Supplementary Information for:

Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: $Au_{36-x}Ag_x(SPh\textit{t}Bu)_{24}$

Shevanuja Theivendran[1,‡], Le Chang[2,‡], Aneek Mukherjee[1], Luca Sementa[3], Mauro Stener[4], Alessandro Fortunelli[3,*], Amala Dass[1,*]

1 Department of Chemistry and Biochemistry, University of Mississippi, Oxford, MS 38677, United States

2 Beijing Key Laboratory of Energy Environmental Catalysis, State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, Beijing 100029, People's Republic of China

3 CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche, via Giuseppe Moruzzi 1, 56124, Pisa, Italy

4 Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, Trieste I-34127, Italy

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Table of contents

	Doping site	Doping Species	Total Energy (Ry)	Relative Energy (eV)
/	$Au_{36}(SCH_3)_{24}$	/	-3983.21483359	/
/	$Ag_{36}(SCH_3)_{24}$	/	-4324.91701202	/
	$Au_{36}(SCH_3)_{24}$_Ag01	Ex-Td	-3992.72266360	0.000
	$Au_{36}(SCH_3)_{24}$_Ag02	Ex-Td	3992.72200419	0.009
	$Au_{36}(SCH_3)_{24}$_Ag03	Ex-Td	-3992.72149918	0.016
	$Au_{36}(SCH_3)_{24}$_Ag04	Ex-Td	-3992.72132501	0.018
	$Au_{36}(SCH_3)_{24}$_Ag05	In-Td	-3992.71382831	0.120
	$Au_{36}(SCH_3)_{24}$_Ag06	In-Td	-3992.71193892	0.146
	$Au_{36}(SCH_3)_{24}$_Ag07	In-Td	-3992.71055014	0.165
One Doping Ag atom	$Au_{36}(SCH_3)_{24}$_Ag08	In-Td	-3992.71034110	0.168
	$Au_{36}(SCH_3)_{24}$_Ag09	Edge	-3992.71140630	0.153
	$Au_{36}(SCH_3)_{24}$_Ag10	Edge	-3992.70919639	0.183
	$Au_{36}(SCH_3)_{24}$_Ag11	Edge	-3992.70800429	0.199
	$Au_{36}(SCH_3)_{24}$_Ag12	Ex-St-near	-3992.70839655	0.194
	$Au_{36}(SCH_3)_{24}$_Ag13	Ex-St-far	-3992.69777108	0.339
	$Au_{36}(SCH_3)_{24}$_Ag14	In-St	-3992.69972761	0.312
	$Au_{36}(SCH_3)_{24}$_Ag15	In-St	-3992.69601530	0.363
	$Au_{36}(SCH_3)_{24}$_Ag0102	Ex-Td& Ex-Td	-4002.22998774	0.000
	$Au_{36}(SCH_3)_{24}$_Ag0103	Ex-Td& Ex-Td	-4002.22949861	0.007
	$Au_{36}(SCH_3)_{24}$_Ag0104	Ex-Td& Ex-Td	-4002.22930947	0.009
	$Au_{36}(SCH_3)_{24}$_Ag0203	Ex-Td& Ex-Td	-4002.22880981	0.016
	$Au_{36}(SCH_3)_{24}$_Ag0204	Ex-Td& Ex-Td	-4002.22866953	0.018
	$Au_{36}(SCH_3)_{24}$_Ag0304	Ex-Td& Ex-Td	-4002.22817767	0.025
Two Doping Ag atom	$Au_{36}(SCH_3)_{24}$_Ag0112	Ex-Td& Ex-St-near	-4002.21625316	0.187
	$Au_{36}(SCH_3)_{24}$_Ag0312	Ex-Td& Ex-St-near	-4002.21260017	0.236
	$Au_{36}(SCH_3)_{24}$_Ag0506	In-Td& In-Td	-4002.20923881	0.282
	$Au_{36}(SCH_3)_{24}$_Ag0507	In-Td& In-Td	-4002.20778053	0.302
	$Au_{36}(SCH_3)_{24}$_Ag0508	In-Td& In-Td	-4002.20682878	0.315
	$Au_{36}(SCH_3)_{24}$_Ag0608	In-Td& In-Td	-4002.20564960	0.331
	$Au_{36}(SCH_3)_{24}$_Ag0607	In-Td& In-Td	-4002.20507634	0.339
	$Au_{36}(SCH_3)_{24}$_Ag0708	In-Td& In-Td	-4002.20420229	0.351
	$Au_{36}(SCH_3)_{24}$_Ag010203	Ex-Td	-4011.73696186	0.000
	$Au_{36}(SCH_3)_{24}$_Ag010204	Ex-Td	-4011.73680699	0.002
	$Au_{36}(SCH_3)_{24}$_Ag010304	Ex-Td	-4011.73633075	0.009
Three Doping Ag atom	$Au_{36}(SCH_3)_{24}$_Ag020304	Ex-Td	-4011.73566179	0.018
	$Au_{36}(SCH_3)_{24}$_Ag050607	In-Td	-4011.70053719	0.496
	$Au_{36}(SCH_3)_{24}$_Ag050608	In-Td	-4011.70037119	0.498
	$Au_{36}(SCH_3)_{24}$_Ag050708	In-Td	-4011.69884775	0.519

	$Au_{36}(SCH_3)_{24}$_Ag060708	In-Td	-4011.69685610	0.546
Four Doping Ag atoms	$Au_{36}(SCH_3)_{24}$_Ag01020304	Ex-Td	-4021.24396649	0.000
	$Au_{36}(SCH_3)_{24}$_Ag05060708	In-Td	-4021.18965746	0.739
Eight Doping Ag atoms	$Au_{36}(SCH_3)_{24}$_Ag0102030405060708	Ex-Td& In-Td	-4059.22451426	0.000
	$Au_{36}(SCH_3)_{24}$_ Ag0102030412 Ex-St else	Ex-Td& Ex-St-near	-4059.20986787	0.199

Table S1. Nomenclature and total and relative energies of $Au_{36}(SCH_3)_{24}$, $Ag_{36}(SCH_3)_{24}$, $Ag_1Au_{35}(SCH_3)_{24}$, $Ag_2Au_{34}(SCH_3)_{24}$, $Ag_3Au_{33}(SCH_3)_{24}$, $Ag_4Au_{32}(SCH_3)_{24}$, and $Ag_8Au_{28}(SCH_3)_{24}$ clusters with doping Ag atoms at different doping sites.

