Supporting Information

Nano-Gymnastics: Visualisation of Inter-Cluster Reactions by High Resolution Trapped Ion Mobility Mass Spectrometry

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Contents

Experimental Details

Synthesis of $[PPh_4][Ag_{44}(4\text{-FTP})_{30}]$

$[PPh_4][Ag_{44}(4\text{-FTP})_{30}]$ clusters were synthesized following a room temperature solid state synthesis route.[1] For this about 20 mg of $AgNO_3$ was ground with 12 mg of PPh_4Br in an agate mortar and pestle and 76 µL of 4-FTP was added to the mixture and ground again to obtain silver thiolates. About 45 mg of dry $NaBH_4$ was then added in order to reduce the thiolates to clusters. A color change to brown indicated successful reduction and formation of the cluster. The reaction mixture was extracted immediately with 7 mL of dichloromethane (DCM) and the resulting solution kept undisturbed at room temperature for a few hours. From time-to-time UV−vis absorption spectra were recorded until all the characteristic absorption features of the clusters appeared. The clusters were then cleaned repeatedly with dimethylformamide (DMF) and toluene by centrifugation and finally rotavapored to achieve powdered clusters. The powder was dissolved in DMF for further study

Synthesis of $[TOA][Au_{25}(PET)_{18}]$ cluster

$[TOA][Au_{25}(PET)_{18}]$ clusters were synthesized following the previously reported method.[1] Briefly, about 40 mg of $HAuCl_4.3H_2O$ in 7.5 ml THF was mixed with 65 mg of TAOBr and stirred for around 15 min at room temperature until the color of the solution changed to orange red. To that, 68 µL of PET was added and stirred for another hour. The resulting thiolate was reduced by 39 mg of $NaBH_4$ in ice-cold water. The color changed from yellow to brown indicating reduction. The solution was stirred for another 5 hours for complete conversion of the thiolates to clusters and size focusing was applied to get $[TOA][Au_{25}(PET)_{18}]$. The as-synthesized clusters were vacuum dried by rotavapor following precipitation using excess MeOH. This step removes free thiol and excess thiolate and was repeated several times. The resulting solid was then dissolved in acetone and centrifuged. The supernatant solution was collected and the precipitate containing larger clusters was discarded. The acetone solution containing $[TOA][Au_{25}(PET)_{18}]$ was vacuum dried and then dissolved in dichloromethane (DCM). Following centrifugation at 1500 rpm the supernatant solution was collected and used for further study.

Instrumental details

Measurements were performed in Nano-ESI mode (NESI) on both the Waters Synapt G2S and the Thermo Fischer Orbitrap instruments. A regular ESI source was used in the Bruker timsTOF measurements. All the measurements were performed in negative ion mode. Both clusters were dissolved in DMF and dilute solutions (10 µM and below) as well as dilute solution mixtures were sprayed. For NESI mode, a 2 kV capillary voltage was applied in the Synapt G2S measurements, while a 3 kV spray voltage was needed to get a stable spray in the case of the Orbitrap platform. All CID experiments were performed on the Synapt G2S platform in ESI mode. To get reasonable signal intensity in regular MS and in CID using ESI mode, the following parameters were used: capillary voltage: 1 kV, cone voltage: 10 V, source offset: 15 V, desolvation temperature 80 ºC, desolvation gas flow: 600 L/h, nebulizer: 2.5 bar. Laboratory collision energy (CE) was varied from nominally 0 to 80 V at 5 mL/min trap gas flow rate. All other parameters were kept the same during CID measurements apart from the CE.

All the ion mobility measurements were performed using a Bruker timsTOF mass spectrometer. The optimized source parameters were as follows: capillary voltage of 2.5 kV, a nebuliser pressure of 0.3 bar, dry gas temperature of 200°C and a dry gas flow of 3.5 l/min. Briefly, in trapped ion mobility spectrometry (TIMS)[2] the ions are held by an electric field gradient (EFG) while exposed to a constant N_2 flow. The source of the flow is a pressure difference between the entrance and the exit of the TIMS-tunnel (here, a pressure difference, Δp, of 2 mbar was attained). Lowering the EFG results in the elution

of the analyte according to its inverse mobility ($1/K_0$). Depending on the difference between start-EFG and end-EFG (ΔEFG) as well as the duration of this reduction (ramp time = t_r), rather high ion mobility resolutions can be achieved. Resolutions of 250 and more have been reported.[3] In this study resolutions were better than 160 throughout. In front of the trapping part of the TIMS-tunnel, a second ramp accumulates the ions for a given period of time (accumulation time = t_a) in order to enhance the overall duty cycle. Since TIMS doesn't operate on first principles, a calibration is necessary. For calibration, Agilent Tune-Mix™ was used as purchased and the reported drift tube $^{DT}CCS_{N2}$-values published by Stow *et al.* have been used.[4] TIMS determines (calibrated) inverse mobilities which were converted to the tabulated $^{TIMS}CCS_{N2}$ values following Mason-Schamp-equation[5]

$$CCS = \left(\frac{3}{16N}\right)\left(\frac{2\pi}{kT}\right)^{0,5}\frac{q}{\sqrt{\mu}K_0}$$

where, q is the charge of the ion, N the number density of the collision gas, μ is the reduced mass of the ion and the N_2 collision gas, k the Boltzmann's constant, T the temperature in Kelvin. Both the analyte solution and the calibrants have been electrosprayed in anionic mode with the same experimental conditions (ΔEFG = 0.1 V s cm^{-2}, t_r = 420 ms, t_a =10 ms). After elution from the TIMS tunnel, the ions are focused into a hexapole ion guide, and can be selected by their m/z in a further quadrupole. Before entering the TOF-region, the ions have to pass a second quadrupole (the collision cell).

Reference

1. Krishnadas, K. R.; Baksi, A.; Ghosh, A.; Natarajan, G.; Pradeep, T. Manifestation of Geometric and Electronic Shell Structures of Metal Clusters in Intercluster Reactions. *ACS Nano* **2017,** *11* (6), 6015-6023.

2. Michelmann, K.; Silveira, J. A.; Ridgeway, M. E.; Park, M. A. Fundamentals of Trapped Ion Mobility Spectrometry. *J. Am. Soc. Mass Spectrom.* **2015,** *26* (1), 14-24.

3. Ridgeway, M. E.; Silveira, J. A.; Meier, J. E.; Park, M. A. Microheterogeneity within conformational states of ubiquitin revealed by high resolution trapped ion mobility spectrometry. *Analyst* **2015,** *140* (20), 6964-6972.

4. Stow, S. M.; Causon, T. J.; Zheng, X.; Kurulugama, R. T.; Mairinger, T.; May, J. C.; Rennie, E. E.; Baker, E. S.; Smith, R. D.; McLean, J. A.; Hann, S.; Fjeldsted, J. C. An Interlaboratory Evaluation of Drift Tube Ion Mobility-Mass Spectrometry Collision Cross Section Measurements. *Anal. Chem.* **2017,** *89* (17), 9048-9055.

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Supporting Information 1

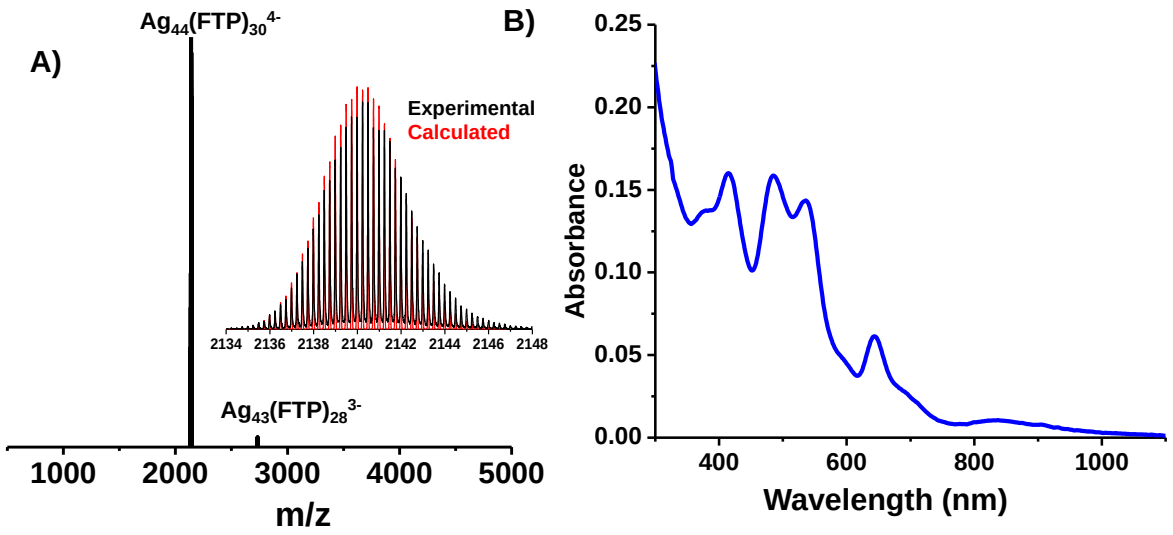

Figure S1. A) Negative ion ESI-MS of pure $[PPh_4]_4[Ag_{44}(FTP)_{30}]$ dissolved in DMF – as obtained under standard ESI conditions[1] (see Experimental Section for details) showing predominantly the 4-charged ion. The peak $Ag_{43}(FTP)_{28}^{3-}$ is a standard fragment formed by $Ag(FTP)_2^-$ loss during electrospray. Experimental isotope pattern exactly matches with the calculated pattern of $Ag_{44}(FTP)_{30}^{4-}$ as shown in inset. No other peaks were found confirming purity of the cluster. B) UV-vis absorption spectrum of the solution in the inset shows all the characteristic bands known from the literature.

