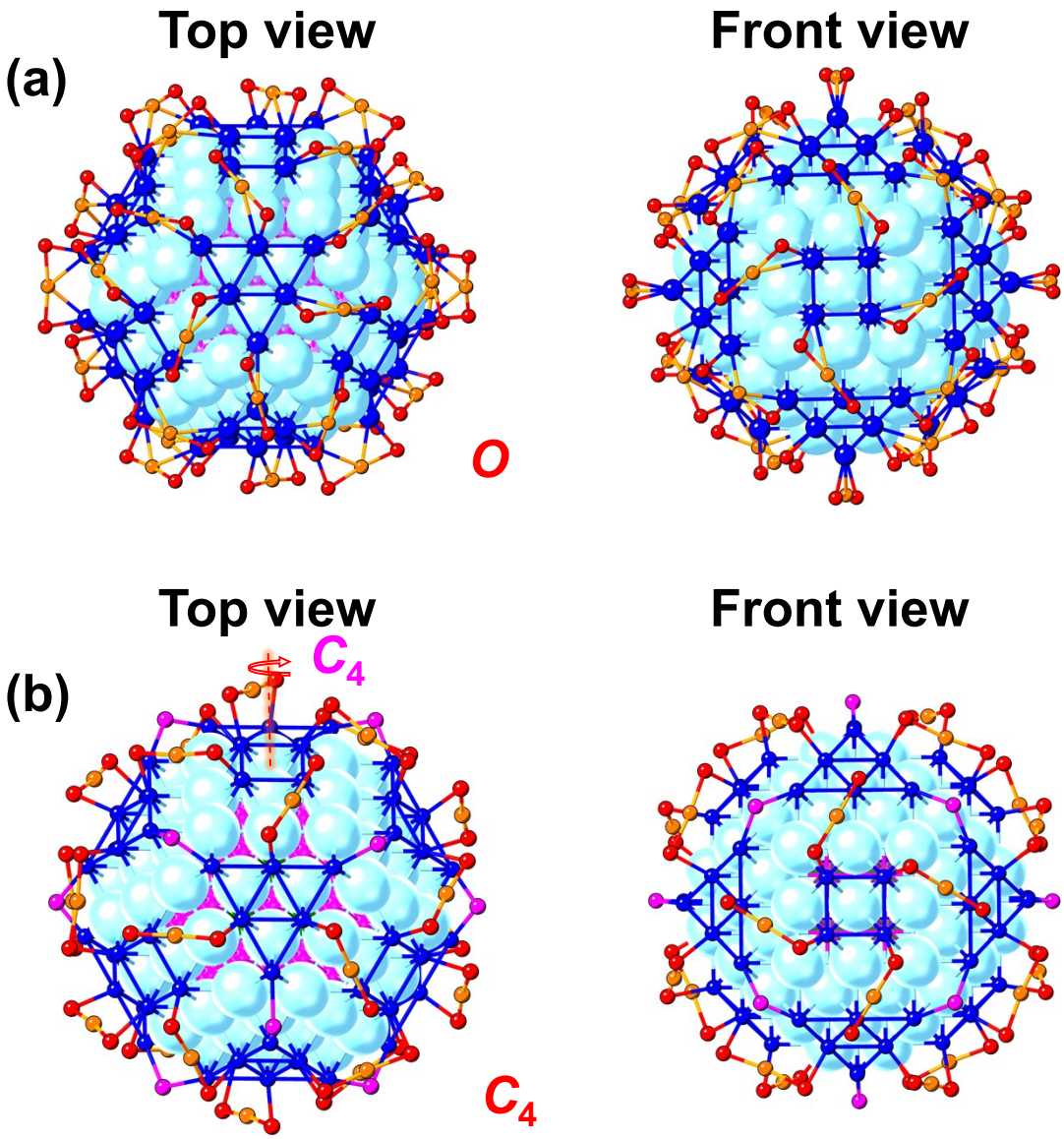

Fig. S3. Comparison of the structures and symmetry between (a) $Au_{224}(SR)_{72}$ and (b) $Au_{212}(SR)_{60}$.

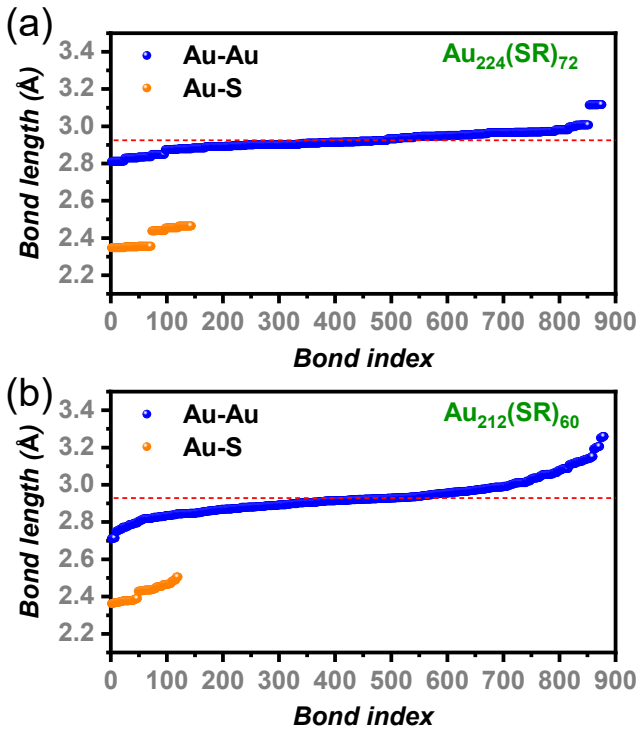

Fig. S4. The bond length distribution of Au-Au and Au-S bonds in (a) $Au_{224}(SH)_{72}$ and (b) $Au_{212}(SH)_{60}$ clusters after energy minimization. The red dashed line indicates the average Au-Au bond length.