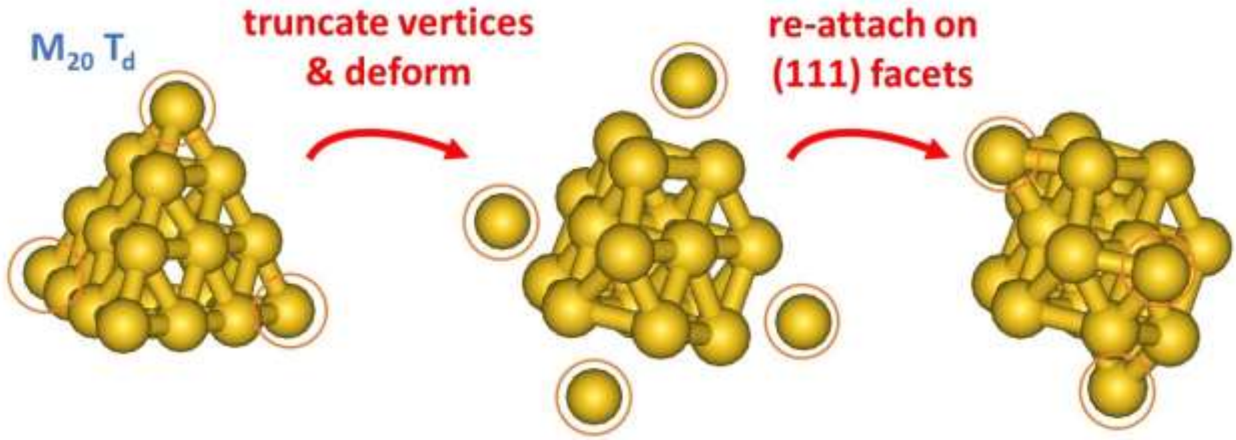


Figure S1. Transformation from a 20-atom tetrahedron (T_d) to the misplaced and deformed metal core of $Au_{36}(SPh\text{-}R)_{24}$. The vertices of M_{20} T_d are truncated and re-attached on fcc (111) facets (in such a way that they still define a 4-atom T_d), while the body of the cluster is slightly deformed.

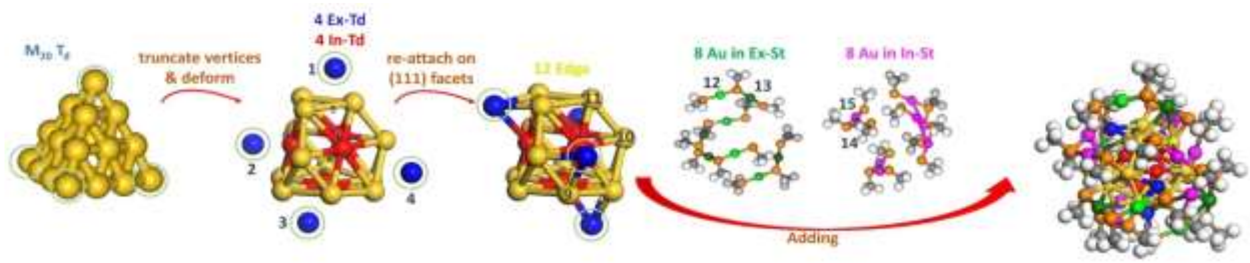


Figure S2: Formation diagram of the $Au_{36}(SCH_3)_{24}$ cluster, going from left to right: 20-atom tetrahedron has its vertexes truncated and re-attached on (111) facets as in Fig.S1. These 4 atoms are named external Td or Ex-Td (labelled as 1, 2, 3, 4, plotted in blue). The atoms on (111) facets are named internal Td or In-Td (labelled as 5, 6, 7, 8, plotted in red), while the 12 atoms on the edges are named Edge (only 3 of them are numbered explicitly, labelled as 9, 10, 11, plotted in yellow). There are two types of staples: external and internal ones, and these are added to the 20-atom core to make up the whole cluster as illustrated in the middle/right section. In the external staples, or Ex-St, there are 8 Au atoms, of which 4 (named Ex-St-near) are close and bind to Ex-Td core Au atoms and are plotted in light green (a representative one of these is labelled as 12) while other 4 (named Ex-St-far) do not bind to any core Au atoms and are plotted in dark green (a representative one of these is labelled as 13). In the internal staples, or In-St, there are 8 Au atoms, plotted in light pink and dark pink, and representative ones labelled as 14 and 15, respectively.

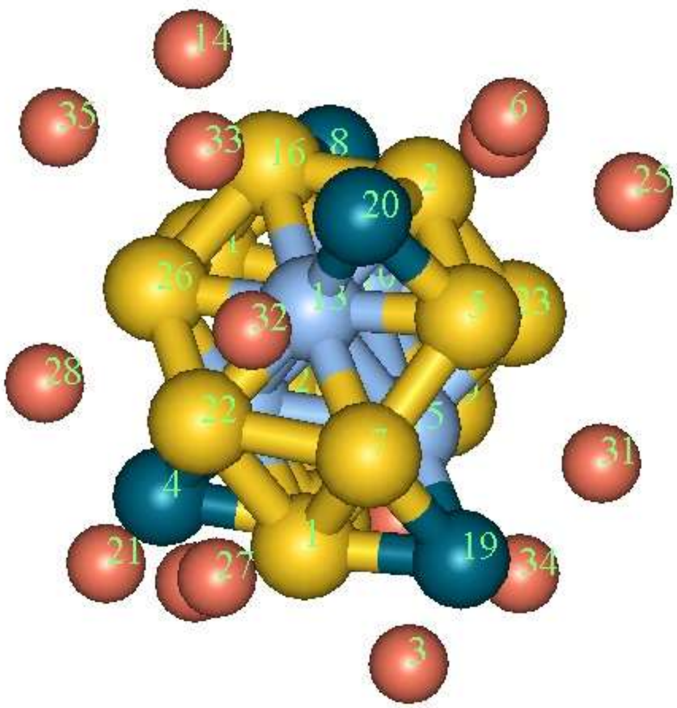


Figure S3. 36-atom metal framework of $Au_{36}(SPh\text{-}R)_{24}$. Atoms of staple motifs are colored in red, atoms in external T_d sites in dark blue, atoms in edge sites in yellow, and atoms in internal T_d sites in light blue. Numbering is consistent with the Cartesian coordinates reported below and with Table S1.