Supporting Information 2

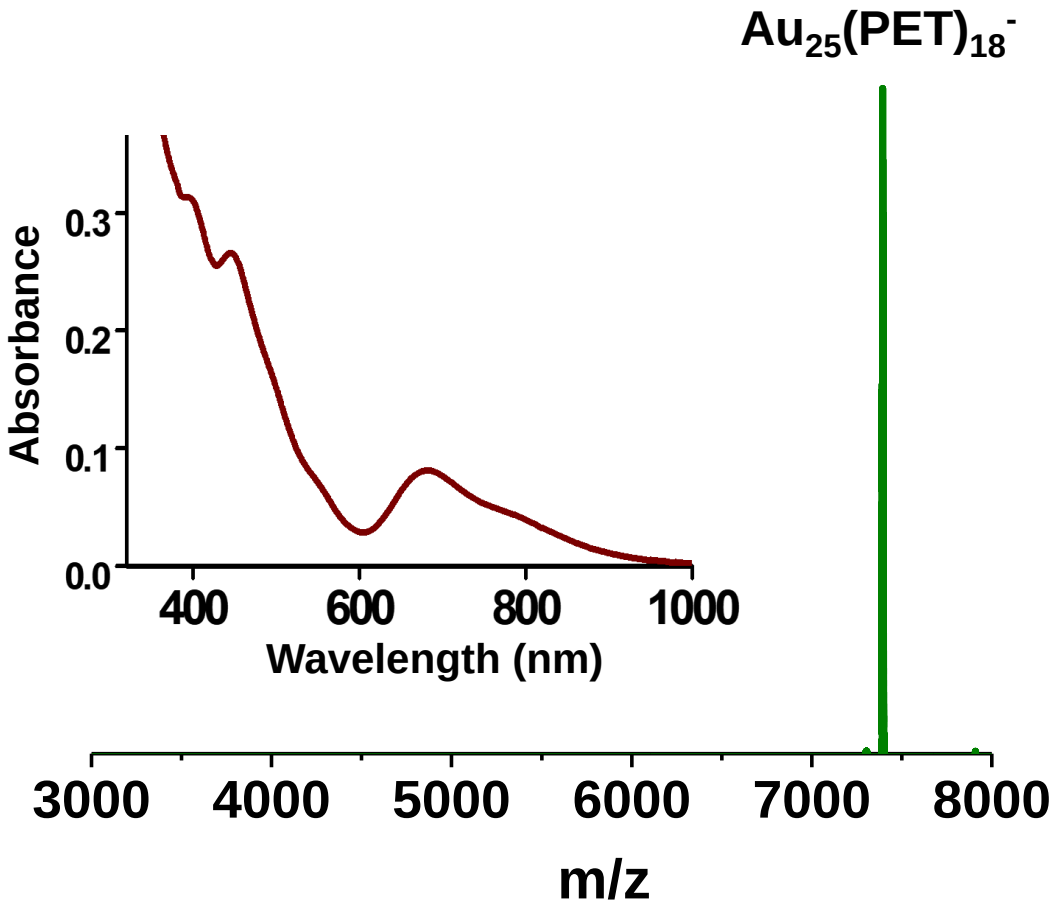

Figure S2. Negative ion ESI-MS of pure [TOA][$Au_{25}(PET)_{18}$] dissolved in DMF - as obtained under standard ESI conditions[1] showing corresponding peak. The inset shows a UV-vis absorption spectrum of the solution showing all the characteristic bands. No other peaks were found confirming the purity of the cluster.

Supporting Information 3

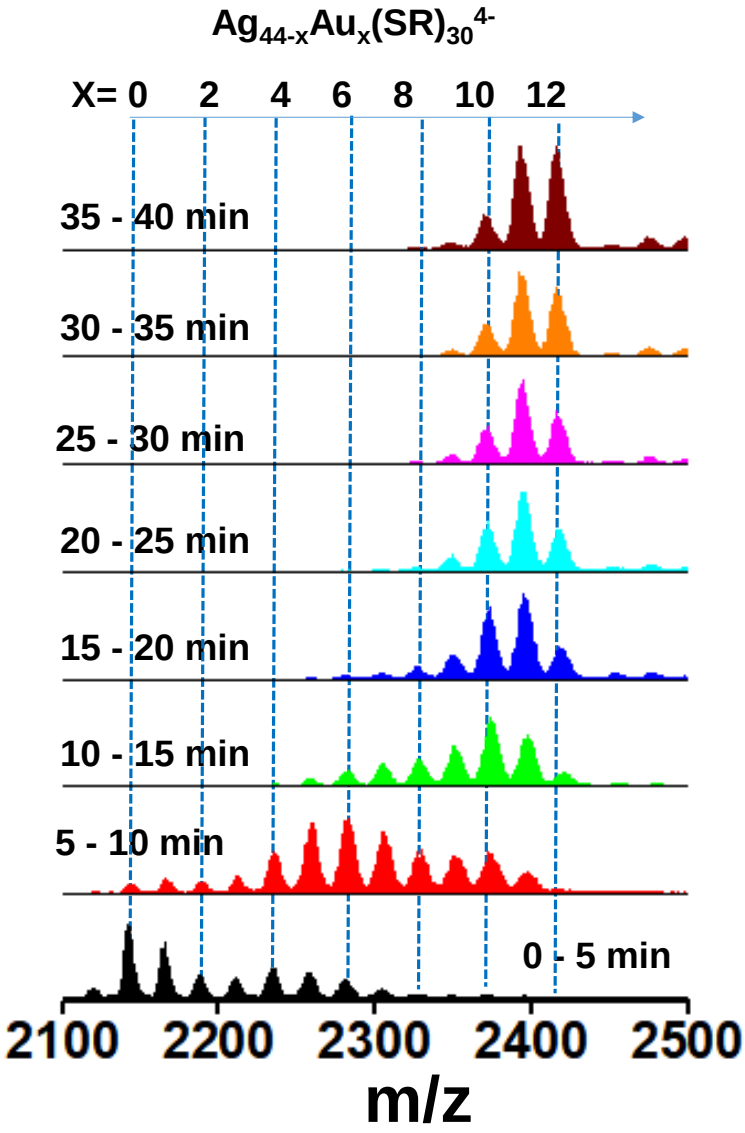

Figure S3. Time-dependent mass spectra (measured in Bruker timsTOF) of *inter-cluster* reaction showing gradual formation of $Au_{12}Ag_{32}(SR)_{30}^{4-}$ over a reaction time of 40 min for 5:1 Ag_{44} : Au_{25} molar ratio (5μM : 1 μM). See also the corresponding "heat map" shown in Figure 1 of the main text. Mass spectra were collected at 1 scan/s and 300 mass spectra were averaged per 5 min reaction time interval. Dashed vertical blue lines are Δm/z = 45 apart which corresponds to replacement of two silver atoms by two gold atoms. Selected $Au_xAg_{44-x}(SR)_{30}^{4-}$ intermediate signals are zoomed in Figures S8-S9 to show their silver isotopomer and ligand compositions. Mass resolution, m/Δm, was ~36,400 in this mass range.

Supporting Information 4

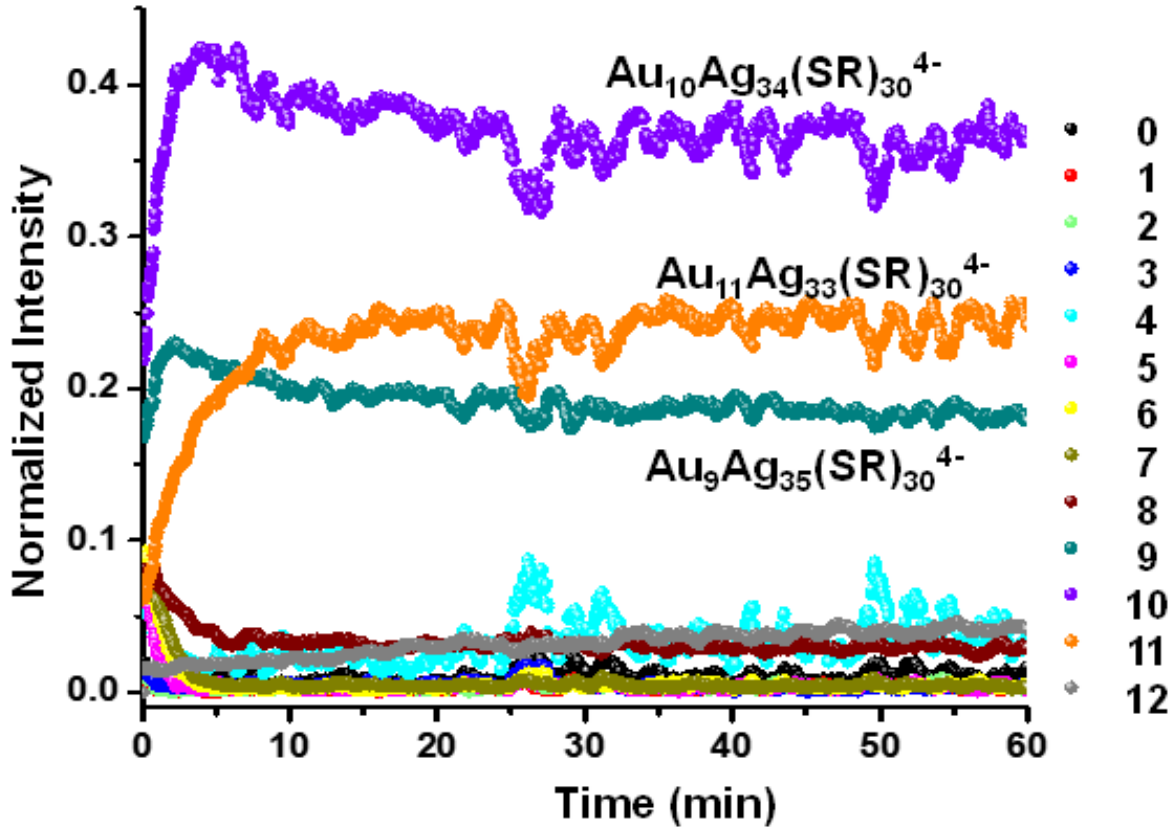

Figure S4. Reaction time dependent variation of total ion intensity of different reaction products $Au_xAg_{44-x}(SR)_{30}^{4-}$, x=0-12, for an 15:1 molar ratio of $Ag_{44}(FTP)_{30}$ (1.5 µM) : $Au_{25}(PET)_{18}$ (100 nM). See also the Figure S2 caption. The reaction was probed using a Thermo Fischer Orbitrap in NESI mode. The time dependent change in intensity of each ion was extracted and was normalized to the total ion intensity (from "TIC" = total ion current) for a mass window of Δm/z = 3 corresponding to 0-2 ligand exchanges.