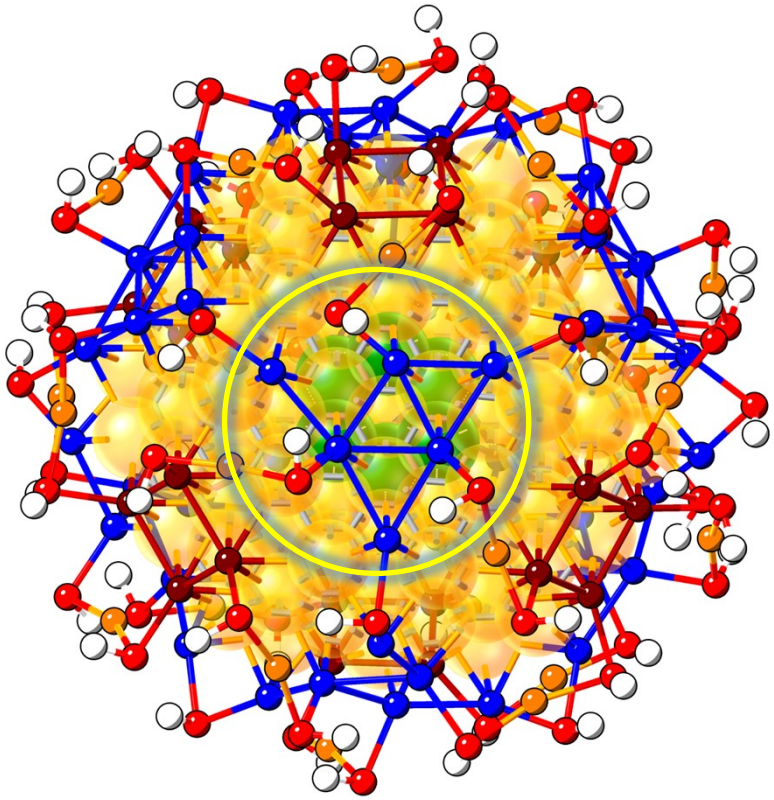

Fig. S5. Shorter SR ligands in $Au_{212}(SR)_{60}$ lead to local compression or stretching of the Au–Au bonds on the core surface. Red balls, S; white balls, H; yellow balls, Au.

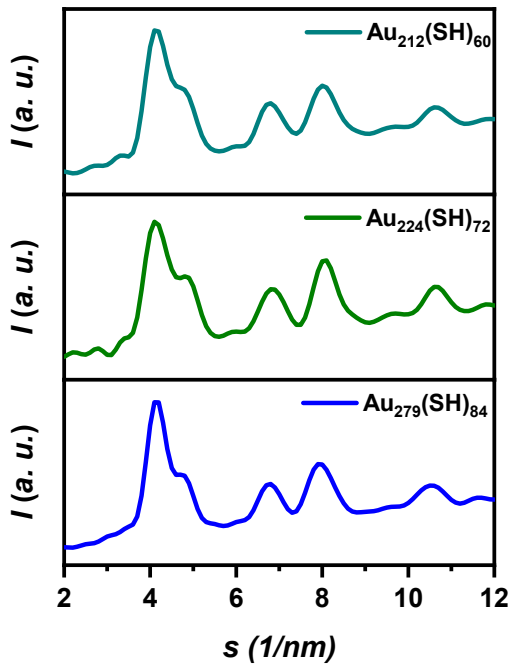

Fig. S6. Simulated XRD patterns of the relaxed (a) $Au_{212}(SH)_{60}$, (b) $Au_{224}(SH)_{72}$ and (c) $Au_{279}(SH)_{84}$ clusters.

Table S1. The Cartesian coordinates of $Au_{224}(SR)_{72}$, R = CH_3.

