

Supporting information

Kinetics of Intercluster Reactions between Atomically Precise Noble Metal Clusters [Ag₂₅(DMBT)₁₈]⁻ and [Au₂₅(PET)₁₈]⁻ in Room Temperature Solutions

Marco Neumaier^{1*†}, Ananya Baksi^{1†}, Patrick Weis², Erik K. Schneider², Papri Chakraborty^{1,2}, Horst Hahn¹, Thalappil Pradeep^{3*} and Manfred M. Kappes^{1,2*}

¹*Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany*

²*Institute of Physical Chemistry, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany*

³*DST Unit of Nanoscience and Thematic Unit of Excellence, Indian Institute of Technology Madras, 600 036 Chennai, India*

*Email: marco.neumaier@kit.edu, manfred.kappes@kit.edu, pradeep@iitm.ac.in

†Contributed equally

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Materials and synthesis of clusters

Materials. Silver nitrate (AgNO_3), dichloromethane (DCM), phenylethanethiol (PET), 2,4-dimethylbenzenethiol (DMBT), 1,3-benzenedithiol (BDT) and sodium borohydride (NaBH_4) were purchased from Sigma Aldrich. Chloroauric acid ($\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$) was prepared in the lab from pure gold and aqua regia.

Synthesis of $[\text{TOA}]^+[\text{Au}_{25}(\text{PET})_{18}]^-$. The cluster was synthesized following the previously reported method.¹⁻³ About 40 mg of $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$ was dissolved in 7.5 mL tetrahydrofuran (THF) and 65 mg of tetraoctylammoniumbromide (TOABr) was added. The mixture was stirred for 15 min. The color changed from golden yellow to orange red confirming successful complexation. 68 μL of PET was directly added and the mixture was stirred for another hour for Au-PET thiolate formation. The yellow thiolates were then reduced using 39 mg of NaBH_4 in ice-cold water. The color of the mixture changed to brown indicating reduction of the thiolates. The solution was stirred for another 5 h for complete conversion and size focusing to achieve high yield of $[\text{Au}_{25}(\text{PET})_{18}]^-$. After 5 h, the as-synthesized cluster was dried using a rotary evaporator and excess methanol was added to precipitate the clusters and to remove the free thiol and excess thiolates. The procedure was repeated several times to get a clean cluster sample. The resulting sample contains a small quantity of larger clusters. To remove the larger clusters, the methanol washed clusters were extracted in acetone and centrifuged for a few times. The supernatant solution was collected leaving behind a smaller quantity of precipitate consisting of larger clusters. The acetone solution was then vacuum dried and the cluster was dissolved in DCM and centrifuged at 10000 rpm. The supernatant solution was collected which consisted of pure $[\text{TOA}]^+[\text{Au}_{25}(\text{PET})_{18}]^-$ clusters. The purified cluster was characterized by UV-vis absorption spectroscopy, where characteristic peaks at 675 nm and 450 nm confirmed the

formation of Au_{25} clusters. The sample was crystallized from solution in a mixture of toluene/ethanol kept at room temperature. This sample was used for detailed characterization by ESI-MS and intercluster reactions.

Synthesis of $[\text{PPh}_4]^+[\text{Ag}_{25}(\text{DMBT})_{18}]^-$. The synthesis followed a reported method with slight modification.⁴ A quantity of 38 mg AgNO_3 was dissolved in a mixture of 2 mL methanol and 17 mL DCM. About 90 μL of 2,4-DMBT was added to the mixture to form yellow insoluble thiolates (Ag-S complex) and the mixture was kept at 0 °C for 15–17 min while stirring. Afterwards 6 mg of PPh_4Br dissolved in 0.5 mL of methanol was added followed by the dropwise addition of 15 mg of NaBH_4 in 0.5 mL of ice–cold water. The reaction mixture was kept for 7–8 h while stirring. After that, stirring was discontinued and the solution was held at 4 °C for about two days. For purification of the cluster, the sample was centrifuged to remove any insoluble impurities and DCM was removed by rotary evaporation. The precipitate was washed twice with methanol. After that, the cluster was redissolved in DCM and again centrifuged to remove any further insoluble contaminants. DCM was again removed by rotary evaporation and the purified cluster was obtained in the powder form. Dark black crystals of the cluster were obtained from a DCM/hexane mixture kept at 4°C over a period of around seven days. The cluster was redissolved in DCM, characterized by UV-vis and then used for ESI-MS (see Figure S1).

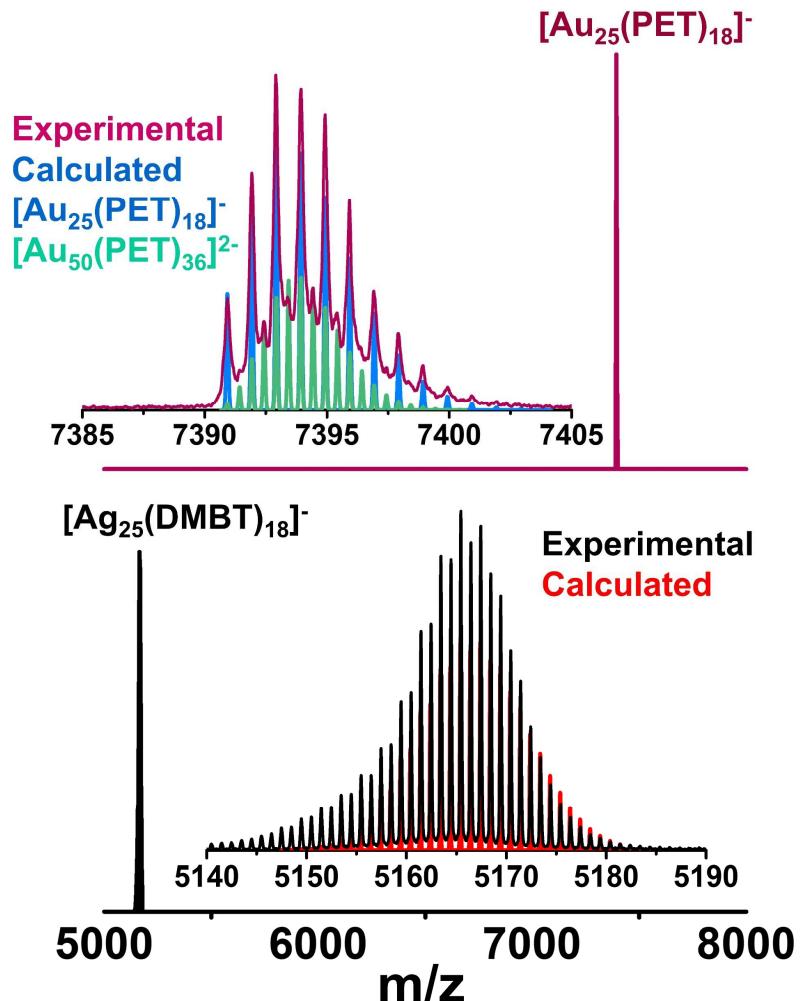


Figure S1. Mass spectra of pure $[\text{Au}_{25}(\text{PET})_{18}]^-$ and $[\text{Ag}_{25}(\text{DMBT})_{18}]^-$ clusters with isotopically resolved patterns and the corresponding calculated isotope distributions. Note that for $[\text{Au}_{25}(\text{PET})_{18}]^-$ dimers are present also in the pure cluster solution.

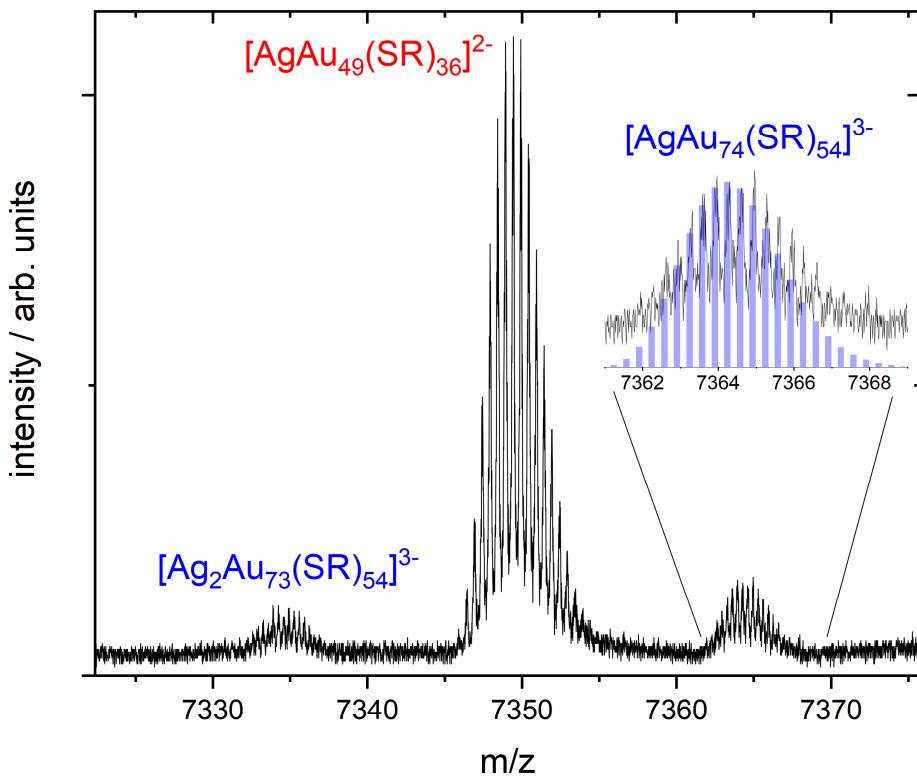


Figure S2. Integrated signal between 0 – 6 min reaction time ($[\text{Ag}_{25}]^-$: $[\text{Au}_{25}]^-$ ratio = 40:40 nmol L⁻¹). Next to the dianion $[\text{AgAu}_{49}(\text{SR})_{36}]^{2-}$ trimer signals are apparent with about tenfold less intensity compared to $[\text{AgAu}_{49}(\text{SR})_{36}]^{2-}$. The inset shows the calculated spectrum of the triply charged trimer $[\text{AgAu}_{74}(\text{SR})_{54}]^{3-}$ ion (blue bars) together with the experimental signal.

Mass spectrometry and collision induced dissociation

High resolution mass spectra as a function of reaction time after mixing were recorded on a Bruker timsTOF-MS in Karlsruhe at a mass resolution exceeding 25000. Briefly, the timsTOF comprises an electrospray ion source (ESI), a trapped ion mobility spectrometer (TIMS), a quadrupole mass filter (QMS), a collision cell (which is a second quadrupole) as well as an orthogonally accelerated time-of-flight mass spectrometer with a reflectron (oa-ReTOF). TIMS is a high resolution variant of ion mobility spectrometry allowing isomer separation based on collision cross section. For (low) intensity reasons we operated the timsTOF in the “TIMS-off” mode in this study, i.e. without isomer separation. Typical measurement conditions were as follows: sample concentration: 40–100 nmol L⁻¹ in DMF, flow rate: 3 µL min⁻¹, capillary voltage: 4.5 kV, nebulizer: 0.3 bar, dry gas: 2 L min⁻¹, dry temperature: 300 °C, ion energy: 1 eV, collision energy: 1 eV, transfer time: 200 µs, pre-pulse storage time: 20 µs and scan time: 1 ms. Different mixing ratios of [Au₂₅(PET)₁₈]⁻ and [Ag₂₅(DMBT)₁₈]⁻ were mixed and injected directly into the mass spectrometer to avoid delay in the measurement. Considering the sample transfer time, a “dead time” of about 20 – 40 s between starting the reaction by mixing and completing the first mass spectral scan is possible in all experiments.

Collision induced dissociation (CID) studies were carried out in Chennai using a Waters Synapt G2Si mass spectrometer system, comprising an ESI source, a quadrupole mass filter for mass-preselection, a travelling wave ion mobility spectrometer (not used in this study), a collision cell and a ReTOF mass analyzer with a specified resolution of 50000. For the CID studies, the [Ag₂₅Au₂₅]²⁻ parent ions were mass selected in the QMS and collided with nitrogen at 0.02 mbar with a laboratory frame collision energy of 30 eV. The fragments were analyzed in the ReTOF. Again, the mass resolution is high enough to allow isotopic resolution of all species.

Data analysis

For best accuracy each mass spectrum was smoothed by a 5 point moving average procedure and recalibrated linearly with respect to calculated m/z values of [Ag₂₅(SR)]₁₈⁻ and [Au₂₅(SR)]₁₈⁻. As monoanions [Ag_mAu_{25-m}]⁻ share the same m/z ratio as dianions [Ag_{2m}Au_{50-2m}]²⁻, their intensities have to be deconvoluted, see Figure S1 as an example. The integer (larger) peaks correspond to both monoanion and dianion isotopologues while the (smaller) half integer peaks (marked with an asterisk) correspond to dianionic dimers only. Therefore, we integrate first the half integer peaks and multiply the result by a factor of 2 to get the dianion intensity (using the fact that the isotopologue distribution is quite wide and almost Gaussian-shaped). The monoanion intensities are obtained by integrating the integer peaks and

subtracting the corresponding dianion intensities. Each ion intensity was normalized to the sum of all ions (strictly speaking the sum of all monomers and the monomeric subunits in the dimers) I_{total} :

$$I_{total} = \sum_{i=1}^{26} I_i^{monoanion} + 2 \cdot \sum_{j=1}^{51} I_j^{dianion} \quad (1)$$

No systematic behavior of I_{total} was found and for some measurement series I_{total} was constant within ~10% on a timescale of up to 60 min. On this basis we can rule out significant dark reaction channels not accessible to mass spectrometry and conclude that the kinetics followed by mass spectrometry largely resemble the kinetics in solution.

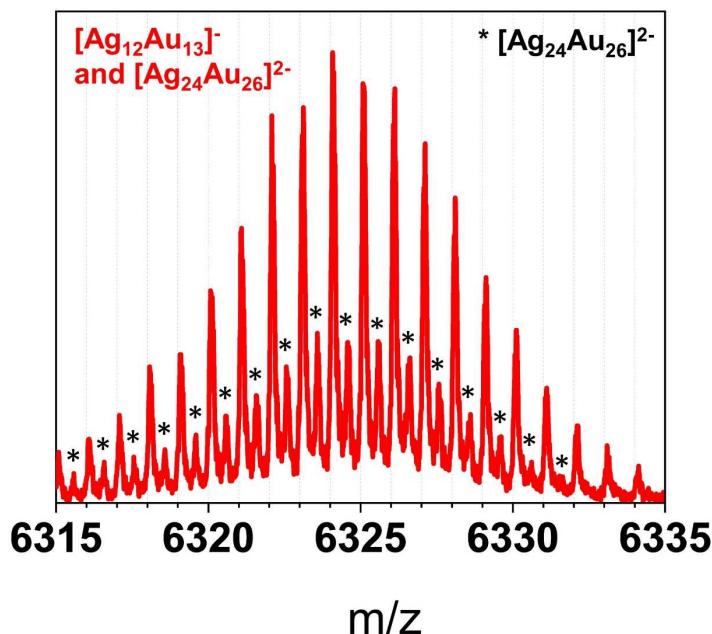


Figure S3. Isotopic distribution for $[Ag_{12}Au_{13}]^-$ with underlying dianion signal of $[Ag_{24}Au_{26}]^{2-}$. The spectrum was taken for a $[Ag_{25}]^-:[Au_{25}]^-$ ratio of 40:40 nmol L⁻¹ and after a reaction time of 54 min. Peaks marked with an asterisk belong to the dianion $[Ag_{24}Au_{26}]^{2-}$ only.

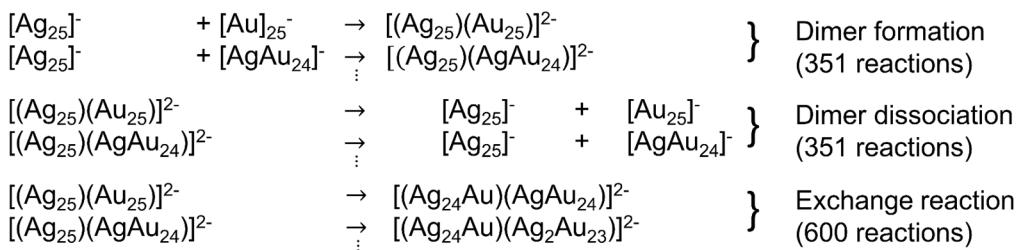
Kinetic Model

The exchange kinetics was modeled by standard matrix algebra suites in MATLAB and solving all kinetic differential equations numerically. According to reaction scheme 1 (see main text for details) all 26 monoanions can form dimers which in turn can dissociate to the monomers. The number of possible dimerization and dissociation steps is given by the number of possible combinations of monoanions with repetition

$$C(n, r) = \frac{(n+r-1)!}{r!(n-1)!} = 351 \quad (2)$$

where $n=26$ is the number of monoanions and $r=2$ is the sample size, i.e. reaction partners. Note that for dianions aside from $[\text{Ag}_{50}]^{2-}$ and $[\text{Au}_{50}]^{2-}$ several constitutional isomers exist with $[\text{Ag}_{25}\text{Au}_{25}]^{2-}$ being the dimer with a maximum of 13 possible isomers ranging from $[(\text{Ag}_{25})(\text{Au}_{25})]^{2-}$, over $[(\text{Ag}_{18}\text{Au}_7)(\text{Ag}_7\text{Au}_{18})]^{2-}$, to fully mixed $[(\text{Ag}_{12}\text{Au}_{13})(\text{Ag}_{13}\text{Au}_{12})]^{2-}$. In total there exist 351 different dianionic species. Note that different isomers of the monomeric subunits (i.e. with well-defined structures where e.g. gold atoms preferably occupy the staple and core positions and silver atoms the icosahedral shell) were not taken into account.

When we allow metal atom exchange exclusively in the dianions the number of physically meaningful exchange reactions amounts to 600. Therefore, the reaction is determined by 1302 ($=351+351+600$) elementary reactions in total and can be written as



Scheme S1. Reaction scheme based on the kinetic model. The kinetics of the intercluster reaction between $[\text{Ag}_{25}]^-$ and $[\text{Au}_{25}]^-$ is described by 1302 reactions.

From the reactions in scheme S1 the stoichiometric matrix α can be calculated.

$\alpha =$	$\begin{array}{c} [\text{Ag}_{25}] + [\text{Au}_{25}] \xrightarrow{\quad} [\text{(Ag}_{25}\text{)(Au}_{25}\text{)]}^2 \\ [\text{Ag}_{25}] + [\text{AgAu}_{24}] \xrightarrow{\quad} [\text{(Ag}_{25}\text{)(AgAu}_{24}\text{)]}^2 \\ \\ [\text{(Ag}_{25}\text{)(Au}_{25}\text{)]}^2 \xrightarrow{\quad} [\text{Ag}_{25}] + [\text{Au}_{25}] \\ [\text{(Ag}_{25}\text{)(AgAu}_{24}\text{)]}^2 \xrightarrow{\quad} [\text{Ag}_{25}] + [\text{AgAu}_{24}] \\ \\ [\text{(Ag}_{25}\text{)(Au}_{25}\text{)]}^2 \xrightarrow{\quad} [\text{(Ag}_{24}\text{Au})(\text{AgAu}_{24}\text{)]}^2 \\ [\text{(Ag}_{25}\text{)(AgAu}_{24}\text{)]}^2 \xrightarrow{\quad} [\text{(Ag}_{24}\text{Au})(\text{Ag}_2\text{Au}_{23}\text{)]}^2 \end{array}$									
-1	-1	...	1	1	...	0	0	...		$[\text{Ag}_{25}]^-$
-1	0	...	1	0	...	0	0	...		$[\text{Au}_{25}]^-$
0	-1	...	0	1	...	0	0	...		$[\text{AgAu}_{24}]^-$
1	0	...	-1	0	...	-1	0	...		$[(\text{Ag}_{25})(\text{Au}_{25})]^2-$
0	1	...	0	-1	...	0	-1	...		$[(\text{Ag}_{25})(\text{AgAu}_{24})]^2-$
0	0	...	0	0	...	1	0	...		$[(\text{Ag}_{24}\text{Au})(\text{AgAu}_{24})]^2-$
0	0	...	0	0	...	0	1	...		$[(\text{Ag}_{24}\text{Au})(\text{Ag}_2\text{Au}_{23})]^2-$
:	:		:	:		:	:			:

Figure S4. Stoichiometric matrix α according to the reactions in scheme S1. Number of columns correspond to the number of elementary reactions (=1302) and number of rows equals the number of species participating in the reaction (=377). The matrix elements represent stoichiometric factors, which are -1 if one unit of the corresponding species is consumed in the reaction, 1 if one unit of the species is produced and 0 if the species does not participate in the reaction. The blue and yellow columns represent the 351 dimerization and dissociation reactions, respectively. The red columns represent the 600 intra-cluster exchange reactions.

The number of columns in α correspond to the number of elementary reactions (=1302) and the number of rows equal the number of participating species (=377). The matrix elements in α represent stoichiometric factors of a definite species at a given elementary step which are positive in case of products, negative in case of reactants and zero if the species does not participate in the reaction.

By introducing the rate vector \vec{r} with the corresponding concentrations c of the clusters

$$\vec{r} = \begin{pmatrix} k_{dim} \cdot c([\text{Ag}_{25}]^-) \cdot c([\text{Au}_{25}]^-) \\ k_{dim} \cdot c([\text{Ag}_{25}]^-) \cdot c([\text{AgAu}_{24}]^-) \\ \vdots \\ k_{diss} \cdot c([(\text{Ag}_{25})(\text{Au}_{25})]^{2-}) \\ k_{diss} \cdot c([(\text{Ag}_{25})(\text{AgAu}_{24})]^{2-}) \\ \vdots \\ k_{ex} P_{ex,1} \cdot c([(\text{Ag}_{25})(\text{Au}_{25})]^{2-}) \\ k_{ex} P_{ex,2} \cdot c([(\text{Ag}_{25})(\text{AgAu}_{24})]^{2-}) \\ \vdots \end{pmatrix} \quad (3)$$

the 377 differential reaction equations are given by

$$\frac{dC(t)}{dt} = \boldsymbol{\alpha} \cdot \vec{r} \quad (4)$$

and are solved numerically in MATLAB by using the Ordinary Differential Equations (ODE) solver ODE45. Simulated concentrations were treated like the experimental data (to allow easy comparison) and have been normalized to the sum of all ion concentrations (counting the dianions twice to account for the monomeric subunits, see above). Time zero was assumed to equal the “dead time” of ~20 s of the experiment.

Calculation of mixing entropy

For the dimer $[(\text{Ag}_{22}\text{Au}_3)(\text{Ag}_4\text{Au}_{21})]^{2-}$ the forward mixing reaction produces $[(\text{Ag}_{21}\text{Au}_4)(\text{Ag}_5\text{Au}_{20})]^{2-}$ and the backward mixing reaction leads to $[(\text{Ag}_{23}\text{Au}_2)(\text{Ag}_3\text{Au}_{22})]^{2-}$. Based on equation 5 and the number of structural isomers W for each monomeric subunit (SU), the configurational entropy change for the forward reaction is $1.04 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and for the backward reaction it is $-1.24 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

$$\Delta S = \frac{1}{25} \cdot R \cdot (\ln W_{SU1,product} + \ln W_{SU2,product} - \ln W_{SU1,educt} - \ln W_{SU2,educt}) \quad (5)$$

The number of structural isomers W can be calculated from the binomial coefficient $\binom{n}{k}$ where n is the number of metal atoms per subunit ($n=25$) and k is the number of silver or gold atoms in the respective subunit ($k=0-25$). The total mixing entropy for the formation of $[(\text{Ag}_{12}\text{Au}_{13})(\text{Ag}_{13}\text{Au}_{12})]^{2-}$ is $10.28 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

DFT Calculations

Method. The quantum chemical calculations were performed with the TURBOMOLE package⁵ with the BP86-functional^{6,7} and def-SVP basis set⁸. We used the published crystal structure coordinates^{4,9} of Ag₂₅(DMBT)₁₈ and Au₂₅(PET)₁₈ as starting points, removed the counterions and optimized the geometries without symmetry restrictions. The mixed clusters were obtained by exchanging gold and silver atoms and reoptimizing the structure.

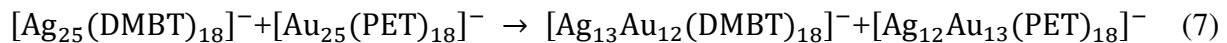
Results.

