Supporting information for the paper:

The Superstable 25-*kDa* Protected Silver Nanoparticle: Measurements & Interpretation as an Icosahedral $Ag_{152}(SCH_2CH_2Ph)_{60}$ Cluster

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Contents

Supporting information 1

Materials and methods:

1. Chemicals

Silver nitrate ($AgNO_3$, 99% Aldrich), sodium borohydride ($NaBH_4$, 99.9%, Aldrich); 2-phenylethanethiol (PETH, 98%, Aldrich); ethanol (Changshu Yangyuan Chemical, China, AR grade), THF (MARC, HPLC grade) and toluene (Ranken, AR grade) were used in this synthesis. All the chemicals were commercially available and were used without further purification.

2. Synthesis of $Ag_{152}(SCH_2CH_2Ph)_{60}$

The synthesis of Ag_{152} cluster protected by PET (2-phenylethanethiolate) involves the following processes. Initially, at room temperature (35-40°C, relative humidity-80%) 23 mg of $AgNO_3$ and 100 µL of PETH were ground well in a clean agate mortar using a pestle. The color of the mixture changes to pale orange showing the formation of silver thiolate. To this mixture, 25 mg of solid $NaBH_4$ were added and the content was mixed well. 3 mL of ethanol was added to the mixture and mixed well after which 2 mL of ethanol was added for the washing the mixture. The mixture was kept for 15-30 sec till there is a color change from pale orange to deep grey. The contents were then taken into a centrifuge tube and centrifuged at 1600 rpm. The centrifugate was removed and the residue was dissolved in 5 mL toluene/THF. The Ag_{152} clusters were obtained from the toluene extract, which was dark brown in color. The toluene extracted cluster is stable for 10 days in the laboratory conditions and in deep freezer, it is stable for one month but THF extracted cluster is stable up to 2 days. The calculated yield is 82%.

The cluster is not stable in presence of excess thiol. It is this thiol that is removed by extraction with ethanol. However, ethanol also adds water and with more water, the cluster size increases. Therefore, it is important to optimize the time of exposure of ethanol. Humidity of the laboratory air is also an important factor.

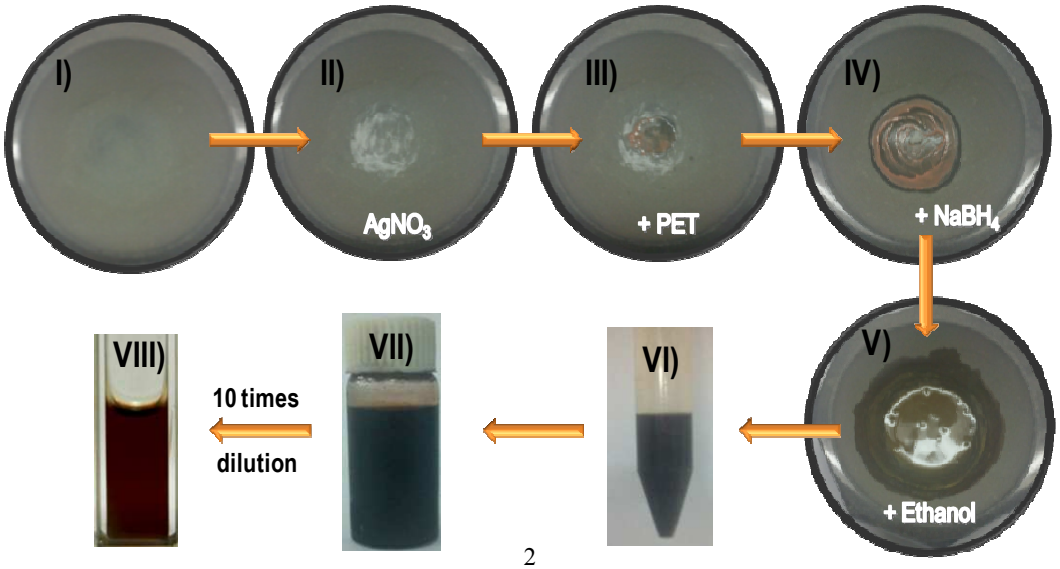

Figure S1. Photographs of various steps during the synthesis. I) Empty mortar, II) ground silver nitrate, III) addition of PETH to II, IV) addition of $NaBH_4$ to III, V) ethanol additionto IV, VI) reaction mixture in centrifuges tube for centrifugation, VII) residue after centrifugation, extracted in toluene and VII) cluster in cuvette after 10 times dilution.

3. Instrumentation:

UV-Vis spectra were measured with a Perkin Elmer Lambda 25 instrument in the range of 200-1100 nm. Luminescence measurements were carried out on a Jobin Vyon NanoLog instrument. The band pass for excitation and emission was set as 2 nm. High resolution transmission electron microscopy of clusters was carried out with a JEOL 3010 instrument. The samples were drop casted on carbon-coated copper grids and allowed to dry under ambient conditions. Matrix-assisted desorption ionization mass spectrometry (MALDI MS) studies were conducted using a Voyager-DE PRO Biospectrometry Workstation from Applied Biosystems. The matrix used was DCTB (at 1:100 ratio of sample to matrix). A pulsed nitrogen laser of 337 nm was used for the MALDI MS studies. Mass spectra were collected in positive ion mode and were averaged for 200 shots. Scanning electron microscopic (SEM) and energy dispersive X-ray (EDAX) analyses were performed with a FEI QUANTA-200 SEM. For measurements, samples were drop casted on an indium tin oxide (ITO) coated glass and dried in vacuum. Transmission small angle X-ray scattering (SAXS) measurements of toluene solution of the clusters were performed with a Rigaku SmartLab X-ray diffractometer operating at 9 kW (200 mA; 45 kV) using Cu-Ka radiation. A NANO-Solver programme of Rigaku was used. Nonlinear least square method was used for finding the best first. For SAXS measurements cluster solutions were taken in a sealed silica glass capillary of 1 mm diameter 1 mm. HPLC measurement was done in Shimadzu HPLC system equipped with a C18 column (Shimadzu).