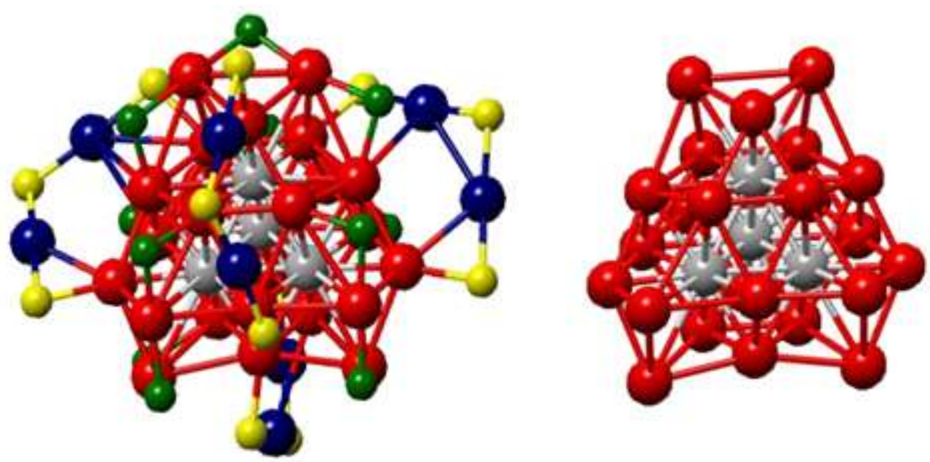


Figure S4. [left] Complete fcc $Au_{36}S_{24}$ motif with 8 dimeric staples. [right] Au_{28} motif only for clarity. Core locations (4 gold atoms in the center) for Ag incorporation are colored in silver color in both cases.

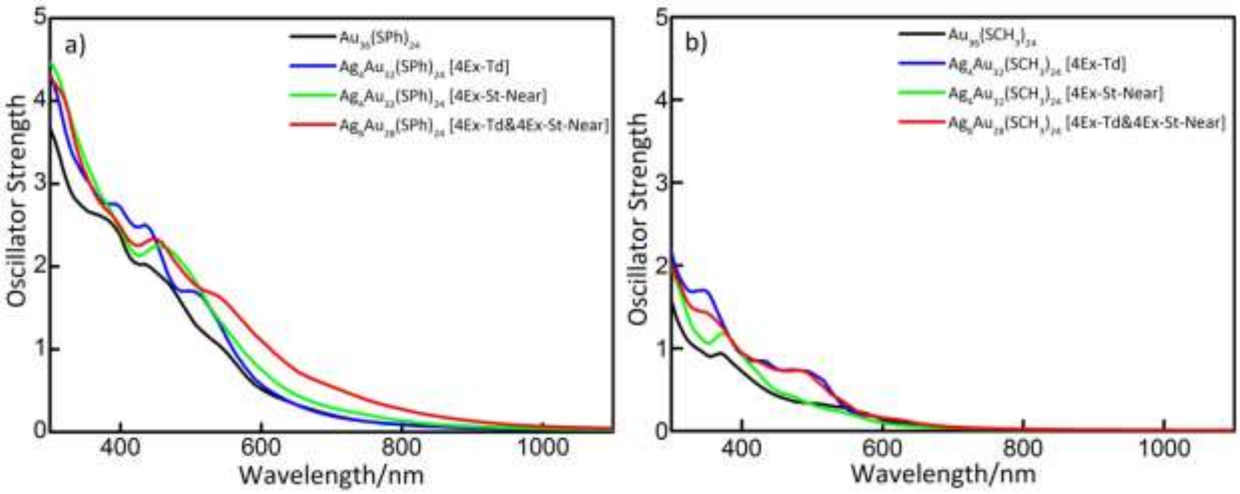
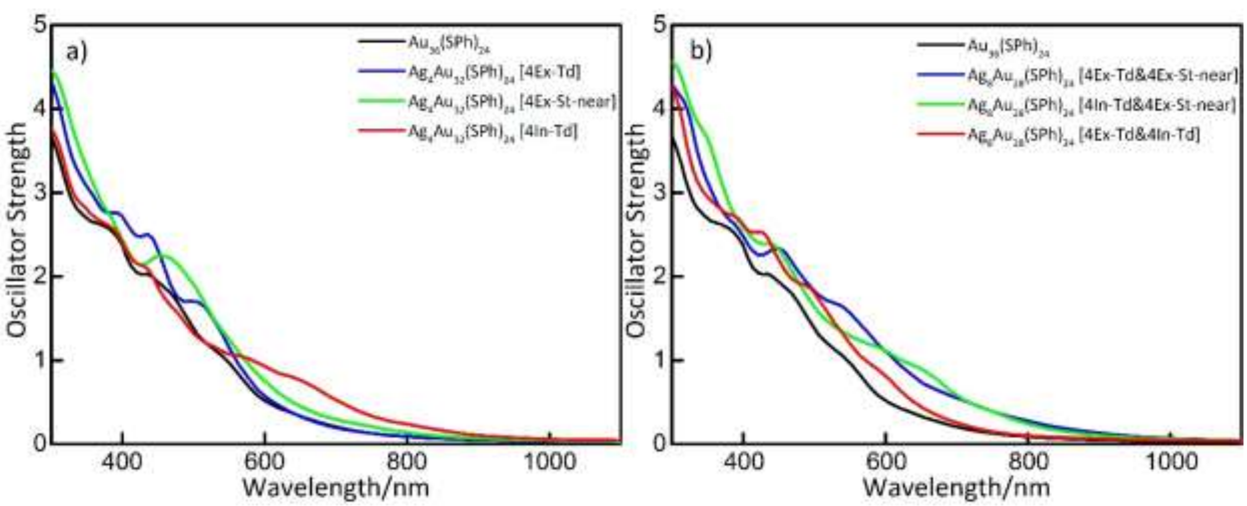


Figure S5: Simulated optical spectra of $Au_{36}(SR)_{24}$, $Ag_4Au_{32}(SR)_{24}$[4Ex-Td], $Ag_4Au_{32}(SR)_{24}$[4Ex-St-near], and $Ag_8Au_{32}(SR)_{24}$[4Ex-Td&4Ex-St-near] alloy nanomolecules with a) R = Ph, and b) R = CH_3.



F**igure S6. a)** Simulated optical spectra of $Au_{36}(SPh)_{24}$, $Ag_4Au_{32}(SPh)_{24}$ [4Ex-Td], $Ag_4Au_{32}(SPh)_{24}$[4Ex-St-near] and $Ag_4Au_{32}(SPh)_{24}$[4In-Td], respectively. **b)** Simulated optical spectra of $Au_{36}(SPh)_{24}$, $Ag_8Au_{32}(SPh)_{24}$[4Ex-Td&4Ex-St-near], $Ag_8Au_{32}(SPh)_{24}$[4In-Td&4Ex-St-near] and $Ag_8Au_{32}(SPh)_{24}$[4Ex-Td&4In-Td] respectively.