(A) Metal atom exchange

In a first step we investigated the exchange of one metal atom, i.e. the reaction



In both pure [Au₂₅(PET)₁₈]⁻ and [Ag₂₅(DMBT)₁₈]⁻ clusters, the metal atoms have topologically the same arrangements: 12 atoms form an icosahedron, one atom is in its core and another 12 atoms form 6 “staples” and are bound to the DMBT and PET molecules covering the cluster. Therefore, we assume that the mixed clusters also have these topologies. For the mixed [AgAu₂₄(PET)₁₈]⁻ clusters 3 isomers have to be considered: The extra metal atom can either be in the core, in the icosahedron or on the staple. It turns out that in the most stable structure of [AgAu₂₄(PET)₁₈]⁻ the silver atom replaces one gold atom on the icosahedron (core: +0.31 eV, staple: +0.20 eV). In [AuAg₂₄(DMBT)₁₈]⁻ the gold atom is in the core (icosahedron: +0.27 eV, staple: +0.28 eV). With these optimized isomers the mixing reaction (7) is exothermic by 0.5 eV. These findings are in line with the calculations by Krishnadas et al.¹⁰ Since the number of possible isomers quickly increases with the number of exchanged metal atoms we did not try to follow all steps but focused on the limiting case of complete mixing, i.e. exchange of 12 atoms:



Even so, there are still a large number of isomers possible for the mixed clusters [Ag₁₃Au₁₂(DMBT)₁₈]⁻ and [Ag₁₂Au₁₃(PET)₁₈]⁻. The obvious limiting cases are the isomers with 12 atoms of the same element on staple and icosahedron, respectively (see Table S1, isomers I and II). In the case [Ag₁₂Au₁₃(PET)₁₈]⁻ the isomer with a Au atom in the core, 12 Ag atoms on the icosahedron and the remaining 12 Au atoms on the staples is the lowest energy isomer that we found. Swapping the elements in icosahedron and staple is highly unfavourable (isomer II, +1.04 eV), moving the Au atom from the core to the icosahedron (isomer III) increases the energy by 0.11 eV. We also calculated several isomers with a “statistical” distribution, i.e.

similar numbers of Au and Ag atoms in icosahedron and staples (isomers IV-VII). They are between 0.41 eV and 0.87 eV higher in energy. Therefore we are confident that isomer I represents the global minimum for $[\text{Ag}_{12}\text{Au}_{13}(\text{PET})_{18}]^-$. For $[\text{Ag}_{13}\text{Au}_{12}(\text{DMBT})_{18}]^-$ we performed similar calculations. We found that the isomer with one Au atom in the core, 12 Ag atoms on the icosahedron and one Ag plus 11 Au atoms on the staples (isomer III) to be the lowest in energy. With these lowest energy structures we obtain for reaction (7) an exothermicity of 1.69 eV.

Table S1. Relative energies for isomers of $[\text{Ag}_{12}\text{Au}_{13}(\text{PET})_{18}]^-$ and $[\text{Ag}_{13}\text{Au}_{12}(\text{DMBT})_{18}]^-$.

$[\text{Ag}_{12}\text{Au}_{13}(\text{PET})_{18}]^-$	core	icosahedron	staple	relative Energy [eV]
I	Au	12 Ag	12 Au	0
II	Au	12 Au	12 Ag	1.27
III	Ag	11 Ag, 1Au	12 Au	0.11
IV	Au	6 Ag, 6 Au	6 Ag, 6 Au	0.41
V	Au	6 Ag, 6 Au	6 Ag, 6 Au	0.56
VI	Au	6 Ag, 6 Au	6 Ag, 6 Au	0.63
VII	Ag	5 Ag, 7Au	6 Ag, 6 Au	0.87
<hr/>				
$[\text{Ag}_{13}\text{Au}_{12}(\text{DMBT})_{18}]^-$				
I	Ag	12 Ag	12 Au	0.40
II	Ag	12 Au	12 Ag	1.04
III	Au	12 Ag	1 Ag, 11 Au	0
IV	Ag	6 Ag, 6 Au	6 Ag, 6 Au	0.56
V	Ag	6 Ag, 6 Au	6 Ag, 6 Au	0.72
VI	Ag	6 Ag, 6 Au	6 Ag, 6 Au	0.66
VII	Au	6Ag, 6 Au	7 Ag, 5 Au	0.34

(B) Ligand exchange

What role do the different ligands DMBT vs. PET play in the nanoalloying chemistry?

In order to shed some light into this issue we compared the DFT-energies of $[\text{Ag}_{25}(\text{DMBT})_{18}]^-$ and $[\text{Au}_{25}(\text{PET})_{18}]^-$ with those of the (experimentally not accessible) ligand-exchanged clusters $[\text{Au}_{25}(\text{DMBT})_{18}]^-$ and $[\text{Ag}_{25}(\text{PET})_{18}]^-$ (obtained by replacing all Ag by Au atoms and vice versa and optimizing the geometries).

For the hypothetical exchange reaction:



we calculate an endothermicity of 1.26 eV, i.e. less than 0.1 eV for each ligand exchange. Note that in reaction (8) we assumed the most basic ligand exchange being well aware that there can be partial ligand exchange or ligand exchange at some specific sites on the cluster surface favouring the formation of the dimers.

Does the ligand shell alter the order of topological isomers?

As a test case we reinvestigated the three isomers of $[\text{Ag}_{24}\text{Au}(\text{SR})_{18}]^-$ and $[\text{AgAu}_{24}(\text{SR})_{18}]^-$ ($\text{SR}=\text{PET}$ and DMBT), now as function of the ligand. The relative energies are summarized in Table S2.

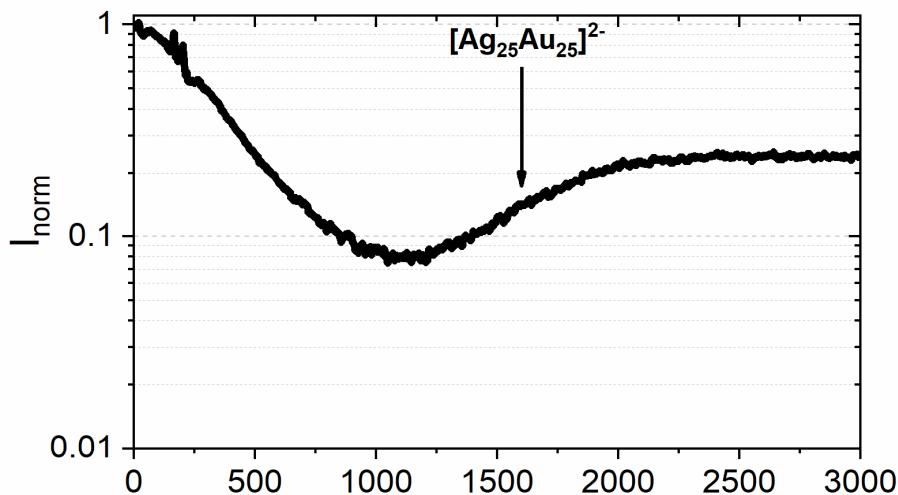
Table S2. Relative energies for isomers of $[\text{Ag}_{24}\text{Au}(\text{SR})_{18}]^-$ and $[\text{AgAu}_{24}(\text{SR})_{18}]^-$ ($\text{SR}=\text{PET}$ and DMBT) as function of the ligand.

	$[\text{AgAu}_{24}\text{PET}_{18}]^-$	$[\text{AgAu}_{24}\text{DMBT}_{18}]^-$
Ag icosahedron	0.00 eV	0.00 eV
Ag staple	0.20 eV	0.20 eV
Ag core	0.31 eV	0.29 eV
	$[\text{Ag}_{24}\text{AuPET}_{18}]^-$	$[\text{Ag}_{24}\text{AuDMBT}_{18}]^-$
Au core	0.00 eV	0.00 eV
Au icosahedron	0.30 eV	0.27 eV
Au staple	0.31 eV	0.28 eV

From this we conclude that the impact of the ligands on the relative energies of the isomers is negligible in this case. We assume that this is the case for all mixed clusters.

a)

Experiment



b)

Simulation

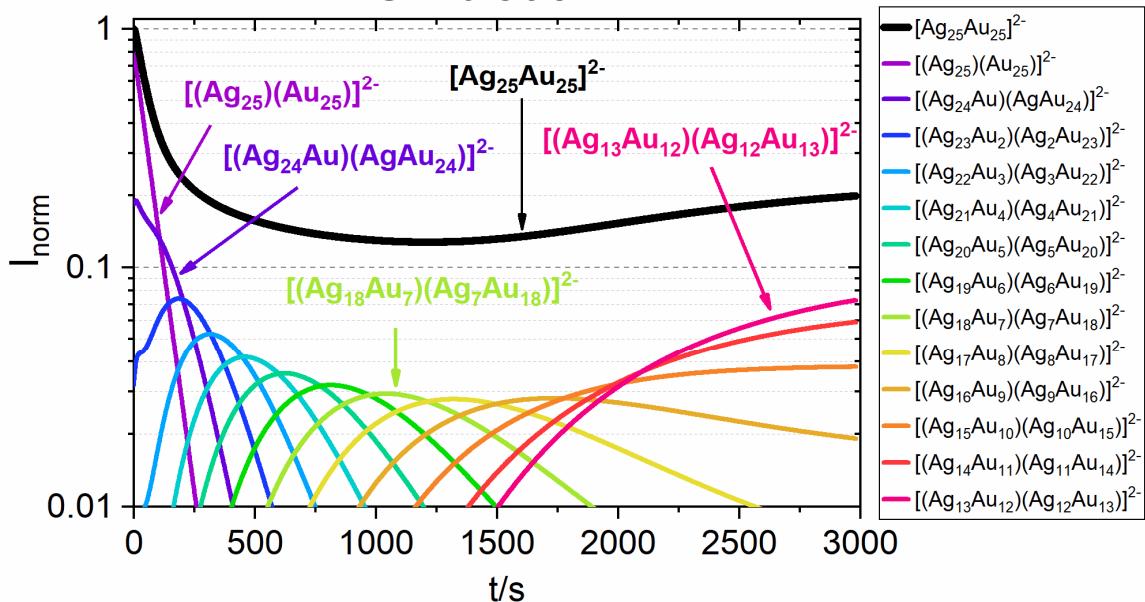


Figure S5. Time dependence of normalized $[Ag_{25}Au_{25}]^{2-}$ solution concentration as observed in a) experiment by ESI-MS (40:40 nmol L⁻¹ ratio of Ag₂₅:Au₂₅) and b) in simulation 2. The intensity of $[Ag_{25}Au_{25}]^{2-}$ in the experiment was normalized to 1 at time zero. In the simulation the integrated signal $[Ag_{25}Au_{25}]^{2-}$ was normalized to 1 after a reaction time of 20s, which is the estimated “dead time” of the experiment. Colored lines in b) refer to isomers of $[Ag_{25}Au_{25}]^{2-}$ starting from $[(Ag_{25})(Au_{25})]^{2-}$ (purple) to fully mixed $[(Ag_{13}Au_{12})(Ag_{12}Au_{13})]^{2-}$ (pink) clusters. The experiment and the simulation have in common that the integrated signal of $[Ag_{25}Au_{25}]^{2-}$ shows a minimum before an equilibrium is reached after ~2500 s in the experiment and after ~3500 s (not shown) in the simulation.

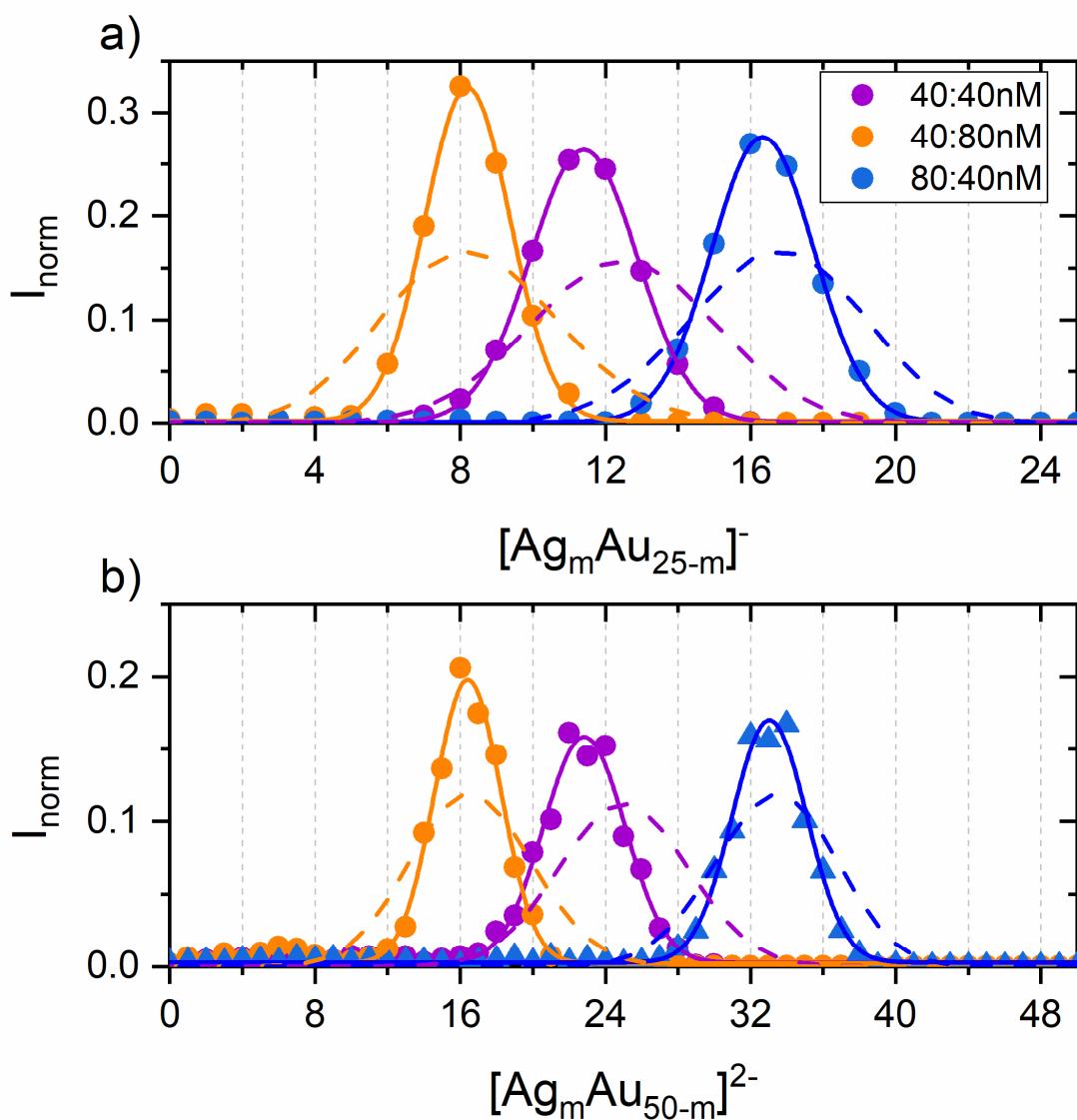


Figure S6. Experimental equilibrium distributions after 54 min for a) monoanions and b) dianions for three different mixing ratios of $[\text{Ag}_{25}]^- : [\text{Au}_{25}]^-$ clusters. The dashed lines show the expected binomial distributions.

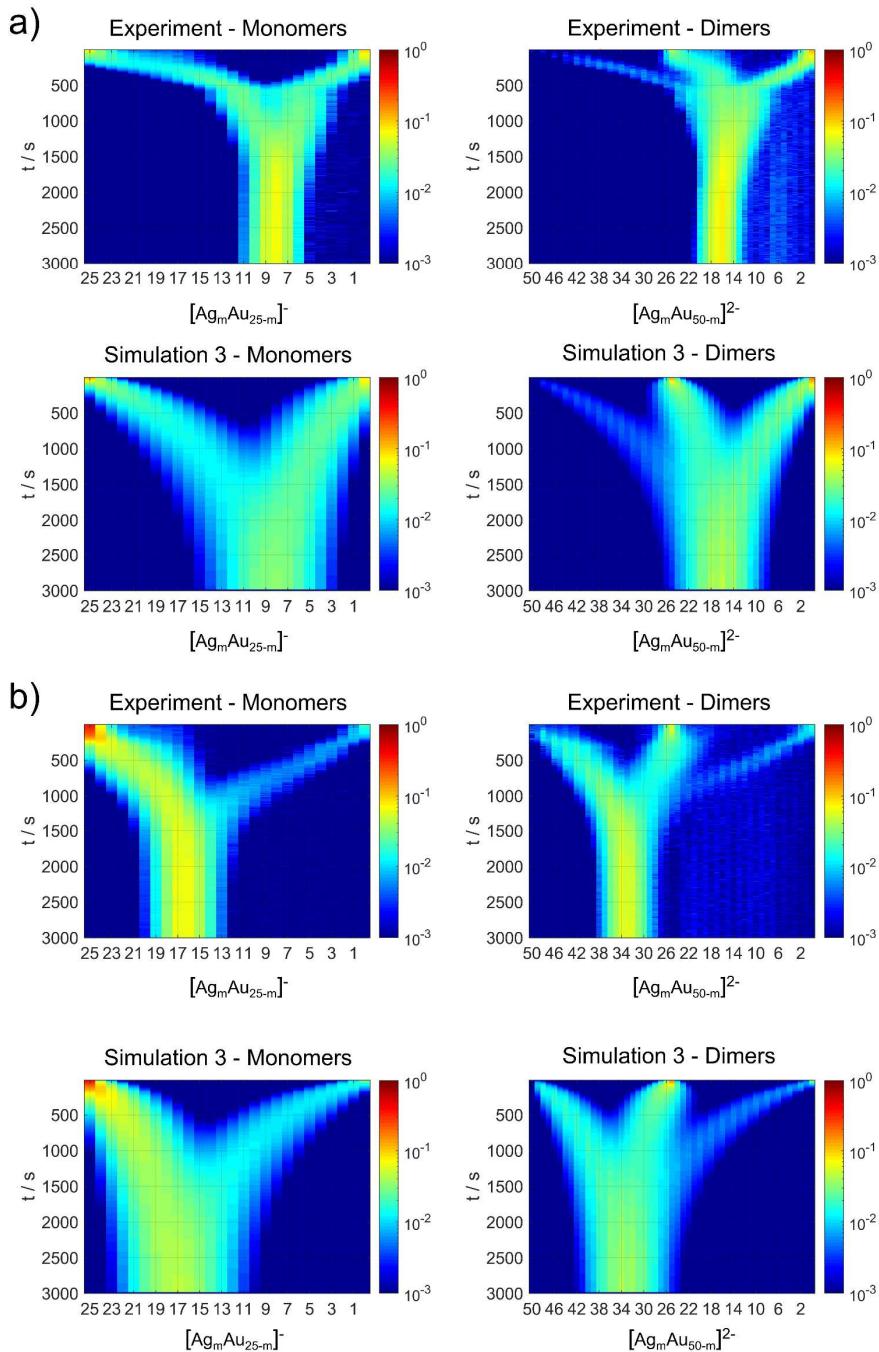


Figure S7. Contour plots of monomers and dimers for the exchange reaction between $[\text{Ag}_{25}]^-$ and $[\text{Au}_{25}]^-$ for a mixing ratio of $[\text{Ag}_{25}]^- : [\text{Au}_{25}]^-$ of a) 40:80 nmol L⁻¹ and b) 80:40 nmol L⁻¹ for experiment (top) and simulation (bottom). For all simulations the optimized rate constants from simulation 3 were applied, i.e. $k_{dim} = 1 \cdot 10^{-2}$ L nmol⁻¹s⁻¹, $k_{diss} = 5.6 \cdot 10^{-2}$ s⁻¹ and $k_{ex} = 3.2 \cdot 10^{-2}$ s⁻¹. Starting conditions of all simulations were chosen as in the experiment.

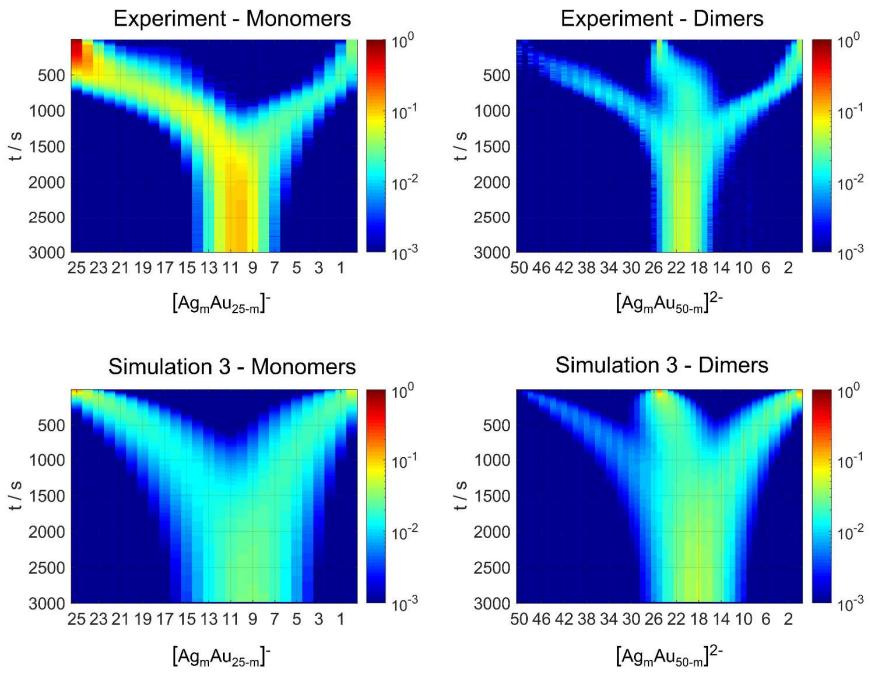


Figure S8. Contour plots of monomers and dimers for the exchange reaction between $[Ag_{25}]^-$ and $[Au_{25}]^-$ for a mixing ratio of $[Ag_{25}]^- : [Au_{25}]^-$ of 60:100 nmol L⁻¹ for experiment (top) and simulation (bottom). For all simulations the optimized rate constants from simulation 3 were applied, i.e. $k_{dim} = 1 \cdot 10^{-2}$ L nmol⁻¹ s⁻¹, $k_{diss} = 5.6 \cdot 10^{-2}$ s⁻¹ and $k_{ex} = 3.2 \cdot 10^{-2}$ s⁻¹. Starting conditions of all simulations were chosen as in the experiment.

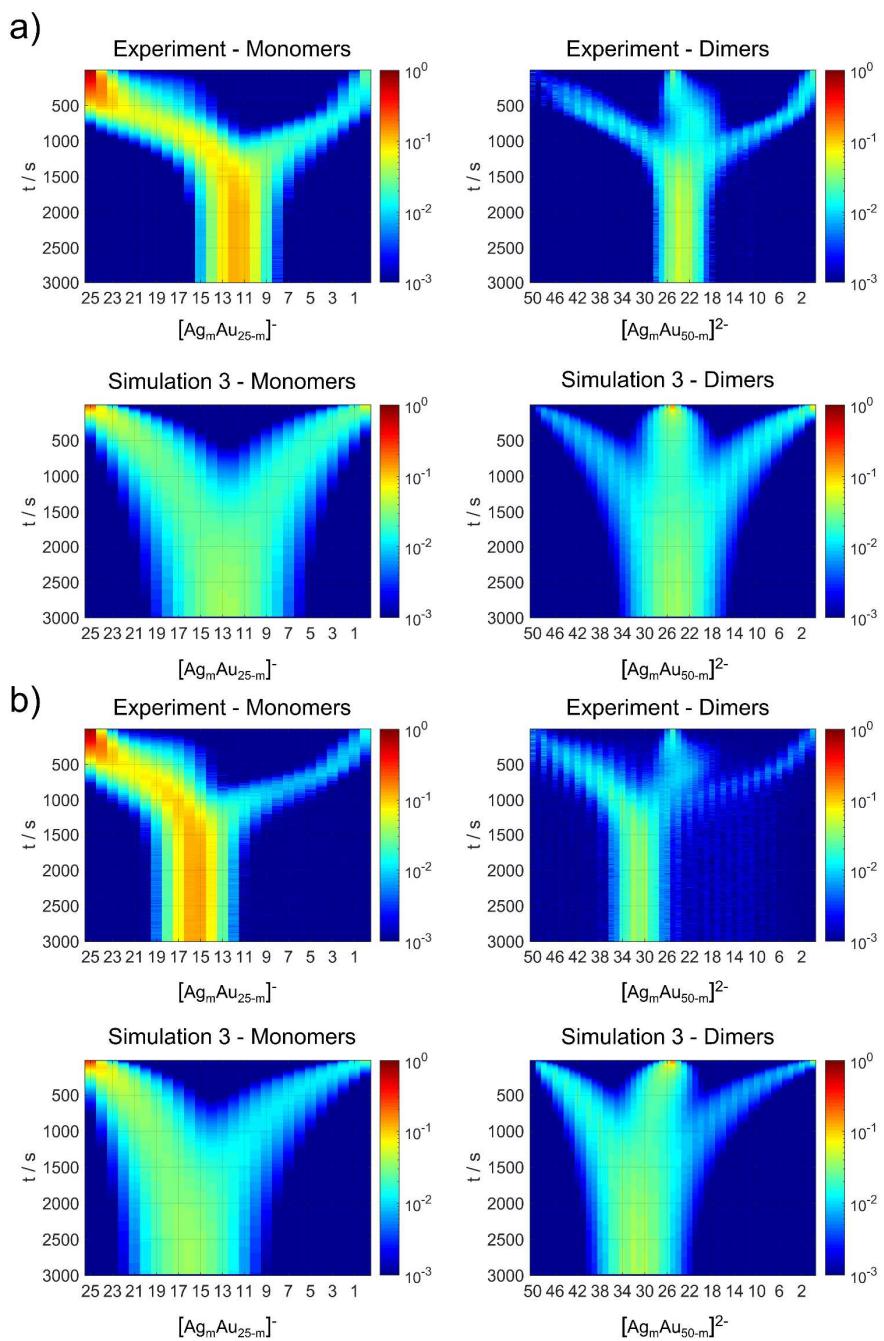


Figure S9. Contour plots of monomers and dimers for the exchange reaction between $[Ag_{25}]^-$ and $[Au_{25}]^-$ for a mixing ratio of $[Ag_{25}]^- : [Au_{25}]^-$ of a) 50:50 nmol L⁻¹ and b) 100:60 nmol L⁻¹ for experiment (top) and simulation (bottom). For all simulations the optimized rate constants from simulation 3 were applied, i.e. $k_{dim} = 1 \cdot 10^{-2}$ L nmol⁻¹ s⁻¹, $k_{diss} = 5.6 \cdot 10^{-2}$ s⁻¹ and $k_{ex} = 3.2 \cdot 10^{-2}$ s⁻¹. Starting conditions of all simulations were chosen as in the experiment.