Supporting information 2

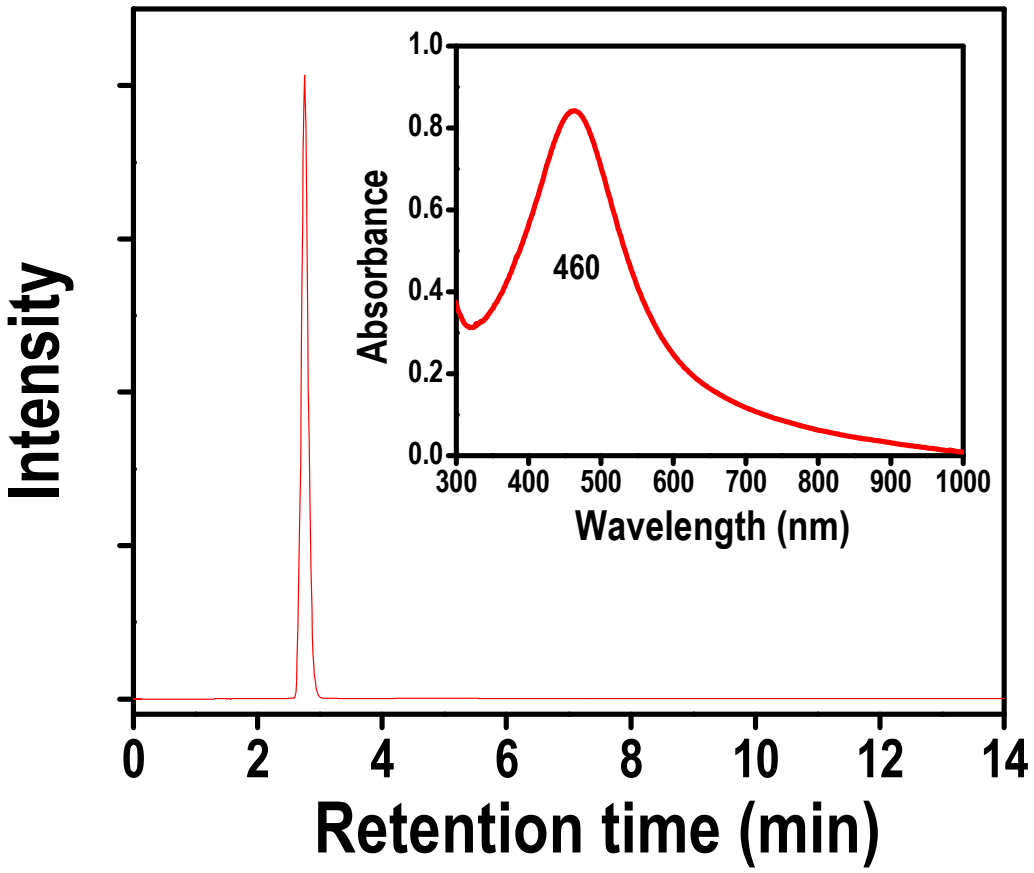

Figure S2. Chromatogram of Ag_{152} cluster extracted in THF. In this experiment, a high-performance liquid chromatography (HPLC) system equipped with a C18 column (250 X 4.6 mm) was used with a flow rate of 1 mL/min. The UV–vis absorbance detector was operated at 400 nm. The spectrum shows the presence of a single cluster. Inset: UV/Vis spectrum of the isolated cluster with a peak maximum at 460 nm.

Supporting information 3

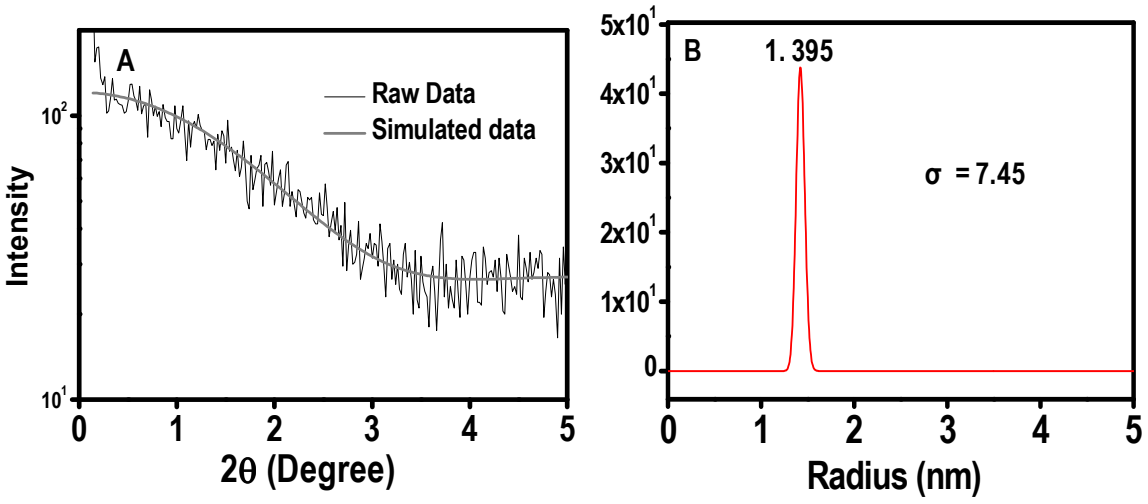

Figure S3. Small angle X-ray scattering (SAXS) analysis of the Ag_{152} cluster. Experimental and simulated (nonlinear least squares method) SAXS curves are shown in the left side (A) and the corresponding particle size distribution obtained from SAXS profile is shown in the right panel (B). Corresponding dispersion (σ) is given in the inset. It shows a great homogeneity in particle size.