Supporting Information 5

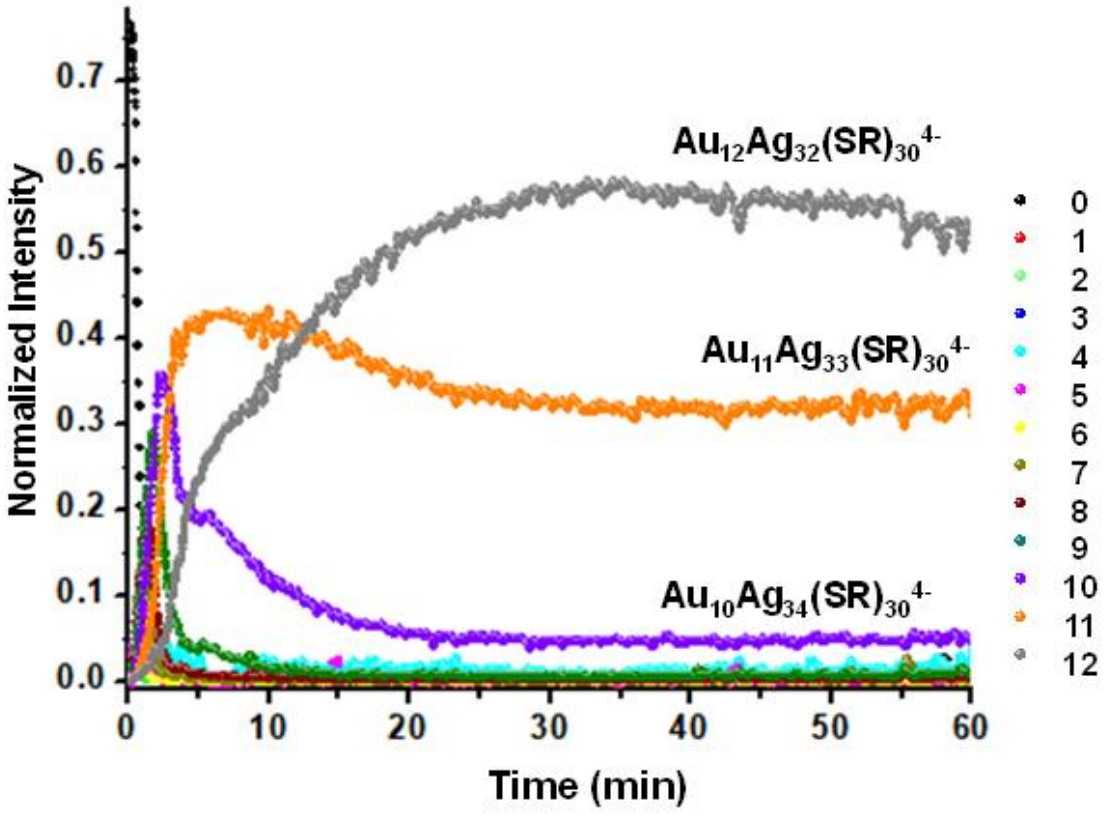

Figure S5. Reaction time dependent variation of total ion intensity of different reaction products $Au_xAg_{44-x}(SR)_{30}^{4-}$, x=0-12, for an 5:1 molar ratio of $Ag_{44}(FTP)_{30}$ (5 µM) : $Au_{25}(PET)_{18}$ (1µM). See also the Figure S2 caption.

Supporting Information 6

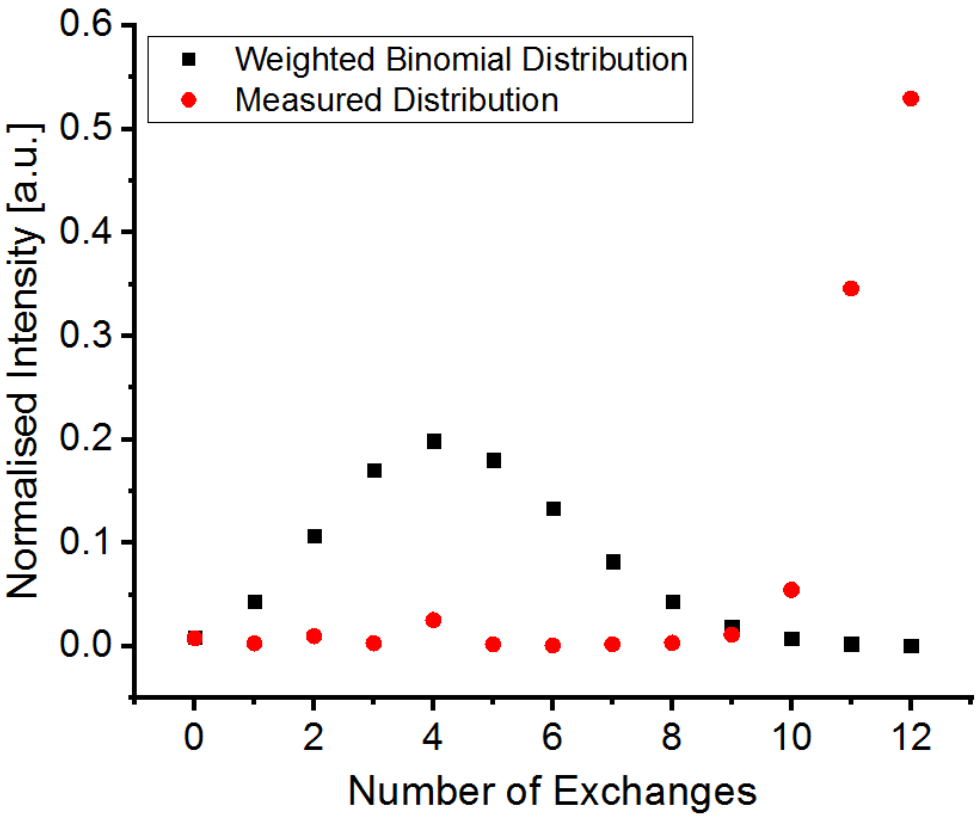

Figure S6. Comparison between the Au exchange distribution at equilibrium determined from the $Au_xAg_{44-x}(SR)_{30}^{4-}$ ion intensity distribution at 40 minute reaction time (red line) with the weighted binomial distribution calculated for an initial Ag_{44}:Au_{25} mixing ratio of 5:1 (black line) using $\binom{n}{k} p^k(1-p)^{n-k}$ where n=44, k is the number of exchanged gold atoms and p is the statistical weight of Au, i.e. 25/245= 0.102. Corresponding mass spectra are presented in Figure S1.

Supporting Information 7

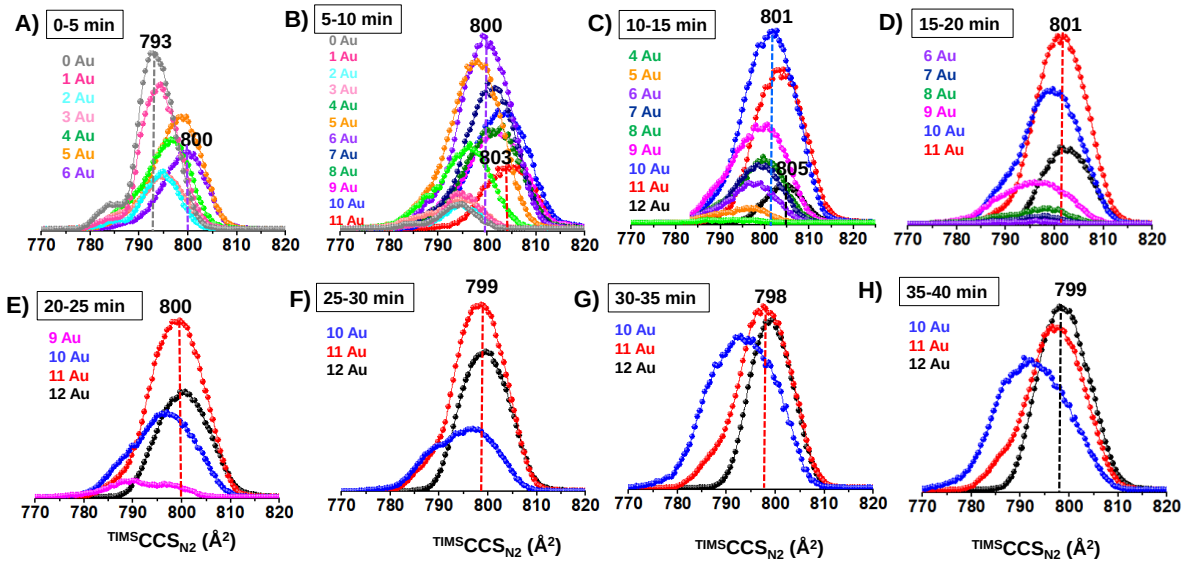

Figure S7. A-H) Change in $^{TIMS}CCS^{N2}$ for different Au exchange products, $Au_xAg_{44-x}(SR)_{30}^{4-}$ (x=0-12), over eight different reaction time ranges. Mobilograms were averaged for 5 min and 2 mobilograms were collected per second. Ion mobility resolution was calculated to be 160. Note, the initial increase in CCS for the Au exchange products. Consequently, the corresponding cluster collision cross sections increase significantly during the first 20 min after mixing. For the final products with x=10 and 11 the CCS then decreases again. The same information is shown in the form of contour plots in Figure 2 of the main text. The vertical dashed lines correspond to the CCS maximum of the most intense ion peak in the specific window. If two vertical dashed lines are shown (A-C), the first corresponds to the CCS of the highest intensity $Au_xAg_{44-x}(SR)_{30}^{4-}$ exchange product whereas the second corresponds to the CCS peak maximum of the product with highest CCS - in that time interval. In each plot, the dashed vertical lines bear the same color code as their respective $Au_xAg_{44-x}(SR)_{30}^{4-}$ (x=0-12) mobilograms.