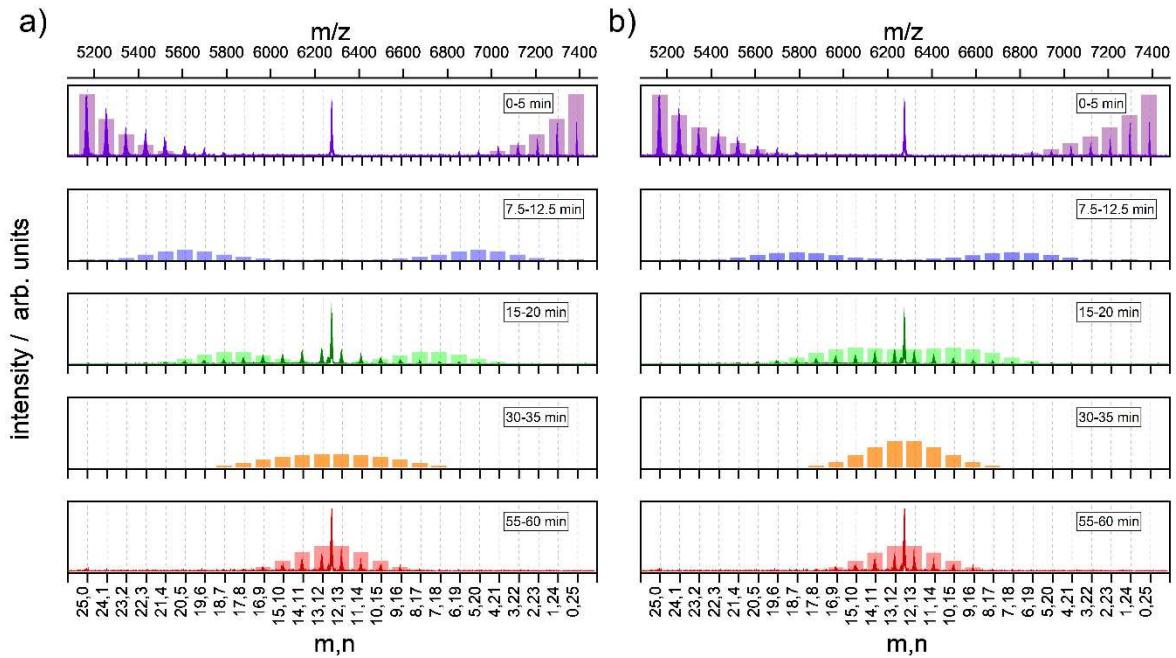


Figure S10. a) Modelled composition of $[Ag_{25}Au_{25}]^{2-}$ isomers (bar plots) based on simulation 3 at five different time intervals ($k_{dim} = 1 \cdot 10^{-2} L nmol^{-1} s^{-1}$, $k_{diss} = 5.6 \cdot 10^{-2} s^{-1}$ and $k_{ex} = 3.2 \cdot 10^{-2} s^{-1}$, mixing ratio 40:40 nmol L⁻¹) together with experimental data (spectrum in the 0–5 min, 15–20 min and 55–60 min time interval) from the CID experiment. Bars correspond to the simulated monomeric subunit constituents of the $[Ag_{25}Au_{25}]^{2-}$ dimers at the respective reaction time intervals. As an example, during the 0–5 min reaction time window, the dominant $[Ag_{25}Au_{25}]^{2-}$ isomer consists of $[Ag_{25}]^-$ and $[Au_{25}]^-$ subunits in good agreement with the experimental data. After a reaction time of 15–20 min the dominant $[Ag_{25}Au_{25}]^{2-}$ isomer in simulation 3 is $[(Ag_{18}Au_7)(Au_7Ag_{18})]^{2-}$, while in the experiment $[(Ag_{13}Au_{12})(Au_{12}Ag_{13})]^{2-}$ is already present, i.e. the experimental kinetics proceeds somewhat faster. b) The same plot as in a) but with $k_{ex} = 5 \cdot 10^{-2} s^{-1}$ (which is still within our estimated range of k_{ex}). This leads to a better agreement for the 15–20 min CID experiment. Note however that the CID data were recorded on a different instrument (Synapt mass spectrometer; IIT Madras) compared to the kinetics data (tims-TOFMS; KIT) which serve as the basis for our determined rate constants. Another reason for the deviation could be further Ag/Au mixing as a result of collisional heating before dissociation.

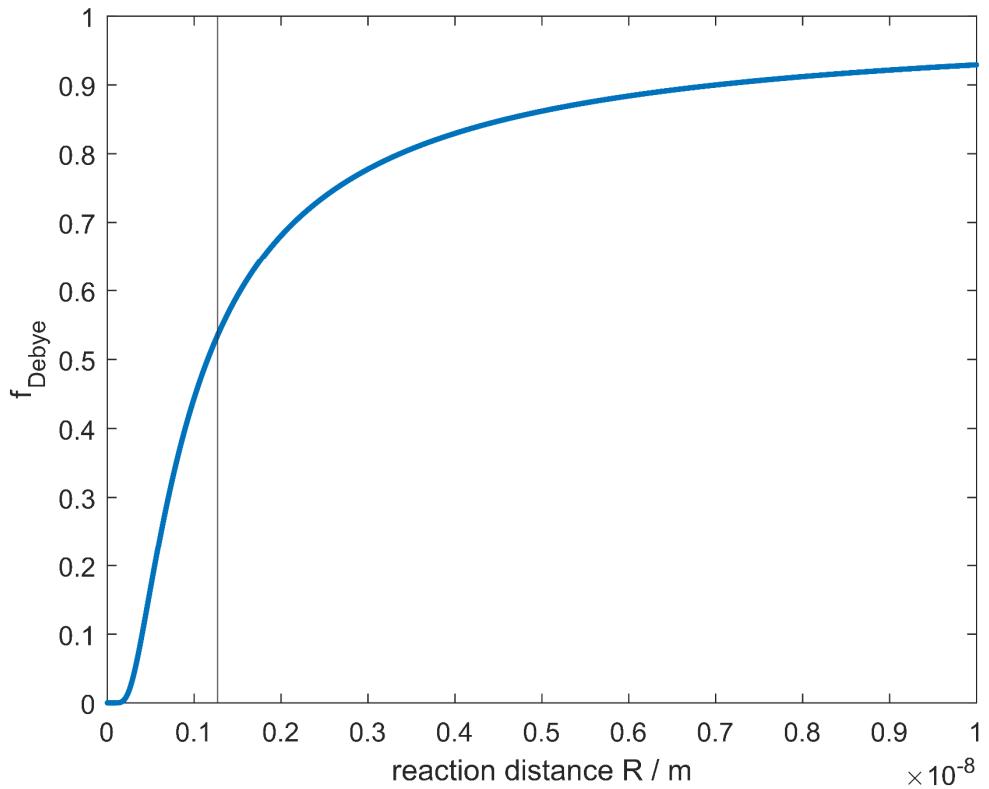


Figure S11: Debye factor f_{Debye} according to equation 6 as a function of the reaction distance R . For $[M_{25}]^-(M = Ag \text{ or } Au)$ clusters the reaction distance is assumed to be twice the radius of $[Au_{25}]^-$ which corresponds to $R=12.7\text{\AA}$ (denoted by the black vertical line).

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Coordinates of calculated structures

Ag₂₅DMBT₁₈

349

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Ag	17.62927	18.71260	15.20890
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Ag	13.35763	16.46562	17.01561
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Ag	13.25717	18.51471	12.34170
Ag	14.84712	15.26213	12.43878
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H	19.74068	20.82268	8.35149
H	21.23029	19.92391	7.91933
H	15.18876	13.05512	7.57378
H	18.93260	15.88407	5.89773
H	19.98753	13.82021	8.54644
H	19.35230	15.32138	9.27097
H	20.26667	15.40374	7.72613
H	14.97211	14.20265	5.37426
H	17.79929	16.15763	3.74561
H	16.22129	16.82126	4.27708
H	16.27722	15.26265	3.39828
H	14.95410	19.69497	9.41255
H	14.12591	20.35733	7.15445
H	12.43369	16.39743	6.65182
H	14.12347	14.77933	9.20433
H	12.57396	14.75551	8.29284
H	12.62576	15.33360	9.99270
H	12.37139	19.84569	5.30798
H	11.90337	18.13519	5.00776
H	13.54994	18.70514	4.59044
H	7.68917	12.82361	17.05682
H	6.30454	10.95999	17.95586
H	9.51432	9.93224	20.68203
H	11.37226	12.85307	20.40754

H	12.08109	11.78106	19.18220
H	11.52541	11.08966	20.74641
H	6.36926	8.67430	19.19385
H	6.24071	9.57935	20.73256
H	7.59195	8.42775	20.48929

Au₂₅PET₁₈

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Au	12.52666	15.34445	12.15412
Au	15.65562	16.52948	13.03461
Au	17.43579	13.43367	13.75694
Au	14.82838	11.10913	13.53645
Au	11.05591	14.02736	14.46309
Au	9.57283	16.70357	12.81880
Au	10.99696	16.36594	9.44567
Au	12.66229	13.38418	9.80075
Au	14.11908	13.94307	14.37415
Au	12.46893	14.10836	17.42111
Au	9.37719	12.30827	16.62987
Au	9.98117	11.36342	13.33849
Au	12.48070	9.61323	12.86629
Au	9.34980	8.42692	11.99139
Au	7.57009	11.52426	11.27080
Au	10.17583	13.84840	11.49552
Au	13.94922	10.93516	10.55846
Au	15.42887	8.25663	12.20738
Au	14.00859	8.59703	15.58163
Au	12.34363	11.57952	15.22761
Au	10.89120	11.01650	10.64978
Au	12.53614	10.85272	7.60107
Au	15.63052	12.64791	8.39279
Au	15.02984	13.58656	11.68643
Au	12.50387	12.47936	12.51372
S	13.51522	17.53363	12.77953
S	17.88107	15.69055	13.14125
S	17.18338	11.14302	14.36268
S	9.64588	17.85116	10.73054
S	12.42067	15.09342	8.01605
S	9.34388	15.74417	14.98149
S	14.69048	14.57228	16.70833
S	10.26253	13.80981	18.26278
S	8.26912	10.88259	15.08395
C	13.66167	18.59030	11.25738
H	14.34578	18.10028	10.53477
H	12.64532	18.60026	10.80815
C	14.10653	20.03297	11.56840
H	13.39404	20.47686	12.29853
H	13.99490	20.60945	10.62014
C	15.52726	20.18356	12.07779
C	16.62246	20.10081	11.18932
H	16.44186	19.93669	10.11248
C	17.94074	20.22746	11.65659
H	18.78001	20.15949	10.94414
C	18.18959	20.44376	13.02392
H	19.22459	20.54976	13.39080
C	17.10949	20.52680	13.91931
H	17.28840	20.68988	14.99528
C	15.79193	20.39612	13.44728
H	14.95065	20.45781	14.15802
C	18.65069	16.48288	14.63469
H	18.61225	17.57745	14.44769
H	18.03365	16.26349	15.52982

C	20.10097	16.00296	14.83156
H	20.09579	14.89834	14.97212
H	20.67807	16.20766	13.90274
C	20.76157	16.67838	16.01892
C	21.48635	17.88003	15.86192
H	21.60328	18.31098	14.85227
C	22.06443	18.52739	16.96686
H	22.63057	19.46275	16.81967
C	21.92591	17.98299	18.25552
H	22.38060	18.48818	19.12422
C	21.20794	16.78651	18.42815
H	21.09846	16.34609	19.43343
C	20.63211	16.14317	17.31959
H	20.07668	15.20024	17.46385
C	17.02613	11.24137	16.20743
H	16.19518	11.93299	16.45497
H	16.73805	10.21979	16.54097
C	18.34025	11.68850	16.87324
H	19.17000	11.03660	16.52257
H	18.57095	12.71946	16.51584
C	18.27442	11.66455	18.38990
C	19.06428	10.76434	19.13772
H	19.74465	10.07668	18.60632
C	18.99873	10.73444	20.54193
H	19.62659	10.02317	21.10473
C	18.13435	11.60609	21.22582
H	18.07930	11.58390	22.32723
C	17.33975	12.50731	20.49389
H	16.65922	13.19758	21.02048
C	17.40914	12.53669	19.09089
H	16.77920	13.24873	18.52827
C	7.93916	17.59974	10.04157
H	7.98359	17.93578	8.98349
H	7.70957	16.51394	10.06355
C	6.88754	18.39249	10.83783
H	7.16508	19.46962	10.84903
H	6.90922	18.03967	11.89446
C	5.49529	18.21738	10.25969
C	4.88192	19.24018	9.50526
H	5.41782	20.19367	9.35448
C	3.60138	19.06520	8.95231
H	3.13963	19.88084	8.37018
C	2.91076	17.85679	9.14387
H	1.90422	17.71754	8.71455
C	3.51065	16.82735	9.89157
H	2.97497	15.87655	10.05265
C	4.79000	17.00608	10.44284
H	5.25227	16.19110	11.02619
C	11.31672	14.36938	6.70735
H	11.75311	13.37159	6.47763
H	10.31063	14.19735	7.13692
C	11.24536	15.22321	5.42767
H	12.27622	15.38510	5.04104
H	10.71261	14.60556	4.66673
C	10.53238	16.55491	5.56874
C	11.24983	17.76901	5.60150
H	12.34926	17.74648	5.51624
C	10.58544	19.00011	5.73726

H	11.16734	19.93710	5.75987
C	9.18531	19.03824	5.84370
H	8.66145	20.00328	5.94935
C	8.45659	17.83574	5.81031
H	7.35631	17.85258	5.88461
C	9.12455	16.60776	5.67193
H	8.53837	15.67324	5.63298
C	10.04831	17.03255	16.11661
H	10.21647	16.51156	17.08397
H	11.02932	17.37463	15.72953
C	9.06489	18.20649	16.28666
H	8.90420	18.68501	15.29483
H	8.08148	17.79871	16.61105
C	9.55022	19.23893	17.28739
C	9.43376	19.00820	18.67690
H	8.97142	18.07050	19.03132
C	9.89086	19.95405	19.60904
H	9.78638	19.75425	20.68901
C	10.47342	21.15622	19.16845
H	10.82661	21.90257	19.89968
C	10.59953	21.39829	17.78969
H	11.05180	22.33849	17.43110
C	10.14466	20.44602	16.86095
H	10.24481	20.64394	15.77982
C	14.85962	16.41719	16.82645
H	15.73969	16.67249	16.19656
H	13.97413	16.89810	16.36458
C	15.06346	16.87727	18.28258
H	14.14704	16.63081	18.86492
H	15.89835	16.29337	18.73002
C	15.36562	18.36175	18.38121
C	16.69881	18.82767	18.37939
H	17.52765	18.10004	18.33381
C	16.98651	20.20171	18.44123
H	18.03650	20.53972	18.44553
C	15.94006	21.13880	18.50367
H	16.16265	22.21805	18.55446
C	14.60797	20.68914	18.50369
H	13.77575	21.41082	18.55397
C	14.32511	19.31426	18.44284
H	13.27485	18.97629	18.44843
C	10.43667	12.80079	19.81316
H	10.96172	11.85270	19.57530
H	11.08034	13.39253	20.49885
C	9.06301	12.52363	20.45179
H	8.55134	13.49282	20.64409
H	8.43637	11.96604	19.71991
C	9.19382	11.73351	21.74083
C	9.22540	10.32167	21.72336
H	9.11320	9.78982	20.76277
C	9.38734	9.58703	22.90996
H	9.40458	8.48496	22.87192
C	9.52214	10.25341	24.14028
H	9.64764	9.67796	25.07276
C	9.49173	11.65833	24.17369
H	9.59186	12.19137	25.13444
C	9.32954	12.38843	22.98429
H	9.30155	13.49161	23.01946

C	8.71401	9.17673	15.65944
H	8.30460	8.49290	14.88392
H	9.81897	9.07499	15.65968
C	8.12610	8.85632	17.04531
H	8.59175	9.54747	17.78631
H	7.03588	9.07593	17.04213
C	8.36220	7.41363	17.45374
C	7.29238	6.49825	17.55247
H	6.26555	6.84713	17.34707
C	7.51425	5.15704	17.91122
H	6.66102	4.46166	17.98686
C	8.81859	4.70314	18.17090
H	8.99611	3.65072	18.44947
C	9.89537	5.60308	18.07301
H	10.92429	5.25910	18.27241
C	9.66948	6.94431	17.72068
H	10.52292	7.64276	17.65476
S	11.49107	7.42353	12.24180
S	7.12492	9.26772	11.88787
S	7.82292	13.81489	10.66538
S	15.35747	7.11018	14.29633
S	12.58573	9.86996	17.01186
S	15.65802	9.21396	10.04379
S	10.31481	10.39129	8.31597
S	14.74212	11.15018	6.75785
S	16.74084	14.07010	9.94047
C	11.34999	6.36609	13.76379
H	10.66847	6.85549	14.48927
H	12.36805	6.35617	14.20907
C	10.90455	4.92334	13.45383
H	11.61262	4.48127	12.71831
H	11.02322	4.34557	14.40046
C	9.48044	4.77179	12.95426
C	8.39187	4.84783	13.85145
H	8.58023	5.00760	14.92763
C	7.07034	4.71995	13.39382
H	6.23649	4.78250	14.11311
C	6.81148	4.50915	12.02751
H	5.77392	4.40222	11.66822
C	7.88485	4.43289	11.12348
H	7.69806	4.27399	10.04824
C	9.20572	4.56494	11.58585
H	10.04161	4.50855	10.86832
C	6.35075	8.47555	10.39673
H	6.38683	7.38111	10.58492
H	6.96656	8.69230	9.50011
C	4.90126	8.95886	10.20239
H	4.90915	10.06321	10.05975
H	4.32596	8.75758	11.13305
C	4.23557	8.28310	9.01809
C	3.50329	7.08670	9.18016
H	3.38481	6.66010	10.19147
C	2.91973	6.43916	8.07821
H	2.34774	5.50802	8.22942
C	3.06018	6.97809	6.78749
H	2.60113	6.47284	5.92112
C	3.78569	8.16929	6.60977
H	3.89670	8.60547	5.60281

C	4.36695	8.81285	7.71536
H	4.92813	9.75176	7.56707
C	7.98138	13.71739	8.82062
H	8.80994	13.02290	8.57304
H	8.27331	14.73819	8.48803
C	6.66551	13.27593	8.15463
H	5.83871	13.93188	8.50466
H	6.42985	12.24637	8.51292
C	6.73068	13.29773	6.63788
C	5.93928	14.19592	5.88927
H	5.25937	14.88438	6.42021
C	6.00202	14.22220	4.48487
H	5.37261	14.93163	3.92147
C	6.86536	13.34910	3.80152
H	6.91820	13.36842	2.69995
C	7.66209	12.45044	4.53427
H	8.34196	11.75916	4.00814
C	7.59544	12.42463	5.93747
H	8.22670	11.71417	6.50059
C	17.06501	7.36096	14.98333
H	17.02179	7.02414	16.04121
H	17.29448	8.44681	14.96189
C	18.11600	6.56922	14.18521
H	17.83998	5.49169	14.17509
H	18.09165	6.92157	13.12849
C	19.50911	6.74676	14.76055
C	20.12427	5.72653	15.51704
H	19.58935	4.77301	15.67112
C	21.40547	5.90402	16.06767
H	21.86868	5.09037	16.65142
C	22.09499	7.11234	15.87152
H	23.10203	7.25354	16.29903
C	21.49325	8.13922	15.12181
H	22.02801	9.08995	14.95726
C	20.21322	7.95803	14.57296
H	19.74945	8.77099	13.98802
C	13.69077	10.59463	18.31932
H	13.25376	11.59181	18.55039
H	14.69573	10.76818	17.88777
C	13.76609	9.74056	19.59858
H	12.73667	9.58191	19.99039
H	14.30449	10.35676	20.35672
C	14.47376	8.40632	19.45476
C	13.75218	7.19445	19.43201
H	12.65358	7.22086	19.52649
C	14.41141	5.96076	19.29454
H	13.82635	5.02558	19.27990
C	15.81044	5.91773	19.17625
H	16.33026	4.95064	19.06938
C	16.54331	7.11796	19.19983
H	17.64289	7.09721	19.11644
C	15.88052	8.34853	19.34009
H	16.47003	9.28123	19.37163
C	14.95065	7.92625	8.90980
H	14.78200	8.44726	7.94252
H	13.96963	7.58547	9.29803
C	15.93243	6.75110	8.73858
H	16.09295	6.27176	9.73006

H	16.91619	7.15771	8.41389
C	15.44506	5.72010	7.73739
C	15.56598	5.94945	6.34804
H	16.03331	6.88491	5.99424
C	15.10705	5.00505	5.41533
H	15.21530	5.20364	4.33551
C	14.51788	3.80585	5.85520
H	14.16303	3.06069	5.12356
C	14.38726	3.56520	7.23380
H	13.92998	2.62721	7.59183
C	14.84401	4.51602	8.16310
H	14.74021	4.31921	9.24409
C	10.14214	8.54681	8.19700
H	9.26319	8.29278	8.82898
H	11.02791	8.06402	8.65634
C	9.93365	8.08802	6.74112
H	10.84904	8.33306	6.15656
H	9.09874	8.67378	6.29617
C	9.62833	6.60420	6.64237
C	8.29418	6.14103	6.64413
H	7.46686	6.87038	6.68993
C	8.00362	4.76760	6.58203
H	6.95294	4.43175	6.57773
C	9.04811	3.82838	6.51945
H	8.82327	2.74960	6.46851
C	10.38112	4.27527	6.51949
H	11.21182	3.55184	6.46902
C	10.66686	5.64954	6.58061
C	14.56737	12.16275	5.20984
H	14.04353	13.11075	5.45067
H	13.92237	11.57337	4.52338
C	15.94059	12.44047	4.57053
H	16.44983	11.47135	4.37151
H	16.56960	12.99238	5.30471
C	15.80928	13.23896	3.28672
C	15.78228	14.65076	3.31322
H	15.89865	15.17613	4.27688
C	15.61951	15.39350	2.13179
H	15.60580	16.49534	2.17703
C	15.47931	14.73541	0.89763
H	15.35312	15.31716	-0.03082
C	15.50525	13.33064	0.85520
H	15.40087	12.80409	-0.10867
C	15.66829	12.59242	2.03948
H	15.69272	11.48940	1.99708
C	16.29588	15.77741	9.36944
H	16.70863	16.45921	10.14495
H	15.19105	15.88039	9.37319
C	16.87929	16.10040	7.98222
H	16.40842	15.41328	7.24082
H	17.96885	15.87746	7.98033
C	16.64612	17.54538	7.58027
C	17.71806	18.45857	7.48400
H	18.74439	18.10608	7.68565
C	17.49879	19.80225	7.13302
H	18.35359	20.49590	7.05943
C	16.19506	20.26079	6.87849
H	16.01957	21.31522	6.60632