Supporting information 4

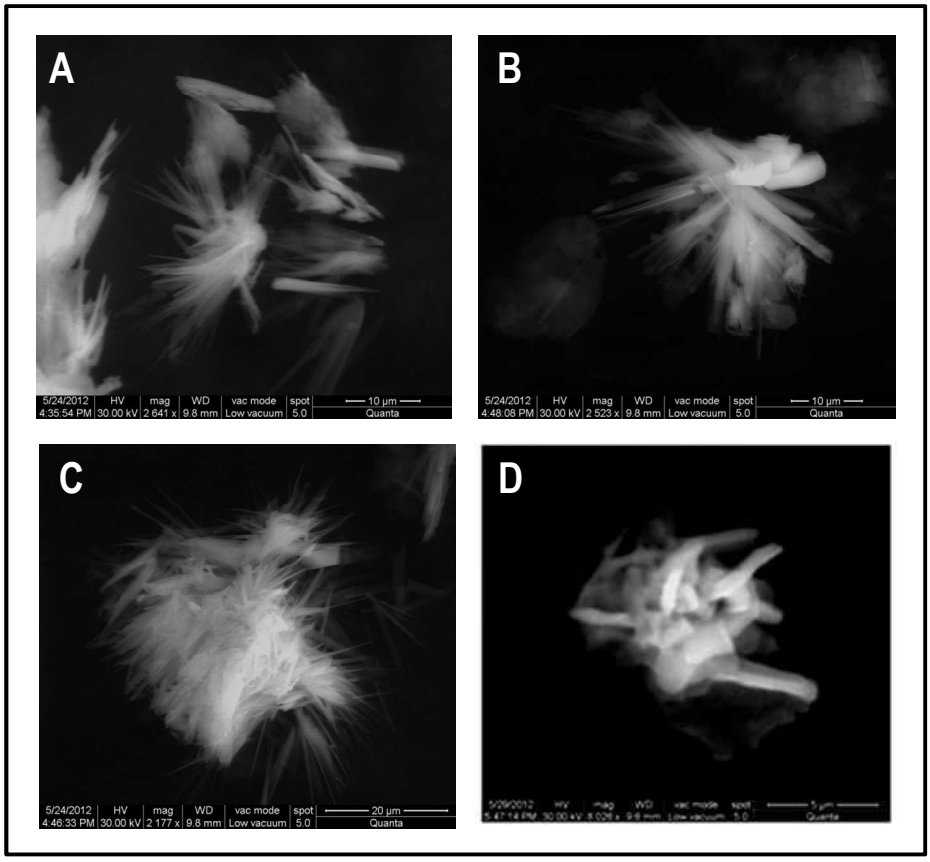

Figure S4. SEM images of as synthesized Ag_{152} cluster. After removal of toluene using rotavapor, the solid mass was taken on an ITO glass plate for imaging.

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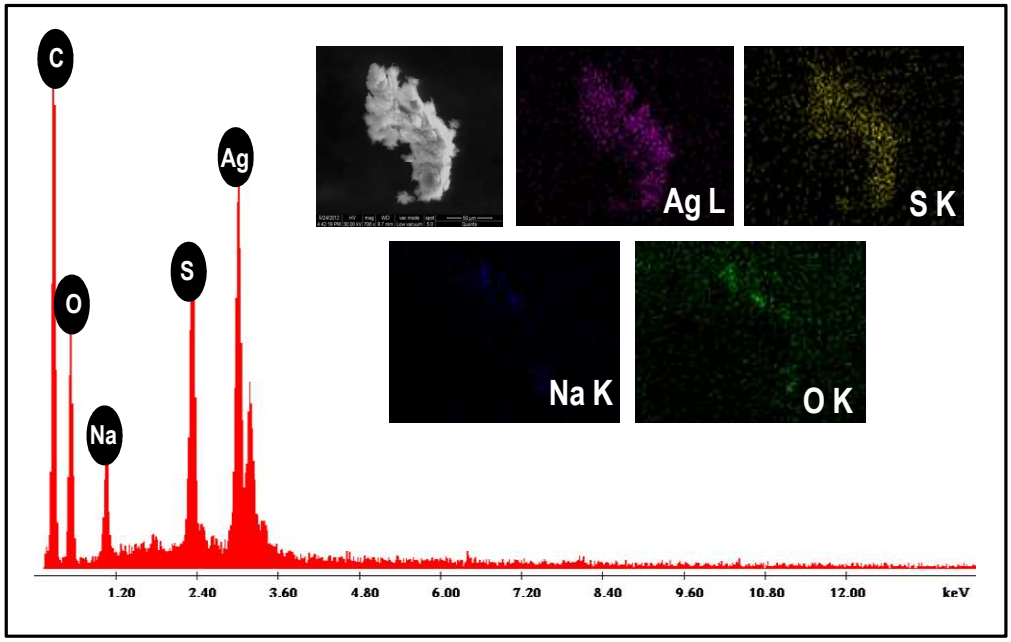

Figure S5. Elemental mapping of a specified area was taken which shows the presence of silver and sulfur at a ratio of 2.2:1. A little excess of thiol was seen compared to the expected composition (2.5:1) which may be needed for cluster stabilization in the solid state.

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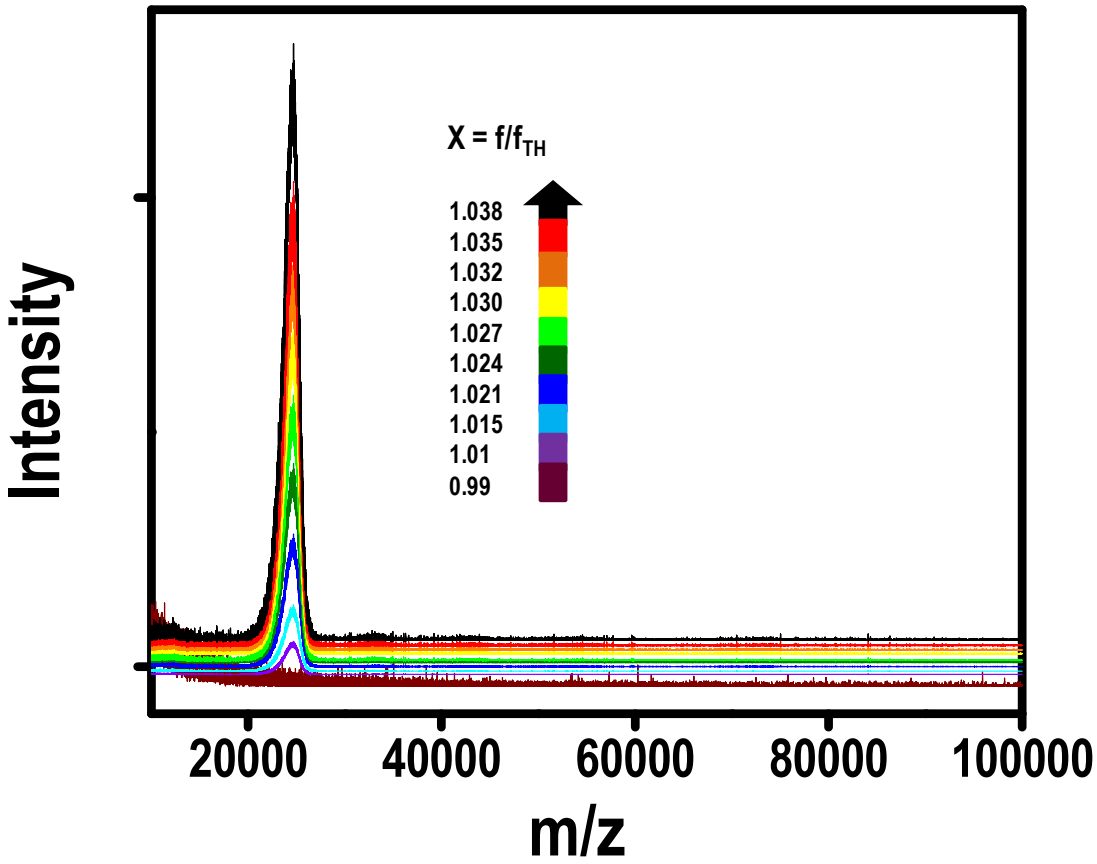