Atoms	x	y	z	Atoms	x	y	z
S	2.269524	-7.46398	8.248521	Au	-0.01073	-0.00163	2.068996
S	-2.26654	-8.20918	7.474728	Au	2.053265	-0.01016	0.011025
S	7.487647	-8.20102	2.30013	Au	-0.00512	-0.01138	-2.05398
S	8.179774	-7.51503	-2.26106	Au	-2.06154	0.004231	0.003987
S	8.199258	-2.25466	7.487602	C	3.048253	-9.07756	7.852405
S	7.480777	2.290462	8.231564	C	-3.05486	-7.81719	9.084084
S	3.897428	-8.712	4.400288	C	9.109789	-7.76699	3.038411
S	3.965561	-9.7839	-0.16976	C	7.761505	-9.14201	-2.99923
S	8.664598	-4.39523	3.957271	C	7.812464	-3.02454	9.10728
S	10.06395	0.077466	3.641583	C	9.103361	3.042616	7.820737
S	4.421572	-3.92043	8.677354	C	5.497954	-9.25914	5.101599
S	-0.05327	-3.64848	10.08	C	3.26502	-11.4652	-0.39177
S	3.909073	4.390089	8.703116	C	9.239965	-5.06582	5.558139
S	3.986506	-0.18179	9.788849	C	11.53028	0.119581	2.536982
S	8.244617	7.445231	2.26903	C	5.092369	-5.51887	9.260234
S	7.496299	8.179549	-2.2754	C	-0.10973	-2.55001	11.55102
S	2.321942	8.224273	7.466246	C	5.501975	5.089834	9.27435
S	-2.21897	7.469835	8.216696	C	3.272611	-0.3731	11.46813
S	8.707894	3.873133	4.375515	C	7.857166	9.070331	3.028954
S	9.774038	3.950602	-0.20299	C	9.099403	7.755128	-3.05929
S	4.426558	8.675274	3.88994	C	3.083527	7.833686	9.089385
S	-0.13916	9.774904	3.992295	C	-2.99085	9.090384	7.838264
S	-4.39417	3.950141	8.692963	C	9.276624	5.466589	5.075388
S	0.084071	3.651729	10.07701	C	11.45018	3.232483	-0.40578
S	-8.20012	2.288264	7.497283	C	5.131561	9.256258	5.476815
S	-7.49944	-2.26957	8.209391	C	-0.36134	11.45424	3.285852
S	-3.88904	8.668994	4.456143	C	-5.05513	5.557532	9.262232
S	-3.64977	10.06656	-0.02	C	0.135274	2.556549	11.55016
S	-8.69359	4.385268	3.91435	C	-7.7855	3.043546	9.117222
S	-9.79898	-0.18095	3.953644	C	-9.12126	-3.01793	7.790165
S	-3.91315	-4.37449	8.704396	C	-5.48919	9.250816	5.124871
S	-3.97078	0.192195	9.799106	C	-2.56939	11.55017	-0.0875
S	-8.19723	-7.48423	2.264938	C	-9.2606	5.084215	5.509212
S	-7.49659	-8.21428	-2.28713	C	-11.4596	-0.40303	3.204702
S	-8.68499	-3.94157	4.412808	C	-5.50801	-5.07603	9.267969
S	-10.0161	-3.71755	-0.08558	C	-3.24886	0.400624	11.47334
S	-3.91696	-8.69998	-4.37992	C	-7.77778	-9.09962	3.026588
S	-4.00365	-9.78257	0.190573	C	-9.11948	-7.7956	-3.0348
S	-2.28304	-7.46346	-8.22642	C	-9.24579	-5.54751	5.085073
S	2.245292	-8.24356	-7.44717	C	-11.5365	-2.68982	-0.16051

S	-8.70033	-4.37008	-3.91786	C	-5.50696	-9.27319	-5.08387
S	-9.80998	0.197487	-3.93705	C	-3.28612	-11.4555	0.42282
S	4.387726	-8.69389	-3.91094	C	-3.07225	-9.07446	-7.84158
S	-0.0878	-10.0875	-3.61433	C	3.033017	-7.86628	-9.06023
S	8.685562	-3.95037	-4.36079	C	-9.26331	-5.06969	-5.51334
S	9.762481	-4.00132	0.213043	C	-11.4685	0.365154	-3.16942
S	7.460566	-2.33841	-8.21534	C	5.058723	-9.2793	-5.50824
S	8.182391	2.212074	-7.49745	C	-0.13814	-11.5458	-2.49875
S	3.867352	-4.408	-8.68791	C	9.243048	-5.54674	-5.06204
S	3.971756	0.162145	-9.77433	C	11.44252	-3.28937	0.405967
S	8.693226	4.345999	-3.95663	C	9.081349	-3.09325	-7.80074
S	10.06021	-0.13986	-3.64966	C	7.776947	2.977814	-9.11407
S	4.410205	3.92986	-8.66701	C	5.452542	-5.12098	-9.26508
S	-0.06427	3.641329	-10.0623	C	3.26688	0.386657	-11.4536
S	3.928419	8.672118	-4.41034	C	9.259256	5.013937	-5.56219
S	3.675607	10.05437	0.071267	C	11.52531	-0.18743	-2.54347
S	-4.37632	-8.69375	3.943635	C	5.07497	5.535877	-9.2357
S	0.105789	-10.084	3.652253	C	-0.11927	2.538461	-11.5302
S	-4.41814	-3.92414	-8.6757	C	5.531461	9.252714	-5.07336
S	0.056743	-3.6533	-10.0772	C	2.574707	11.52286	0.140776
S	-8.2349	7.447999	-2.23827	C	-5.06139	-9.27553	5.536307
S	-7.43165	8.245638	2.284721	C	0.15409	-11.5501	2.547171
S	-2.29649	8.244011	-7.44111	C	-5.09441	-5.52073	-9.25782
S	2.241442	7.467862	-8.1958	C	0.113787	-2.54216	-11.5385
S	-7.47251	2.286339	-8.19884	C	-7.87052	9.05998	-3.03526
S	-8.20748	-2.26491	-7.49105	C	-9.03378	7.852894	3.088366
S	-4.40901	8.69409	-3.85733	C	-3.07294	7.852705	-9.05678
S	0.158888	9.794865	-3.95308	C	3.029915	9.076689	-7.80204
S	-3.89787	4.398302	-8.68719	C	-9.09433	3.043345	-7.79501
S	-3.98351	-0.17135	-9.77075	C	-7.79975	-3.01487	-9.11477
S	-8.66719	3.925901	-4.40792	C	-5.11078	9.27521	-5.44632
S	-10.0492	3.683869	0.073581	C	0.38118	11.4674	-3.23063
Au	8.240418	2.026417	-0.11097	C	-5.49431	5.095761	-9.2513
Au	8.230863	-2.07295	0.103234	C	-3.27343	-0.39357	-11.4485
Au	8.210848	0.09582	2.043076	C	-9.24596	5.526485	-5.07722
Au	8.206765	-0.13524	-2.05168	C	-11.5341	2.607321	0.170056
Au	4.250114	6.230937	4.188087	H	2.781387	-9.41265	6.841918
Au	6.204846	6.08215	2.000187	H	2.719314	-9.81556	8.599212
Au	4.180416	6.233841	-4.20612	H	4.138959	-8.94605	7.920702
Au	6.111711	6.165709	-2.00114	H	-2.72868	-8.56509	9.8222
Au	4.191824	4.215648	6.256756	H	-4.14478	-7.88661	8.946488
Au	6.104634	1.984139	6.201477	H	-2.79119	-6.80695	9.422408
Au	6.257413	4.142055	4.22397	H	9.420162	-6.75355	2.753415