C	15.11625	19.36296	6.97346
H	14.08784	19.71054	6.77764
C	15.33952	18.01927	7.31807
H	14.48454	17.32251	7.38198
H	11.71783	5.98531	6.57513

Ag₁Au₂₄PET₁₈_Ag_in_core

349

Au	12.51257	15.33570	12.15114
Au	15.66944	16.51337	13.02760
Au	17.43849	13.43126	13.75032
Au	14.81156	11.10482	13.53072
Au	11.06620	14.01726	14.46669
Au	9.57365	16.70528	12.80733
Au	10.99444	16.37304	9.45101
Au	12.66117	13.36821	9.80472
Au	14.12037	13.93966	14.35677
Au	12.46194	14.10908	17.42208
Au	9.38140	12.32316	16.64026
Au	9.98667	11.36491	13.33335
Au	12.48572	9.62291	12.87280
Au	9.33052	8.44279	11.99883
Au	7.56134	11.52577	11.27718
Au	10.18584	13.85357	11.49856
Au	13.93247	10.94427	10.55871
Au	15.42198	8.25329	12.22045
Au	14.00720	8.59090	15.57774
Au	12.33814	11.59442	15.22359
Au	10.88138	11.01994	10.66889
Au	12.53535	10.85035	7.60270
Au	15.61691	12.63321	8.38374
Au	15.01512	13.58888	11.69286
Ag	12.49958	12.47979	12.51387
S	13.53222	17.52056	12.78298
S	17.89783	15.68306	13.12949
S	17.17617	11.14771	14.36567
S	9.63860	17.86199	10.72513
S	12.41938	15.10167	8.02657
S	9.34472	15.74582	14.96684
S	14.68203	14.56383	16.70772
S	10.25954	13.82369	18.27711
S	8.27638	10.89522	15.09877
C	13.67677	18.57897	11.26209
H	14.35712	18.08823	10.53639
H	12.65907	18.59202	10.81588
C	14.12614	20.02040	11.57286
H	13.41843	20.46459	12.30741
H	14.01091	20.59864	10.62606
C	15.54990	20.16699	12.07477
C	16.63973	20.08928	11.17924
H	16.45265	19.93222	10.10244
C	17.96087	20.21283	11.63925
H	18.79581	20.14770	10.92147
C	18.21799	20.42193	13.00617
H	19.25514	20.52732	13.36710
C	17.14337	20.49907	13.90866
H	17.32883	20.65544	14.98450
C	15.82293	20.37079	13.44400
H	14.98610	20.42727	14.16040
C	18.66024	16.47362	14.62789
H	18.62451	17.56836	14.44145
H	18.03710	16.25460	15.51888

C	20.10852	15.99147	14.83368
H	20.10043	14.88690	14.97482
H	20.69205	16.19470	13.90862
C	20.76231	16.66595	16.02535
C	21.50729	17.85540	15.87086
H	21.64598	18.27709	14.86005
C	22.07839	18.50213	16.97988
H	22.65955	19.42855	16.83477
C	21.91309	17.96879	18.26994
H	22.36314	18.47283	19.14175
C	21.17454	16.78448	18.44015
H	21.04276	16.35340	19.44678
C	20.60595	16.14177	17.32759
H	20.03479	15.20802	17.47012
C	17.01669	11.25326	16.20959
H	16.18421	11.94428	16.45397
H	16.73010	10.23227	16.54622
C	18.32923	11.70445	16.87599
H	19.16101	11.05520	16.52528
H	18.55694	12.73605	16.51832
C	18.26428	11.68067	18.39269
C	19.06088	10.78603	19.14006
H	19.74798	10.10531	18.60839
C	18.99401	10.75328	20.54412
H	19.62873	10.04784	21.10659
C	18.12083	11.61586	21.22837
H	18.05963	11.58660	22.32930
C	17.32271	12.51454	20.49714
H	16.64030	13.20248	21.02437
C	17.39277	12.54619	19.09420
H	16.75820	13.25456	18.53212
C	7.93317	17.60167	10.03566
H	7.97537	17.94286	8.97914
H	7.71114	16.51418	10.05251
C	6.87620	18.38321	10.83585
H	7.14823	19.46165	10.85520
H	6.89778	18.02294	11.88993
C	5.48600	18.20545	10.25361
C	4.87074	19.22968	9.50261
H	5.40434	20.18514	9.35617
C	3.59152	19.05335	8.94708
H	3.12870	19.86973	8.36684
C	2.90395	17.84231	9.13300
H	1.89683	17.70343	8.70494
C	3.50687	16.81051	9.87496
H	2.97512	15.85623	10.02833
C	4.78476	16.99071	10.42916
H	5.24905	16.17422	11.00877
C	11.31916	14.38536	6.71085
H	11.76015	13.39182	6.47201
H	10.31393	14.20406	7.13865
C	11.24302	15.24958	5.43827
H	12.27308	15.41975	5.05307
H	10.71331	14.63553	4.67231
C	10.52348	16.57648	5.58979
C	11.23582	17.79285	5.64414
H	12.33596	17.77560	5.56726
C	10.56561	19.01957	5.79035

H	11.14370	19.95835	5.82980
C	9.16451	19.05102	5.88580
H	8.63616	20.01247	6.00115
C	8.44071	17.84638	5.82977
H	7.33974	17.85820	5.89414
C	9.11456	16.62281	5.68088
H	8.53215	15.68697	5.62180
C	10.04854	17.03454	16.10179
H	10.22169	16.51221	17.06759
H	11.02754	17.37996	15.71253
C	9.06325	18.20583	16.27862
H	8.90079	18.68983	15.28980
H	8.08073	17.79418	16.60107
C	9.54661	19.23350	17.28537
C	9.46129	18.97967	18.67323
H	9.02789	18.02615	19.02193
C	9.91364	19.92212	19.61104
H	9.83194	19.70487	20.68960
C	10.46177	21.14318	19.17822
H	10.81405	21.88540	19.91407
C	10.55586	21.40873	17.80129
H	10.97848	22.36495	17.44886
C	10.10626	20.45964	16.86661
H	10.18348	20.67493	15.78694
C	14.85529	16.40821	16.82591
H	15.74608	16.65911	16.20943
H	13.97899	16.89119	16.34873
C	15.03816	16.87329	18.28332
H	14.11256	16.63052	18.85256
H	15.86507	16.28965	18.74547
C	15.34141	18.35763	18.38028
C	16.67528	18.82092	18.40591
H	17.50334	18.09122	18.38623
C	16.96450	20.19488	18.46275
H	18.01481	20.53085	18.48968
C	15.91891	21.13453	18.49212
H	16.14264	22.21390	18.53495
C	14.58614	20.68745	18.46747
H	13.75462	21.41115	18.49561
C	14.30173	19.31268	18.41168
H	13.25084	18.97688	18.39766
C	10.43884	12.80742	19.82261
H	10.96052	11.85946	19.57713
H	11.08740	13.39406	20.50805
C	9.06781	12.52944	20.46647
H	8.56023	13.49845	20.67044
H	8.43540	11.98012	19.73331
C	9.20351	11.72655	21.74711
C	9.22467	10.31476	21.71562
H	9.09977	9.79317	20.75096
C	9.39228	9.56722	22.89333
H	9.40066	8.46550	22.84416
C	9.54390	10.22052	24.12867
H	9.67557	9.63510	25.05405
C	9.52329	11.62523	24.17617
H	9.63590	12.14795	25.14120
C	9.35483	12.36826	22.99564
H	9.33334	13.47119	23.04237

C	8.71996	9.18981	15.67588
H	8.31263	8.50600	14.89918
H	9.82497	9.08802	15.67885
C	8.12926	8.86791	17.06033
H	8.59240	9.55936	17.80264
H	7.03879	9.08612	17.05479
C	8.36655	7.42529	17.46853
C	7.29785	6.50826	17.56476
H	6.27073	6.85603	17.35888
C	7.52122	5.16674	17.92152
H	6.66872	4.47040	17.99659
C	8.82599	4.71408	18.18113
H	9.00536	3.66017	18.45285
C	9.90130	5.61631	18.08833
H	10.93006	5.27403	18.29143
C	9.67402	6.95770	17.73760
H	10.52649	7.65760	17.67385
S	11.46837	7.43636	12.24119
S	7.10244	9.27411	11.89898
S	7.82223	13.80954	10.66216
S	15.35945	7.09836	14.30392
S	12.58382	9.86304	17.00287
S	15.65237	9.21352	10.06157
S	10.31549	10.39732	8.31868
S	14.73733	11.13399	6.74635
S	16.72458	14.05815	9.92600
C	11.32795	6.37827	13.76262
H	10.64964	6.86906	14.49020
H	12.34692	6.36558	14.20586
C	10.87832	4.93649	13.45383
H	11.58304	4.49295	12.71602
H	10.99853	4.35833	14.40007
C	9.45234	4.78824	12.95875
C	8.36674	4.86697	13.85933
H	8.55887	5.02609	14.93494
C	7.04345	4.74216	13.40589
H	6.21194	4.80731	14.12767
C	6.77985	4.53101	12.04053
H	5.74096	4.42566	11.68464
C	7.85023	4.45207	11.13317
H	7.65977	4.29241	10.05869
C	9.17286	4.58167	11.59122
H	10.00630	4.52359	10.87101
C	6.33851	8.48474	10.40070
H	6.37350	7.38986	10.58646
H	6.96128	8.70381	9.50947
C	4.89056	8.96825	10.19582
H	4.89900	10.07374	10.06208
H	4.30551	8.75890	11.11855
C	4.23873	8.30205	8.99844
C	3.49734	7.10904	9.14251
H	3.36061	6.67764	10.14948
C	2.92788	6.47059	8.02788
H	2.34871	5.54168	8.16493
C	3.09174	7.01560	6.74251
H	2.64341	6.51775	5.86628
C	3.82661	8.20362	6.58273
H	3.95660	8.64425	5.58001

C	4.39344	8.83811	7.70087
H	4.96195	9.77469	7.56657
C	7.98404	13.70505	8.81841
H	8.81654	13.01375	8.57487
H	8.27166	14.72611	8.48283
C	6.67245	13.25470	8.14971
H	5.84068	13.90559	8.49742
H	6.44262	12.22390	8.50826
C	6.74133	13.27602	6.63315
C	5.94871	14.17099	5.88197
H	5.26092	14.85356	6.41039
C	6.01933	14.20079	4.47801
H	5.39075	14.90943	3.91270
C	6.89033	13.33297	3.79761
H	6.94990	13.35555	2.69644
C	7.68668	12.43601	4.53287
H	8.37188	11.74824	4.00906
C	7.61273	12.40718	5.93564
H	8.24326	11.69762	6.50077
C	17.06648	7.35892	14.98962
H	17.02600	7.02180	16.04751
H	17.28974	8.44609	14.96822
C	18.12109	6.57327	14.19025
H	17.84988	5.49451	14.17827
H	18.09546	6.92732	13.13415
C	19.51332	6.75590	14.76614
C	20.13180	5.73803	15.52313
H	19.60022	4.78263	15.67725
C	21.41234	5.92003	16.07375
H	21.87744	5.10889	16.65951
C	22.09845	7.13000	15.87582
H	23.10591	7.27395	16.30143
C	21.49310	8.15475	15.12612
H	22.02492	9.10698	14.96067
C	20.21321	7.96952	14.57829
H	19.74593	8.78142	13.99468
C	13.68540	10.58484	18.31445
H	13.24267	11.57813	18.55116
H	14.68940	10.76719	17.88415
C	13.76597	9.72479	19.58956
H	12.73695	9.55001	19.97545
H	14.29242	10.34383	20.35380
C	14.49336	8.40176	19.44136
C	13.79007	7.17943	19.40690
H	12.69090	7.18871	19.49780
C	14.46830	5.95659	19.26468
H	13.89719	5.01303	19.23985
C	15.86849	5.93510	19.15414
H	16.40324	4.97663	19.04355
C	16.58325	7.14590	19.18945
H	17.68342	7.14228	19.11193
C	15.90141	8.36555	19.33366
H	16.47690	9.30665	19.37399
C	14.94725	7.92641	8.92565
H	14.77529	8.44966	7.96013
H	13.96746	7.58248	9.31429
C	15.93018	6.75326	8.74813
H	16.09541	6.27117	9.73743

H	16.91218	7.16251	8.42100
C	15.44075	5.72447	7.74547
C	15.51688	5.97717	6.35687
H	15.95194	6.92855	6.00438
C	15.05180	5.03697	5.42303
H	15.12175	5.25545	4.34390
C	14.50322	3.81779	5.86057
H	14.14762	3.07426	5.12765
C	14.41753	3.55371	7.23833
H	13.98883	2.60163	7.59457
C	14.88051	4.50026	8.16903
H	14.81348	4.28445	9.24927
C	10.14217	8.55275	8.20197
H	9.25365	8.30174	8.82169
H	11.02030	8.07046	8.67646
C	9.95478	8.08654	6.74553
H	10.87890	8.32812	6.17338
H	9.12681	8.67012	6.28518
C	9.65075	6.60219	6.65126
C	8.31672	6.13914	6.62972
H	7.48883	6.86900	6.65022
C	8.02720	4.76509	6.57683
H	6.97678	4.42908	6.55478
C	9.07255	3.82521	6.54642
H	8.84851	2.74587	6.50430
C	10.40544	4.27205	6.56755
H	11.23683	3.54821	6.53992
C	10.69015	5.64690	6.61944
C	14.55757	12.15070	5.20121
H	14.03847	13.09983	5.44762
H	13.90651	11.56551	4.51690
C	15.92812	12.42528	4.55497
H	16.43237	11.45497	4.34902
H	16.56363	12.97198	5.28742
C	15.79227	13.22975	3.27535
C	15.77369	14.64155	3.30832
H	15.90001	15.16189	4.27347
C	15.60708	15.39061	2.13143
H	15.60004	16.49228	2.18183
C	15.45429	14.73887	0.89540
H	15.32467	15.32549	-0.02950
C	15.47147	13.33417	0.84657
H	15.35686	12.81263	-0.11886
C	15.63867	12.58961	2.02631
H	15.65714	11.48668	1.97855
C	16.28395	15.76488	9.35081
H	16.69665	16.44694	10.12619
H	15.17929	15.87039	9.35214
C	16.87084	16.08533	7.96439
H	16.39535	15.40272	7.22174
H	17.95859	15.85385	7.96325
C	16.64985	17.53264	7.56385
C	17.73067	18.43480	7.46287
H	18.75439	18.07115	7.65771
C	17.52362	19.78116	7.11479
H	18.38515	20.46610	7.03842
C	16.22350	20.25340	6.86698
H	16.05747	21.31016	6.59793

C	15.13604	19.36643	6.96546
H	14.11050	19.72485	6.77425
C	15.34702	18.02011	7.30767
H	14.48533	17.33193	7.37444
H	11.74109	5.98269	6.63026

Ag₁Au₂₄PET₁₈_Ag_in_icosahedron

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Ag	12.46424	15.33834	12.14229
Au	15.54410	16.54944	13.06282
Au	17.38598	13.46559	13.73962
Au	14.80708	11.09648	13.54235
Au	11.03963	14.01553	14.44116
Au	9.60432	16.69409	12.80234
Au	11.02410	16.34437	9.41578
Au	12.60959	13.36342	9.81423
Au	14.09092	13.96114	14.34869
Au	12.43965	14.09604	17.40937
Au	9.35422	12.28825	16.62562
Au	9.98426	11.32159	13.35768
Au	12.49679	9.57731	12.88870
Au	9.31009	8.44065	12.00417
Au	7.52050	11.54841	11.26881
Au	10.12670	13.75463	11.52559
Au	13.94527	10.92751	10.57963
Au	15.42186	8.24162	12.22234
Au	13.99417	8.57997	15.59973
Au	12.34254	11.57298	15.23137
Au	10.89236	10.96060	10.66265
Au	12.52688	10.80686	7.61230
Au	15.60469	12.65421	8.38852
Au	14.96903	13.62829	11.66810
Au	12.48345	12.46761	12.51614
S	13.40892	17.57404	12.89160
S	17.78159	15.72211	13.09297
S	17.16102	11.17504	14.35306
S	9.70023	17.83927	10.71327
S	12.42408	15.04556	7.99183
S	9.35296	15.75734	14.97216
S	14.66386	14.54411	16.70293
S	10.23070	13.80464	18.24828
S	8.25927	10.84544	15.08671
C	13.53116	18.70352	11.42197
H	14.18091	18.23701	10.65339
H	12.50152	18.75554	11.00708
C	14.01102	20.12503	11.77664
H	13.33875	20.54341	12.55818
H	13.86466	20.74674	10.86189
C	15.45494	20.23855	12.22609
C	16.50835	20.17289	11.28698
H	16.27823	20.04611	10.21453
C	17.84779	20.27213	11.69728
H	18.65329	20.21407	10.94597
C	18.16021	20.44793	13.05745
H	19.21159	20.53789	13.37943
C	17.12258	20.51210	14.00319
H	17.35159	20.64355	15.07390
C	15.78385	20.40424	13.58827
H	14.97634	20.44707	14.33845
C	18.60446	16.53417	14.54656
H	18.54792	17.62665	14.35141
H	18.02714	16.31812	15.46860
C	20.06604	16.06841	14.68641

H	20.07864	14.96187	14.81049
H	20.60765	16.29323	13.74100
C	20.76086	16.73442	15.85936
C	21.45482	17.95341	15.69664
H	21.51968	18.40668	14.69208
C	22.06677	18.59058	16.78913
H	22.60794	19.53988	16.63722
C	21.99362	18.01867	18.07123
H	22.47540	18.51568	18.92997
C	21.30653	16.80506	18.24962
H	21.24856	16.34301	19.24957
C	20.69669	16.17190	17.15337
H	20.16619	15.21516	17.30139
C	17.01338	11.26825	16.19903
H	16.17980	11.95413	16.45353
H	16.73442	10.24389	16.53143
C	18.32869	11.72230	16.85768
H	19.16146	11.08037	16.49585
H	18.54770	12.75789	16.50646
C	18.27485	11.68633	18.37465
C	19.08395	10.79303	19.11004
H	19.76840	10.11735	18.56864
C	19.03205	10.75481	20.51464
H	19.67779	10.05211	21.06791
C	18.15996	11.60854	21.21124
H	18.11426	11.57838	22.31290
C	17.34468	12.50119	20.49161
H	16.65659	13.17616	21.02812
C	17.40242	12.54076	19.08837
H	16.75841	13.24746	18.53503
C	7.98957	17.61651	10.02292
H	8.03944	17.95623	8.96628
H	7.74349	16.53426	10.04089
C	6.95007	18.42166	10.82249
H	7.23912	19.49579	10.83109
H	6.97199	18.06991	11.87944
C	5.55382	18.26028	10.24986
C	4.94864	19.28775	9.49513
H	5.49347	20.23559	9.34081
C	3.66453	19.12448	8.94684
H	3.20950	19.94309	8.36359
C	2.96190	17.92392	9.14433
H	1.95218	17.79449	8.71947
C	3.55373	16.89000	9.89220
H	3.00882	15.94528	10.05776
C	4.83685	17.05671	10.43835
H	5.29307	16.23801	11.02127
C	11.30115	14.32943	6.69476
H	11.72121	13.32349	6.46996
H	10.29487	14.17580	7.13080
C	11.23642	15.17625	5.41016
H	12.26765	15.32167	5.01807
H	10.69209	14.56105	4.65546
C	10.54268	16.51876	5.54490
C	11.27591	17.72386	5.55311
H	12.37423	17.68614	5.45921
C	10.62839	18.96537	5.67548
H	11.22221	19.89509	5.67714

C	9.22990	19.02322	5.79375
H	8.71917	19.99661	5.88644
C	8.48577	17.82971	5.78731
H	7.38644	17.86225	5.87060
C	9.13695	16.59121	5.66360
H	8.53923	15.66335	5.65019
C	10.08476	17.04036	16.09658
H	10.25877	16.51838	17.06238
H	11.06477	17.37046	15.69630
C	9.11648	18.22513	16.27709
H	8.96283	18.71608	15.29032
H	8.12754	17.82692	16.59675
C	9.61385	19.24046	17.28954
C	9.50339	18.98987	18.67617
H	9.04333	18.04685	19.01927
C	9.96609	19.92162	19.61966
H	9.85887	19.71010	20.69711
C	10.55467	21.12615	19.19352
H	10.91689	21.85923	19.93374
C	10.67626	21.38705	17.81786
H	11.13360	22.32903	17.47062
C	10.21217	20.45056	16.87775
H	10.30904	20.66324	15.79919
C	14.86607	16.38211	16.85995
H	15.75944	16.63207	16.24690
H	13.99683	16.88936	16.39557
C	15.05915	16.81041	18.32725
H	14.13054	16.57026	18.89261
H	15.87699	16.20228	18.77422
C	15.38754	18.28674	18.45906
C	16.72881	18.72888	18.47222
H	17.54495	17.98772	18.41607
C	17.04073	20.09599	18.56323
H	18.09655	20.41497	18.57654
C	16.01085	21.04996	18.64251
H	16.25222	22.12372	18.71774
C	14.67105	20.62421	18.62787
H	13.85159	21.35963	18.68846
C	14.36404	19.25612	18.53728
H	13.30789	18.93702	18.53122
C	10.40742	12.80345	19.80375
H	10.93100	11.85368	19.56937
H	11.05359	13.39832	20.48431
C	9.03542	12.53168	20.44814
H	8.53301	13.50325	20.65242
H	8.39959	11.98586	19.71534
C	9.16786	11.72905	21.72930
C	9.18710	10.31720	21.69924
H	9.06416	9.79480	20.73481
C	9.35052	9.57076	22.87825
H	9.35850	8.46899	22.83025
C	9.49899	10.22508	24.11347
H	9.62415	9.64037	25.04023
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C	9.31789	12.37178	22.97745
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C	9.87923	5.60254	18.13704
H	10.90846	5.26345	18.34316
C	9.65063	6.93950	17.77061
H	10.50223	7.63981	17.70077
S	11.43965	7.41642	12.26395
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S	7.77581	13.83871	10.65314
S	15.34628	7.09603	14.31303
S	12.58044	9.86988	17.02638
S	15.66361	9.21381	10.06496
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S	14.72824	11.13310	6.76940
S	16.69906	14.09159	9.93102
C	11.28680	6.36356	13.78802
H	10.61210	6.86302	14.51287
H	12.30483	6.34226	14.23294
C	10.82319	4.92583	13.48152
H	11.53128	4.46960	12.75477
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C	9.40193	4.79178	12.96907
C	8.30513	4.89466	13.85349
H	8.48434	5.06642	14.92937
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H	6.14632	4.86098	14.09291
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H	9.98109	4.49635	10.89238
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H	6.36897	7.40603	10.56118
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C	4.88913	8.98394	10.15906
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H	2.66275	6.54510	5.81200
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H	10.90216	8.23154	6.19727
H	9.15321	8.59003	6.30535
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H	6.95934	4.37508	6.56670
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C	10.68552	5.55207	6.65615
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Ag₁Au₂₄PET₁₈_Ag_in_staple

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Au	14.82335	11.16484	13.54420
Au	11.05654	14.04567	14.45841
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Au	11.00689	16.37535	9.42536
Au	12.67015	13.38665	9.78793
Au	14.11021	13.98511	14.37072
Au	12.47140	14.13445	17.42420
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Au	9.98823	11.38560	13.34415
Au	12.47394	9.63690	12.87940
Au	9.37891	8.43166	11.99998
Au	7.58550	11.52282	11.25659
Au	10.18395	13.85990	11.47212
Au	13.96352	10.92832	10.55655
Ag	15.26298	8.49289	12.18837
Au	14.01308	8.60199	15.55507
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Au	12.55205	10.87179	7.59853
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H	17.25388	20.68974	15.04613
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C	21.48778	8.11156	14.86989
H	22.02663	9.06570	14.74272
C	20.19061	7.97149	14.34978
H	19.71769	8.81979	13.82539
C	13.70994	10.60248	18.30988
H	13.28332	11.60559	18.53453
H	14.72076	10.76116	17.88625
C	13.76358	9.75193	19.59252
H	12.72869	9.60477	19.97416
H	14.29988	10.36550	20.35437
C	14.45981	8.41033	19.46134
C	13.72790	7.20465	19.44716
H	12.62930	7.24140	19.53848
C	14.37699	5.96418	19.32320
H	13.78408	5.03389	19.31546
C	15.77587	5.90817	19.20940
H	16.28773	4.93588	19.11181
C	16.51879	7.10224	19.22402
H	17.61835	7.07131	19.14325
C	15.86625	8.33950	19.35104
H	16.46362	9.26735	19.37583
C	14.91632	7.93511	8.85469
H	14.71836	8.39451	7.86228
H	13.94558	7.61673	9.28679
C	15.88784	6.74531	8.72222
H	16.06337	6.31057	9.73138