Figure S6. MALDI MS spectra for as-synthesized Ag_{152} cluster measured at varying laser fluence, expressed interms of the threshold fluence f_{TH} corresponding the detection of ions; f = x f_{TH}, x= 0.99 to x = 1.04. The ion signal increases with increase in laser fluence in this window. Subsequently, no further increase in ion intensity was observed; however at still higher laser intensity, frangmentation commences (see Figure S7).

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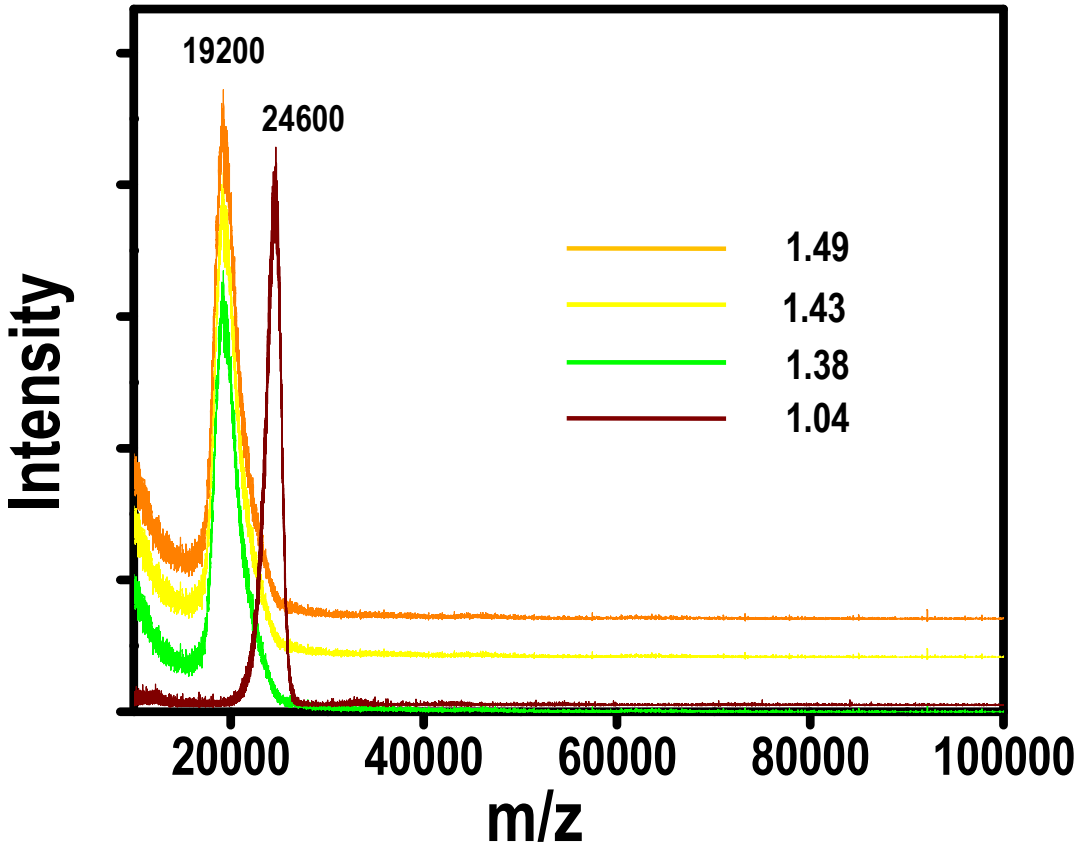

Figure S7. MALDI MS data for as-synthesized Ag_{152} cluster measured at varying laser fluence, expressed in terms of the threshold fluence f_{TH} corresponding the detection of ions; f = x f_{TH}, x= 1.04 to x = 1.49. In this fluence-window fragmentation occurs. The fragment-ion signal increases with increase in laser fluence (see peak at m/z 19200). Beyond a critical value no further change happens. The spectrum at a lower laser power showing the feature at m/z 24,600 is shown for comparison. Data corresponding to in-between laser intensities are shown in Figure 2 of the text.