Au	6.244234	4.188188	-4.15941	H	9.852231	-8.50547	2.700274
Au	4.206602	4.155415	-6.22527	H	9.004846	-7.82737	4.132558
Au	6.164635	1.984422	-6.1108	H	8.503093	-9.87901	-2.65628
Au	6.169341	-2.02521	6.118438	H	7.826963	-9.03817	-4.09322
Au	6.09363	-2.02035	-6.18518	H	6.74842	-9.45774	-2.71903
Au	4.139775	-6.26395	4.226672	H	7.87647	-4.11634	8.981766
Au	4.195756	-4.19264	6.241122	H	6.805002	-2.75212	9.446491
Au	6.218209	-4.24075	4.178559	H	8.566902	-2.69358	9.836582
Au	6.081659	-6.19709	2.010029	H	9.425153	2.769002	6.807596
Au	4.204176	-6.25363	-4.16575	H	9.842753	2.702646	8.561203
Au	6.164506	-6.11979	-1.98513	H	8.990618	4.135394	7.889923
Au	6.232589	-4.1884	-4.21679	H	6.326713	-9.0069	4.425773
Au	4.162283	-4.23775	-6.24135	H	5.456483	-10.3496	5.253779
Au	2.020448	6.185274	6.107275	H	5.633488	-8.75458	6.069669
Au	-0.09108	8.247143	2.062929	H	4.010522	-12.2058	-0.06266
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Au	2.000822	6.091053	-6.17032	H	10.32755	-5.22977	5.495777
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Au	1.991605	-6.20156	-6.0932	H	4.394175	-6.3388	9.042361
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Au	-6.0824	6.20359	2.006579	H	2.811356	6.825075	9.425723

Au	-6.17822	2.01022	6.118612	H	2.747665	8.583943	9.820745
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Au	-8.22442	2.060451	0.132319	H	-2.72299	9.432914	6.830791
Au	-6.11002	-1.98206	6.192644	H	-2.65656	9.817714	8.593308
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Au	0.000325	-7.81306	7.838886	H	6.09361	8.745	5.627586
Au	7.797806	-7.82336	0.019271	H	-1.43789	11.57962	3.089937
Au	7.803919	0.015418	7.834314	H	0.200296	11.58205	2.352379
Au	3.934317	-9.28486	2.129344	H	-0.02782	12.19752	4.026325
Au	9.372508	-2.16881	3.828752	H	-4.35595	6.37262	9.029868
Au	2.19341	-3.80023	9.382596	H	-5.21668	5.501802	10.35056
Au	3.95562	2.112246	9.24822	H	-6.01567	5.723308	8.752259
Au	7.846923	7.779129	-0.00468	H	1.1947	2.311636	11.72315
Au	0.048534	7.822897	7.806414	H	-0.4307	1.631309	11.38723
Au	9.245403	3.923468	2.095239	H	-0.26718	3.099137	12.4197
Au	2.157998	9.25853	3.926647	H	-7.84488	4.1365	8.999854
Au	-2.16355	3.822313	9.388697	H	-6.77553	2.762178	9.441368
Au	-7.81936	0.009696	7.824145	H	-8.53205	2.712492	9.854724
Au	-3.77733	9.37542	2.22826	H	-9.01089	-4.11125	7.856629
Au	-9.28831	2.118656	3.933976	H	-9.43796	-2.74132	6.776402
Au	-3.94321	-2.10587	9.287364	H	-9.8615	-2.67878	8.530257
Au	-7.81249	-7.82213	-0.00883	H	-5.65812	8.735909	6.082078
Au	-9.3541	-3.85084	2.172137	H	-6.30849	9.031378	4.426432
Au	-3.95498	-9.27979	-2.11005	H	-5.42283	10.33753	5.292649
Au	-0.01832	-7.82871	-7.8135	H	-2.334	11.71995	-1.14957
Au	-9.26114	-2.09579	-3.94644	H	-1.63871	11.39903	0.472783
Au	2.159128	-9.39524	-3.78588	H	-3.11786	12.41631	0.314635
Au	9.232044	-3.99517	-2.08336	H	-9.02302	4.40456	6.339149
Au	7.787577	-0.06008	-7.83239	H	-10.3499	5.23978	5.453335
Au	3.916805	-2.13788	-9.26799	H	-8.75501	6.050173	5.654482
Au	9.387161	2.113472	-3.83729	H	-11.5773	-1.4794	3.00332
Au	2.182013	3.805695	-9.36858	H	-11.5647	0.161888	2.270464
Au	3.814246	9.363569	-2.17783	H	-12.2229	-0.07435	3.926965
Au	-2.14761	-9.40294	3.834529	H	-5.65264	-6.04013	8.758442
Au	-2.19018	-3.80905	-9.38104	H	-6.33845	-4.39629	9.031815
Au	-4.21455	6.254774	-4.17083	H	-5.45256	-5.23604	10.35664