H	16.86844	7.13283	8.36502
C	15.38816	5.66915	7.77620
C	15.43957	5.85915	6.37639
H	15.85836	6.79813	5.97437
C	14.97495	4.87076	5.49354
H	15.02849	5.03927	4.40456
C	14.45077	3.66528	5.99456
H	14.09249	2.88548	5.30167
C	14.38993	3.46299	7.38400
H	13.98363	2.52089	7.78959
C	14.85117	4.45824	8.26335
H	14.80216	4.29098	9.35324
C	10.17783	8.54490	8.21463
H	9.29542	8.29011	8.84142
H	11.06342	8.07329	8.68597
C	9.98539	8.06921	6.76209
H	10.90726	8.30644	6.18461
H	9.15570	8.64971	6.30088
C	9.67951	6.58445	6.68042
C	8.34468	6.12339	6.66665
H	7.51796	6.85462	6.68576
C	8.05264	4.74954	6.62350
H	7.00154	4.41538	6.60692
C	9.09644	3.80784	6.59590
H	8.87068	2.72862	6.56024
C	10.43010	4.25260	6.61139
H	11.26066	3.52772	6.58833
C	10.71727	5.62732	6.65311
C	14.57105	12.20064	5.20312
H	14.04541	13.14787	5.44327
H	13.92712	11.60921	4.51731
C	15.94333	12.48091	4.56258
H	16.45523	11.51259	4.36642
H	16.57076	13.03613	5.29566
C	15.81140	13.27557	3.27658
C	15.78315	14.68742	3.29863
H	15.89823	15.21576	4.26082
C	15.62124	15.42636	2.11469
H	15.60683	16.52835	2.15639
C	15.48298	14.76438	0.88238
H	15.35765	15.34316	-0.04805
C	15.50987	13.35949	0.84440
H	15.40709	12.82982	-0.11794
C	15.67211	12.62513	2.03116
H	15.69752	11.52200	1.99231
C	16.31190	15.80933	9.37773
H	16.71534	16.48838	10.16057
H	15.20740	15.91438	9.36643
C	16.91435	16.13439	7.99924
H	16.45701	15.44522	7.25132
H	18.00467	15.91576	8.01322
C	16.68060	17.57831	7.59421
C	17.74881	18.49786	7.51877
H	18.77321	18.15116	7.73941
C	17.52819	19.84062	7.16506
H	18.38006	20.53940	7.10826
C	16.22679	20.29157	6.88616
H	16.05019	21.34515	6.61147

C	15.15167	19.38732	6.96007
H	14.12519	19.72913	6.74489
C	15.37640	18.04476	7.30797
H	14.52446	17.34308	7.35631
H	11.76897	5.96086	6.65989

Ag₁₂Au₁₃PET₁₈_I

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Ag	12.52056	15.30216	12.14424
Au	15.50937	16.52431	13.06865
Au	17.37204	13.40093	13.74501
Ag	14.83860	11.20121	13.52054
Ag	11.05634	14.03487	14.40502
Au	9.60057	16.60829	12.84168
Au	11.09187	16.25818	9.40496
Ag	12.62399	13.35812	9.82271
Ag	14.08056	13.96432	14.35276
Au	12.49593	14.11103	17.34321
Au	9.38406	12.23503	16.55008
Ag	10.03544	11.37451	13.39261
Ag	12.48410	9.66145	12.88583
Au	9.49635	8.43819	11.96148
Au	7.63415	11.56109	11.28431
Ag	10.16695	13.76201	11.51105
Ag	13.95033	10.92975	10.62651
Au	15.40206	8.35394	12.18960
Au	13.91158	8.70648	15.62662
Ag	12.38239	11.60696	15.20944
Ag	10.92710	10.99955	10.67778
Au	12.51150	10.85547	7.68765
Au	15.62402	12.73209	8.48160
Ag	14.97154	13.58777	11.63817
Au	12.50312	12.48195	12.51590
S	13.38013	17.56025	12.94335
S	17.72970	15.65919	13.06965
S	17.23676	11.12449	14.41192
S	9.78440	17.73273	10.74566
S	12.46012	15.02298	7.90203
S	9.26240	15.72913	15.01943
S	14.74294	14.57037	16.73620
S	10.26387	13.81192	18.11653
S	8.23969	10.75420	15.09744
C	13.49329	18.74402	11.51632
H	14.11332	18.29546	10.71320
H	12.45375	18.82999	11.13262
C	14.00980	20.14173	11.91155
H	13.36838	20.54143	12.72802
H	13.84889	20.80146	11.02610
C	15.46829	20.21320	12.32089
C	16.49129	20.15168	11.34824
H	16.22669	20.05390	10.28079
C	17.84420	20.21898	11.71898
H	18.62492	20.17026	10.94137
C	18.20127	20.35463	13.07282
H	19.26352	20.41785	13.36397
C	17.19444	20.41276	14.05161
H	17.45840	20.51333	15.11753
C	15.84159	20.33917	13.67602
H	15.05835	20.38160	14.45140
C	18.57487	16.46860	14.51388
H	18.50875	17.56194	14.32715
H	18.01572	16.24112	15.44443
C	20.04114	16.00932	14.62205

H	20.06095	14.90418	14.75782
H	20.55848	16.22547	13.66125
C	20.76265	16.68943	15.77062
C	21.46615	17.89784	15.57414
H	21.51960	18.33159	14.56034
C	22.10268	18.54826	16.64461
H	22.65055	19.48910	16.46653
C	22.04556	18.00011	17.93777
H	22.54671	18.50742	18.77922
C	21.34964	16.79689	18.14958
H	21.30438	16.35298	19.15834
C	20.71519	16.15053	17.07534
H	20.17846	15.20171	17.24950
C	17.08306	11.25126	16.25466
H	16.23485	11.92180	16.50275
H	16.82573	10.22721	16.60599
C	18.38365	11.74199	16.91812
H	19.23118	11.11530	16.56442
H	18.58156	12.77910	16.55909
C	18.32172	11.71605	18.43479
C	19.11813	10.81902	19.17955
H	19.80239	10.13699	18.64578
C	19.05453	10.78530	20.58373
H	19.68735	10.07656	21.14417
C	18.18577	11.65024	21.27066
H	18.13354	11.62636	22.37219
C	17.38329	12.54693	20.54170
H	16.69822	13.23080	21.07079
C	17.45049	12.57973	19.13866
H	16.81409	13.28757	18.57776
C	8.07985	17.58886	10.02149
H	8.16032	17.95061	8.97407
H	7.79681	16.51571	10.01008
C	7.05552	18.41046	10.82384
H	7.38594	19.47151	10.87141
H	7.04053	18.02654	11.86972
C	5.66600	18.32189	10.21938
C	5.11157	19.39998	9.49691
H	5.69245	20.33274	9.39013
C	3.83275	19.30531	8.92058
H	3.41747	20.16296	8.36439
C	3.08476	18.12358	9.05610
H	2.07944	18.04801	8.60847
C	3.62560	17.03983	9.77147
H	3.04491	16.10939	9.88873
C	4.90328	17.13830	10.34641
H	5.31904	16.28131	10.90415
C	11.29806	14.32436	6.63109
H	11.71252	13.32464	6.37201
H	10.30729	14.15478	7.09662
C	11.17752	15.18813	5.36104
H	12.19282	15.34729	4.93419
H	10.60926	14.58039	4.61805
C	10.47955	16.52214	5.54332
C	11.20821	17.72946	5.58671
H	12.30534	17.69989	5.47881
C	10.55704	18.96279	5.76110
H	11.14727	19.89447	5.78956

C	9.15961	19.01038	5.89738
H	8.64620	19.97741	6.03205
C	8.41993	17.81486	5.85491
H	7.32161	17.83954	5.95221
C	9.07464	16.58455	5.67763
H	8.48008	15.65561	5.63074
C	9.94668	17.05587	16.12319
H	10.07971	16.56865	17.11326
H	10.94484	17.37007	15.75545
C	8.98481	18.25546	16.22881
H	8.86027	18.70380	15.21805
H	7.98477	17.87956	16.54036
C	9.46934	19.30916	17.20742
C	9.28859	19.14052	18.59899
H	8.77194	18.23829	18.97025
C	9.74839	20.10375	19.51184
H	9.59259	19.95263	20.59355
C	10.39936	21.26170	19.04915
H	10.75355	22.02283	19.76459
C	10.59043	21.44196	17.66831
H	11.09867	22.34618	17.29268
C	10.13161	20.47263	16.75957
H	10.28295	20.62236	15.67661
C	14.92500	16.40826	16.91866
H	15.84134	16.67017	16.34555
H	14.07415	16.91649	16.42183
C	15.05755	16.83684	18.39266
H	14.11226	16.58132	18.92277
H	15.86668	16.23894	18.86788
C	15.35807	18.31758	18.53810
C	16.69117	18.78178	18.58656
H	17.52027	18.05404	18.54731
C	16.97778	20.15359	18.68920
H	18.02726	20.49071	18.73185
C	15.93057	21.09038	18.74318
H	16.15252	22.16786	18.82500
C	14.59875	20.64287	18.69341
H	13.76608	21.36455	18.73593
C	14.31716	19.27012	18.59137
H	13.26723	18.93279	18.55728
C	10.41491	12.86369	19.70830
H	10.94145	11.90667	19.51296
H	11.04920	13.48070	20.38014
C	9.03133	12.61203	20.33587
H	8.52139	13.58845	20.49177
H	8.41211	12.03492	19.61287
C	9.14088	11.86042	21.64973
C	9.18083	10.44886	21.67318
H	9.09154	9.88986	20.72579
C	9.32247	9.74958	22.88343
H	9.34667	8.64699	22.87777
C	9.42821	10.45181	24.09665
H	9.53776	9.90396	25.04763
C	9.38941	11.85685	24.08917
H	9.46707	12.41772	25.03601
C	9.24750	12.55157	22.87622
H	9.21272	13.65506	22.87882
C	8.75159	9.06221	15.65674

H	8.30970	8.37062	14.90661
H	9.85633	8.97077	15.59458
C	8.25176	8.72214	17.07308
H	8.76160	9.40310	17.79320
H	7.16294	8.93867	17.13731
C	8.51537	7.27358	17.44109
C	7.46009	6.34078	17.53463
H	6.42432	6.68176	17.36319
C	7.70774	4.99209	17.84490
H	6.86567	4.28294	17.91840
C	9.02370	4.54855	18.06072
H	9.22146	3.49024	18.30091
C	10.08593	5.46624	17.96862
H	11.12352	5.13113	18.13518
C	9.83425	6.81471	17.66456
H	10.67603	7.52766	17.60266
S	11.62555	7.40218	12.08764
S	7.27583	9.30265	11.95834
S	7.76990	13.83731	10.61717
S	15.21532	7.22925	14.28522
S	12.54588	9.94293	17.13085
S	15.74203	9.23268	10.01203
S	10.26364	10.39791	8.29345
S	14.74364	11.15583	6.91476
S	16.76777	14.21264	9.93509
C	11.51147	6.21929	13.51536
H	10.89085	6.66844	14.31770
H	12.55072	6.13348	13.89987
C	10.99511	4.82131	13.12088
H	11.63655	4.42136	12.30454
H	11.15627	4.16211	14.00665
C	9.53665	4.74926	12.71159
C	8.51361	4.80997	13.68423
H	8.77816	4.90691	14.75177
C	7.16074	4.74246	13.31335
H	6.37997	4.79046	14.09096
C	6.80379	4.60737	11.95943
H	5.74156	4.54445	11.66813
C	7.81067	4.54984	10.98065
H	7.54676	4.44941	9.91471
C	9.16346	4.62369	11.35638
H	9.94678	4.58179	10.58104
C	6.43462	8.49386	10.51144
H	6.50149	7.40039	10.69716
H	6.99579	8.72279	9.58245
C	4.96810	8.95157	10.39988
H	4.94762	10.05581	10.25707
H	4.45034	8.74104	11.36170
C	4.24820	8.26363	9.25497
C	3.54544	7.05592	9.45831
H	3.49128	6.62850	10.47476
C	2.91089	6.39807	8.39120
H	2.36334	5.45807	8.57465
C	2.96958	6.93773	7.09454
H	2.47000	6.42458	6.25570
C	3.66495	8.14005	6.87587
H	3.71157	8.57725	5.86425
C	4.29727	8.79392	7.94679

H	4.83401	9.74171	7.76714
C	7.92564	13.70949	8.77474
H	8.77676	13.04210	8.52804
H	8.17928	14.73426	8.42287
C	6.62790	13.21289	8.10997
H	5.77640	13.83232	8.46688
H	6.43727	12.17287	8.46450
C	6.68943	13.24645	6.59344
C	5.88605	14.14074	5.85286
H	5.19574	14.81421	6.38969
C	5.95037	14.18241	4.44891
H	5.31207	14.88880	3.89174
C	6.82679	13.32838	3.75806
H	6.88053	13.35943	2.65678
C	7.63560	12.43398	4.48281
H	8.32629	11.75822	3.95061
C	7.56764	12.39316	5.88559
H	8.20918	11.68740	6.44325
C	16.92044	7.36500	15.00955
H	16.83856	7.00116	16.05614
H	17.20811	8.43689	15.02325
C	17.94065	6.54031	14.20511
H	17.60811	5.47978	14.16089
H	17.95238	6.92199	13.15839
C	19.33255	6.62694	14.80438
C	19.88717	5.54832	15.52589
H	19.30362	4.61781	15.63768
C	21.16935	5.63961	16.09522
H	21.58450	4.78165	16.65102
C	21.92068	6.81848	15.95351
H	22.92903	6.89099	16.39478
C	21.37955	7.90298	15.23945
H	21.96267	8.83131	15.11768
C	20.09838	7.80793	14.67164
H	19.68222	8.66553	14.11512
C	13.71042	10.63958	18.40061
H	13.29994	11.64153	18.65742
H	14.70212	10.80403	17.93524
C	13.82659	9.77753	19.67221
H	12.81039	9.62281	20.09852
H	14.39661	10.38412	20.41480
C	14.51980	8.44070	19.49214
C	13.78708	7.23575	19.45152
H	12.69026	7.26902	19.56143
C	14.43394	6.00005	19.27787
H	13.84058	5.07030	19.25189
C	15.83097	5.94767	19.13934
H	16.34093	4.97887	19.00428
C	16.57469	7.14078	19.17928
H	17.67283	7.11229	19.08088
C	15.92429	8.37348	19.35581
H	16.52198	9.30052	19.40031
C	15.05345	7.90822	8.90822
H	14.92171	8.39625	7.91838
H	14.05443	7.59684	9.27604
C	16.01175	6.70588	8.80155
H	16.13390	6.25516	9.81154
H	17.01323	7.07932	8.49172

C	15.52503	5.65590	7.82003
C	15.71135	5.82576	6.42934
H	16.23332	6.72622	6.06126
C	15.25012	4.86613	5.51343
H	15.41108	5.01779	4.43255
C	14.59159	3.71086	5.97208
H	14.23502	2.95315	5.25422
C	14.39495	3.52945	7.35199
H	13.88161	2.62682	7.72453
C	14.85530	4.49516	8.26383
H	14.69906	4.34475	9.34600
C	10.07738	8.56063	8.10932
H	9.16062	8.30070	8.68267
H	10.92713	8.04970	8.60525
C	9.94222	8.13392	6.63498
H	10.88774	8.38678	6.10404
H	9.13461	8.73510	6.16132
C	9.63571	6.65456	6.48814
C	8.30056	6.19643	6.43836
H	7.47477	6.92797	6.47682
C	8.00759	4.82600	6.33537
H	6.95655	4.49390	6.29223
C	9.05051	3.88443	6.28197
H	8.82373	2.80798	6.19997
C	10.38435	4.32589	6.33263
H	11.21352	3.60016	6.29025
C	10.67234	5.69729	6.43513
C	14.59076	12.10526	5.32384
H	14.06270	13.06123	5.52023
H	13.95718	11.48789	4.65166
C	15.97362	12.35987	4.69588
H	16.48804	11.38500	4.54517
H	16.58980	12.94340	5.41633
C	15.86124	13.10449	3.37829
C	15.81416	14.51569	3.34790
H	15.89877	15.07974	4.29272
C	15.67077	15.20832	2.13406
H	15.64122	16.31079	2.13428
C	15.57010	14.49967	0.92415
H	15.45949	15.04234	-0.02968
C	15.61549	13.09488	0.93857
H	15.54181	12.52902	-0.00562
C	15.75903	12.40681	2.15511
H	15.79829	11.30346	2.15809
C	16.25651	15.90494	9.37625
H	16.69844	16.59648	10.12639
H	15.15176	15.99653	9.43835
C	16.75598	16.24491	7.95976
H	16.24901	15.56101	7.24041
H	17.84562	16.03234	7.89629
C	16.48644	17.69182	7.58953
C	17.53705	18.63003	7.49807
H	18.57399	18.29514	7.67448
C	17.28330	19.97672	7.18402
H	18.12181	20.69024	7.11185
C	15.96576	20.41276	6.96261
H	15.76323	21.46934	6.71882
C	14.90809	19.48971	7.05329

H	13.86929	19.81896	6.88268
C	15.16585	18.14328	7.36121
H	14.32757	17.42617	7.42279
H	11.72384	6.02968	6.46944

Ag₁₂Au₁₃PET₁₈_II

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Au	12.56519	15.33962	12.14111
Ag	15.54364	16.37676	13.00758
Ag	17.22941	13.43408	13.66401
Au	14.82658	11.12556	13.56857
Au	11.07049	14.07541	14.44262
Ag	9.78143	16.55305	12.78465
Ag	11.08999	16.15704	9.57454
Au	12.65596	13.35870	9.76672
Au	14.14319	13.95659	14.37653
Ag	12.44639	14.02682	17.21910
Ag	9.52658	12.42286	16.47772
Au	9.98908	11.38907	13.38443
Au	12.43543	9.62106	12.88737
Ag	9.45805	8.58271	12.02092
Ag	7.77233	11.52497	11.36437
Au	10.17464	13.83528	11.46085
Au	13.93098	10.88558	10.58647
Ag	15.21931	8.40781	12.24443
Ag	13.91107	8.80433	15.45400
Au	12.34535	11.60279	15.26285
Au	10.85869	11.00378	10.65260
Ag	12.55576	10.93466	7.81008
Ag	15.47423	12.53853	8.55097
Au	15.01262	13.57057	11.64457
Au	12.50069	12.48033	12.51473
S	13.43562	17.58182	12.68525
S	17.87869	15.72251	13.15971
S	17.18620	11.07345	14.32604
S	9.78902	17.86713	10.73272
S	12.45837	14.96887	7.89930
S	9.33836	15.72239	15.04906
S	14.75785	14.62712	16.66907
S	10.30208	13.79753	18.34504
S	8.17233	10.99839	15.01573
C	13.66200	18.52440	11.09882
H	14.37199	17.98014	10.44286
H	12.67002	18.53547	10.59822
C	14.13077	19.97309	11.34258
H	13.39395	20.47942	12.00492
H	14.08541	20.49203	10.35664
C	15.52712	20.11327	11.91779
C	16.66288	19.97530	11.08921
H	16.53154	19.78001	10.01054
C	17.95908	20.08707	11.61830
H	18.83090	19.97544	10.95222
C	18.14435	20.34294	12.98862
H	19.16205	20.43498	13.40420
C	17.02335	20.48158	13.82508
H	17.15275	20.67770	14.90264
C	15.72807	20.36601	13.29151
H	14.85407	20.47367	13.95553
C	18.53381	16.46818	14.72751
H	18.47944	17.57119	14.60422
H	17.88022	16.18699	15.57913
C	19.98567	16.02340	14.99527

H	20.00638	14.91480	15.09789
H	20.60794	16.27609	14.10840
C	20.56002	16.67435	16.23969
C	21.29082	17.87989	16.15925
H	21.47699	18.33151	15.16917
C	21.78832	18.50532	17.31500
H	22.36125	19.44407	17.22689
C	21.56144	17.93442	18.57943
H	21.95339	18.42184	19.48802
C	20.83576	16.73401	18.67652
H	20.65659	16.27252	19.66207
C	20.34118	16.11286	17.51731
H	19.77961	15.16658	17.60454
C	17.10401	11.20639	16.17449
H	16.26127	11.87352	16.44867
H	16.88126	10.18811	16.56287
C	18.42582	11.73235	16.76509
H	19.26752	11.10577	16.39711
H	18.59542	12.76222	16.37146
C	18.41899	11.74702	18.28319
C	19.20705	10.83952	19.02386
H	19.85150	10.12298	18.48594
C	19.18478	10.83936	20.42967
H	19.80989	10.12174	20.98739
C	18.36773	11.74925	21.12214
H	18.34856	11.75150	22.22495
C	17.57522	12.65793	20.39731
H	16.93110	13.37728	20.93074
C	17.60028	12.65654	18.99233
H	16.97110	13.37285	18.43404
C	8.07101	17.64175	10.07186
H	8.08739	17.98340	9.01455
H	7.82169	16.55888	10.08855
C	7.03339	18.43466	10.88892
H	7.32999	19.50644	10.92004
H	7.05352	18.06154	11.93852
C	5.63558	18.29692	10.31437
C	5.05372	19.33082	9.54960
H	5.61746	20.26727	9.39352
C	3.77055	19.18857	8.99338
H	3.33438	20.01264	8.40334
C	3.04414	18.00233	9.19239
H	2.03520	17.88926	8.76097
C	3.61165	16.96213	9.95047
H	3.04776	16.02884	10.11772
C	4.89427	17.10835	10.50413
H	5.33195	16.28506	11.09483
C	11.25766	14.23501	6.68356
H	11.65064	13.22745	6.42083
H	10.27781	14.08836	7.17891
C	11.11196	15.08424	5.40605
H	12.11543	15.21783	4.94336
H	10.50842	14.47870	4.69025
C	10.44659	16.43370	5.59784
C	11.20545	17.62198	5.65312
H	12.30114	17.56501	5.54166
C	10.58567	18.86905	5.84229
H	11.19869	19.78522	5.88292

C	9.18977	18.94976	5.97941
H	8.70119	19.92761	6.12674
C	8.42008	17.77407	5.92406
H	7.32292	17.82549	6.02345
C	9.04384	16.52950	5.73407
H	8.42680	15.61579	5.67813
C	10.05901	17.02679	16.15676
H	10.24779	16.53866	17.13717
H	11.02903	17.37547	15.74738
C	9.06508	18.19505	16.30865
H	8.89120	18.65161	15.30894
H	8.08828	17.78267	16.64803
C	9.53946	19.25631	17.28452
C	9.49789	19.02463	18.67834
H	9.10716	18.06341	19.05518
C	9.93750	20.00064	19.58745
H	9.89301	19.79957	20.67125
C	10.42572	21.23412	19.11953
H	10.76463	22.00360	19.83333
C	10.47626	21.47752	17.73632
H	10.85426	22.44186	17.35655
C	10.04079	20.49482	16.83003
H	10.08129	20.69399	15.74524
C	14.82911	16.48239	16.74434
H	15.70834	16.78668	16.13589
H	13.92812	16.91098	16.26023
C	14.97564	16.97632	18.19699
H	14.04898	16.72098	18.75910
H	15.81060	16.42159	18.67987
C	15.24425	18.46876	18.27034
C	16.56845	18.95985	18.28740
H	17.41179	18.24768	18.27992
C	16.82832	20.34033	18.32021
H	17.87135	20.69874	18.34015
C	15.76303	21.25811	18.33420
H	15.96407	22.34247	18.36175
C	14.44010	20.78298	18.31614
H	13.59307	21.48867	18.32954
C	14.18462	19.40166	18.28471
H	13.14075	19.04433	18.27702
C	10.56640	12.62644	19.75964
H	11.02887	11.68979	19.38237
H	11.28235	13.10892	20.46020
C	9.23893	12.31852	20.48114
H	8.76456	13.27822	20.78459
H	8.54618	11.83023	19.75905
C	9.44317	11.43201	21.69542
C	9.46458	10.02511	21.57186
H	9.29084	9.56500	20.58373
C	9.69304	9.20355	22.68865
H	9.69977	8.10732	22.56743
C	9.90632	9.77590	23.95474
H	10.08328	9.13231	24.83275
C	9.88766	11.17449	24.09388
H	10.04906	11.63422	25.08375
C	9.65852	11.99149	22.97401
H	9.63976	13.08911	23.09267
C	8.48843	9.27494	15.62720