Supporting information 8

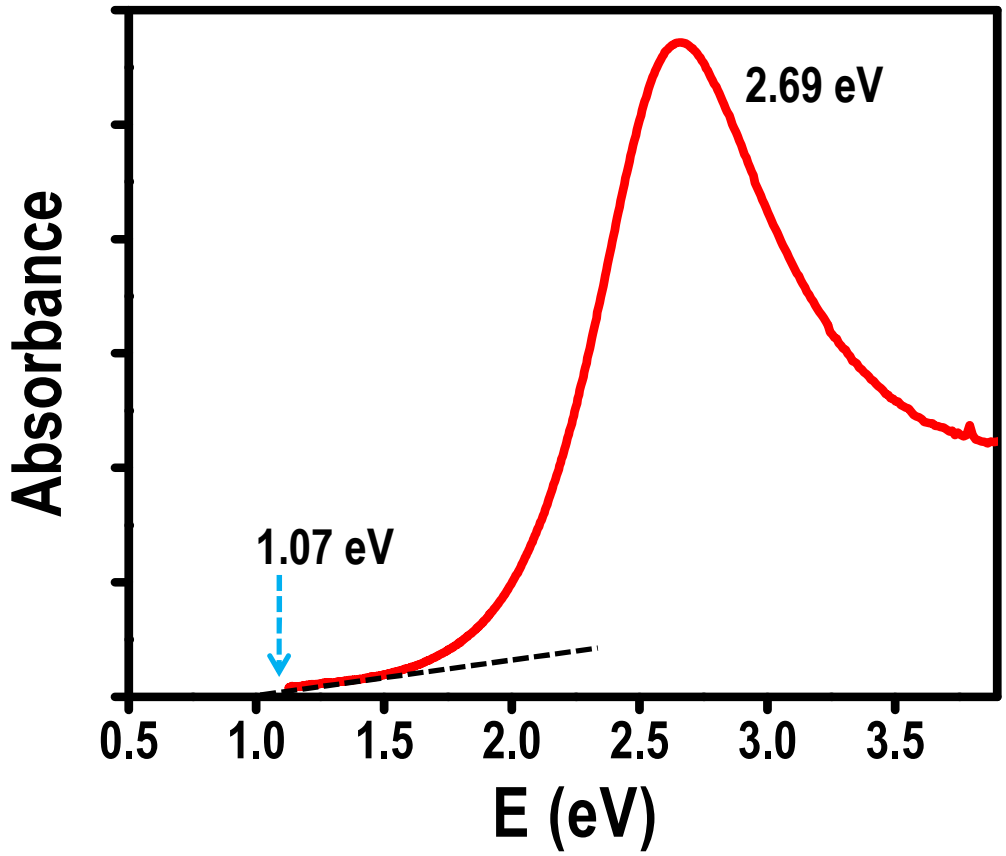

Figure S8. Absorbance spectrum in terms of energy in eV. A band at 2.66 eV was observed along with a threshold of 1.07 eV.

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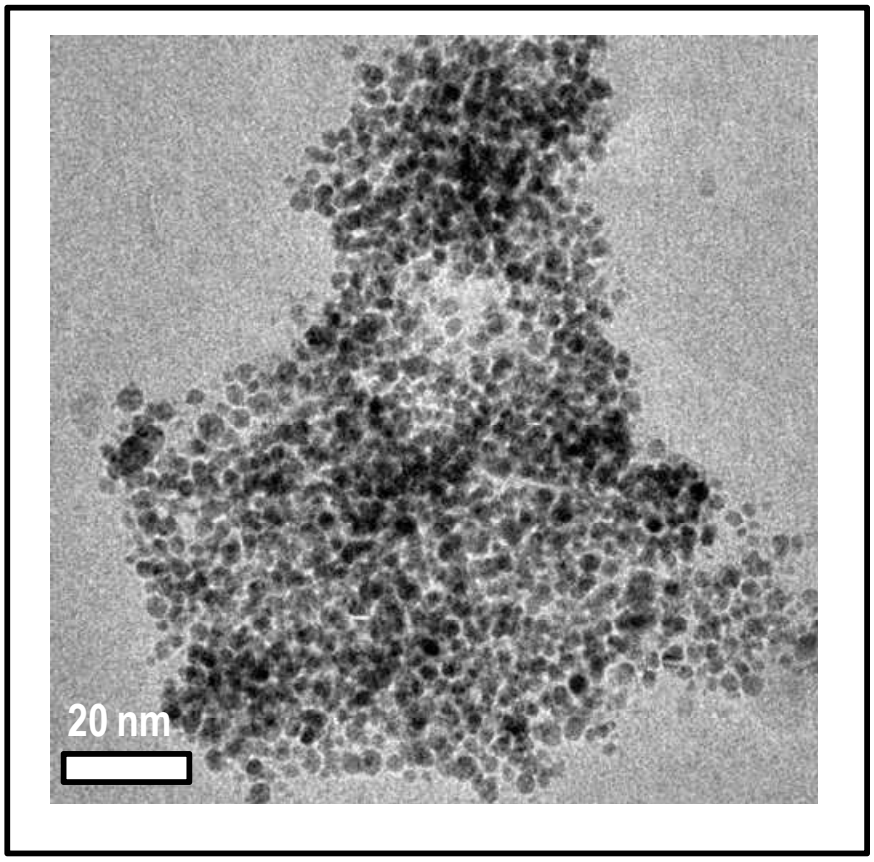
TEM image of Ag@PET nanoparticles