Supporting Information 8

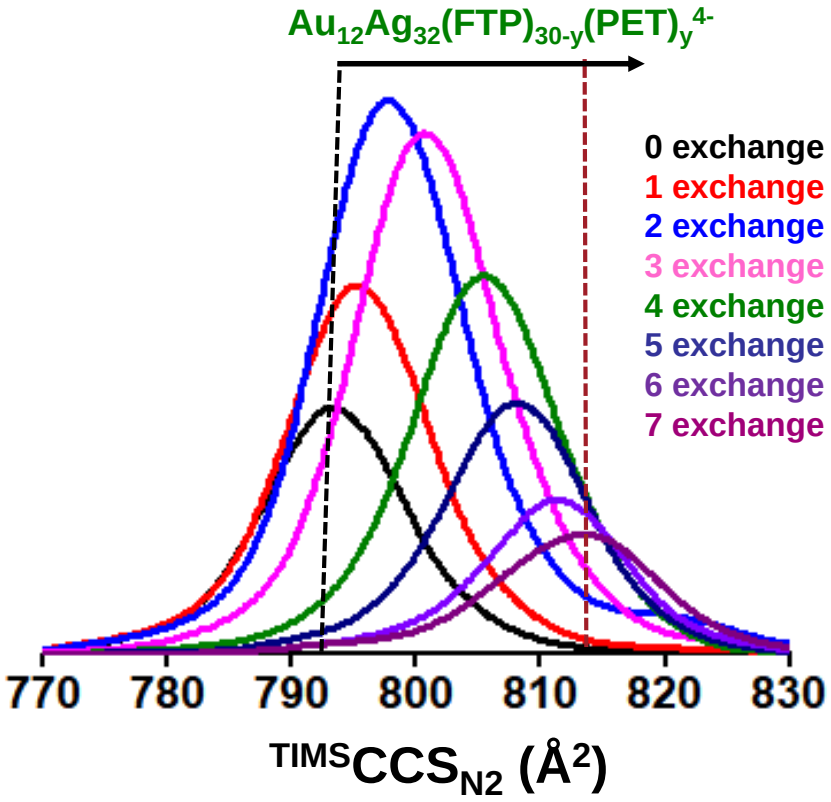

Figure S8. $^{TIMS}CCS_{N2}$ of different ligand exchange products of $Au_{12}Ag_{32}(SR)_{30}^{4-}$ showing a sequential increase in overall cross section as FTP ligands are exchanged by PET ligands Each such ligand exchange leads to an increase in $^{TIMS}CCS_{N2}$ of roughly 2 Å^2.

Supporting Information 9

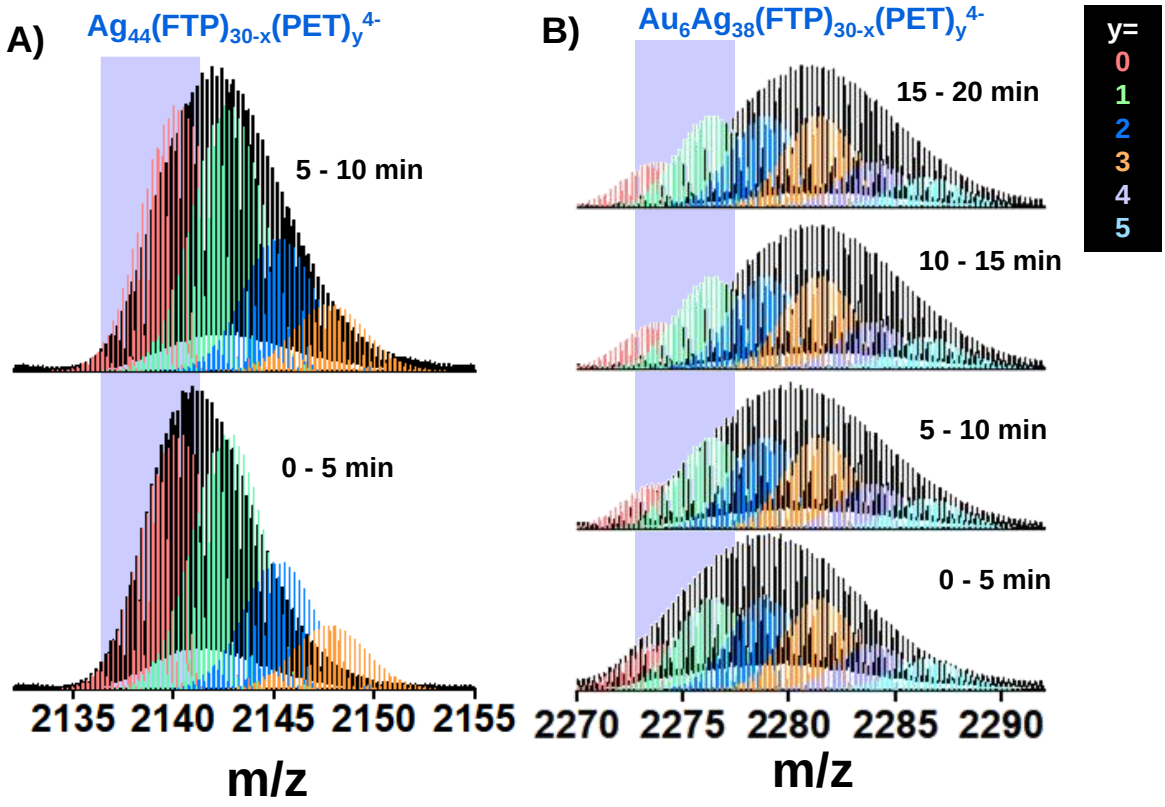

Figure S9. Time-dependent, high-resolution mass spectra of A) $Ag_{44}(SR)_{30}^{4-}$ and B) $Au_6Ag_{38}(SR)_{30}^{4-}$, recorded with the Bruker timsTOF over different reaction time intervals between 0 and 20 min after mixing the cluster reagents (black traces). The calculated isotope patterns for different numbers of ligand exchange, x, are overlaid on the plots (colored traces). The mass range used to extract the mobilograms (and hence $^{TIMS}CCS_{N2}$) shown in Figure 2 and Figure S5 are highlighted (purple rectangle). This corresponds to 0-1 ligand exchanges.

Supporting Information 10

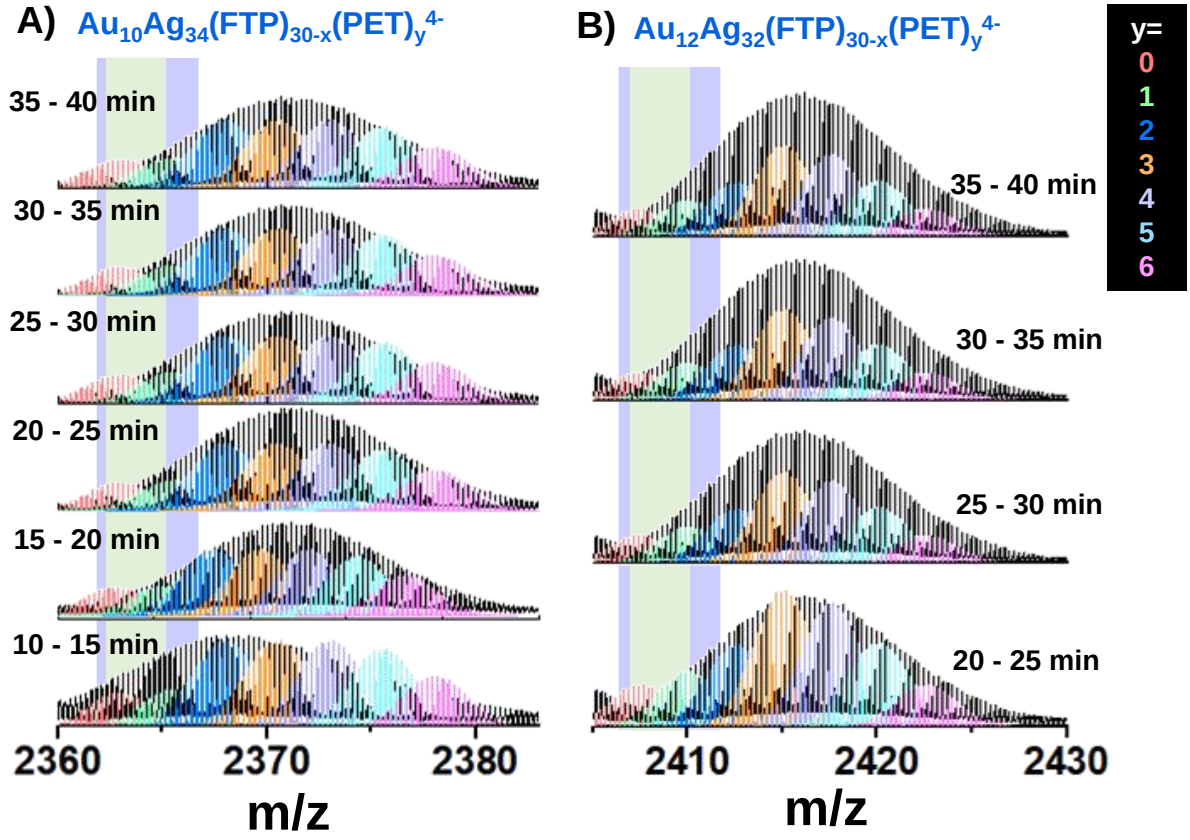

Figure S10. Time-dependent, high-resolution mass spectra of of A) $Au_{10}Ag_{34}(SR)_{30}^{4-}$ and B) $Au_{12}Ag_{32}(SR)_{30}^{4-}$ recorded with the Bruker timsTOF over different reaction time intervals between 0 and 40 min after mixing the cluster reagents (black traces). The calculated isotope patterns for different numbers of ligand exchange, x, are overlaid on the plots (colored traces). Mass range used to extract the mobilograms (and hence $^{TIMS}CCS_{N2}$) shown in Figure 2 and Figure S6 are highlighted in purple (0-2 ligand exchange). The mass ranges used in Figure 3 and Figure S11 are highlighted in green (0-1 ligand exchange).