H	7.99394	8.59407	14.90088
H	9.57963	9.07541	15.60109
C	7.93084	9.05814	17.04585
H	8.46748	9.74599	17.73978
H	6.85759	9.34967	17.06699
C	8.08763	7.62124	17.50789
C	6.97924	6.74981	17.57382
H	5.97811	7.13221	17.31001
C	7.13143	5.41034	17.97284
H	6.24946	4.74941	18.02077
C	8.40273	4.91488	18.30988
H	8.52508	3.86416	18.62210
C	9.51713	5.77087	18.24709
H	10.51977	5.39353	18.50975
C	9.36071	7.11004	17.85111
H	10.24245	7.77438	17.80968
S	11.56623	7.37804	12.34417
S	7.12293	9.23622	11.86689
S	7.81517	13.88581	10.70334
S	15.21158	7.09355	14.29623
S	12.54262	9.99189	17.12966
S	15.66377	9.23917	9.98055
S	10.24424	10.33357	8.35977
S	14.69981	11.16365	6.68337
S	16.82819	13.96364	10.01246
C	11.33938	6.43597	13.93081
H	10.62957	6.98068	14.58661
H	12.33134	6.42460	14.43145
C	10.87004	4.98743	13.68729
H	11.60679	4.48062	13.02524
H	10.91498	4.46869	14.67336
C	9.47375	4.84763	13.11184
C	8.33785	4.98592	13.94018
H	8.46899	5.18118	15.01886
C	7.04173	4.87451	13.41080
H	6.16981	4.98632	14.07671
C	6.85669	4.61872	12.04044
H	5.83905	4.52706	11.62463
C	7.97782	4.47974	11.20423
H	7.84859	4.28365	10.12664
C	9.27302	4.59489	11.73809
H	10.14714	4.48688	11.07427
C	6.46980	8.49120	10.29800
H	6.52426	7.38815	10.42090
H	7.12436	8.77287	9.44729
C	5.01817	8.93570	10.02855
H	4.99725	10.04433	9.92630
H	4.39480	8.68245	10.91448
C	4.44576	8.28494	8.78312
C	3.71528	7.07911	8.86216
H	3.52704	6.62763	9.85191
C	3.22058	6.45330	7.70542
H	2.64781	5.51435	7.79243
C	3.44994	7.02412	6.44140
H	3.06058	6.53616	5.53200
C	4.17503	8.22500	6.34574
H	4.35585	8.68660	5.36054
C	4.66678	8.84656	7.50594

H	5.22772	9.79331	7.41983
C	7.89876	13.75404	8.85486
H	8.74173	13.08709	8.58095
H	8.12192	14.77259	8.46739
C	6.57749	13.22866	8.26260
H	5.73534	13.85435	8.63108
H	6.40796	12.19805	8.65429
C	6.58553	13.21678	6.74447
C	5.79705	14.12477	6.00486
H	5.15079	14.83907	6.54358
C	5.82145	14.12847	4.59909
H	5.19576	14.84622	4.04220
C	6.64101	13.22161	3.90560
H	6.66257	13.22278	2.80283
C	7.43348	12.31205	4.62936
H	8.07897	11.59453	4.09511
C	7.40623	12.30986	6.03430
H	8.03542	11.59288	6.59173
C	16.92959	7.31926	14.95695
H	16.91328	6.97761	16.01426
H	17.17867	8.40218	14.94026
C	17.96740	6.52654	14.13994
H	17.67167	5.45449	14.10988
H	17.94643	6.89878	13.09005
C	19.36539	6.66585	14.71370
C	19.94872	5.63285	15.47857
H	19.38619	4.69574	15.63501
C	21.23184	5.77686	16.03446
H	21.66928	4.95339	16.62440
C	21.95670	6.96398	15.83506
H	22.96544	7.07857	16.26655
C	21.38779	8.00323	15.07675
H	21.95052	8.93713	14.90901
C	20.10526	7.85523	14.52335
H	19.66652	8.67772	13.93230
C	13.74265	10.72566	18.34607
H	13.34921	11.73295	18.60907
H	14.72267	10.87283	17.85122
C	13.88797	9.87590	19.62328
H	12.88390	9.73901	20.08371
H	14.48823	10.48262	20.34083
C	14.55781	8.52862	19.43169
C	13.80274	7.33802	19.37375
H	12.70662	7.39152	19.48257
C	14.42683	6.09304	19.18488
H	13.81678	5.17498	19.14232
C	15.82328	6.01681	19.05073
H	16.31524	5.04063	18.90356
C	16.58916	7.19486	19.10868
H	17.68668	7.14695	19.01154
C	15.96113	8.43729	19.29845
H	16.57516	9.35288	19.35626
C	14.94386	7.93487	8.87222
H	14.75486	8.42332	7.89200
H	13.97399	7.58555	9.28141
C	15.93829	6.76713	8.71978
H	16.11337	6.31094	9.71945
H	16.91455	7.17990	8.37929

C	15.46325	5.70545	7.74467
C	15.50354	5.93663	6.35073
H	15.89289	6.89815	5.97324
C	15.06384	4.95999	5.44235
H	15.10705	5.16080	4.35845
C	14.57698	3.72630	5.91111
H	14.23868	2.95604	5.19786
C	14.52759	3.48344	7.29446
H	14.15066	2.51894	7.67490
C	14.96299	4.46684	8.20003
H	14.92265	4.26840	9.28495
C	10.17376	8.47831	8.28403
H	9.29553	8.17330	8.89356
H	11.07567	8.05013	8.76679
C	10.02576	7.98480	6.83139
H	10.95133	8.24153	6.26813
H	9.18941	8.53862	6.34986
C	9.75915	6.49200	6.75786
C	8.43565	5.99898	6.74274
H	7.59125	6.70987	6.75216
C	8.17778	4.61814	6.70937
H	7.13522	4.25830	6.69116
C	9.24439	3.70194	6.69277
H	9.04495	2.61731	6.66460
C	10.56666	4.17900	6.70892
H	11.41465	3.47449	6.69333
C	10.82014	5.56068	6.74109
C	14.43505	12.33481	5.26891
H	13.97211	13.27120	5.64624
H	13.71938	11.85205	4.56826
C	15.76238	12.64351	4.54748
H	16.23713	11.68410	4.24368
H	16.45497	13.13186	5.26968
C	15.55763	13.53031	3.33349
C	15.53518	14.93714	3.45757
H	15.70878	15.39702	4.44584
C	15.30586	15.75894	2.34113
H	15.29830	16.85512	2.46276
C	15.09279	15.18690	1.07487
H	14.91505	15.83068	0.19716
C	15.11260	13.78838	0.93520
H	14.95145	13.32889	-0.05483
C	15.34258	12.97114	2.05471
H	15.36224	11.87357	1.93563
C	16.50989	15.68709	9.40212
H	17.00431	16.36805	10.12840
H	15.41850	15.88550	9.42930
C	17.06597	15.90534	7.98309
H	16.53001	15.21675	7.28937
H	18.13974	15.61582	7.96099
C	16.90611	17.34214	7.52177
C	18.01275	18.21577	7.45550
H	19.01491	17.83504	7.71783
C	17.85754	19.55531	7.05788
H	18.73817	20.21801	7.00969
C	16.58496	20.04859	6.72251
H	16.46022	21.09941	6.41156
C	15.47232	19.19032	6.78547

H	14.46870	19.56591	6.52403
C	15.63174	17.85111	7.18006
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Ag₁₂Au₁₃PET₁₈_III

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Ag	12.52287	15.31799	12.17197
Au	15.51968	16.52082	13.10237
Au	17.38203	13.40364	13.76969
Ag	14.84046	11.19392	13.54771
Ag	11.00936	14.00358	14.39132
Au	9.60385	16.60757	12.81228
Au	11.11635	16.26440	9.38241
Ag	12.68848	13.43757	9.83867
Ag	14.03993	13.94151	14.38166
Au	12.48697	14.10008	17.34808
Au	9.39576	12.23039	16.52482
Ag	10.02990	11.33347	13.30477
Ag	12.49881	9.65488	12.85235
Au	9.46849	8.44669	11.95901
Au	7.59534	11.55891	11.30754
Ag	10.17834	13.78466	11.48967
Ag	14.03358	10.96746	10.64491
Au	15.43238	8.36921	12.17282
Au	13.90889	8.69550	15.59984
Ag	12.34109	11.57396	15.18956
Au	11.02913	11.05745	10.58209
Ag	12.52192	10.94957	7.83935
Au	15.63453	12.75949	8.48152
Ag	15.00217	13.61487	11.67126
Au	12.51924	12.48884	12.51141
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S	17.74194	15.66009	13.08952
S	17.23687	11.12988	14.44137
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S	12.48657	15.03590	7.87126
S	9.24605	15.73689	14.99148
S	14.74024	14.53828	16.74829
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H	12.43953	18.84762	11.22581
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H	13.38599	20.53745	12.83004
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C	15.47698	20.21437	12.37529
C	16.47918	20.16806	11.38040
H	16.19236	20.08466	10.31755
C	17.83951	20.23342	11.72321
H	18.60348	20.19768	10.92849
C	18.22504	20.35157	13.07086
H	19.29314	20.41321	13.34011
C	17.23919	20.39410	14.07155
H	17.52550	20.48185	15.13280
C	15.87878	20.32239	13.72381
H	15.11228	20.35288	14.51621
C	18.58544	16.46923	14.53543
H	18.51902	17.56260	14.34898
H	18.02537	16.24165	15.46537
C	20.05182	16.01089	14.64598

H	20.07266	14.90620	14.78474
H	20.57003	16.22520	13.68519
C	20.77039	16.69528	15.79385
C	21.45778	17.91314	15.59858
H	21.50136	18.35109	14.58610
C	22.09013	18.56806	16.66871
H	22.62566	19.51615	16.49155
C	22.04475	18.01521	17.96039
H	22.54253	18.52624	18.80158
C	21.36515	16.80251	18.17090
H	21.32967	16.35469	19.17832
C	20.73476	16.15166	17.09693
H	20.21010	15.19590	17.27006
C	17.08151	11.25410	16.28422
H	16.23210	11.92309	16.53238
H	16.82554	10.22893	16.63311
C	18.38012	11.74566	16.95069
H	19.22996	11.12315	16.59517
H	18.57538	12.78504	16.59670
C	18.31608	11.71236	18.46721
C	19.12136	10.82126	19.20950
H	19.81487	10.14992	18.67414
C	19.05456	10.77969	20.61333
H	19.69455	10.07590	21.17185
C	18.17355	11.63043	21.30235
H	18.11805	11.59960	22.40354
C	17.36249	12.52139	20.57589
H	16.66796	13.19431	21.10665
C	17.43307	12.56219	19.17325
H	16.78973	13.26506	18.61410
C	8.10043	17.58975	9.98525
H	8.18600	17.94939	8.93753
H	7.81735	16.51669	9.97495
C	7.07305	18.41346	10.78153
H	7.39909	19.47622	10.82041
H	7.05980	18.03790	11.83045
C	5.68373	18.31423	10.17826
C	5.12658	19.38233	9.44317
H	5.70533	20.31503	9.32482
C	3.84756	19.27793	8.86896
H	3.42984	20.12802	8.30310
C	3.10228	18.09630	9.01931
H	2.09693	18.01303	8.57311
C	3.64598	17.02235	9.74724
H	3.06746	16.09209	9.87601
C	4.92391	17.13043	10.31998
H	5.34206	16.28117	10.88775
C	11.30754	14.29680	6.63756
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H	10.32700	14.12852	7.12465
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H	12.16477	15.27950	4.89856
H	10.57268	14.51049	4.63546
C	10.46928	16.47276	5.52116
C	11.20495	17.67661	5.53843
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C	10.56202	18.91585	5.70050
H	11.15726	19.84470	5.70696

C	9.16635	18.97289	5.85100
H	8.65938	19.94462	5.97598
C	8.42001	17.78091	5.83499
H	7.32296	17.81301	5.94382
C	9.06635	16.54448	5.66947
H	8.46638	15.61827	5.64252
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H	10.04897	16.58469	17.08853
H	10.97189	17.32818	15.73496
C	9.03609	18.29338	16.14878
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H	8.01748	17.96299	16.45057
C	9.54413	19.35172	17.10963
C	9.23039	19.29201	18.48600
H	8.58866	18.47385	18.85688
C	9.71340	20.25929	19.38272
H	9.45107	20.19505	20.45239
C	10.52218	21.31155	18.91760
H	10.89616	22.07618	19.61920
C	10.84674	21.38247	17.55143
H	11.47791	22.20481	17.17426
C	10.36410	20.40956	16.65954
H	10.62184	20.47243	15.58826
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H	15.86368	16.62685	16.37061
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H	17.56944	17.95255	18.57086
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H	16.28722	22.08865	18.91419
C	14.70225	20.59728	18.77127
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S	15.23402	7.23497	14.26198
S	12.51837	9.90465	17.10442
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S	14.74694	11.19382	6.90907
S	16.77929	14.23810	9.94435
C	11.52271	6.21690	13.46664
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C	11.01141	4.82042	13.05957
H	11.63661	4.44242	12.22031
H	11.20185	4.14672	13.92853
C	9.54375	4.73863	12.68597
C	8.54613	4.75868	13.68626
H	8.83756	4.83182	14.74862
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H	5.72532	4.50677	11.73751
C	7.77526	4.56030	10.99638
H	7.48517	4.48351	9.93533
C	9.13650	4.64379	11.33816
H	9.89900	4.63361	10.54150
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H	6.48759	7.39960	10.68839
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C	4.94330	8.93989	10.39493
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C	21.16937	5.64984	16.12650
H	21.57842	4.79041	16.68455
C	21.92248	6.82886	15.99563
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C	21.38966	7.91490	15.27769
H	21.97450	8.84316	15.16391
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H	7.47571	6.85477	6.59167
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H	8.88119	2.75273	6.32750
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H	11.26017	3.58096	6.37752
C	10.68994	5.67079	6.51365
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H	14.04499	13.12086	5.55303
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C	15.76134	13.16484	3.34857
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C	16.46882	17.72001	7.60664
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C	17.25705	20.00991	7.21229
H	18.09271	20.72724	7.14482
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H	15.73179	21.49821	6.75010
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Au	12.53527	13.30613	9.79285
Ag	14.18620	14.03976	14.28952
Au	12.55403	14.21114	17.35008
Ag	9.61613	12.35740	16.46706
Au	10.06518	11.41905	13.48213
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Ag	7.76791	11.57462	11.49001
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C	8.44239	4.75589	13.63284
H	8.64894	4.85359	14.71315
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Ag₁₂Au₁₃PET₁₈_V

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Ag	14.77150	11.09480	13.65296
Au	10.95998	14.03491	14.32630
Ag	9.74096	16.51930	12.81360
Au	11.05533	16.31308	9.42350
Ag	12.79447	13.38539	9.79710
Au	14.03501	13.85725	14.44761
Ag	12.42986	14.02612	17.17087
Au	9.34121	12.24650	16.54939
Ag	9.93431	11.40862	13.27493
Au	12.37245	9.66818	12.89874
Ag	9.57703	8.58436	11.93016
Au	7.61202	11.55811	11.25235
Ag	10.23445	13.86794	11.37313
Au	14.04714	10.92897	10.69952
Ag	15.26425	8.44346	12.21217
Au	13.95029	8.65059	15.60265
Ag	12.21218	11.57881	15.22935
Au	10.97237	11.10588	10.57810
Ag	12.57794	10.93832	7.85485
Au	15.66677	12.71749	8.47745
Ag	15.07272	13.55339	11.75061
Au	12.50332	12.48164	12.51311
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S	9.30260	15.72835	15.08206
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C	14.74399	4.45895	8.27349
H	14.69143	4.28421	9.36199
C	10.11693	8.54469	8.22039
H	9.22009	8.26535	8.81539
H	10.99675	8.08408	8.71382
C	9.97159	8.06222	6.76307
H	10.91666	8.28146	6.21662
H	9.16905	8.65537	6.27098
C	9.63975	6.58363	6.67317
C	8.29576	6.15061	6.63334
H	7.48403	6.89867	6.63903
C	7.97570	4.78341	6.58102
H	6.91825	4.47205	6.54455
C	8.99992	3.81998	6.57009
H	8.75251	2.74587	6.52666
C	10.34201	4.23673	6.61177
H	11.15729	3.49445	6.60156
C	10.65755	5.60511	6.66277
C	14.59285	12.15402	5.30478
H	14.07985	13.11348	5.52429
H	13.93382	11.55350	4.64093
C	15.95592	12.40870	4.63315
H	16.46047	11.43202	4.46191
H	16.59590	12.98346	5.33954
C	15.81020	13.16157	3.32389
C	15.76748	14.57320	3.30211
H	15.88057	15.13177	4.24727
C	15.59391	15.27331	2.09645
H	15.56883	16.37591	2.10348
C	15.45794	14.57203	0.88568
H	15.32362	15.12045	-0.06179
C	15.49861	13.16699	0.89120
H	15.39781	12.60671	-0.05385
C	15.67251	12.47167	2.09965
H	15.70900	11.36820	2.09527
C	16.33908	15.86170	9.43971
H	16.77606	16.53827	10.20634
H	15.23498	15.97178	9.47009
C	16.88570	16.19880	8.03993
H	16.39441	15.51979	7.30527
H	17.97424	15.97344	8.01078
C	16.64499	17.64789	7.65923
C	17.70718	18.57676	7.61564
H	18.73185	18.23253	7.83909
C	17.48025	19.92514	7.28862
H	18.32733	20.63126	7.25593
C	16.17853	20.37199	7.00396
H	15.99717	21.42961	6.74845
C	15.10950	19.45852	7.04627

H	14.08317	19.79695	6.82517
C	15.34062	18.11055	7.36850
H	14.49391	17.40103	7.39150
H	11.71608	5.91554	6.68948

Ag₁₂Au₁₃PET₁₈_VI

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Ag	12.53225	15.31120	12.12741
Ag	15.44817	16.38981	13.00410
Ag	17.20532	13.42206	13.62092
Ag	14.79399	11.10038	13.51519
Ag	11.03740	14.04789	14.37850
Ag	9.70420	16.46779	12.82670
Ag	11.05861	16.17581	9.54558
Ag	12.63257	13.35809	9.74498
Ag	14.10414	13.91648	14.33865
Ag	12.49371	13.95390	17.18647
Ag	9.47753	12.45331	16.44638
Ag	9.93428	11.40515	13.31524
Au	12.34845	9.64947	12.87677
Au	9.30717	8.45130	12.02843
Au	7.53999	11.58098	11.21955
Au	10.16770	13.79820	11.43361
Au	13.92160	10.87943	10.61684
Au	15.42217	8.28346	12.16607
Au	13.94508	8.63922	15.55625
Au	12.31486	11.60038	15.18365
Au	10.92513	11.02022	10.59592
Au	12.48517	10.82048	7.58163
Au	15.61068	12.62684	8.38578
Au	14.94305	13.57312	11.60744
Au	12.47542	12.49018	12.49044
S	13.32623	17.56821	12.86488
S	17.77663	15.71010	13.04150
S	17.18138	11.09654	14.32348
S	9.74433	17.80265	10.78993
S	12.47392	15.05891	7.90441
S	9.25030	15.65566	15.08138
S	14.80106	14.52975	16.66443
S	10.33822	13.79742	18.29483
S	8.12740	11.02726	15.01714
C	13.49249	18.66250	11.36983
H	14.18060	18.19027	10.63893
H	12.48367	18.71041	10.90638
C	13.95812	20.08936	11.72317
H	13.24513	20.52417	12.45818
H	13.86716	20.69506	10.79093
C	15.37494	20.19879	12.25193
C	16.47790	20.14518	11.37075
H	16.30465	20.03474	10.28588
C	17.79361	20.23540	11.85438
H	18.63864	20.19155	11.14696
C	18.03155	20.38602	13.23232
H	19.06394	20.46460	13.61304
C	16.94401	20.43772	14.12133
H	17.11513	20.54917	15.20510
C	15.62949	20.34237	13.63269
H	14.78218	20.38016	14.33758
C	18.52301	16.48143	14.55618
H	18.45928	17.58189	14.41588
H	17.92006	16.21535	15.44882
C	19.98837	16.04033	14.74330

H	20.01633	14.93375	14.86417
H	20.55506	16.27696	13.81563
C	20.63753	16.71351	15.93813
C	21.34792	17.92530	15.79306
H	21.46201	18.36519	14.78692
C	21.91524	18.57136	16.90437
H	22.47020	19.51476	16.76582
C	21.78032	18.01543	18.18846
H	22.22678	18.51934	19.06223
C	21.07645	16.80895	18.34975
H	20.96987	16.35895	19.35113
C	20.51154	16.16724	17.23462
H	19.96753	15.21651	17.37107
C	17.10180	11.24222	16.17009
H	16.25340	11.90018	16.44960
H	16.88859	10.22234	16.56059
C	18.41676	11.78046	16.76572
H	19.26663	11.17658	16.37897
H	18.56596	12.82029	16.39001
C	18.42235	11.76511	18.28376
C	19.26058	10.88295	18.99977
H	19.93452	10.20990	18.44208
C	19.25016	10.85215	20.40544
H	19.91567	10.15593	20.94338
C	18.39412	11.70496	21.12303
H	18.38281	11.68214	22.22579
C	17.55206	12.58835	20.42301
H	16.87818	13.26434	20.97617
C	17.56609	12.61827	19.01824
H	16.89820	13.31411	18.47899
C	8.03126	17.61905	10.10316
H	8.06188	18.00432	9.06127
H	7.76949	16.54003	10.07069
C	6.99277	18.38789	10.94146
H	7.29927	19.45449	11.01850
H	6.99870	17.97305	11.97548
C	5.59968	18.28740	10.34776
C	5.03165	19.36117	9.62899
H	5.60283	20.30007	9.52311
C	3.75249	19.25498	9.05567
H	3.32692	20.10988	8.50290
C	3.01660	18.06547	9.19021
H	2.01091	17.98077	8.74497
C	3.57046	16.98569	9.90149
H	2.99932	16.04922	10.01836
C	4.84888	17.09610	10.47296
H	5.27515	16.24227	11.02748
C	11.31438	14.35566	6.63325
H	11.71367	13.35210	6.36519
H	10.31670	14.19721	7.08820
C	11.20457	15.22815	5.36729
H	12.22255	15.37931	4.94335
H	10.62984	14.63443	4.61823
C	10.52293	16.56833	5.56487
C	11.26751	17.76316	5.65735
H	12.36593	17.71894	5.57048
C	10.63108	19.00055	5.85475
H	11.23385	19.92176	5.92484

C	9.23191	19.06526	5.96424
H	8.73034	20.03538	6.11901
C	8.47601	17.88287	5.87236
H	7.37649	17.92157	5.94967
C	9.11672	16.64834	5.67334
H	8.51057	15.72948	5.58967
C	9.94814	16.98761	16.17241
H	10.11804	16.51986	17.16622
H	10.92795	17.32597	15.77738
C	8.96176	18.16667	16.28753
H	8.80218	18.60018	15.27525
H	7.97853	17.76943	16.62575
C	9.43658	19.24635	17.24243
C	9.33527	19.06890	18.64105
H	8.89386	18.13750	19.03648
C	9.77912	20.06059	19.53104
H	9.68622	19.90219	20.61890
C	10.33291	21.25615	19.03820
H	10.67403	22.03901	19.73640
C	10.44478	21.44521	17.64997
H	10.87617	22.37882	17.25079
C	10.00340	20.44719	16.76384
H	10.09217	20.60380	15.67487
C	14.89720	16.37719	16.83672
H	15.79372	16.69860	16.26296
H	14.01580	16.84675	16.35474
C	15.01899	16.80464	18.31240
H	14.08953	16.50653	18.84845
H	15.85658	16.23981	18.77875
C	15.25811	18.29607	18.46289
C	16.57128	18.81469	18.50194
H	17.42963	18.12229	18.45333
C	16.80118	20.19694	18.60730
H	17.83615	20.57729	18.64242
C	15.71634	21.08924	18.67363
H	15.89429	22.17471	18.75802
C	14.40388	20.58716	18.63370
H	13.54157	21.27233	18.68571
C	14.17906	19.20418	18.52901
H	13.14364	18.82391	18.50292
C	10.56675	12.63813	19.72621
H	10.99436	11.67920	19.36540
H	11.30293	13.10579	20.41571
C	9.23414	12.38710	20.45967
H	8.79949	13.36631	20.75974
H	8.51718	11.92052	19.74688
C	9.41729	11.50161	21.67812
C	9.39886	10.09404	21.56120
H	9.20653	9.63414	20.57641
C	9.61154	9.27162	22.68041
H	9.58760	8.17510	22.56411
C	9.84809	9.84377	23.94253
H	10.01294	9.19962	24.82250
C	9.86865	11.24296	24.07515
H	10.04868	11.70262	25.06183
C	9.65563	12.06087	22.95269
H	9.66841	13.15915	23.06611
C	8.47025	9.31690	15.64728