Supporting information 10
Assembly of Ag_{92} (core) cluster

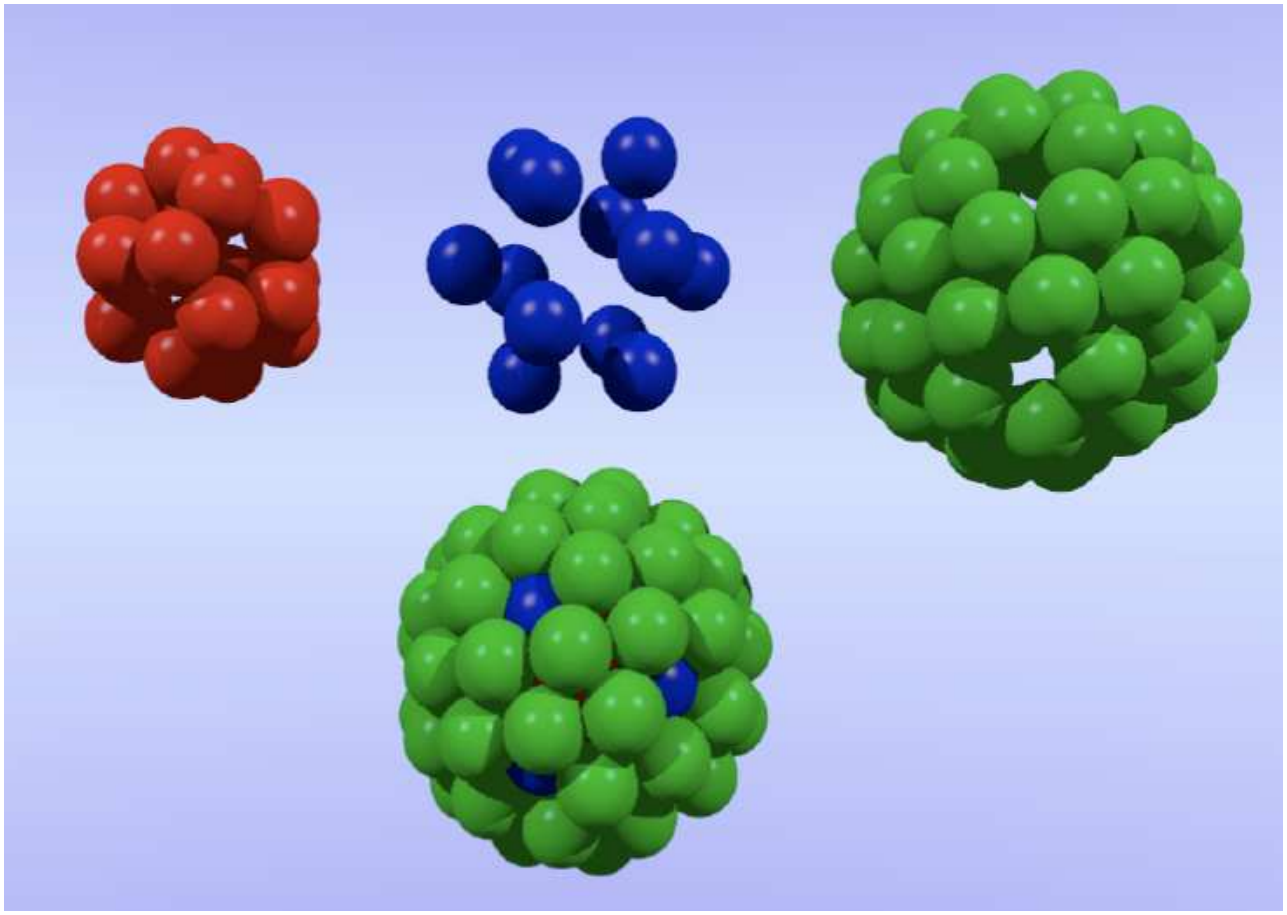


Figure S10. Schematic illustration of the assembly of the ideal 92 atom core, *Icosahedral I-92*. TOP ROW: (left, red) 20 Ag atom Pentagonal Dodecahedron and (middle, blue) surrounding 12 Ag atom Icosahedron, with the two forming the first (inner) 32 Ag atom shell; (right, green) 60 Ag atom encapsulating (second shell) Snub Dodecahedron. BOTTOM ROW: 92 Ag atom assembled Core. Source: Adapted from T. G. Schaaff, unpublished (2006).