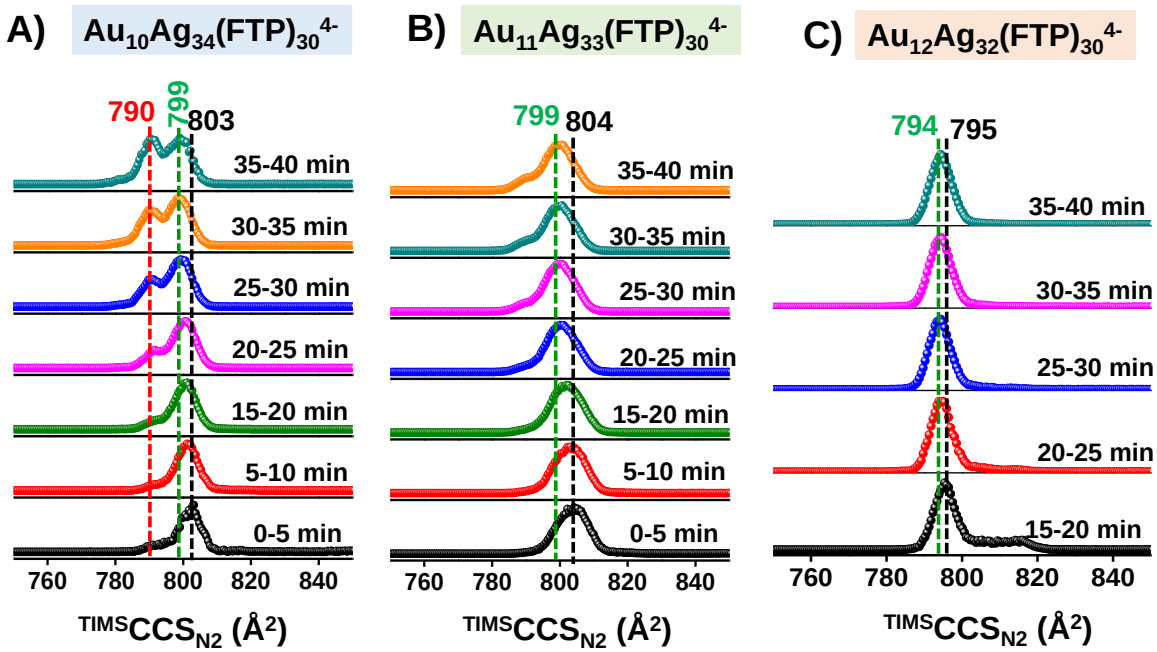

Figure S11. Time dependent change in $^{TIMS}CCS_{N2}$ of A) $Au_{10}Ag_{34}(SR)_{30}^{4-}$, B) $Au_{11}Ag_{33}(SR)_{30}^{4-}$ and C) $Au_{12}Ag_{32}(SR)_{30}^{4-}$. Each of the mobilograms was extracted for the corresponding mass range taking into account only contributions from 0-1 ligand exchange products (see Fig. S9 and S10 as well as Fig. 3 in the main text). Note that $^{TIMS}CCS_{N2}$ of $Au_{10}Ag_{34}(SR)_{30}^{4-}$ and $Au_{11}Ag_{33}(SR)_{30}^{4-}$ change significantly with time while $^{TIMS}CCS_{N2}$ of $Au_{12}Ag_{32}(SR)_{30}^{4-}$ remains almost the same after it begins to be formed 15 min into the reaction. The black and green dashed lines in each plot correspond to the initial and final CCS, respectively. The red dotted line in A) is for the second isomer. Mobilograms are plotted normalized to the respective signal maxima.

Supporting Information 12

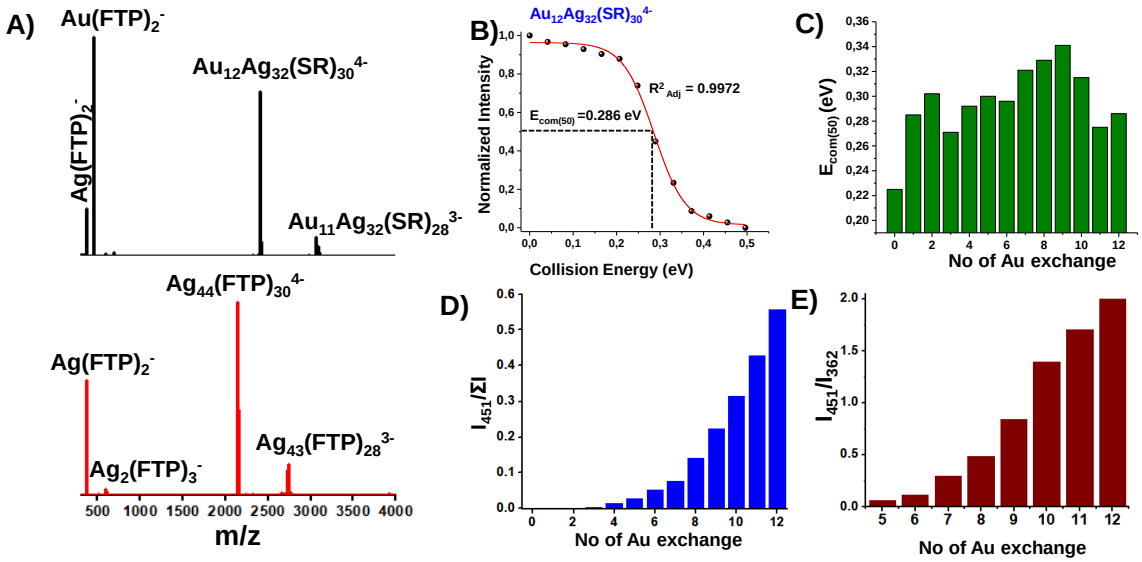

Figure S12. A) Collision induced dissociation measurements in Ar for mass-selected $Ag_{44}(FTP)_{30}^{4-}$ $Au_{12}Ag_{32}(SR)_{30}^{4-}$. Mass spectrum of primary anionic fragments resulting at a lab frame collision energy setting of 6 V. B) Residual $Au_{12}Ag_{32}(SR)_{30}^{4-}$ parent ion intensity after collision with Ar at systematically increasing centre of mass collision energy (normalized to the intensity at CE=0 eV). The collision energy providing 50% survival yield ($E_{com(50)}$) was determined from a fit to the data of the function y = (a-b)/ (1+ exp((x-x_0)/dx)) +b.[6] Relative intensity of parent ion was calculated as:

$$Ip = \frac{Ip}{Ip + \frac{\Sigma If}{n}}$$

Where, I_p is the intensity of the parent ion and ΣI_f is sum of intensities of the fragment ions and n represents to the number of fragments. C) Plot of $E_{com(50)}$ versus the number of Au atom exchanged (x= 0-12 Au). The main fragmentation channels correspond to $Ag(FTP)_2^-$ and for Au containing ions also $Au(FTP)_2^-$ loss. D) Plots of the relative $Au(FTP)_2^-$ fragment intensity (m/z = 451) after back ground subtraction at 0 V normalized to the intensity of the mass selected $Au_xAg_{44-x}(SR)_{30}^{4-}$ ion subjected to CID versus x -- for a nominal lab frame collision energy setting of 6 V. E) Shows the $Au(FTP)_2^-$/ $Ag(FTP)_2^-$ 0 V back ground subtracted fragment intensity ratio ($I_{m/z451}$/ $I_{m/z362}$) for 5-12 Au exchange products at the same lab frame collision energy setting of 6 V. Note that at x=12, this observed ratio is larger than expected for a random distribution of 12 Au and 32 Ag atoms throughout the cluster – assuming dissociation only from the staple regions. However, the x=10-12 measurements are subject to significant contributions from "upstream" fragmentation (presumably during ion transfer from the Synapt quadrupole mass filter to the collision cell region) which causes large $M(FTP)_2^-$ background signals even for low nominal collision energies. Therefore quantitative inferences concerning the $Au(FTP)_2^-$/ $Ag(FTP)_2^-$ ratio cannot be drawn at this stage.