DFT and TDDFT approaches and further methodological and computational details

In the TDFT approach here employed, the photoabsorption spectrum $\sigma(\omega)$ is calculated for each value of the photon energy ω, from the imaginary part of the isotropic complex dynamical polarizability $\alpha(\omega)$:

$$\sigma(\omega) = \frac{4\pi\omega}{c}\,\mathrm{Im}[\alpha(\omega)] \qquad \text{(S1)}$$

Complex frequencies are employed: the real part ω_r corresponds to the actual photon frequency (energy) while the imaginary part ω_i corresponds to the broadening of the discrete lines and is interpreted as the excited state finite lifetime[1]. The TDDFT equations are represented in matrix form, using the density fitting f_μ auxiliary basis set. Within this formalism, the induced density is expanded according to the expression:

$$\rho_z^{(1)}(\omega,\vec{r}) = \sum_{\mu}^{K} f_\mu(\bar{r})\, b_\mu(\omega) \qquad \text{(S2)}$$

The TDDFT equations therefore reduce to the following non-homogeneous system of linear algebraic equations in matrix form:

$$[\mathbf{S} - \mathbf{M}(\omega)]\mathbf{b} = \mathbf{d}(\omega) \qquad \text{(S3)}$$

In equation (S3) $\mathbf{S}$ is the overlap matrix between fitting functions, $\mathbf{b}$ is the unknown vector with the expansion coefficients $b_\mu(\omega)$ of $\rho_z^{(1)}$ as in expression (S2), $\mathbf{M}(\omega)$ and $\mathbf{d}(\omega)$ are frequency-dependent matrix and vector whose elements are given in Refs.[2,3,4], where it is also shown that the approach is fully consistent with and produces an accuracy similar to alternative TDDFT approaches (such as the traditional Casida one). In practice, equation (S3) is solved for each value of the photon energy. We recall that present TDDFT implementation should be employed only below the ionization threshold, due to the localized nature of the basis set of Slater Type Orbitals (STO), which is suited for describing the long-range behavior in real space of the bound states only.

In relation to Independent Component Mapping of Oscillatory Strength (ICM-OS) plots plots, we add that in the main text we use the zz-diagonal element of the complex dynamical polarizability defined in Eq. (S1), i.e., $\alpha_{zz}(\omega) = \sum_{i}^{occ}\sum_{a}^{virt} \langle \varphi_i | z | \varphi_a \rangle P_i^a(z)$. Moreover, we note that in the ICM-OS plots we report the energies of the occupied orbitals (ε_i) on the X axis and the energies of the virtual orbitals (ε_a) on the Y axis. In the main text we report two-dimensional (contour) ICM-OS plots but full three-dimensional ICM plots can also be produced with the Z axis corresponding to ICM values. The ICM-OS values have been smeared by a Gaussian function with FWHM=0.12 eV to make them visually clearer. A complete description of the merits and usefulness of the ICM-OS analysis together with a comparison with previous alternative analyses will be given in a forthcoming article.

From the complex dynamical polarizability TDDFT approach we derive the simulated optical spectra reported in the main text and above. In particular in Figs. S5,S6 we report and compare the simulated optical spectra of alternative homotops with respect to those considered in the main text. In the main text it is shown how the spectrum of $Ag_4Au_{32}(SPh)_{24}$[4Ex-St-near] fairly reproduce the experimental one at low doping levels. In contrast, the spectrum of $Ag_4Au_{32}(SPh)_{24}$[4Ex-Td] in Fig. S5 exhibits an increase in intensity around 520 nm and below 450 nm and is thus in worse agreement with experiment. Note also that, as also shown in Figure S5, the $Ag_4Au_{32}(SPh)_{24}$[4In-Td] homotop only produces increased intensity beyond 600 nm and is thus in complete disagreement with experiment. The fact that Ag replacement in the internal core sites (In-Td) produces a spectrum in complete disagreement with experiment is also demonstrated by the optical spectrum of $Ag_8Au_{28}(SPh)_{24}$[4Ex-Td&4In-Td] in Fig. S6.

As for the DFT calculations, we report in Table S1 results obtained for simplified $(Ag\text{-}Au)_{36}(SCH_3)_{24}$ models at (atom numbering as in Figure S2). An analysis of these exploratory results can be summarized in terms of three main conclusions: 1) single-atom replacements indicate the following order of energetic preference of Ag doping: external T_d (Ex-Td) < internal T_d (In-Td, $\Delta E \approx 0.12\text{-}0.17$ eV) ≈ external staples close to external Td (Ex-St-near, $\Delta E \approx 0.19$ eV) < edges (Edge, $\Delta E \approx 0.16\text{-}0.2$ eV) < external staples far from external Td (Ex-St-far, $\Delta E \approx 0.34$ eV) ≈ internal staples (In-St, $\Delta E \approx 0.31\text{-}0.36$ eV), where ΔE is the energy difference with respect to the most stable external T_d configuration; 2) the energetic order is preserved when multiple Ag replacements are considered, so that the most stable homotops at higher Ag content can be predicted by occupying the most stable sites from single-replacement in ascending order ('aufbau' principle). Ag-Ag interactions in fact appear to be modest, and energy differences between multiple-replacement homotops can be roughly predicted as the sum of independent energy difference exchanges – e.g., the mixing energy for the first four replacements is nearly exactly linear in their number: $\Delta_{mixing}(01) = -0.22$ eV; $\Delta_{mixing}(01, 02) = -0.43$ eV; $\Delta_{mixing}(01, 02, 03) = -0.64$ eV; $\Delta_{mixing}(01, 02, 03, 04) = -0.85$ eV, with the mixing energy Δ_{mixing} defined above; 3) as mentioned in the main text, it is known from literature that Ag doping into staple sites is not usually favorable – however in the $Au_{36}(SR)_{24}$ cluster the four external staple sites close to external Td (Ex-St-near) represent an exception: doping into these sites is actually roughly as favorable as doping into the inner core (edge and internal Td) sites. To make one example, in the eight doping case the energy difference between the 4Ex-Td&4In-Td and 4Ex-Td&4Ex-St-near is only 0.2 eV. It is important to note that this energy difference is preserved when using the complete $(Ag\text{-}Au)_{36}(SCH_3)_{24}$ models and performing a full geometry relaxation. To summarize, the most favorable Ag doping into outer core sites (i.e., Ex-Td) is consistent with previous findings, but is not in agreement with experimental crystal structures[5] in which Ag at low doping occupies 4 staple metal atoms close to the external Td atoms, thus showing the the difficulty of theory in describing these aromatic and doped MPC (work is in progress to improve accuracy of theoretical approaches for these systems).