Supporting information 11
Inner core structures of Ag_{92}^{2+} and Ag_{94}^{2+}

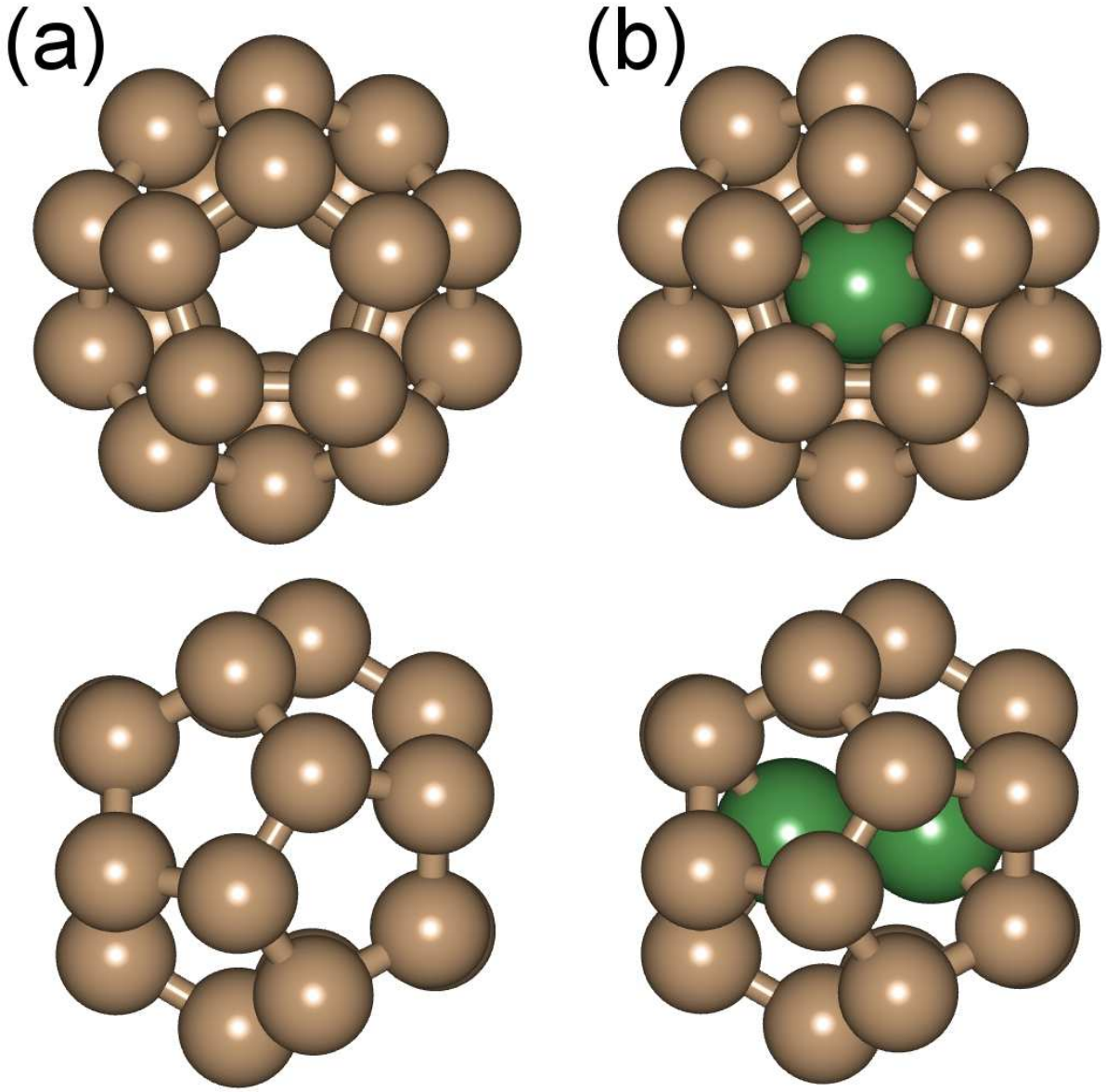


Figure S11. **(a)** Two views of the Pentagonal dodecahedral inner core of the relaxed Ag_{92}^{2+} cluster. **(a)** (b) Two views of the Pentagonal dodecahedral inner core of the relaxed Ag_{94}^{2+} cluster. The two extra atoms inside the dodecahedron are colored green. The interatomic distance between the two inner Ag atom d(Ag-Ag) = 2.83Å, and the mean distance between an inner Ag atom and an Ag atom on the nearest pentagonal face is 2.94 Å.

Supporting information 12
Radial distances for $Ag_{152}(SH)_{60}^{2+}$ and $Ag_{154}(SH)_{60}^{2+}$

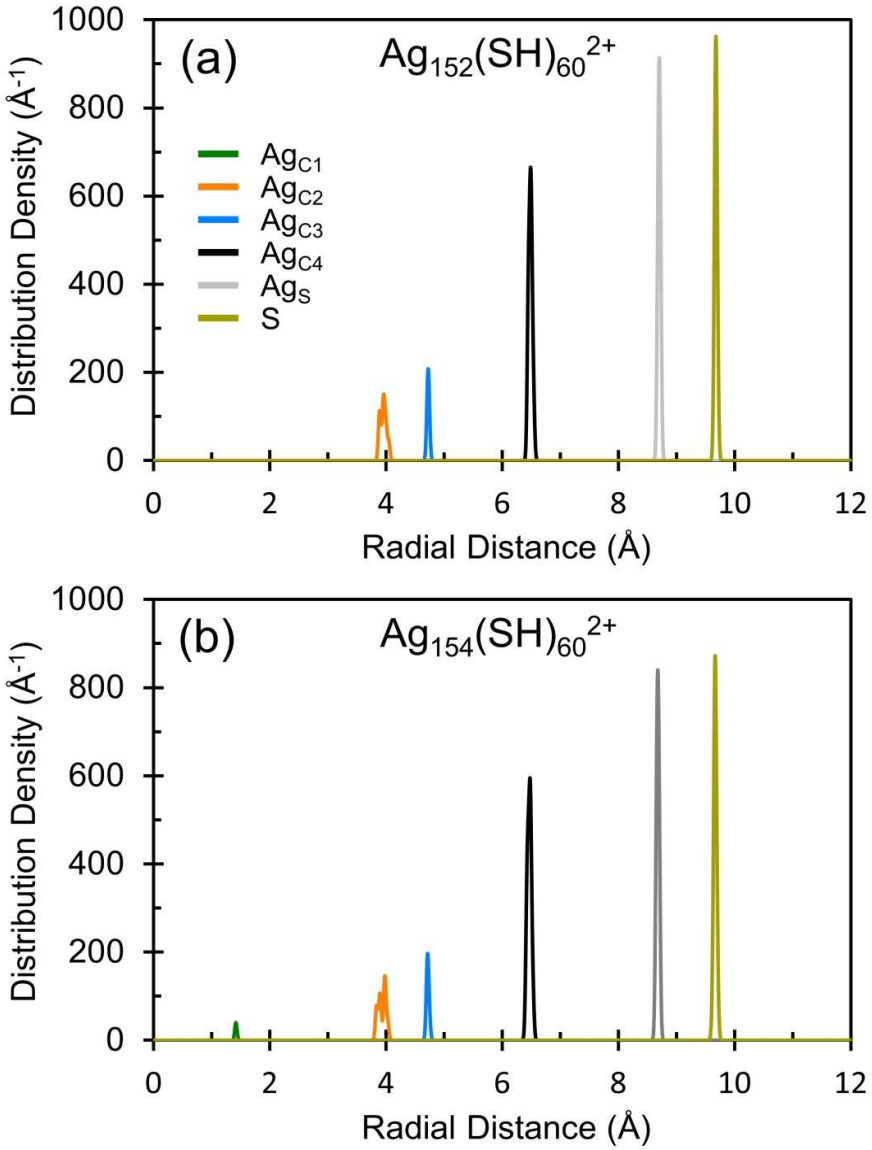


Figure S12. Radial distances for (a) $Ag_{152}(SH)_{60}^{2+}$ and (b) $Ag_{154}(SH)_{60}^{2+}$, measured from the center of the clusters.

Ag_{C1} : Ag dimer in the core

Ag_{C2} : 20-atom dodecahedron in the core

Ag_{C3}: 12 capping Ag atoms on the faces of dodecahedron

Ag_{C4} : 60-Ag-atom shell in the core

Ag_S : 60-Ag-atom outer shell

S : sulfur atoms

Supporting information 13

Projected density of states

The projected local density of states (PDOS) (1), $w_{i,\,l}(R_0)$ was calculated from the Kohn-Sham (KS) orbitals $\psi_i(\mathbf{r}+\mathbf{R}_{cm})$, where $\mathbf{R}_{cm}$ is the center of mass of the cluster (taken from here on as the origin, $\mathbf{R}_{cm} = 0$), using

$$w_{i,\,l}(R_0) = \sum_{m=-l}^{l} \int_0^{R0} r^2 dr \; |\varphi_{i,lm}(r)|^2$$

$$\varphi_{i,lm}(r) = \int d\Omega \; Y_{lm}(\Omega) \; \psi_i(\mathbf{r})$$

Here, Y_{lm} is the spherical harmonic function with angular momentum number l and magnetic quantum number m, and the angular momenta up to l = 6 (I symmetry) are included; the symmetries associated with the angular momentum numbers l = 0,1,2…..,6 are denoted as S,P,D,F,G,H and I, respectively. The integration is taken in a sphere of radius R_0, chosen as follows for Ag_{92}^{++} : R_0 = 11.4 Å and for $Au_{92}(AgSH)_{60}$: R_0 = 7.6 Å.