Au	-1.98718	6.200284	-6.08904	H	-2.32058	-0.17132	11.59179
Au	-4.16194	4.236441	-6.23901	H	-3.98691	0.071493	12.22099
Au	-6.18356	6.107067	-1.99033	H	-3.04165	1.474776	11.60168
Au	-6.22706	4.180728	-4.21444	H	-8.51845	-9.84221	2.693891
Au	-6.08998	2.000832	-6.17726	H	-7.84263	-8.98002	4.118966
Au	-7.81096	7.824378	0.022731	H	-6.76453	-9.41891	2.751101
Au	-0.0253	7.835379	-7.79038	H	-9.85893	-8.53781	-2.69856
Au	-7.80683	0.010291	-7.81249	H	-9.00785	-7.85825	-4.12803
Au	-2.13826	9.271392	-3.89227	H	-9.43995	-6.78399	-2.75441
Au	-3.92908	2.127623	-9.26224	H	-8.73302	-5.70671	6.045206
Au	-9.37021	3.812164	-2.17928	H	-9.01323	-6.36595	4.389698
Au	-4.13503	2.102662	-4.14719	H	-10.3339	-5.49453	5.249308
Au	-4.14899	4.153544	-2.0956	H	-12.3887	-3.27539	0.219885
Au	-2.10174	4.163274	-4.13522	H	-11.6989	-2.44311	-1.22127
Au	4.111018	6.168491	0.063724	H	-11.4273	-1.76443	0.417813
Au	4.143416	2.09435	4.169494	H	-5.45884	-10.3668	-5.20631
Au	4.16632	4.126905	2.108218	H	-5.63384	-8.79484	-6.06645
Au	6.237061	2.118601	2.064897	H	-6.34441	-9.00677	-4.42455
Au	6.175611	4.072491	-0.05721	H	-4.02533	-12.2055	0.101117
Au	4.146145	2.084006	-4.13893	H	-3.08446	-11.5708	1.499568
Au	4.139866	4.14928	-2.09986	H	-2.35597	-11.5839	-0.14342
Au	6.226959	2.04334	-2.13925	H	-2.81018	-9.4165	-6.83209
Au	4.142739	-2.11029	4.153666	H	-2.74507	-9.81013	-8.59136
Au	4.098929	-0.06897	6.189688	H	-4.16194	-8.93632	-7.9121
Au	6.186712	0.034728	4.113669	H	2.770409	-6.85863	-9.40704
Au	6.222463	-2.07914	2.146671	H	2.704246	-8.61926	-9.79209
Au	6.242397	-0.0181	3.55E-05	H	4.12292	-7.93708	-8.92401
Au	4.129064	-2.12046	-4.15872	H	-8.75967	-6.0372	-5.65563
Au	6.222249	-2.1542	-2.0601	H	-9.02161	-4.39175	-6.34349
Au	6.176587	-0.07299	-4.10714	H	-10.3532	-5.22238	-5.46063
Au	4.074633	0.035486	-6.16935	H	-11.5506	-0.22162	-2.24643
Au	4.07459	-6.17872	-0.04942	H	-12.2307	0.033524	-3.89144
Au	4.121486	-4.16924	2.11061	H	-11.6096	1.434146	-2.94443
Au	6.158396	-4.10163	0.064183	H	5.226628	-10.3657	-5.43858
Au	4.138787	-4.15033	-2.09281	H	6.016498	-8.76527	-5.67698
Au	-0.04104	6.164203	4.100527	H	4.361484	-9.06124	-6.32899
Au	0.011881	6.2555	0.00408	H	0.265989	-12.4222	-3.02879
Au	2.07944	6.222605	2.153619	H	-1.19767	-11.717	-2.25307
Au	0.06257	6.181011	-4.07729	H	0.426674	-11.3699	-1.57526
Au	2.144612	6.232516	-2.05131	H	8.738113	-5.68794	-6.0291
Au	0.070666	4.095662	6.19761	H	8.998859	-6.37662	-4.38466
Au	2.148356	2.060132	6.248115	H	10.33287	-5.49676	-5.21588
Au	2.113905	4.15483	4.152061	H	11.56457	-2.36501	-0.17133