Cartesian coordinates of $Au_{36}(SCH_3)_{24}$ as predicted at the DFT/PBE-D2 level.

Au	0.101200000	-2.792500000	-1.501900000
Au	-0.140200000	3.555800000	-0.396100000
Au	-0.279100000	-3.464600000	-5.355100000
Au	0.468800000	-3.519100000	2.663400000
Au	-0.508000000	2.104600000	-2.655900000
Au	0.582500000	5.813300000	-3.216600000
Au	0.600300000	-0.605800000	-3.072900000
Au	-0.706600000	2.854900000	3.583300000
Au	0.760800000	-1.264300000	1.076600000
Au	-0.853200000	1.227400000	1.408000000
Au	0.972200000	0.641000000	3.493100000
Au	-1.143700000	-1.338300000	3.137500000
Au	1.236900000	1.087000000	-0.650100000
Au	1.287900000	3.530400000	5.762500000
Au	-1.288000000	-0.430900000	-0.997200000
Au	1.469700000	2.789200000	1.900500000
Au	-1.546300000	-2.870800000	0.918000000
Au	-1.638200000	-5.114100000	3.953600000
Au	-1.824100000	-1.906700000	-3.262500000
Au	1.951500000	3.222100000	-2.175400000
Au	2.404200000	-4.449600000	0.555700000
Au	2.668000000	-1.272100000	-0.968200000
Au	-2.712300000	1.903100000	-0.542600000
Au	-2.729400000	4.260700000	1.952100000
Au	-2.901800000	4.922500000	-2.364900000
Au	3.046600000	0.281600000	1.310100000
Au	3.059900000	-3.207100000	-3.861600000
Au	3.065800000	-2.309700000	3.451600000
Au	-3.124700000	-0.326200000	1.070200000
Au	-3.235100000	1.396400000	4.113000000
Au	-3.445600000	0.476800000	-3.765100000
Au	3.800900000	0.995900000	-3.128400000
Au	4.197800000	3.187700000	-0.257400000
Au	-4.208500000	-2.274200000	-1.502400000
Au	4.245700000	1.932300000	4.214500000
Au	-4.490800000	-2.913800000	3.092300000
S	0.631600000	-5.019000000	-0.819600000
S	0.677800000	-5.567700000	3.896800000
S	-0.884900000	4.349000000	5.446200000
S	-1.227100000	5.445100000	0.646100000
S	-1.530000000	6.717000000	-2.881800000
S	-1.631200000	1.566000000	-4.699700000
S	-1.955600000	-0.259600000	5.107400000
S	1.974200000	-3.464900000	-5.888900000
S	2.193200000	-0.792200000	4.983800000
S	2.289000000	0.084700000	-4.637700000
S	-2.600500000	-3.328900000	-5.013600000
S	2.770800000	5.038300000	-3.512400000
S	2.903200000	4.539300000	1.112700000
S	3.353000000	2.616200000	6.249100000
S	-3.391200000	-3.959600000	-0.125300000

S	-3.957200000	-4.953800000	4.084200000
S	4.147800000	-3.643500000	1.862900000
S	4.194300000	-2.851500000	-1.883200000
S	-4.303300000	3.184200000	-1.753400000
S	-4.442100000	3.033800000	2.971300000
S	5.098500000	1.062800000	2.246100000
S	-5.123700000	-0.845500000	2.251600000
S	-5.238900000	-0.536500000	-2.686500000
S	5.387100000	1.683800000	-1.561800000
C	-0.038367702	6.119618126	1.862069983
C	0.819517857	-6.818489183	2.565344508
C	1.000251264	-1.782396435	5.949571744
C	1.301056136	-5.845865962	-2.304298213
C	1.657404500	1.550325566	-5.529456450
C	-1.868620119	3.382443701	6.651831221
C	-2.057559083	7.223679237	-4.564641822
C	-2.234243847	3.150641104	-5.378977123
C	2.313894447	-5.199052876	-6.382792199
C	-2.715435861	-5.135019890	-1.354062455
C	-3.091790284	-1.426933938	5.929541730
C	-3.118282709	-2.115440414	-6.292526028
C	3.751362263	6.020040104	-2.315982665
C	3.913472108	5.028823903	2.569464852
C	4.372617289	4.055316293	6.758639106
C	-4.478796885	-6.158582491	2.802019932
C	4.619918626	-5.094718588	2.882037991
C	-5.105851720	4.165961782	4.267125162
C	-5.432045800	3.920138188	-0.515438919
C	5.698320789	-1.927564396	-2.367966679
C	6.022826585	-0.426218120	2.777494793
C	-6.106564070	-1.470675604	-4.003863986
C	-6.432759949	-1.214168963	1.030141996
C	6.498199250	2.737098433	-2.572635160
H	0.357846849	-2.377893590	5.290793431
H	-0.542760380	6.915336809	2.422821080
H	0.188094372	-6.550511950	1.712712449
H	0.300025620	5.333342856	2.546199770
H	0.386146343	-1.089257234	6.534889770
H	0.544207292	-5.764659178	-3.096128602
H	0.525231947	-7.793521563	2.971786369
H	0.807768228	1.228754309	-6.141691084
H	0.817967126	6.516750669	1.305338551
H	1.331790758	2.321781104	-4.822657868
H	-1.378173479	8.010916344	-4.912128915
H	-1.353905838	3.780239145	-5.563433708
H	1.574383946	-2.442882250	6.610278216
H	-1.545050111	2.337070696	6.658848026
H	1.492679674	-6.897503344	-2.056263815
H	1.754803068	-5.407237782	-7.302684607
H	1.866904711	-6.838937825	2.235192740
H	-2.080998038	-4.601849568	-2.071336105
H	-1.748875596	3.834380191	7.643806309
H	-2.030194750	6.373711663	-5.253376022
H	2.011017062	-5.895476958	-5.595249150