Reference

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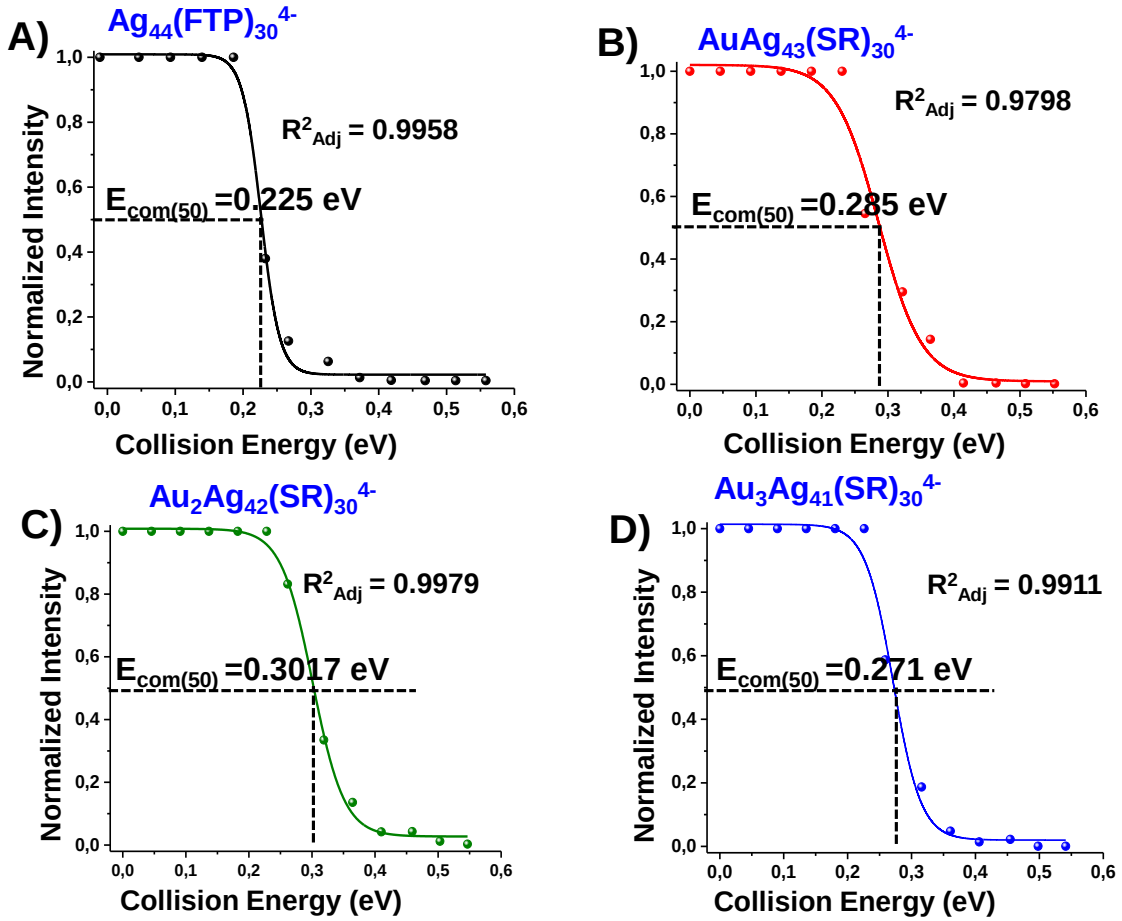

Figure S13. Determination of $E_{com(50)}$ values for $Ag_{44-x}Au_x(SR)_{30}^{4-}$ (x = 0-3) following the same procedure as described in the caption of Figure S10.

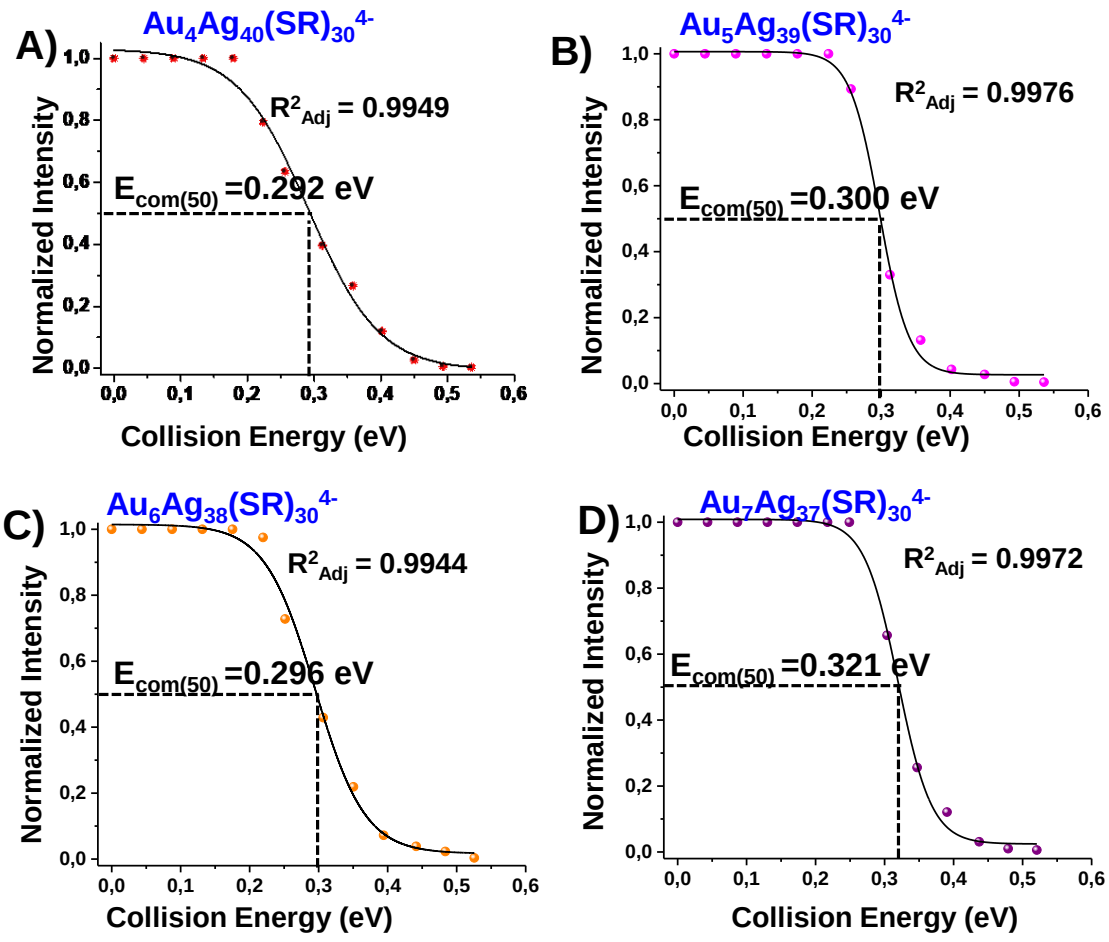

Figure S14. Determination of $E_{com(50)}$ values for $Ag_{44-x}Au_x(SR)_{30}^{4-}$ (x = 4-7) following the same procedure as described in the caption of Figure S10.

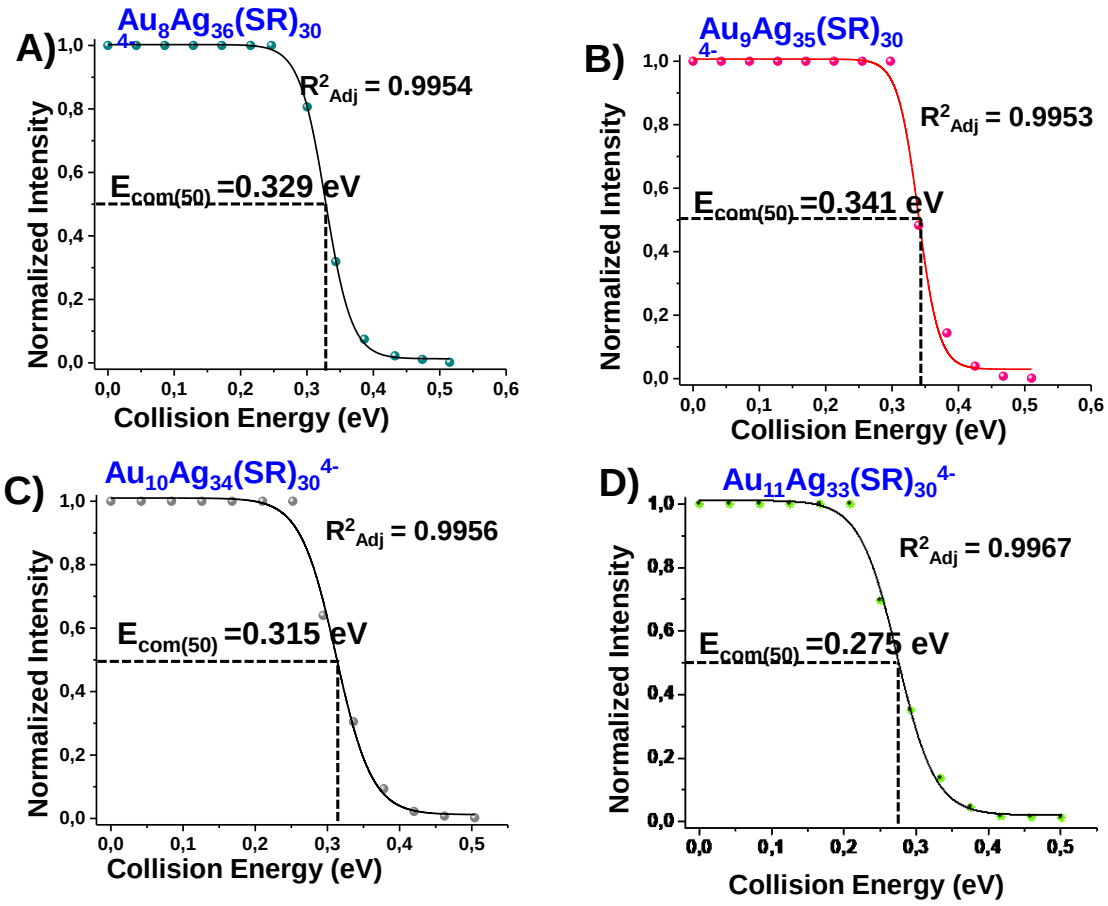

Figure S15. Determination of $E_{com(50)}$ values for $Ag_{44-x}Au_x(SR)_{30}^{4-}$ (x = 8-11) following the same procedure as described in the caption of Figure S10.