Au	2.102633	4.130986	-4.14119	H	12.184	-4.03396	0.077325
Au	-0.05947	4.095022	-6.17813	H	11.57719	-3.07764	1.478447
Au	2.059851	2.126768	-6.22977	H	9.822424	-2.75587	-8.54063
Au	0.001977	-0.00344	6.268619	H	8.965391	-4.18577	-7.86845
Au	2.056985	-2.14107	6.251244	H	9.401739	-2.81959	-6.78723
Au	-0.01029	-0.00825	-6.2519	H	8.526252	2.649344	-9.84992
Au	2.121769	-2.07728	-6.23561	H	7.837555	4.070038	-8.9901
Au	0.04123	-6.19774	4.110594	H	6.767628	2.701479	-9.44405
Au	-0.06528	-4.09582	6.192546	H	5.387713	-5.27779	-10.3537
Au	2.08788	-4.15605	4.169215	H	5.594322	-6.08696	-8.7587
Au	-0.02465	-6.25746	0.011051	H	6.289481	-4.44749	-9.03471
Au	2.114219	-6.24487	2.065459	H	4.008598	0.055778	-12.1969
Au	-0.07427	-6.20539	-4.09776	H	3.070726	1.463394	-11.5772
Au	2.043228	-6.24972	-2.13064	H	2.33441	-0.17576	-11.5841
Au	2.088084	-4.17489	-4.13545	H	8.749913	5.975629	-5.72318
Au	0.041454	-4.11304	-6.17608	H	9.025137	4.318843	-6.38031
Au	-4.0801	6.190909	-0.0539	H	10.3478	5.174197	-5.50759
Au	-2.12162	6.239663	2.066222	H	12.40174	0.201947	-3.08466
Au	-2.05752	6.243499	-2.13149	H	11.6897	-1.24502	-2.28418
Au	-4.1559	2.111438	4.152523	H	11.35979	0.39092	-1.62639
Au	-2.05635	2.147495	6.250992	H	4.377027	6.35243	-9.00468
Au	-2.08813	4.137627	4.15638	H	5.238114	5.479663	-10.3237
Au	-4.13023	4.159973	2.114288	H	6.03516	5.700178	-8.7244
Au	-2.14507	2.059709	-6.23436	H	0.283654	3.074845	-12.4032
Au	-4.14713	-2.09638	4.165493	H	-1.17958	2.295258	-11.7005
Au	-4.09326	0.067943	6.183058	H	0.443876	1.612329	-11.3627
Au	-2.14359	-2.05539	6.246761	H	5.699481	8.745177	-6.03479
Au	-4.16678	-2.10547	-4.13464	H	6.349533	9.023987	-4.37614
Au	-4.09195	-0.064	-6.16877	H	5.468972	10.3409	-5.23226
Au	-2.07218	-2.1509	-6.23487	H	1.643727	11.35837	-0.41533
Au	-2.11534	-4.14871	4.147407	H	3.109042	12.39708	-0.26243
Au	-4.11168	-6.17015	0.064056	H	2.340475	11.68952	1.203694
Au	-4.16029	-4.13215	2.107489	H	-4.37088	-9.05635	6.362371
Au	-2.07841	-6.23951	2.146576	H	-5.22959	-10.362	5.46696
Au	-4.15388	-4.15656	-2.09538	H	-6.0205	-8.76111	5.696499
Au	-2.1564	-6.2439	-2.0615	H	-0.23765	-12.4254	3.088323
Au	-2.11604	-4.15139	-4.14989	H	1.211941	-11.7155	2.289991
Au	-6.23396	2.076143	2.149509	H	-0.42317	-11.3849	1.629253
Au	-6.17115	4.104839	0.068592	H	-5.26283	-5.45275	-10.3443
Au	-6.23286	2.15265	-2.05278	H	-6.05279	-5.68493	-8.74333
Au	-6.18155	-0.04145	4.099001	H	-4.39989	-6.34292	-9.03753
Au	-6.24037	-2.13184	2.065955	H	-0.28971	-3.07328	-12.4144
Au	-6.25576	0.01003	0.007104	H	1.174078	-2.29815	-11.7071