H	2.225672137	-5.361736506	-2.638696908
H	-2.118615809	-5.884334093	-0.823124566
H	2.468111100	1.934888441	-6.159294001
H	-2.322465822	-1.385449476	-6.465050311
H	-2.535462932	-2.354409506	6.115156759
H	-2.900213079	3.655456420	-4.669828805
H	-2.919181417	3.426125922	6.337756457
H	-2.763338203	2.945740967	-6.318090486
H	-3.080685988	7.610987581	-4.493361601
H	3.227375617	6.094173427	-1.358093024
H	3.390640117	-5.291961633	-6.566143495
H	-3.560508256	-5.603197041	-1.872553342
H	-3.416223063	-0.979811766	6.877436179
H	3.563624442	4.482897360	3.452730414
H	-3.350183364	-2.658453404	-7.216745010
H	3.775541688	6.108005615	2.717340562
H	3.742258174	-5.473042886	3.418857471
H	-3.960781502	-1.643250195	5.298252204
H	-4.059784775	-5.881389528	1.828608494
H	-4.005769301	-1.586265204	-5.924625443
H	3.942420811	4.465500004	7.680401817
H	3.923564651	7.015985243	-2.741865215
H	-4.133262526	-7.152924418	3.107509224
H	4.383705618	4.821522521	5.976994504
H	4.705078091	5.499092280	-2.158131106
H	-4.767396524	5.187204821	4.068396377
H	-4.885844449	4.584126478	0.162995748
H	-4.765061833	3.848461301	5.256404935
H	4.967971189	4.799696754	2.391441647
H	5.018836503	-5.867085456	2.214311780
H	5.496186106	-0.943221921	3.587114133
H	5.391959204	3.695415239	6.942192744
H	5.483043225	-1.233915916	-3.187805742
H	-5.432822157	-2.212069858	-4.446598387
H	-5.573581655	-6.136558868	2.751190509
H	5.388084265	-4.779351232	3.598244782
H	-5.879245682	3.101192601	0.059632740
H	-6.196287975	-2.115396490	0.454882351
H	6.042620013	-1.362246026	-1.494410189
H	6.107928501	-1.095773428	1.913831613
H	5.914762861	3.476285658	-3.131301967
H	-6.206028263	4.479298557	-1.055642777
H	-6.200655312	4.117431250	4.222119615
H	-6.447363592	-0.759715308	-4.765562969
H	6.455221116	-2.658882885	-2.677849186
H	-6.511982224	-0.358277119	0.350141540
H	7.015672672	-0.104116312	3.115666570
H	-6.965464402	-1.979598525	-3.550308851
H	7.200126314	3.240717545	-1.898001030
H	7.043023147	2.089790740	-3.270347756
H	-7.370935811	-1.355136433	1.581700143

Cartesian coordinates of $Au_{36}(SPh)_{24}$ as predicted at the DFT/PBE-D3 level.

Au	17.6979648035	14.0725272251	20.3010846178
Au	15.5585923700	14.6651380316	18.5748627302
Au	13.9760857042	17.2462547368	18.6277367017
Au	16.0280658345	16.2998806850	20.7792291602
Au	16.4022969680	20.4756861747	21.1619184264
Au	18.1860388199	18.2771621577	21.1159576852
Au	16.2866084514	18.8228438939	18.9446602600
Au	14.4560397105	19.5102558241	16.9267895452
Au	15.8557025991	17.1095879869	16.5587165205
Au	17.9372536417	16.3192380617	18.6751417799
Au	17.2350982267	14.6779594105	16.1682444224
Au	15.2467668517	15.5138536966	14.3591025632
Au	19.8630989895	16.1943886058	16.6164745861
Au	17.7820000297	16.8036396064	14.4347701667
Au	16.7625779553	19.6003022074	14.8167621046
Au	18.4399861676	18.6070905000	16.8919128714
Au	20.2719535930	17.8684646750	18.9126463235
Au	18.5937884975	20.4244211678	19.3998046812
Au	17.0355217897	21.2100669616	17.0466309034
Au	19.2683226701	20.7500291635	15.3543210065
Au	15.6385886967	12.2257645880	21.5647899092
Au	12.7800762463	14.3201903931	20.6216857571
Au	13.0241928908	15.3645411406	16.3770448662
Au	13.9243516040	18.9161276227	21.3363721020
Au	14.4705367101	21.6281104292	19.1912529384
Au	18.2738743725	20.8874183310	23.5595558008
Au	13.7467015030	18.0110420151	14.1828167900
Au	20.2100471113	15.5377654664	20.8770506963
Au	19.5953644567	13.3428145069	18.1486438735
Au	16.7198972819	14.1252291351	12.0634242256
Au	19.9781334554	14.3477531174	13.5485134881
Au	21.2372975351	19.4921036998	21.9327794253
Au	14.7027348572	22.5584902202	15.1189144142
Au	20.7927004244	18.2917132787	14.5667026986
Au	21.3283680507	20.3975228476	17.3694284630
Au	18.2432481970	23.4681580389	14.5544738420
S	13.2888771269	12.2359030303	21.6079446846
S	12.0928881790	16.4638525333	19.9754401838
S	17.9808430441	11.9825690593	21.5688396096
S	13.6550749393	13.4832838187	17.6467565913
S	11.8630954217	17.0770186339	15.2334139651
S	15.0896779199	17.3972284343	22.7103686635
S	12.6415102454	20.3494795730	19.9685713893
S	17.7669357687	12.4609477343	16.9611397806
S	14.4101639512	14.1253676972	12.5236010919
S	13.0527850190	20.9513699703	15.5332441678
S	16.1295860636	21.7987186639	23.2113917701
S	20.3527091333	19.9442471021	24.0638479709
S	19.4538766812	16.8828763666	22.6591614198
S	21.4427012263	14.2514778441	19.3135587187
S	21.2429178011	14.5026200296	15.5053039842

S	18.9635597221	14.2768866019	11.4303620464
S	22.3023522278	18.7533366445	19.9914081362
S	22.4724897792	18.7086912611	16.1777580224
S	19.4499245300	17.5143043233	12.7920322899
S	15.4282687836	19.0488457429	12.9088640143
S	15.9447262014	23.1125318319	18.1135290050
S	20.1836905539	22.0442118914	18.6008169212
S	20.4070963480	22.6129673729	14.1972561968
S	16.1264710368	24.4201486283	14.8481313592
C	12.9183813827	10.9429654712	20.4228976201
C	11.9107661654	11.1127329031	19.4635942557
C	11.5833389962	10.0632986257	18.6022086850
C	12.2468299508	8.8369029193	18.6939800861
C	13.2416331768	8.6612340329	19.6607747478
C	13.5789591759	9.7061976955	20.5236285288
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C	10.2698223844	15.1007116015	18.3293448314
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C	18.3445615763	10.7446922414	20.3346495140
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C	17.7450008644	9.1324999942	18.6282171403
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C	14.0443205677	12.1585869158	16.5239627593
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H	19.5203061223	22.1494352460	11.0820227389
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H	16.7102684423	19.4441854715	9.2405150767
H	17.4501338562	17.6341006782	10.7750732112
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H	24.0460064658	24.9569308828	17.8687488764
H	21.7107391584	25.8051900311	17.7635729094
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H	12.9000300339	26.3240875157	11.6898205380

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H	17.6986970530	25.3599829958	12.5625677545

Cartesian coordinates of $Ag_4Au_{32}(SPh)_{24}$[4Ex-Td] as predicted at the DFT/PBE-D3 level.