(1) B.Yoon *et al.* Size-Dependent Structural Evolution and Chemical Reactivity of Gold Clusters. *ChemPhysChem* **8**, 157- 161 (2007).

Supporting information 14

Coordinate file for the optimized $Ag_{152}(SH)_{60}^{2+}$ cluster

Coordinates of Ag_{92}^{++} cluster (element x y z):

Ag	0.752565	2.283295	3.133637
Ag	2.357669	0.001888	3.080903
Ag	1.185169	3.646204	0.730142
Ag	-1.887624	1.398449	3.109269
Ag	3.838411	0.002623	0.716517
Ag	0.747340	-2.279548	3.132133
Ag	-1.176478	3.645008	-0.737800
Ag	3.095906	2.257852	-0.749036
Ag	-1.889690	-1.393433	3.119143
Ag	-3.095603	2.271838	0.744787
Ag	3.078952	-2.249063	-0.750801
Ag	1.182329	-3.650029	0.731682
Ag	-0.750477	2.285118	-3.146674
Ag	1.888804	1.398986	-3.114206
Ag	-3.078210	-2.257184	0.747978
Ag	-3.800016	0.002038	-0.718364
Ag	1.895171	-1.392033	-3.126091
Ag	-1.182178	-3.655543	-0.738161
Ag	-2.353206	0.000769	-3.098757
Ag	-0.742955	-2.281619	-3.136094
Ag	3.467682	2.517425	2.128473
Ag	-1.316506	4.089817	2.149922
Ag	0.021939	0.002692	4.808978
Ag	3.465158	-2.510643	2.129846
Ag	1.317465	4.089561	-2.158360
Ag	-4.248013	0.004343	2.153448
Ag	4.257215	0.003135	-2.160201
Ag	-1.308450	-4.088341	2.149553
Ag	-3.457026	2.521503	-2.138536
Ag	1.313433	-4.083525	-2.155046
Ag	-0.014006	0.003132	-4.813318
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Ag	1.380317	2.209858	5.939215
Ag	2.539478	-0.623028	5.906376
Ag	3.983755	1.691730	4.774006
Ag	2.551184	4.280482	4.149097
Ag	-0.355265	4.335520	4.803262
Ag	-1.644978	1.991213	5.921998
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Ag	2.867388	-3.282198	4.793081
Ag	4.840921	-1.065269	4.122254
Ag	5.869777	1.067690	2.463722
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Ag	-3.277550	3.704241	4.142177
Ag	-4.188497	0.967659	4.807155
Ag	-2.369805	-0.980867	5.935834
Ag	-2.199192	-3.713279	4.802754
Ag	0.499656	-4.954496	4.148620
Ag	2.846819	-5.241823	2.472214
Ag	6.070752	-1.696460	1.409148
Ag	6.409609	0.604556	-0.420153
Ag	5.555416	3.257022	0.378086
Ag	3.918299	4.924926	-1.437916
Ag	1.398500	6.294301	-0.399647
Ag	-1.382628	6.295002	0.390958

Ag	-3.916568	4.942704	1.431590
Ag	-5.365895	2.572848	2.490832
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Ag	-0.208880	-2.588337	-5.938435
Ag	-2.528281	-0.627120	-5.918263

Coordinates of $Ag_{92}(AgSH)_{60}^{++}$ cluster (element x y z):

Ag	0.771598	2.294144	3.177294
Ag	2.417707	0.001673	3.144356
Ag	1.201710	3.622222	0.732302
Ag	-1.892728	1.379798	3.101799
Ag	3.879332	0.012595	0.726156
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Ag	-3.222895	2.325688	0.775359
Ag	3.098384	-2.251853	-0.747873
Ag	1.205768	-3.693893	0.745488
Ag	-0.768402	2.286000	-3.163730
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Ag	-3.089166	-2.254103	0.759849
Ag	-3.868379	0.005266	-0.718883
Ag	1.946348	-1.441430	-3.190002
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Ag	-2.421666	-0.003918	-3.149597
Ag	-0.753687	-2.289541	-3.140011
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Ag	-1.371047	6.284833	0.461699
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Ag	1.456422	6.507570	5.598155
Ag	0.067686	4.174048	7.614236
Ag	4.047495	1.229957	7.621216
Ag	6.660883	0.630838	5.595890
Ag	4.892354	-1.946890	6.941671
Ag	-2.757795	4.429172	6.940977
Ag	-5.667540	3.352978	5.666609
Ag	-3.926734	1.343633	7.637041
Ag	2.459162	-3.399585	7.616114
Ag	2.671895	-6.093996	5.625362
Ag	-0.352339	-5.227993	6.963301
Ag	8.018983	-0.631562	3.338610
Ag	8.606882	-1.298359	0.084006
Ag	8.408361	1.906876	1.220093
Ag	3.077018	7.395833	3.343284
Ag	0.770056	8.549110	1.233241
Ag	3.803451	7.819734	0.220997
Ag	-2.467614	-3.357012	7.646065
Ag	-4.988618	-4.473236	5.596615
Ag	-5.033303	-1.272037	6.992165
Ag	1.883146	-7.805031	3.380893
Ag	1.474156	-8.591253	0.169490
Ag	4.445939	-7.363949	1.225945
Ag	6.172763	6.154773	-0.053326
Ag	6.083286	5.192686	-3.439492
Ag	7.942893	3.381901	-1.258267
Ag	-0.736319	8.544532	-1.251412
Ag	-3.083680	7.371343	-3.369227

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Ag	-6.076614	5.209233	3.443493
Ag	-7.966038	3.336048	1.258925
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Ag	-6.823402	-4.217461	3.344361
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Ag	7.685334	-4.042038	-0.177982
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H	-10.311729	-2.250187	-2.178837
H	-4.162444	-9.884856	0.034617
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H	-4.370622	-9.102424	-3.675255
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H	-2.315862	4.245437	-9.602132
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