H	7.94225	8.62513	14.95537
H	9.55731	9.10550	15.57306
C	7.97775	9.11220	17.09254
H	8.55515	9.79709	17.75635
H	6.91114	9.42043	17.16166
C	8.13494	7.67610	17.55615
C	7.01793	6.82172	17.67961
H	6.01129	7.21890	17.46265
C	7.16814	5.48153	18.07689
H	6.27919	4.83495	18.17110
C	8.44634	4.96708	18.35442
H	8.56723	3.91576	18.66536
C	9.56928	5.80575	18.23483
H	10.57735	5.41383	18.45165
C	9.41487	7.14585	17.84085
H	10.30346	7.79682	17.75579
S	11.41630	7.40042	12.36099
S	7.10381	9.33012	11.85857
S	7.77971	13.86593	10.59246
S	15.27482	7.15086	14.25414
S	12.57089	9.91522	17.03404
S	15.69643	9.24303	10.00875
S	10.26571	10.32905	8.29176
S	14.69245	11.14001	6.75703
S	16.76099	14.02794	9.92309
C	11.20779	6.43162	13.93385
H	10.52373	6.97895	14.61388
H	12.21460	6.41668	14.40453
C	10.72387	4.98867	13.68882
H	11.43256	4.48641	12.99368
H	10.80382	4.45825	14.66674
C	9.30602	4.85697	13.16600
C	8.20239	5.02146	14.03243
H	8.37356	5.23465	15.10213
C	6.88707	4.91352	13.55242
H	6.04134	5.04566	14.24787
C	6.64958	4.63468	12.19451
H	5.61663	4.54332	11.81812
C	7.73818	4.46992	11.32108
H	7.56830	4.25569	10.25262
C	9.05304	4.58206	11.80542
H	9.90113	4.45447	11.11172
C	6.36942	8.51997	10.35557
H	6.39862	7.42811	10.55889
H	7.01002	8.72568	9.47376
C	4.92643	9.00131	10.11460
H	4.93906	10.10330	9.95429
H	4.32546	8.81545	11.03207
C	4.29337	8.30692	8.92309
C	3.54574	7.12018	9.08538
H	3.39051	6.71546	10.10070
C	2.99275	6.45494	7.97818
H	2.40788	5.53186	8.12944
C	3.17987	6.96620	6.68217
H	2.74469	6.44712	5.81168
C	3.92117	8.14760	6.50422
H	4.06858	8.56242	5.49296
C	4.47172	8.80893	7.61499

H	5.04557	9.74000	7.46576
C	7.93295	13.75419	8.74800
H	8.77289	13.07249	8.50213
H	8.20277	14.77680	8.40229
C	6.62548	13.28226	8.08520
H	5.78880	13.93233	8.42200
H	6.40403	12.25490	8.45795
C	6.70181	13.28288	6.56894
C	5.94717	14.19754	5.80272
H	5.28301	14.91224	6.31873
C	6.02755	14.20812	4.39902
H	5.42722	14.93110	3.82137
C	6.87116	13.30171	3.73458
H	6.93760	13.30858	2.63362
C	7.63074	12.38585	4.48513
H	8.29525	11.66903	3.97379
C	7.54701	12.37644	5.88758
H	8.15002	11.65313	6.46504
C	16.97777	7.35369	14.96871
H	16.91053	7.00623	16.02181
H	17.22783	8.43565	14.95914
C	18.01903	6.54647	14.17368
H	17.71796	5.47590	14.14592
H	18.01685	6.91291	13.12139
C	19.41011	6.68222	14.76553
C	19.99785	5.63194	15.50239
H	19.44147	4.68706	15.63151
C	21.27923	5.76874	16.06429
H	21.72081	4.93220	16.63226
C	21.99642	6.96557	15.89910
H	23.00385	7.07437	16.33503
C	21.42194	8.02215	15.16939
H	21.97862	8.96409	15.02908
C	20.14149	7.88187	14.60955
H	19.69859	8.71770	14.04063
C	13.73656	10.62034	18.30048
H	13.29792	11.60126	18.58815
H	14.71339	10.82410	17.81998
C	13.89567	9.73336	19.55024
H	12.88931	9.52462	19.97691
H	14.44094	10.34790	20.30422
C	14.64930	8.43480	19.33621
C	13.96814	7.20620	19.20344
H	12.86707	7.19255	19.26530
C	14.67115	6.00642	18.99894
H	14.11743	5.05778	18.89712
C	16.07414	6.01478	18.92449
H	16.62852	5.07426	18.76738
C	16.76665	7.23180	19.05643
H	17.86809	7.25097	19.00585
C	16.05999	8.42870	19.26063
H	16.61746	9.37465	19.37480
C	15.01929	7.94504	8.86647
H	14.85146	8.46500	7.89858
H	14.04025	7.58849	9.24505
C	16.02133	6.78597	8.70377
H	16.18291	6.31000	9.69655
H	17.00089	7.20857	8.38618

C	15.55948	5.74495	7.70043
C	15.63976	5.99480	6.31164
H	16.05453	6.95500	5.95865
C	15.20655	5.03949	5.37786
H	15.28152	5.25484	4.29847
C	14.68533	3.80861	5.81565
H	14.34995	3.05560	5.08297
C	14.59705	3.54661	7.19360
H	14.19517	2.58292	7.54990
C	15.02690	4.50861	8.12448
H	14.95614	4.29525	9.20497
C	10.15971	8.47588	8.23607
H	9.27121	8.21473	8.85147
H	11.04724	8.04163	8.73912
C	10.01121	7.95346	6.79454
H	10.93933	8.19745	6.22993
H	9.17776	8.49863	6.29868
C	9.74520	6.45950	6.75215
C	8.42335	5.96372	6.71799
H	7.57842	6.67352	6.69044
C	8.16789	4.58201	6.71246
H	7.12666	4.21932	6.67840
C	9.23557	3.66763	6.74388
H	9.03802	2.58233	6.73785
C	10.55659	4.14735	6.77946
H	11.40511	3.44355	6.80052
C	10.80746	5.52971	6.78324
C	14.52035	12.16422	5.21626
H	14.00815	13.11542	5.46957
H	13.86697	11.58524	4.52899
C	15.89464	12.42998	4.57448
H	16.39949	11.45690	4.38382
H	16.52650	12.98562	5.30339
C	15.76813	13.21652	3.28272
C	15.73136	14.62824	3.29614
H	15.83398	15.16348	4.25583
C	15.57676	15.35861	2.10595
H	15.55597	16.46069	2.14050
C	15.45408	14.68810	0.87658
H	15.33457	15.26039	-0.05860
C	15.48901	13.28323	0.84752
H	15.39854	12.74699	-0.11239
C	15.64402	12.55728	2.04040
H	15.67616	11.45411	2.00875
C	16.40308	15.74969	9.33244
H	16.84342	16.41608	10.10568
H	15.30447	15.90741	9.31959
C	17.01490	16.03140	7.94839
H	16.53215	15.34874	7.21108
H	18.09690	15.77516	7.96713
C	16.82964	17.47686	7.52487
C	17.91694	18.37661	7.50423
H	18.92218	18.01219	7.77804
C	17.73860	19.72240	7.13855
H	18.60434	20.40608	7.12572
C	16.46164	20.19494	6.79025
H	16.31833	21.25059	6.50437
C	15.36816	19.31016	6.80907

H	14.36100	19.67034	6.53955
C	15.55051	17.96506	7.17137
H	14.68466	17.27872	7.18126
H	11.84972	5.89115	6.80474

Ag₁₂Au₁₃PET₁₈_VII

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Au	12.64198	15.26386	12.14164
Au	15.64980	16.52734	13.00122
Au	17.41357	13.42929	13.79401
Au	14.79076	11.09341	13.59015
Au	11.09327	14.04029	14.42152
Au	9.58288	16.64663	12.85414
Au	11.05285	16.30173	9.47759
Au	12.67111	13.31640	9.83861
Au	14.07160	13.90741	14.39945
Au	12.50559	14.08535	17.44282
Au	9.38598	12.31188	16.64626
Au	10.02408	11.40878	13.39002
Au	12.48209	9.62624	12.86000
Ag	9.44182	8.60280	12.05282
Ag	7.75963	11.56978	11.39977
Ag	10.18809	13.82911	11.51636
Ag	13.94231	10.89960	10.61152
Ag	15.32171	8.46190	12.18354
Ag	13.95185	8.71405	15.43354
Ag	12.33841	11.57524	15.26571
Ag	10.87126	11.03294	10.68719
Ag	12.48580	10.98227	7.82040
Ag	15.50194	12.47704	8.56149
Ag	15.04179	13.52495	11.70960
Ag	12.50760	12.45038	12.52521
S	13.52479	17.54335	12.68198
S	17.86336	15.67397	13.14426
S	17.17365	11.14645	14.41097
S	9.72737	17.79617	10.77638
S	12.42270	15.03490	7.99416
S	9.31338	15.69443	15.01159
S	14.73160	14.54156	16.74169
S	10.29522	13.80579	18.27187
S	8.23900	10.90205	15.11910
C	13.72382	18.53475	11.12230
H	14.41248	18.00288	10.43441
H	12.71661	18.54666	10.65254
C	14.19301	19.97960	11.38499
H	13.48274	20.46383	12.09120
H	14.10090	20.52280	10.41517
C	15.61256	20.12109	11.90044
C	16.71207	19.98527	11.02387
H	16.53615	19.78579	9.95228
C	18.02926	20.10418	11.49614
H	18.87155	19.99467	10.79264
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Au	12.46470	13.51241	16.27536
Au	14.94264	11.97254	15.89437
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349

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Ag	13.32501	16.54925	17.02212
Au	11.46562	18.84743	15.24478
Au	13.27334	18.62498	12.16756
Ag	14.87963	15.32043	12.42872
Ag	16.39540	16.72867	16.84571
Au	14.69038	16.92731	19.81841
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Au	18.05772	10.91493	15.18029
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Au	15.04750	12.83314	10.56469
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H	14.64650	20.60837	7.16741
H	13.00224	16.68995	6.30461
H	14.31868	14.93224	8.95302
H	12.86604	15.01036	7.90075
H	12.78150	15.51307	9.62725
H	13.20695	20.20326	5.08633
H	12.65521	18.53590	4.69649
H	14.37383	18.99083	4.47523
H	7.58858	13.12966	17.56754
H	6.23394	11.22797	18.45253
H	9.79886	9.60003	20.30842
H	11.83965	12.42653	20.05269

H	12.17017	11.50905	18.57726
H	11.89181	10.62447	20.12381
H	6.23326	8.88633	19.40137
H	6.71023	9.39633	21.05078
H	7.71931	8.21473	20.16018

Ag₁₃Au₁₂DMBT₁₈_IV

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Ag	14.73669	17.65561	14.58387
Au	17.80124	19.10035	15.21880
Ag	19.53118	16.12455	16.04021
Au	17.35048	13.83743	16.32896
Ag	13.45873	16.59781	17.03896
Au	11.43414	18.83933	15.28589
Ag	13.03539	18.45541	12.33330
Au	14.85362	15.32454	12.42311
Ag	16.50159	16.75066	16.79165
Au	14.82216	16.95987	19.76043
Ag	11.78261	15.06729	19.11993
Au	12.59696	13.68246	16.38255
Ag	15.05120	12.10687	15.96601
Au	12.07262	10.55733	14.97769
Ag	10.25020	13.51649	14.52400
Au	12.48846	15.94506	14.16006
Ag	16.27188	13.07508	13.46281
Au	17.98894	10.84225	15.26954
Ag	16.54074	11.51748	18.42404
Au	15.02232	14.35454	18.05388
Ag	13.27708	13.03656	13.64250
Au	15.05772	12.83240	10.56530
Ag	17.75264	14.64793	11.43009
Au	17.23501	16.03637	14.11362
Ag	14.90698	14.87396	15.25384
S	15.61549	20.01819	14.96464
S	20.08177	18.47348	15.52121
S	19.85060	13.72478	16.50250
S	11.55288	20.14582	13.29600
S	14.79081	17.44550	10.99321
S	11.15289	17.70693	17.35150
S	17.07767	17.49337	19.15259
S	12.64607	16.69147	20.72362
S	10.30836	13.90441	17.54120
S	14.35186	9.85283	15.01566
S	9.76107	11.11996	14.83888
S	9.99506	15.87012	13.86208
S	17.75005	9.68961	17.34350
S	14.97864	12.59017	19.96484
S	18.35919	11.67007	13.06805
S	12.78240	12.45478	11.19376
S	17.28404	12.95793	9.68570
S	19.35460	16.05040	12.70524
C	19.37984	9.55066	18.09752
C	20.54987	9.92002	17.40497
C	19.48252	8.95587	19.38775
C	21.81496	9.70804	17.97119
C	20.76961	8.76193	19.92629
C	18.25935	8.54566	20.17089
C	21.95001	9.12601	19.24650
C	23.30704	8.91798	19.88316
C	14.52493	8.26487	15.84964
C	15.23943	7.28482	15.12869
C	14.02764	7.96615	17.14756

C	15.46354	6.01255	15.67330
C	14.26296	6.67340	17.65837
C	13.28807	8.98370	17.97206
C	14.97361	5.68129	16.95144
C	15.20346	4.31483	17.56042
C	18.11151	10.20206	12.04454
C	16.82783	9.76893	11.66513
C	19.26046	9.49725	11.58658
C	16.66351	8.65118	10.83301
C	19.05996	8.37839	10.75445
C	20.65890	9.91721	11.97588
C	17.78024	7.93543	10.35984
C	17.62575	6.73520	9.45021
C	12.53289	10.74787	10.65402
C	11.95180	10.51542	9.37714
C	12.88194	9.65482	11.47147
C	11.75239	9.17772	8.97442
C	11.56226	11.64972	8.45922
C	12.66541	8.33833	11.04249
C	12.09755	8.07428	9.77877
C	11.88368	6.65375	9.30173
C	9.15872	10.43311	13.28544
C	8.85508	9.04522	13.20878
C	8.88256	11.27082	12.18633
C	8.27853	8.56114	12.01703
C	9.13845	8.10613	14.35642
C	8.30379	10.75713	11.01782
C	7.99270	9.38677	10.91108
C	7.40755	8.81266	9.63924
C	9.42169	15.83136	12.16105
C	8.06986	15.46798	11.89778
C	10.24841	16.23680	11.09267
C	7.61655	15.51844	10.56256
C	7.13225	15.04368	13.00243
C	9.76312	16.28817	9.78021
C	8.43176	15.92501	9.48827
C	7.89860	15.99210	8.07313
C	9.95590	20.05034	12.46790
C	9.84019	20.58367	11.15445
C	8.81259	19.55058	13.12483
C	8.56431	20.58654	10.55356
C	11.03508	21.12216	10.40526
C	7.56111	19.57087	12.49652
C	7.41281	20.08882	11.19357
C	6.06935	20.07788	10.49706
C	10.84072	18.96489	18.60588
C	9.62635	18.82782	19.31069
C	11.72636	20.03061	18.92405
C	9.27434	19.73215	20.32258
C	11.33684	20.92494	19.94261
C	13.04490	20.21127	18.22453
C	10.12513	20.80516	20.65405
C	9.75110	21.81303	21.72041
C	17.15017	19.25951	19.52259
C	16.68265	20.22693	18.61486
C	17.71365	19.67165	20.76443
C	16.75422	21.59457	18.91959
C	17.76819	21.05217	21.03945

C	18.23793	18.67449	21.77070
C	17.29427	22.03394	20.14341
C	17.35743	23.50319	20.50237
C	20.73647	19.39944	16.92049
C	20.17757	20.64306	17.28249
C	21.89755	18.93027	17.59626
C	20.74453	21.41808	18.30131
C	22.43958	19.73554	18.61966
C	22.54569	17.61195	17.25470
C	21.88921	20.97595	18.99545
C	22.48449	21.78772	20.12532
C	20.48452	13.70144	18.18396
C	19.63459	13.67847	19.30906
C	21.89533	13.65950	18.37010
C	20.15880	13.62487	20.60687
C	22.38936	13.61659	19.69048
C	22.84927	13.64899	17.19860
C	21.55241	13.59773	20.82292
C	22.12223	13.52142	22.22306
C	15.82736	12.31613	21.54090
C	15.70189	11.01490	22.07987
C	16.52598	13.30886	22.27992
C	16.26037	10.68506	23.32287
C	17.08040	12.94110	23.52448
C	16.67298	14.71805	21.77736
C	16.96695	11.64713	24.07165
C	17.56242	11.31992	25.42422
C	12.95229	15.97996	22.34879
C	13.32028	16.84744	23.41475
C	12.76771	14.60449	22.59743
C	13.48569	16.28289	24.69673
C	13.53591	18.32574	23.19679
C	12.93944	14.07746	23.88367
C	13.30394	14.91121	24.96128
C	13.51338	14.34208	26.34754
C	15.68569	21.14133	13.55654
C	14.91086	22.33209	13.61338
C	16.50013	20.88621	12.43370
C	14.98795	23.22285	12.52074
C	14.03417	22.66184	14.79805
C	16.55904	21.79915	11.37318
C	15.79859	22.98796	11.39458
C	15.86498	23.97652	10.25020
C	19.61387	17.46500	11.62350
C	20.93181	17.99811	11.51769
C	18.58090	18.00268	10.82857
C	21.14955	19.04908	10.60423
C	22.07671	17.45730	12.34088
C	18.83785	19.04266	9.92268
C	20.13109	19.58671	9.79073
C	20.43217	20.68829	8.79688
C	17.19397	13.69616	8.04741
C	18.30724	14.41406	7.52671
C	16.07174	13.46165	7.22262
C	18.22458	14.89103	6.20128
C	19.55110	14.66903	8.34189
C	16.02528	13.94835	5.91068
C	17.10365	14.68292	5.37471

C	17.04573	15.24646	3.97157
C	14.22730	17.82451	9.31450
C	14.46196	19.15157	8.88294
C	13.61244	16.89966	8.43106
C	14.09217	19.56948	7.59800
C	13.25582	17.35573	7.14198
C	13.34378	15.47468	8.82765
C	13.48019	18.67273	6.69683
C	13.10600	19.10355	5.29499
C	9.49386	12.46636	18.24509
C	8.13779	12.30210	17.87948
C	10.09654	11.53406	19.13111
C	7.37991	11.23640	18.37786
C	9.30293	10.47167	19.61484
C	11.53091	11.66171	19.55573
C	7.95153	10.29618	19.26090
C	7.13374	9.15619	19.82834
H	20.45967	10.38201	16.40793
H	22.71469	10.00491	17.40541
H	20.84818	8.29916	20.92667
H	17.59764	7.87630	19.57664
H	17.64104	9.43182	20.45077
H	18.54337	8.02301	21.10926
H	24.12610	9.01996	19.13880
H	23.39292	7.91124	20.35045
H	23.49647	9.66724	20.68681
H	15.62720	7.53404	14.12763
H	16.03064	5.26653	15.09014
H	13.87378	6.43547	18.66518
H	13.92814	9.87239	18.17946
H	12.96388	8.55557	18.94395
H	12.38845	9.36968	17.43786
H	15.73450	3.63973	16.85554
H	14.24354	3.82430	17.84210
H	15.81624	4.37893	18.48893
H	15.94232	10.31482	12.02764
H	15.64321	8.34379	10.54682
H	19.95030	7.83022	10.39637
H	20.79757	9.88481	13.08039
H	20.87155	10.96510	11.66786
H	21.41770	9.25290	11.50891
H	16.55544	6.49539	9.27333
H	18.11061	5.82887	9.88010
H	18.09818	6.91303	8.45652
H	13.33418	9.83612	12.45914
H	11.30367	8.99454	7.98123
H	10.84839	12.34704	8.95104
H	11.09658	11.26469	7.52645
H	12.44815	12.26440	8.17942
H	12.94300	7.50534	11.71104
H	11.24948	6.61886	8.38977
H	11.39385	6.03068	10.08322
H	12.85076	6.15721	9.05291
H	9.12949	12.34464	12.25131
H	8.03822	7.48450	11.95494
H	8.66441	8.45928	15.29919
H	10.23213	8.04778	14.56602
H	8.77239	7.08057	14.13484

H	8.09565	11.43929	10.17634
H	6.77909	7.91794	9.84249
H	8.21273	8.49719	8.93507
H	6.78094	9.55920	9.10379
H	11.29386	16.51987	11.30718
H	6.56893	15.23075	10.35876
H	7.50179	14.12955	13.52503
H	6.11707	14.82799	12.60532
H	7.04624	15.82856	13.78723
H	10.43685	16.61883	8.97153
H	6.88594	15.54004	7.99569
H	8.56458	15.45814	7.35823
H	7.82318	17.04542	7.71598
H	8.91462	19.13990	14.14294
H	8.47251	21.00060	9.53325
H	11.57788	21.89555	10.99358
H	10.72933	21.56773	9.43458
H	11.77793	20.31730	10.19058
H	6.68332	19.17209	13.03343
H	6.04121	20.79499	9.64782
H	5.24337	20.33944	11.19516
H	5.83805	19.06753	10.08563
H	8.95320	17.99354	19.05512
H	8.32014	19.60015	20.86141
H	12.02343	21.75364	20.19206
H	12.91418	20.32399	17.12325
H	13.69612	19.31652	18.36602
H	13.59193	21.09567	18.61255
H	8.90845	21.44998	22.34806
H	9.43526	22.78374	21.27097
H	10.60844	22.03358	22.39480
H	16.25131	19.90946	17.65337
H	16.38114	22.32736	18.18369
H	18.20326	21.37388	22.00327
H	17.43110	17.99140	22.12077
H	18.66698	19.19085	22.65646
H	19.02435	18.02384	21.32780
H	17.07837	24.14567	19.63962
H	18.37768	23.80224	20.83350
H	16.66285	23.74880	21.33922
H	19.28083	21.00307	16.75250
H	20.28120	22.38498	18.56107
H	23.34009	19.36836	19.14427
H	22.82003	17.55091	16.17757
H	21.85084	16.76000	17.45119
H	23.46320	17.44831	17.85920
H	22.39473	22.88040	19.93630
H	23.56069	21.55283	20.27700
H	21.96364	21.58180	21.09006
H	18.54307	13.70738	19.15178
H	19.46649	13.60096	21.46539
H	23.48468	13.59167	19.83580
H	22.67496	12.76552	16.54385
H	23.90530	13.62511	17.54433
H	22.71429	14.54205	16.54708
H	21.62118	14.24083	22.90883
H	23.21182	13.74250	22.23464
H	21.98361	12.50660	22.66453

H	15.15058	10.25204	21.50582
H	16.14623	9.65840	23.71243
H	17.62624	13.71510	24.09381
H	15.68012	15.21701	21.69043
H	17.12147	14.75461	20.76165
H	17.30347	15.32710	22.45824
H	17.62948	10.22227	25.58583
H	16.94721	11.73952	26.25479
H	18.58526	11.74413	25.53585
H	12.49421	13.93936	21.76274
H	13.76827	16.95442	25.52744
H	14.38472	18.51151	22.49775
H	13.75578	18.84352	24.15512
H	12.64664	18.80260	22.72805
H	12.79493	12.99594	24.04676
H	13.63176	15.14520	27.10655
H	14.42733	13.70508	26.38722
H	12.65967	13.69931	26.65972
H	17.10246	19.96448	12.39637
H	14.38920	24.15024	12.56385
H	13.21195	21.91964	14.91341
H	13.57036	23.66480	14.68174
H	14.61275	22.64687	15.74888
H	17.22027	21.57889	10.51756
H	15.20471	24.85263	10.42827
H	15.55231	23.51091	9.28748
H	16.90071	24.35900	10.10040
H	17.55636	17.60308	10.91676
H	22.17163	19.46160	10.52345
H	22.23197	16.36961	12.15996
H	21.87180	17.57308	13.42969
H	23.02249	17.99086	12.10443
H	18.00951	19.42572	9.30251
H	21.07727	21.47806	9.24309
H	19.50129	21.17395	8.43252
H	20.97133	20.29602	7.90262
H	15.22887	12.87586	7.62485
H	19.08627	15.45380	5.79984
H	19.99981	13.72199	8.71661
H	19.33027	15.28675	9.24556
H	20.31690	15.20791	7.74456
H	15.13331	13.74939	5.29159
H	18.05673	15.51626	3.59668
H	16.42126	16.16948	3.93218
H	16.59705	14.52138	3.25627
H	14.93549	19.86281	9.58035
H	14.28274	20.61345	7.29394
H	12.77677	16.63521	6.45548
H	14.29119	14.92719	9.03648
H	12.80481	14.92817	8.02597
H	12.74338	15.40471	9.75960
H	12.69329	20.13676	5.28007
H	12.34697	18.42585	4.84713
H	13.99222	19.09888	4.61743
H	7.68005	13.02784	17.18788
H	6.32557	11.13137	18.06803
H	9.77382	9.74522	20.30122
H	11.71307	12.62479	20.09169