Ag	17.7035465216	14.0700915422	20.3049467544
Au	15.5604014231	14.6727847165	18.5401022529
Au	13.9735346953	17.2787792732	18.5763724669
Au	15.9741846483	16.2882505521	20.7345526150
Ag	16.3456685968	20.5493632055	21.1292309722
Au	18.1057532445	18.2949996118	21.0676132223
Au	16.2810084396	18.8525689729	18.9258690454
Au	14.4554992557	19.5123269619	16.8932003601
Au	15.8379505644	17.1031264106	16.4976090203
Au	17.8832641632	16.3208349247	18.6488728304
Au	17.1978865135	14.6856418597	16.0910525683
Ag	15.1759380019	15.4954099014	14.2796252225
Au	19.8093724715	16.2111476554	16.5998999941
Au	17.7266105217	16.8105704020	14.3992344832
Au	16.7482891428	19.6323460121	14.7891271457
Au	18.4162850074	18.6442337385	16.8402630997
Au	20.2212824763	17.8702080135	18.8701149061
Au	18.5935148185	20.4300463875	19.4043307498
Au	17.0652129463	21.1885598751	17.0211585544
Ag	19.2971493755	20.7776576205	15.2742633125
Au	15.7568934518	12.2627190370	21.5540141524
Au	12.8607577546	14.3914375673	20.5940474805
Au	13.0403623338	15.3624037484	16.3529401579
Au	13.9478312591	18.9286742174	21.3251722406
Au	14.4872926199	21.6616397022	19.1328844140
Au	18.1865295531	21.0176539610	23.4557320098
Au	13.7837172420	18.0188199087	14.1421675056
Au	20.1434555081	15.5750411211	20.8808476072
Au	19.5067790790	13.3459004519	18.1303014349
Au	16.5844657370	14.1516243239	12.0228586039
Au	19.8563231049	14.3783115702	13.5632997439
Au	21.1574868506	19.5437534029	21.8815231031
Au	14.7906721430	22.5189768745	15.0585584886
Au	20.7152330686	18.2881386624	14.5087626803
Au	21.2657558665	20.4160102217	17.3259564729
Au	18.3516711168	23.4325253749	14.4444002094
S	13.4036834389	12.3210332415	21.5839360206
S	12.1064925046	16.5097562386	19.9499687592
S	18.0851389745	11.9304112429	21.5962828544
S	13.6673491339	13.4626301379	17.5919864560
S	11.9044386184	17.0775283371	15.1945115212
S	15.0973885983	17.3984885051	22.6982861455
S	12.6843360934	20.3836127471	19.9611550268
S	17.7044491261	12.4649227310	16.9005299141
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S	13.0902770165	20.9655302412	15.4764624332
S	16.0460765824	21.9439627994	23.1938680880
S	20.2449222337	20.0398725890	23.9874514122
S	19.3647483011	16.9207843008	22.6520388027
S	21.3360991517	14.2570443233	19.3198075737
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S	22.3909381322	18.7293530689	16.1143361284
S	19.3735367449	17.5282136875	12.7278259290
S	15.4561610304	19.0518423170	12.8507770503
S	15.9747050103	23.1251601162	18.0486614417
S	20.1461160853	22.0770430937	18.5577406270
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H	16.4419355730	21.6926510221	12.2134600649
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H	23.2273141859	22.1496209536	14.7721752056
H	24.7890701160	23.1853810520	16.3750968140
H	24.0296729605	25.0682582057	17.8370240481
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H	20.1273580302	24.8676188726	16.0066687009
H	13.6593880445	25.1073518375	13.8252525199
H	12.9142653819	26.3629443677	11.8174406023

H	14.5835814430	27.1291293949	10.1294917421
H	17.0028225452	26.6535666362	10.4882323070
H	17.7474235209	25.4100348697	12.5130256482

Cartesian coordinates of $Ag_4Au_{32}(SPh)_{24}$[4Ex-St-near] as predicted at the DFT/PBE-D3 level.

Au	17.8160750980	14.1466641876	20.2703600404
Au	15.5790776925	14.6712621951	18.5925364363
Au	13.9857671055	17.2544494403	18.6245067519
Au	16.0618409745	16.3265570320	20.7845534724
Au	16.4032058767	20.5395342646	21.1357579684
Au	18.1999136148	18.3377573385	21.1271805746
Au	16.2849011456	18.8554162893	18.9408720767
Au	14.4641553081	19.5371498471	16.9092444399
Au	15.8719050026	17.1450033839	16.5682401479
Au	17.9490038022	16.3820209093	18.6606924563
Au	17.2396581900	14.7147916573	16.1941313390
Au	15.1874555928	15.5221054843	14.4301370749
Au	19.8786679808	16.2264188984	16.5987860039
Au	17.7731479082	16.8017253392	14.4103776119
Au	16.7762055677	19.5909412946	14.8002400283
Au	18.4607578309	18.6419638145	16.8742776645
Au	20.2882371113	17.9118694811	18.9046643104
Au	18.5902922176	20.4545888482	19.3556444146
Au	17.0606531632	21.2547192505	16.9856507975
Au	19.3046781901	20.7387475566	15.2944243983
Ag	15.3968989660	12.9295025258	21.0903469400
Au	12.6626019716	14.3103648144	20.6337125243
Au	12.9934063257	15.3905046503	16.3894791790
Au	13.9551359202	18.9179498889	21.3203064336
Au	14.4980975531	21.6460391496	19.1542603094
Ag	18.3508519758	20.8152750687	23.2767678609
Au	13.7275374644	18.0293321879	14.1987890215
Au	20.2581468508	15.5827986136	20.8886002436
Au	19.6543661688	13.3905171157	18.1068161571
Ag	17.0156807147	14.3465382155	12.5615813108
Au	20.0785510574	14.4295054294	13.4443317916
Au	21.2562933956	19.5135683012	22.0080978044
Au	14.6382343808	22.6493545428	15.1186497610
Au	20.8128972398	18.3139515329	14.5384344050
Au	21.3643230326	20.4165972914	17.3328686825
Ag	18.0333931276	23.2631682209	14.7157581596
S	13.0858355395	12.2145731094	21.6026518129
S	12.0920174394	16.4788883306	19.9584718101
S	17.7700680230	12.0955869666	21.5620696160
S	13.6682362365	13.5154639580	17.6452955787
S	11.8290217163	17.0898575603	15.2229100612
S	15.1003289782	17.4047354414	22.7168748050
S	12.6840435907	20.3561083349	19.9454622868
S	17.8250042967	12.4906800437	16.9274652303
S	14.5264836144	14.0619329918	12.6094008188
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S	16.1465990054	21.8930850373	23.1461776557
S	20.4118430748	19.9386074711	24.1544628514
S	19.4535693063	16.9125961538	22.6632759284
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C	19.6713445266	11.3048227504	15.1931538206