Au	-6.24068	-2.05745	-2.12911	H	-0.45005	-1.61727	-11.3666
Au	-6.17095	0.060103	-4.08454	H	-7.94261	8.917406	-4.12431
Au	-6.19505	-4.09371	-0.05498	H	-6.86468	9.415088	-2.77685
Au	-2.08774	2.092656	-2.08124	H	-8.62808	9.788025	-2.70871
Au	4.115603	2.031574	0.003799	H	-9.37407	6.842595	2.827444
Au	4.10943	-2.05812	0.01259	H	-9.77524	8.600503	2.769344
Au	4.127223	-0.00836	2.064712	H	-8.88584	7.922198	4.17694
Au	4.11786	-0.01858	-2.05013	H	-2.80594	6.843034	-9.39405
Au	0.012736	2.043744	4.136331	H	-2.74204	8.60075	-9.79276
Au	0.001554	4.126671	2.050079	H	-4.16375	7.922086	-8.92701
Au	2.088079	2.083935	2.101221	H	2.708673	9.812119	-8.55479
Au	2.05048	4.122758	0.013553	H	4.120225	8.938151	-7.86491
Au	-0.01488	2.051895	-4.12534	H	2.76016	9.416085	-6.79402
Au	0.004767	4.118658	-2.04101	H	-9.42208	2.767564	-6.78469
Au	2.084404	2.07818	-2.08043	H	-9.82863	2.708428	-8.54293
Au	-0.00949	-2.04826	4.139976	H	-8.97732	4.135976	-7.86028
Au	2.050206	-0.00466	4.134702	H	-8.54267	-2.67305	-9.85099
Au	2.081587	-2.09743	2.101014	H	-7.8695	-4.10799	-9.00452
Au	-0.01021	-2.06959	-4.12432	H	-6.78664	-2.74162	-9.43637
Au	2.078245	-2.10009	-2.08495	H	-5.27705	10.36215	-5.37739
Au	2.030025	-0.01562	-4.1134	H	-6.07104	8.761644	-5.59993
Au	-0.00671	-4.13796	2.064473	H	-4.42711	9.054644	-6.27769
Au	2.022244	-4.13706	-0.00181	H	-0.18615	11.58963	-2.3
Au	-0.01614	-4.13737	-2.04484	H	0.053536	12.21728	-3.96736
Au	-4.12142	2.057121	0.010892	H	1.457227	11.58806	-3.02999
Au	-2.09132	2.090277	2.100555	H	-6.32219	4.412034	-9.01804
Au	-2.04442	4.130538	0.003388	H	-5.43861	5.258101	-10.3397
Au	-2.05451	0.012674	4.136485	H	-5.64296	6.057711	-8.73934
Au	-4.1332	-2.04339	-0.00408	H	-4.01479	-0.0652	-12.1935
Au	-4.12997	0.00226	2.054534	H	-3.07375	-1.46963	-11.5725
Au	-2.09004	-2.08706	2.094043	H	-2.34303	0.172454	-11.5766
Au	-4.13077	0.016866	-2.0369	H	-10.3327	5.461714	-5.24596
Au	-2.09894	-2.09349	-2.08589	H	-8.73012	5.695499	-6.03391
Au	-2.04729	-0.0114	-4.11904	H	-9.02576	6.344757	-4.37803
Au	-2.06619	-4.12477	0.013038	H	-11.3897	1.669696	-0.38049
Au	0.000358	2.055728	0.008603	H	-12.4039	3.152418	-0.22833
Au	-0.01055	-2.06494	0.009713	H	-11.6906	2.385395	1.236922

Table S2. The Cartesian coordinates of $Au_{212}(SR)_{60}$, R = CH_3.

Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Au	17.57356	8.729671	16.67207	S	12.45516	11.65242	4.647218
Au	20.50939	11.71047	16.75988	Au	19.2664	6.524172	10.38474
Au	18.93481	10.2319	18.58613	S	17.30439	5.438343	9.656635
Au	17.59625	8.67345	12.43772	S	21.42678	7.127462	11.11755
Au	16.23705	7.454073	14.56139	S	9.392653	9.223569	7.102446
Au	20.65025	11.69855	12.45705	S	20.04537	9.343009	7.167767
Au	19.04539	10.21808	14.57215	S	14.7134	4.1512	15.07005
Au	21.82288	13.10366	14.71516	S	9.337574	9.383855	21.94118
Au	19.05107	10.24922	10.61667	S	19.81017	9.419651	22.01529
Au	14.66127	11.72001	20.85004	S	19.86046	19.90684	21.92271
Au	17.51233	14.71402	20.84175	S	9.347111	19.89238	21.91749
Au	17.51239	11.85456	20.81158	S	14.5851	25.09111	15.0097
Au	11.68218	8.700827	16.75138	S	4.146765	14.63892	15.00742
Au	13.16269	10.23832	18.77611	S	25.06229	14.59083	15.0529
Au	14.64087	8.837543	16.69557	S	19.82277	19.95762	7.095891
Au	16.06721	10.28767	18.75558	S	9.268366	19.87334	7.061046
Au	18.9808	13.20534	18.77839	C	21.76173	23.61689	16.92439
Au	20.47437	17.60364	16.64784	C	16.91669	24.40944	20.89168
Au	18.93703	16.11279	18.74438	C	13.0988	25.17667	19.48163
Au	20.38915	14.6719	16.69335	C	11.01249	25.04588	13.75326
Au	11.676	8.55633	12.42192	C	15.37992	22.12873	23.74781
Au	13.08301	7.395208	14.71255	C	11.3763	18.3141	24.71549
Au	14.55577	8.683328	12.54038	C	21.36924	7.223397	19.51469
Au	20.56684	17.59837	12.41092	C	24.3595	12.23338	20.90932
Au	20.53127	14.56229	12.53514	C	25.13136	16.10763	19.56882
Au	21.75978	16.25708	14.55542	C	25.12656	18.25213	13.9852
Au	14.62512	11.50348	8.319003	C	22.13549	13.95259	23.74551
Au	13.19507	10.14763	10.41841	C	18.24801	17.84443	24.7495
Au	16.13573	10.12188	10.4782	C	7.474799	5.608771	16.97365
Au	17.70794	14.59473	8.306114	C	12.29467	4.922851	21.01198
Au	17.43073	11.76906	8.456975	C	16.09104	4.090152	19.57186
Au	19.07321	13.1834	10.41457	C	21.04454	4.786468	15.50002
Au	19.09442	16.12136	10.45507	C	13.92256	7.199954	23.83319
Au	11.66941	14.56098	20.83584	C	15.40283	12.76128	26.14376
Au	11.81286	11.70228	20.80146	C	5.590609	21.75554	16.94114
Au	14.51729	17.55173	20.83425	C	4.821521	16.93266	20.89541
Au	14.58775	14.63618	20.82124	C	4.058144	13.07776	19.53681
Au	17.36659	17.57435	20.80005	C	4.105176	11.0719	13.89927
Au	8.708724	11.64007	16.63818	C	7.09667	15.4536	23.75461
Au	10.19036	10.29153	18.5594	C	10.90716	11.43547	24.7412
Au	10.24986	13.15273	18.73627	C	12.06686	15.51045	3.211078