Table S1. Coordinates and NBO-based partial charges of the DFT optimized structures:

$Ag_{44}(FTP)_{30}^{4-}$

atom	x	y	z	charge
Ag	-0.1982	-2.7379	-0.1630	-0.170
Ag	0.3503	-1.5034	2.4049	-0.174
Ag	2.3196	-1.3859	0.2958	-0.176
Ag	0.1223	2.7607	0.3961	-0.166
Ag	-0.4605	1.5130	-2.1612	-0.175
Ag	-2.4061	1.3861	-0.0464	-0.177
Ag	-1.8946	-0.9596	-1.6951	-0.172
Ag	-2.2631	-1.2186	1.1879	-0.173
Ag	-3.8921	0.8698	2.3742	0.541
Ag	-0.9944	1.0657	2.4792	-0.172
Ag	-4.5128	-0.5322	-0.5813	0.390
Ag	4.4379	0.5083	0.8135	0.395
Ag	2.1158	-3.5896	-1.6419	0.379
Ag	2.1922	1.2256	-0.9467	-0.169
Ag	-2.2351	3.5940	1.8491	0.396
Ag	-0.9074	-0.3656	-4.3393	0.408
Ag	0.7228	3.3213	3.2016	0.517
Ag	1.8742	1.2750	-3.8099	0.374
Ag	1.8284	0.9845	1.9203	-0.177
Ag	-3.2884	1.3210	-2.8243	0.514
Ag	-2.0385	-1.1413	4.0662	0.396
Ag	1.3339	3.7819	-2.0582	0.512
Ag	-2.9623	-3.4007	-0.5667	0.385
Ag	0.9420	-1.0309	-2.2306	-0.173
Ag	-1.8801	3.8912	-1.3888	0.377
Ag	3.8233	-0.8652	-2.1226	0.544
Ag	2.8933	3.4465	0.7554	0.405
Ag	-1.5854	0.7259	6.5902	0.547
Ag	-0.2128	-1.9216	6.5007	0.545
Ag	3.1839	-1.2865	3.0932	0.517
Ag	-1.4161	-3.8053	2.2508	0.516
Ag	-0.7293	-3.2990	-2.9682	0.512
Ag	0.9028	0.3029	4.5685	0.396
Ag	1.7663	-3.8971	1.6505	0.425
Ag	5.8355	3.1516	-0.4328	0.555
Ag	1.7875	-6.4203	-0.3768	0.541
Ag	-5.5441	-2.9435	-2.3481	0.545
Ag	-1.8290	6.4139	0.5229	0.554
Ag	5.5163	2.8891	2.5220	0.546
Ag	1.5779	-0.6113	-6.3256	0.544
Ag	0.1228	1.9855	-6.2906	0.542
Ag	-4.4427	5.0654	0.0049	0.551
Ag	-5.8855	-3.1901	0.6158	0.559
Ag	4.3418	-4.9797	0.0595	0.541
S	0.1133	2.5049	5.7201	-0.432
S	-4.4155	3.7281	-2.1547	-0.410

S	5.8257	0.7176	-1.3559	-0.440
S	-3.9598	-4.5132	1.6025	-0.426
S	3.9047	4.4705	-1.4385	-0.421
S	-4.8064	3.3574	1.9606	-0.434
S	4.7139	-3.3650	-1.8569	-0.427
S	-5.8696	-0.7750	1.6021	-0.436
S	-3.3728	-4.1333	-3.0327	-0.430
S	-0.6770	5.5413	2.6834	-0.442
S	5.2107	0.4346	3.3275	-0.423
S	-2.2902	1.5418	-5.3780	-0.444
S	0.1433	-5.9211	1.6252	-0.437
S	-0.2389	5.9285	-1.4345	-0.430
S	3.5789	-0.4342	-4.7639	-0.428
S	-4.1362	7.4491	0.7937	-0.388
S	-5.2624	-0.4684	-3.1076	-0.428
S	0.5781	-5.6141	-2.4426	-0.403
S	2.2068	-1.7019	5.5975	-0.437
S	3.9570	-7.4460	0.4469	-0.367
S	-7.6913	-3.5363	-1.1404	-0.382
S	-3.6140	0.7117	5.0378	-0.423
S	7.6620	3.4733	1.2800	-0.388
S	-1.4812	-3.5341	4.9840	-0.425
S	1.1672	3.7060	-4.7611	-0.397
S	4.2697	-3.6586	2.3089	-0.433
S	3.3959	4.1309	3.2141	-0.430
S	0.0540	-2.5515	-5.4349	-0.436
S	-0.8099	-0.6104	8.5974	-0.382
S	0.5501	0.5462	-8.3277	-0.368
F	3.6341	4.4082	10.1448	-0.341
F	2.4237	-8.6631	-7.2162	-0.341
F	-2.9500	-4.9697	-9.9817	-0.341
F	6.9956	-10.7338	-3.4956	-0.343
C	-1.2457	6.4260	4.1394	-0.160
F	-5.8642	-6.2349	7.9911	-0.340
C	0.8538	2.7953	8.4000	-0.208
H	-0.0604	2.2268	8.6370	0.240
F	-6.1429	7.1833	-6.6978	-0.340
C	2.2658	-7.4058	-3.7871	-0.208
H	2.7743	-7.5544	-2.8194	0.233
F	4.5167	9.8729	4.3572	-0.340
C	1.2045	-6.4776	-3.8823	-0.159
F	-7.0159	5.7424	6.9527	-0.341
C	-6.8564	0.3077	-3.3935	-0.157
C	-0.8992	-3.2028	-6.8090	-0.156
C	-4.8788	4.8051	-3.5123	-0.158
C	-3.3138	0.9541	-6.7273	-0.152
C	4.4221	-4.2379	-4.5164	-0.195
H	3.3668	-3.9313	-4.4481	0.249
C	5.2717	-4.0967	-3.3952	-0.162
C	7.6002	-1.1618	-0.2406	-0.197

H	6.7567	-1.5201	0.3701	0.246
F	6.7309	-5.6586	-6.9699	-0.338
C	-3.5297	-5.9188	-3.1101	-0.159
C	-5.4229	4.1036	3.4683	-0.153
C	7.4139	-0.0857	-1.1372	-0.153
F	1.0306	-9.9579	5.9193	-0.341
C	2.6827	-8.1420	-4.9070	-0.291
H	3.5112	-8.8634	-4.8327	0.236
F	4.6518	2.7570	-12.0514	-0.343
F	-8.4541	-1.3204	7.8554	-0.340
C	-4.5841	4.4284	4.5574	-0.197
H	-3.4996	4.2498	4.4850	0.244
C	1.6695	3.2592	9.4440	-0.291
H	1.4033	3.0747	10.4968	0.231
C	3.7492	5.8716	3.4779	-0.155
C	-7.4648	0.0273	1.4325	-0.151
C	6.7914	-0.3850	3.5523	-0.157
C	-1.0539	-3.7663	-9.1901	-0.293
H	-0.6428	-3.7455	-10.2118	0.231
C	-0.5956	6.9902	-2.8362	-0.158
C	-5.0648	0.0521	5.8586	-0.160
F	11.1447	-1.8995	-0.7587	-0.342
C	4.9012	-9.7865	-0.6509	-0.217
H	4.3969	-10.2559	0.2093	0.232
C	8.8556	-1.7778	-0.1122	-0.289
H	9.0095	-2.6076	0.5943	0.240
C	6.2538	-5.1497	-5.8067	0.395
C	1.2063	3.0221	7.0492	-0.158
F	-11.2225	1.8004	1.1395	-0.341
C	4.7558	-4.8179	3.5901	-0.155
C	0.4620	-7.1042	2.9353	-0.158
C	2.8438	3.9574	9.1360	0.393
F	-3.8267	-10.0589	-3.4684	-0.338
C	-5.7702	5.8829	-3.3008	-0.213
H	-6.1292	6.0964	-2.2804	0.239
C	8.5111	0.3553	-1.9133	-0.207
H	8.3714	1.1872	-2.6214	0.239
C	8.1303	5.1878	1.4932	-0.162
C	4.2668	8.5701	4.0678	0.395
C	3.2523	-1.1644	6.9526	-0.153
C	4.8117	-8.3810	-0.8157	-0.169
C	-2.1508	-3.8266	-6.5991	-0.220
H	-2.5842	-3.8544	-5.5841	0.245
C	0.5742	-6.2936	-5.1348	-0.200
H	-0.2525	-5.5734	-5.2306	0.240
C	-7.7385	0.9624	0.4100	-0.196
H	-6.9562	1.2194	-0.3220	0.244
C	-6.8136	4.3351	3.5857	-0.206
H	-7.4775	4.0721	2.7469	0.240
C	-5.0076	-5.4163	5.9271	-0.295