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H	17.7304973887	21.6810253190	9.2986559203
H	16.6882273574	19.4227672849	9.2148160216
H	17.4254394664	17.6438994408	10.7830451956
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H	15.4087823047	23.6042454067	11.0846382900
H	13.0499006954	23.4889166562	10.3239072345
H	11.6989958961	21.4366277089	10.7762355761
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H	17.0966774590	25.1112056476	22.4435538080
H	15.7490623569	23.6555448280	20.9563408220
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H	19.4518172053	22.9389326376	21.1667336034
H	23.0060343656	22.0314585874	14.8603929290
H	24.5742771725	23.0806069029	16.4531227485
H	23.8513228634	25.0518874421	17.8149994758
H	21.5522755123	25.9608717164	17.5286325995
H	19.9813274281	24.9066995866	15.9168414678
H	13.5517791857	25.3340182274	13.6809614696

H	13.0436201927	26.4543985898	11.5209888183
H	14.8862610213	27.0040445650	9.9342046575
H	17.2393782889	26.4459221955	10.5364222975
H	17.7425059784	25.3309435540	12.7032134016

Cartesian coordinates of $Ag_8Au_{28}(SPh)_{24}$[4Ex-Td&4Ex-St-near] as predicted at the DFT/PBE-D3 level.

Ag	17.7445595511	14.0555725462	20.2591444985
Au	15.5774495478	14.5799374668	18.5681945698
Au	13.9742060959	17.2625503222	18.6986853581
Au	15.9893271214	16.1790103371	20.8310402315
Ag	16.3986197262	20.5153573261	21.1369790168
Au	18.0819498496	18.2564560000	21.1375625478
Au	16.3291541189	18.8461631334	18.9521707402
Au	14.4327130705	19.5087956407	17.0106384388
Au	15.8150501623	17.0897109291	16.6117398238
Au	17.8869361126	16.3173561455	18.6625208859
Au	17.1768706440	14.6280219142	16.0837205935
Ag	15.1381504259	15.5502788575	14.3824227054
Au	19.8784583690	16.2257587340	16.6657391178
Au	17.6602461833	16.8958295167	14.4918629248
Au	16.7466377154	19.8891085781	14.9064933371
Au	18.4185632562	18.6158823490	16.9089273180
Au	20.2256174917	17.8657046545	18.9396130494
Au	18.7839975352	20.5267643831	19.6814474869
Au	17.2634315841	21.2195038293	17.2910655046
Ag	19.3556812796	20.7545933857	15.4456341129
Ag	15.6795011913	12.2915534933	21.5466473651
Au	12.7552900130	14.3608417259	20.6312436665
Au	12.9514902723	15.2972424770	16.4328757047
Au	13.9270850384	18.9797393422	21.4023218149
Au	14.5578425438	21.8372510399	19.2497191217
Ag	18.3061534769	21.1413962330	23.4727285511
Au	13.6890426332	18.0730112667	14.3024144760
Au	20.2371738248	15.5033448973	20.8921584372
Au	19.5502922599	13.1937313491	18.1409198245
Ag	16.5841975347	14.1662381659	12.1615556935
Au	19.8911719053	14.3532909827	13.7104933209
Au	21.2653343818	19.6401577055	21.8628727949
Au	14.7053888737	22.5768326338	15.1909861128
Au	20.8667679045	18.3610723986	14.6418960666
Au	21.4607258099	20.5931708353	17.4312694990
Ag	18.2824911970	23.3858977867	14.5098352516
S	13.3246795653	12.2791229785	21.5805039380
S	12.0529123607	16.5033401063	20.0036228478
S	18.0266337716	11.9745160380	21.5726414113
S	13.6547295059	13.4135022569	17.6505028275
S	11.8176298393	17.0201289097	15.2728742852
S	15.0546782958	17.3715147244	22.7146100239
S	12.7627843915	20.5056665885	20.0215749804
S	17.7377432139	12.4028442000	16.8661413358
S	14.2507171439	14.1754788734	12.5151980210
S	13.0524056840	21.0004804482	15.6592079540
S	16.1175140746	21.9478266376	23.1269705468
S	20.3833370664	20.2015433088	23.9606170425
S	19.4548409796	16.8985993367	22.6266834247
S	21.3681971030	14.1335304976	19.3253718361

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S	22.2785544731	18.7510793957	19.9570486227
S	22.5403773949	18.8431027359	16.2458411147
S	19.4175063478	17.5842975191	12.9542076576
S	15.3655217260	19.2033474081	13.0830555193
S	16.1141502314	23.2030196172	18.1354516858
S	20.2643394906	22.1753825257	18.7183042960
S	20.4738623176	22.5794944719	14.1831711195
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H	19.6045225666	22.1166024977	10.9979027851
H	17.7806255756	21.6352884309	9.3454515708
H	16.6667609389	19.4166447405	9.3600160384
H	17.3453765330	17.6799680147	11.0049758664
H	16.3331261336	21.7717089439	12.1725469425
H	15.2418923200	23.5785322923	10.8670873382
H	12.8326266858	23.4351629839	10.2878944813
H	11.5041824236	21.4421220622	11.0047021097
H	12.6050357429	19.6156410922	12.2812933673
H	18.1846488906	25.0723674672	17.6166176879
H	19.2507178694	26.8276071066	19.0095254321
H	18.7017428016	27.0085597586	21.4391120884
H	17.1661955144	25.3125838540	22.4764309376
H	16.0703909459	23.6026616686	21.0670566290
H	23.1703635336	22.3054623232	19.0694169460
H	24.5565840067	23.3078779490	20.8794322198
H	23.4588070483	24.2924723905	22.8915521422
H	20.9793518855	24.2515191678	23.0893778650
H	19.5964159197	23.2778895948	21.2732921632
H	23.1716992379	22.0885816293	14.8742713774
H	24.7574417672	23.1800661591	16.4198138877
H	24.0342689296	25.1571589680	17.7732790300
H	21.7112209694	26.0237256998	17.5427688334
H	20.1061973804	24.8934806488	16.0103671302
H	13.6221165048	25.1736288212	13.8480265755

H	12.8960273198	26.3066495506	11.7644973299
H	14.5682533076	26.8553225267	9.9941464432
H	16.9767833681	26.3231772361	10.3616767959
H	17.6961446983	25.1935893729	12.4587909602

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