Au	17.51246	20.5427	16.71855	C	6.472834	15.90417	6.307517
Au	16.02281	19.02416	18.75657	C	5.305511	11.98823	8.100725
Au	18.99254	18.97645	18.55438	C	5.612878	7.287642	12.44347
Au	8.650976	11.61487	12.40318	C	3.973905	15.68982	9.95021
Au	17.54163	20.648	12.39698	C	4.831622	21.01462	13.27189
Au	10.24943	10.1625	10.58213	C	20.81189	24.4773	13.20336
Au	11.53434	14.57237	8.292366	C	15.59722	25.23697	9.869693
Au	10.13046	13.06957	10.44122	C	15.97342	22.75313	6.333927
Au	11.80895	11.77709	8.440188	C	18.60019	17.50067	4.70011
Au	14.61169	17.67135	8.290814	C	12.00593	23.8193	8.080843
Au	14.62392	14.58397	8.380408	C	7.035432	21.13625	9.634383
Au	16.02942	19.04595	10.39335	C	17.18562	13.66849	3.227279
Au	17.42335	17.38949	8.439422	C	22.78305	13.28625	6.362609
Au	18.97985	19.02909	10.57294	C	23.93502	17.17959	8.129922
Au	11.65945	17.40817	20.78498	C	23.61021	21.9193	12.41833
Au	8.679789	17.53303	16.70748	C	25.24101	13.45285	10.19492
Au	8.81548	14.57278	16.66165	C	24.28613	8.052303	13.728
Au	10.2034	16.05548	18.75302	C	8.421272	4.724109	13.28378
Au	11.61665	20.5162	16.61803	C	13.61284	3.994217	9.929669
Au	10.25834	19.02524	18.52694	C	15.88611	7.831515	5.269295
Au	13.11851	18.97052	18.72199	C	10.61056	11.68796	4.696516
Au	14.5538	20.40709	16.65655	C	17.35305	3.857412	10.61739
Au	7.448945	12.98528	14.52481	C	22.26146	8.057203	9.757905
Au	8.563703	17.52693	12.37389	C	8.316534	7.967343	7.886823
Au	7.385927	16.13068	14.66388	C	19.58219	9.578917	5.414625
Au	8.684562	14.65455	12.49532	C	13.03045	3.516099	15.41656
Au	11.6161	20.54688	12.38141	C	7.919546	8.382517	21.35873
Au	12.97193	21.76984	14.50117	C	19.34172	10.0356	23.68476
Au	14.66169	20.52876	12.49436	C	21.27578	20.89645	21.31374
Au	16.11933	21.83377	14.66973	C	8.357079	21.32553	21.35396
Au	10.15909	16.01452	10.3758	C	16.2909	25.63684	15.38731
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Au	16.02284	16.09796	18.6798	H	11.31172	26.03183	14.13757
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Au	11.66655	17.51635	16.56345	H	24.58	13.26939	21.20708
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Au	13.13301	16.05446	18.67195	H	25.05286	15.37089	18.75693
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S	21.11698	22.32593	18.05561	H	23.66239	13.71045	6.868956
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Au	14.47097	18.90865	23.63845	H	23.86995	21.1375	13.14212
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Au	18.87994	14.75953	23.66683	H	8.264453	5.451624	12.47703
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Au	18.20796	5.228126	17.19969	H	15.62327	7.505726	4.250868
S	17.39468	5.372676	19.40412	H	16.27968	8.855604	5.249872
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S	14.37529	7.714186	6.320835	H	9.004537	20.2226	4.698345

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