H	12.21961	11.67839	18.68191
H	11.83791	10.83450	20.22844
H	6.42450	8.74648	19.07528
H	6.52300	9.48708	20.70160
H	7.78091	8.32253	20.17758

Ag₁₃Au₁₂DMBT₁₈_V

349

Au	14.78132	17.67624	14.61980
Ag	17.60988	18.90890	15.45758
Au	19.76633	16.10769	16.25483
Ag	17.25148	13.80513	16.47629
Au	13.19786	16.45182	16.91096
Ag	11.61267	18.68671	15.11232
Au	13.26398	18.73182	12.19359
Ag	15.13704	15.48407	12.38297
Au	16.26180	16.62957	16.98628
Ag	14.63889	16.84078	19.65313
Au	11.63170	15.06546	19.40905
Ag	12.45988	13.60566	16.17571
Au	14.97456	12.12995	15.92546
Ag	12.34171	10.77506	14.95177
Au	10.16008	13.48633	14.15930
Ag	12.57514	16.02213	13.92072
Au	16.52082	13.29295	13.53412
Ag	17.74604	10.96704	15.24228
Au	16.58025	11.13900	18.37367
Ag	14.73313	14.29442	18.05098
Au	13.44640	13.21254	13.46545
Ag	15.18635	12.89497	10.69480
Au	18.01104	14.65954	11.08187
Ag	17.35447	16.09656	14.33431
Ag	14.88874	14.89028	15.22821
S	15.47757	20.06676	15.12466
S	19.99394	18.41439	15.62190
S	19.77844	13.75309	16.68172
S	11.74057	20.24878	13.24581
S	14.95759	17.60645	10.95711
S	10.92168	17.53522	17.13187
S	17.00901	17.41070	19.24936
S	12.51523	16.71966	20.87860
S	10.44500	13.83593	17.75574
S	14.58750	9.76764	14.99050
S	9.94781	11.21240	14.88034
S	10.04831	15.81811	13.63836
S	17.86509	9.49444	17.21139
S	15.09472	12.39305	19.75247
S	18.47096	11.77892	13.03469
S	12.79578	12.57153	11.12193
S	17.34265	12.95906	9.52534
S	19.22145	16.08683	12.55968
C	19.56323	9.52785	17.81058
C	20.61426	9.87864	16.93796
C	19.86242	9.06643	19.12261
C	21.95130	9.78006	17.34466
C	21.21851	8.98709	19.50096
C	18.77922	8.66651	20.09421
C	22.27879	9.33845	18.64274
C	23.71696	9.27376	19.10811
C	14.63735	8.26977	15.98344
C	15.40439	7.21952	15.43072
C	13.96682	8.07211	17.22212

C	15.50908	5.98231	16.07965
C	14.09325	6.81304	17.84491
C	13.15219	9.15370	17.87538
C	14.85159	5.75463	17.30465
C	14.96826	4.43424	18.03553
C	18.06090	10.42388	11.92186
C	16.74279	9.96239	11.73803
C	19.12425	9.82436	11.18802
C	16.46303	8.92092	10.84053
C	18.80870	8.77926	10.29814
C	20.55211	10.29511	11.33866
C	17.49352	8.30996	10.09979
C	17.20773	7.20062	9.11008
C	12.53802	10.84453	10.67579
C	12.01070	10.55638	9.38562
C	12.80549	9.78543	11.56511
C	11.77440	9.20599	9.05096
C	11.70310	11.65033	8.39015
C	12.55489	8.45581	11.20406
C	12.03207	8.13878	9.93278
C	11.75308	6.70360	9.54200
C	9.29074	10.23170	13.51888
C	8.92525	8.88307	13.78249
C	9.05992	10.78324	12.24161
C	8.32751	8.14460	12.73979
C	9.17066	8.24408	15.12862
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349

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H	22.70690	17.74065	16.41089
H	21.67718	17.04807	17.69195
H	23.25290	17.80064	18.12973
H	21.99830	23.38463	19.62530
H	23.17001	22.12065	20.14206
H	21.53295	22.18499	20.86963
H	18.59417	13.41369	19.10840
H	19.54317	13.16320	21.39553
H	23.52958	13.70852	19.77575
H	22.75657	13.17282	16.40716
H	23.92302	14.01320	17.49878
H	22.64780	14.93242	16.61339
H	21.64520	13.85035	22.89998
H	23.26821	13.57697	22.17608
H	22.16497	12.19323	22.47268
H	15.08341	10.21159	21.54122

H	16.04701	9.68700	23.78177
H	17.61885	13.72116	24.00841
H	15.74244	15.17723	21.55745
H	17.15198	14.62628	20.61540
H	17.38359	15.25750	22.28322
H	17.51988	10.29532	25.64558
H	16.87415	11.85977	26.23871
H	18.51833	11.78689	25.53785
H	12.46391	13.91508	21.83566
H	14.11386	16.90370	25.47235
H	14.61778	18.39788	22.38126
H	14.12506	18.77085	24.07427
H	12.91612	18.77233	22.73032
H	12.85132	12.98444	24.11189
H	13.96846	15.12491	27.08751
H	14.65215	13.63740	26.35033
H	12.90341	13.72436	26.71749
H	17.00368	19.97360	12.51851
H	14.58148	24.33328	12.64590
H	13.12617	22.13679	14.86515
H	13.60702	23.86162	14.69742
H	14.51532	22.75881	15.80142
H	17.32706	21.60489	10.68748
H	15.55735	25.01957	10.57071
H	15.87618	23.67993	9.41887
H	17.23133	24.41650	10.32402
H	17.50162	17.71115	10.72741
H	22.07521	19.70575	10.55662
H	22.13063	16.57923	12.17176
H	21.72890	17.79579	13.41742
H	22.91003	18.20708	12.11921
H	17.97107	19.57431	9.15566
H	20.98397	21.70553	9.25779
H	19.45031	21.37432	8.37836
H	20.96293	20.54097	7.89816
H	15.29561	13.06880	7.64859
H	19.57414	14.53687	5.55325
H	20.12876	12.97087	8.67906
H	19.87839	14.71082	8.96449
H	20.78006	14.17017	7.49812
H	15.33694	13.68127	5.23267
H	18.53123	14.59715	3.35862
H	17.07493	15.60953	3.61720
H	16.88973	13.89849	3.12573
H	14.83470	20.12756	9.84797
H	14.36161	20.98432	7.55587
H	13.32366	16.96584	6.30219
H	14.67864	15.20646	8.94909
H	13.33548	15.16066	7.75433
H	13.01604	15.51262	9.49092
H	13.04930	20.52172	5.34507
H	12.92117	18.82380	4.76631
H	14.50861	19.65537	4.77583
H	7.73473	13.00175	17.19543
H	6.33583	11.13689	18.08007
H	9.73065	9.72642	20.37851
H	11.73054	12.57857	20.12098
H	12.23045	11.56308	18.76052

H	11.80700	10.78919	20.33107
H	6.37471	8.76809	19.13239
H	6.47279	9.53551	20.74605
H	7.71154	8.33701	20.25570

Ag₂₄Au₁DMBT₁₈_Au_in_core

349

Ag	14.77020	17.54086	14.62672
Ag	17.62339	18.72086	15.21657
Ag	19.38242	16.07237	16.21527
Ag	17.25377	13.71036	16.38706
Ag	13.33587	16.47310	17.01662
Ag	11.70406	18.55114	15.22178
Ag	13.25123	18.51224	12.33438
Ag	14.83829	15.28428	12.42870
Ag	16.37056	16.54787	16.91639
Ag	14.75035	16.74734	19.71035
Ag	11.61654	15.10778	19.16760
Ag	12.47429	13.60372	16.39810
Ag	14.91304	12.00848	15.99139
Ag	12.14942	10.66347	15.10681
Ag	10.24451	13.59329	14.43715
Ag	12.44329	15.82780	14.13405
Ag	16.28327	13.03800	13.55742
Ag	17.71743	10.90336	15.22617
Ag	16.63790	11.18178	18.24454
Ag	14.87357	14.21414	18.09641
Ag	13.29515	12.99550	13.60768
Ag	15.16492	12.79870	10.64195
Ag	17.92914	14.34527	11.47060
Ag	17.21139	15.87939	14.14635
Au	14.82942	14.77076	15.27824
S	15.51434	19.95226	14.97815
S	20.01641	18.35251	15.51540
S	19.75575	13.66203	16.59074
S	11.83814	20.17938	13.40211
S	14.84300	17.33993	10.93216
S	11.07910	17.61293	17.39402
S	17.08871	17.28621	19.23204
S	12.56731	16.66306	20.78769
S	10.22849	13.83162	17.60651
S	14.36922	9.64578	15.23660
S	9.80467	11.20171	14.77872
S	9.92941	15.96721	13.87261
S	17.92032	9.41207	17.16551
S	15.09005	12.28035	19.76864
S	18.34804	11.68866	12.97666
S	12.85144	12.27629	11.21127
S	17.33310	12.93298	9.53787
S	19.35846	15.86040	12.78515
C	19.64045	9.50230	17.68336
C	20.64994	9.86350	16.76591
C	20.00394	9.09189	18.99748
C	22.00277	9.82618	17.12920
C	21.37333	9.06968	19.33016
C	18.96859	8.68892	20.01949
C	22.39108	9.43150	18.42516
C	23.84462	9.42990	18.84486
C	14.39533	8.19275	16.29706
C	15.15085	7.10572	15.80406
C	13.72064	8.07030	17.54274
C	15.24807	5.90787	16.52443

C	13.83708	6.84795	18.23769
C	12.90780	9.19192	18.12926
C	14.59049	5.75602	17.76128
C	14.70308	4.48027	18.56817
C	18.00496	10.31679	11.86240
C	16.72459	9.74132	11.74547
C	19.07398	9.82576	11.05957
C	16.48598	8.69484	10.84175
C	18.80117	8.76960	10.16874
C	20.45969	10.42238	11.13599
C	17.52264	8.18970	10.03329
C	17.28205	7.07139	9.04178
C	12.73118	10.53625	10.75759
C	12.46288	10.19424	9.40127
C	12.84809	9.51016	11.71555
C	12.32746	8.82908	9.07266
C	12.33130	11.24703	8.32800
C	12.70422	8.16318	11.35782
C	12.44189	7.79450	10.02219
C	12.31212	6.34035	9.62279
C	9.33298	10.45564	13.21176
C	9.03104	9.06519	13.16927
C	9.16530	11.23959	12.05118
C	8.56902	8.52498	11.95193
C	9.19483	8.18073	14.38229
C	8.70161	10.67034	10.85801
C	8.39637	9.29611	10.78523
C	7.93805	8.66335	9.48951
C	9.34927	15.98321	12.17180
C	8.04003	15.51005	11.87168
C	10.13295	16.54431	11.14102
C	7.58863	15.60607	10.53768
C	7.14303	14.91974	12.93271
C	9.65112	16.63536	9.82976
C	8.36427	16.15988	9.50091
C	7.83768	16.25605	8.08497
C	10.23534	20.19469	12.58557
C	10.11895	20.72528	11.27032
C	9.07488	19.77865	13.27333
C	8.83135	20.80283	10.69940
C	11.32394	21.18887	10.48868
C	7.81176	19.87083	12.67594
C	7.66625	20.38344	11.37044
C	6.30906	20.44772	10.70428
C	10.86289	18.98834	18.53427
C	9.61806	19.02700	19.20154
C	11.83118	19.99555	18.79831
C	9.31889	20.04613	20.11521
C	11.49394	21.00883	19.72090
C	13.18165	20.00570	18.13696
C	10.25433	21.06525	20.38838
C	9.93175	22.19952	21.33776
C	17.09246	19.04671	19.61620
C	16.86385	20.02443	18.62987
C	17.37435	19.45532	20.95322
C	16.89733	21.39051	18.94366
C	17.40004	20.83555	21.23459
C	17.63367	18.45119	22.05131

C	17.16177	21.82419	20.25730
C	17.16716	23.29366	20.62044
C	20.50360	19.50553	16.80895
C	20.18096	20.87021	16.63195
C	21.30438	19.11715	17.91942
C	20.63422	21.84461	17.52926
C	21.73863	20.12502	18.80656
C	21.70477	17.68436	18.16581
C	21.42264	21.48739	18.64244
C	21.88565	22.52275	19.64378
C	20.40055	13.55424	18.26334
C	19.56406	13.31896	19.37492
C	21.80680	13.66032	18.45865
C	20.09267	13.19757	20.66633
C	22.30600	13.54426	19.77305
C	22.75109	13.88057	17.30129
C	21.48051	13.31384	20.89059
C	22.05803	13.17666	22.28284
C	15.88199	11.99197	21.36710
C	15.85977	10.66065	21.84423
C	16.46840	13.00825	22.16911
C	16.41030	10.32567	23.08845
C	17.01358	12.63543	23.41724
C	16.52397	14.44430	21.72364
C	17.00109	11.31307	23.90368
C	17.57502	10.97588	25.26297
C	12.89794	15.96270	22.41182
C	13.14601	16.85507	23.49255
C	12.87845	14.57234	22.64896
C	13.36116	16.30107	24.77259
C	13.17903	18.35232	23.29428
C	13.09629	14.05579	23.93256
C	13.34160	14.91545	25.02409
C	13.58093	14.36085	26.41174
C	15.78355	21.03050	13.56153
C	15.19657	22.32688	13.58527
C	16.58535	20.65022	12.46380
C	15.44623	23.18794	12.49462
C	14.33434	22.79211	14.73421
C	16.81609	21.53358	11.40158
C	16.24713	22.82491	11.39507
C	16.50222	23.78390	10.25163
C	19.67979	17.22273	11.65137
C	21.00815	17.73500	11.57461
C	18.68578	17.74280	10.79784
C	21.27427	18.74793	10.63131
C	22.11392	17.20993	12.45866
C	18.99048	18.74429	9.86298
C	20.29463	19.26742	9.76015
C	20.64791	20.33190	8.74303
C	17.18212	13.88412	8.02170
C	18.27827	14.65126	7.53309
C	16.01657	13.76826	7.23198
C	18.13499	15.29072	6.28355
C	19.56881	14.78599	8.30279
C	15.90839	14.41481	5.99465
C	16.96937	15.20018	5.49820
C	16.84809	15.93947	4.18355

C	14.14174	17.66537	9.29942
C	14.38617	18.95130	8.76379
C	13.40087	16.72114	8.54117
C	13.90342	19.31140	7.49913
C	12.92956	17.11829	7.27001
C	13.11234	15.33761	9.05541
C	13.16210	18.39542	6.72352
C	12.66157	18.76133	5.34263
C	9.38690	12.42018	18.33732
C	8.08676	12.16749	17.84210
C	9.90906	11.59739	19.37165
C	7.30923	11.12014	18.34931
C	9.09636	10.55180	19.86199
C	11.27701	11.81842	19.95258
C	7.80151	10.28857	19.37668
C	6.95627	9.17607	19.95858
H	20.36385	10.17572	15.74726
H	22.76844	10.11017	16.38663
H	21.65509	8.75056	20.34987
H	18.30287	7.88456	19.63410
H	18.30237	9.54450	20.28143
H	19.44932	8.33277	20.95582
H	24.52134	9.26571	17.97774
H	24.05443	8.63996	19.59923
H	24.13061	10.40564	19.30354
H	15.67188	7.21187	14.83888
H	15.85034	5.07838	16.11544
H	13.30984	6.75178	19.20395
H	13.53492	10.09425	18.30878
H	12.45023	8.89358	19.09587
H	12.08192	9.50902	17.44603
H	15.08261	3.63832	17.94957
H	13.72149	4.17543	18.99524
H	15.40523	4.60205	19.42603
H	15.90088	10.10875	12.37939
H	15.46811	8.27631	10.76767
H	19.63114	8.38848	9.54636
H	20.86753	10.38316	12.17113
H	20.44932	11.49731	10.84500
H	21.16191	9.88578	10.46191
H	16.24738	6.67436	9.12261
H	17.98660	6.22285	9.19938
H	17.42506	7.41921	7.99250
H	13.06424	9.76923	12.76476
H	12.11851	8.56673	8.01972
H	11.55003	11.99541	8.58654
H	12.07784	10.79025	7.34734
H	13.28054	11.81957	8.20896
H	12.80085	7.38939	12.13877
H	11.83731	6.23102	8.62370
H	11.70211	5.76816	10.35672
H	13.30776	5.84028	9.57267
H	9.40508	12.31616	12.08808
H	8.33143	7.44652	11.91814
H	8.63249	8.57627	15.25745
H	10.26217	8.12682	14.70175
H	8.84637	7.14643	14.17360
H	8.57887	11.31172	9.96895

H	7.34980	7.73702	9.66972
H	8.80867	8.38317	8.85134
H	7.30827	9.36014	8.89351
H	11.14097	16.92513	11.38246
H	6.57525	15.23202	10.30395
H	7.58179	13.99138	13.37054
H	6.14531	14.66391	12.51592
H	7.00360	15.62228	13.78464
H	10.29237	17.08508	9.05255
H	6.82501	15.80690	7.99403
H	8.50552	15.73247	7.36333
H	7.76855	17.31543	7.74647
H	9.17014	19.37521	14.29526
H	8.74046	21.21274	9.67737
H	11.92843	21.92721	11.06100
H	11.02059	21.64917	9.52407
H	12.01133	20.33990	10.25839
H	6.92432	19.53206	13.23744
H	6.31090	21.14083	9.83499
H	5.52033	20.78668	11.41228
H	5.99803	19.44495	10.32875
H	8.87913	18.23596	18.99441
H	8.34008	20.04569	20.62577
H	12.24630	21.79124	19.92532
H	13.10219	20.07387	17.02679
H	13.74360	19.06322	18.34406
H	13.80382	20.85272	18.49255
H	9.16056	21.90311	22.08162
H	9.53543	23.08820	20.79150
H	10.83366	22.53736	21.89429
H	16.65210	19.71398	17.59375
H	16.71606	22.12749	18.14253
H	17.62128	21.15007	22.27069
H	16.74455	17.80131	22.22371
H	17.88094	18.96031	23.00762
H	18.46889	17.76530	21.78768
H	17.27941	23.93500	19.71974
H	17.99435	23.54084	21.32252
H	16.21689	23.59387	21.12178
H	19.56834	21.16607	15.76417
H	20.36838	22.90225	17.35910
H	22.36098	19.82289	19.66793
H	22.26881	17.26248	17.30392
H	20.81327	17.02837	18.31194
H	22.33995	17.59528	19.07231
H	22.03393	23.51634	19.16661
H	22.84232	22.22716	20.12762
H	21.13518	22.65942	20.45749
H	18.47587	13.22825	19.21521
H	19.40807	13.00831	21.51071
H	23.39699	13.63523	19.92509
H	22.68533	13.04736	16.56592
H	23.80292	13.95777	17.65184
H	22.49937	14.80642	16.73570
H	21.52089	13.82141	23.01451
H	23.13376	13.45594	22.30938
H	21.97589	12.12938	22.65642
H	15.40207	9.87775	21.21745

H	16.38089	9.27564	23.42785
H	17.47404	13.42700	24.03494
H	15.49912	14.86341	21.59381
H	17.03832	14.55565	20.74479
H	17.05582	15.07583	22.46468
H	17.88464	9.90976	25.32275
H	16.82959	11.14701	26.07518
H	18.46185	11.60376	25.50080
H	12.70258	13.88618	21.80542
H	13.55093	16.99339	25.61271
H	13.97738	18.65237	22.57729
H	13.36149	18.87799	24.25630
H	12.22548	18.72752	22.86087
H	13.08136	12.96290	24.08265
H	13.75378	15.17142	27.15200
H	14.46907	13.68853	26.43242
H	12.71370	13.75810	26.76684
H	17.04494	19.64871	12.44298
H	14.99368	24.19559	12.51636
H	13.41286	22.17189	14.81853
H	14.02350	23.85018	14.59566
H	14.86821	22.70624	15.70739
H	17.46291	21.20591	10.57006
H	15.96688	24.74664	10.39870
H	16.16796	23.35854	9.27774
H	17.58743	24.01418	10.14590
H	17.65561	17.35352	10.85479
H	22.30504	19.14233	10.57205
H	22.24771	16.11148	12.33426
H	21.87832	17.38041	13.53407
H	23.07889	17.71090	12.22813
H	18.19216	19.11059	9.19499
H	21.19827	21.17964	9.21035
H	19.73944	20.74494	8.25421
H	21.30372	19.92671	7.93708
H	15.18485	13.14481	7.59934
H	18.98537	15.88771	5.90850
H	20.00733	13.79207	8.54473
H	19.40951	15.30414	9.27864
H	20.31743	15.37234	7.72894
H	14.98257	14.30337	5.40468
H	17.84501	16.20003	3.76637
H	16.28284	16.89300	4.30737
H	16.30388	15.33701	3.42247
H	14.96014	19.67658	9.36401
H	14.10648	20.32483	7.11135
H	12.34647	16.38585	6.68348
H	14.05651	14.77567	9.24241
H	12.50574	14.75437	8.33236
H	12.56570	15.35709	10.02290
H	12.33618	19.82396	5.29335
H	11.80215	18.12587	5.03642
H	13.45764	18.62904	4.57233
H	7.68835	12.81043	17.04115
H	6.30114	10.94581	17.93436
H	9.50527	9.91199	20.66481
H	11.36016	12.83805	20.40216
H	12.07467	11.76596	19.18030

H	11.51256	11.07476	20.74226
H	6.34929	8.66990	19.17534
H	6.24097	9.56303	20.72267
H	7.58190	8.40440	20.45759

Ag₂₄Au₁DMBT₁₈_Au_in_icosahedron

349

Au	14.75200	17.53698	14.66575
Ag	17.65258	18.72449	15.23026
Ag	19.36861	16.06924	16.21409
Ag	17.24305	13.73691	16.37634
Ag	13.33940	16.47533	17.04335
Ag	11.74009	18.60271	15.21857
Ag	13.27810	18.52803	12.32297
Ag	14.83380	15.29582	12.42297
Ag	16.37623	16.54952	16.92188
Ag	14.73737	16.75128	19.73312
Ag	11.60592	15.13309	19.17381
Ag	12.46794	13.61912	16.39955
Ag	14.89871	12.05031	15.98769
Ag	12.16025	10.68350	15.11439
Ag	10.25519	13.57266	14.43889
Ag	12.45200	15.87428	14.12509
Ag	16.25590	13.06544	13.54690
Ag	17.69303	10.92643	15.23085
Ag	16.63137	11.20292	18.22502
Ag	14.86487	14.23811	18.09062
Ag	13.27315	13.02559	13.61916
Ag	15.15754	12.81996	10.63637
Ag	17.91273	14.35159	11.46509
Ag	17.19540	15.89126	14.14981
Ag	14.81598	14.77756	15.27904
S	15.53638	19.94827	14.99276
S	20.03913	18.34862	15.53529
S	19.75382	13.65694	16.58619
S	11.85357	20.20121	13.37338
S	14.84644	17.34148	10.90313
S	11.08151	17.63386	17.36699
S	17.07518	17.27800	19.24985
S	12.55221	16.68051	20.80490
S	10.21236	13.87116	17.60741
S	14.38839	9.67550	15.22459
S	9.80362	11.18747	14.80893
S	9.93990	15.94376	13.87637
S	17.92758	9.42949	17.16529
S	15.07437	12.28421	19.75235
S	18.33199	11.70931	12.98474
S	12.84396	12.30092	11.21059
S	17.32738	12.93541	9.53012
S	19.34112	15.86822	12.77799
C	19.64986	9.53790	17.67049
C	20.65020	9.89648	16.74188
C	20.02560	9.14146	18.98552
C	22.00595	9.86935	17.09500
C	21.39764	9.12846	19.30739
C	19.00041	8.74372	20.01974
C	22.40633	9.48761	18.39126
C	23.86314	9.49594	18.79926
C	14.42627	8.22127	16.28318
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C	12.91645	9.19626	18.11145
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C	16.47889	8.70671	10.85466
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C	17.51843	8.19890	10.05156
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C	12.82951	9.53548	11.71336
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H	7.01433	15.59958	13.79452
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H	21.85112	17.40026	13.54682
H	23.06578	17.72280	12.25209
H	18.21297	19.08926	9.15026
H	21.21156	21.16827	9.18888
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Ag	14.84919	15.29924	12.43166
Ag	16.38240	16.62287	16.86734
Ag	14.74079	16.78986	19.70570
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C	20.81133	21.74161	17.54632
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