H	-5.9012	-5.7944	5.4054	0.237
C	-6.1979	6.6871	-4.3692	-0.291
H	-6.8841	7.5326	-4.2051	0.235
C	6.6262	-4.4891	-3.5103	-0.219
H	7.2998	-4.3633	-2.6478	0.242
C	7.1209	-5.0192	-4.7132	-0.306
H	8.1750	-5.3237	-4.8145	0.230
F	-5.7245	-0.2646	-9.9008	-0.341
C	-6.4953	5.2069	5.8179	0.392
C	2.0327	-7.9448	-6.1318	0.393
C	-5.1160	4.9824	5.7333	-0.292
H	-4.4637	5.2446	6.5804	0.242
C	2.7507	6.8542	3.2853	-0.209
H	1.7562	6.5565	2.9109	0.246
C	0.9853	-7.0242	-6.2608	-0.292
H	0.4943	-6.8836	-7.2363	0.237
C	-0.3651	-3.1770	-8.1188	-0.205
H	0.6015	-2.6806	-8.3007	0.239
F	-5.2150	-3.2527	11.6297	-0.342
C	4.9097	-4.7656	-5.7227	-0.284
H	4.2495	-4.8851	-6.5952	0.244
C	-3.6090	1.8373	-7.7924	-0.214
H	-3.1838	2.8538	-7.7838	0.231
C	-5.4023	-1.3190	5.8386	-0.194
H	-4.7527	-2.0352	5.3109	0.242
C	-9.0033	1.5644	0.3088	-0.288
H	-9.2257	2.2826	-0.4950	0.241
C	-8.4779	-0.2740	2.3723	-0.207
H	-8.2662	-0.9875	3.1845	0.240
C	1.4431	1.6865	-10.6637	-0.219
H	0.3829	1.6229	-10.9585	0.233
C	-2.1696	-1.4170	9.4355	-0.166
C	-3.9850	-4.7603	5.2229	-0.217
H	-4.0816	-4.6153	4.1333	0.246
C	5.0163	0.3780	-5.4650	-0.156
C	-2.7345	-4.4811	7.2911	-0.209
H	-1.8512	-4.1026	7.8319	0.235
C	-4.4239	4.5502	-4.8276	-0.224
H	-3.7261	3.7150	-5.0132	0.247
C	-7.3536	4.8888	4.7570	-0.299
H	-8.4353	5.0721	4.8575	0.228
C	3.5871	-2.0996	7.9595	-0.212
H	3.1925	-3.1262	7.8960	0.231
C	3.7692	0.1470	7.0433	-0.196
H	3.5246	0.8868	6.2655	0.246
C	0.4620	-6.7281	4.2980	-0.205
H	0.2900	-5.6751	4.5748	0.248
C	5.2768	7.6204	4.2624	-0.293
H	6.2626	7.9402	4.6347	0.234
F	-1.3666	9.5527	-6.0294	-0.338

C	3.7332	2.2672	-11.1772	0.385
C	5.6308	-10.5804	-1.5495	-0.301
H	5.7051	-11.6724	-1.4197	0.225
C	-5.2995	10.8771	-1.0763	-0.303
H	-5.8327	11.8020	-0.8026	0.223
C	-4.8298	10.7108	-2.3853	0.387
C	-4.1489	9.5495	-2.7700	-0.285
H	-3.7850	9.4438	-3.8036	0.241
C	-3.9321	8.5353	-1.8238	-0.208
H	-3.3889	7.6261	-2.1263	0.245
C	-4.3877	8.6712	-0.4923	-0.163
C	-5.0769	9.8568	-0.1373	-0.222
H	-5.4377	9.9755	0.8976	0.230
C	-2.2865	-4.3863	-8.9503	0.394
C	5.0135	6.2734	3.9671	-0.216
H	5.8042	5.5184	4.1126	0.238
C	9.7695	-0.2537	-1.7888	-0.298
H	10.6322	0.0875	-2.3829	0.227
C	-2.8331	-4.2902	5.8938	-0.156
C	-6.5465	-1.7864	6.5057	-0.289
H	-6.8010	-2.8577	6.5070	0.241
C	-2.9812	-6.7671	-2.1218	-0.192
H	-2.4649	-6.3327	-1.2514	0.248
C	-5.9128	0.9549	6.5431	-0.207
H	-5.6694	2.0296	6.5451	0.243
C	-2.8894	-2.9287	11.2355	-0.306
H	-2.6594	-3.6254	12.0581	0.225
C	6.2762	-9.9686	-2.6321	0.386
C	1.8239	1.2422	-9.3725	-0.170
C	-7.3574	-0.8725	7.1899	0.389
C	-7.0575	0.4959	7.2137	-0.298
H	-7.7213	1.1910	7.7521	0.231
C	0.6527	-7.6873	5.3055	-0.288
H	0.6459	-7.4022	6.3692	0.234
C	-1.1020	8.7125	-4.9970	0.395
C	-5.7324	6.4097	-5.6605	0.393
C	2.4010	3.7251	6.7678	-0.218
H	2.7038	3.8956	5.7204	0.245
C	3.1896	1.3299	-9.0132	-0.213
H	3.5113	0.9917	-8.0144	0.242
F	5.6712	-0.0627	10.1604	-0.341
C	-3.7536	-5.1334	8.0022	-0.289
H	-3.6867	-5.2719	9.0924	0.234
C	2.3894	2.1963	-11.5666	-0.302
H	2.0954	2.5424	-12.5708	0.225
C	-2.8448	-4.4193	-7.6669	-0.294
H	-3.8176	-4.9119	-7.5103	0.231
C	-3.0791	-8.1621	-2.2387	-0.278
H	-2.6544	-8.8245	-1.4695	0.243
C	4.8899	-0.4220	9.1100	0.398

C	5.4676	-7.7995	-1.9269	-0.217
H	5.4099	-6.7094	-2.0825	0.240
C	3.2200	4.1952	7.8084	-0.296
H	4.1480	4.7473	7.5915	0.237
C	-4.8779	-5.5985	7.3090	0.395
C	-3.7280	-8.7115	-3.3508	0.400
C	9.9257	-1.3138	-0.8863	0.394
C	-4.2255	-2.6509	10.9184	0.388
C	3.0063	8.2027	3.5806	-0.289
H	2.2276	8.9695	3.4435	0.236
C	4.1439	1.8420	-9.9076	-0.291
H	5.2053	1.9108	-9.6219	0.240
C	0.6595	-8.4656	2.6048	-0.210
H	0.6670	-8.7694	1.5459	0.237
C	-4.4220	1.4321	-8.8623	-0.296
H	-4.6507	2.1119	-9.6984	0.227
C	6.1966	-8.5854	-2.8348	-0.292
H	6.7064	-8.1242	-3.6952	0.239
C	-1.8692	-2.3105	10.4941	-0.224
H	-0.8138	-2.5186	10.7359	0.232
C	4.0785	-4.8860	4.8288	-0.207
H	3.2075	-4.2353	5.0095	0.248
C	-3.8528	-0.3516	-6.7590	-0.195
H	-3.6357	-1.0512	-5.9371	0.246
C	-4.8499	5.3494	-5.9014	-0.295
H	-4.5053	5.1505	-6.9285	0.234
C	-9.7447	0.3231	2.2783	-0.298
H	-10.5427	0.0896	3.0013	0.228
C	-4.5574	-1.7720	9.8807	-0.284
H	-5.6151	-1.5847	9.6389	0.239
C	-3.5297	-1.1592	9.1460	-0.203
H	-3.7881	-0.4758	8.3210	0.239
C	-1.6224	7.4131	-5.0190	-0.286
H	-2.2307	7.0793	-5.8735	0.240
C	-0.0740	8.3051	-2.8480	-0.206
H	0.5349	8.6530	-1.9989	0.236
C	0.8534	-9.4292	3.6067	-0.296
H	1.0149	-10.4899	3.3570	0.228
C	-9.9929	1.2319	1.2413	0.394
C	7.3192	0.1754	-6.2734	-0.295
H	8.2172	-0.4274	-6.4822	0.231
C	4.4036	-1.7334	9.0405	-0.296
H	4.6634	-2.4535	9.8327	0.226
C	4.5859	0.5221	8.1221	-0.282
H	4.9796	1.5468	8.2033	0.239
C	-1.3630	6.5538	-3.9391	-0.201
H	-1.7720	5.5312	-3.9501	0.243
C	-4.1810	-6.5031	-4.2221	-0.226
H	-4.6086	-5.8530	-5.0027	0.232
C	-4.6660	-0.7655	-7.8261	-0.283

H	-5.0826	-1.7838	-7.8592	0.237
C	-0.3257	9.1700	-3.9244	-0.293
H	0.0697	10.1980	-3.9372	0.231
C	0.8474	-9.0268	4.9480	0.395
C	-4.9420	0.1319	-8.8646	0.398
C	4.1549	6.3443	-5.7106	-0.292
H	4.7742	7.0938	-5.1939	0.236
C	4.2834	6.1636	-7.0938	0.389
C	3.5100	5.2169	-7.7777	-0.295
H	3.6346	5.0867	-8.8641	0.237
C	2.5839	4.4436	-7.0592	-0.214
H	1.9746	3.6931	-7.5905	0.235
C	2.4240	4.6085	-5.6636	-0.164
C	3.2273	5.5660	-5.0002	-0.199
H	3.1243	5.7035	-3.9128	0.242
F	-2.3347	8.6347	7.5025	-0.342
F	-10.5124	2.1063	-4.2832	-0.342
C	-0.5742	6.2415	5.3709	-0.204
H	0.2437	5.5078	5.4436	0.242
C	-2.3058	7.3591	4.0748	-0.211
H	-2.8500	7.5114	3.1276	0.243
F	6.0650	-7.4114	6.5806	-0.341
C	-0.9401	6.9804	6.5076	-0.292
H	-0.4185	6.8384	7.4669	0.238
C	-1.9839	7.9083	6.4095	0.391
C	3.3431	7.0982	-0.6101	-0.202
H	2.4400	6.6906	-0.1293	0.251
C	8.0077	0.2227	3.1668	-0.209
H	7.9993	1.2016	2.6595	0.243
F	-4.9686	-10.3847	1.4604	-0.341
C	-2.6746	8.1027	5.2068	-0.293
H	-3.5006	8.8298	5.1612	0.232
C	-8.0718	-0.3100	-3.0211	-0.211
H	-8.0605	-1.2756	-2.4891	0.243
C	-6.9048	1.5492	-4.0701	-0.201
H	-5.9675	2.0439	-4.3695	0.240
C	-8.1324	2.1598	-4.3714	-0.292
H	-8.1697	3.1273	-4.8956	0.237
C	5.3769	6.7758	-1.9083	-0.222
H	6.0766	6.1069	-2.4349	0.242
C	-9.3201	1.5217	-3.9936	0.391
C	9.2355	-0.4087	3.4211	-0.294
H	10.1855	0.0575	3.1159	0.232
C	-9.3038	0.2927	-3.3227	-0.294
H	-10.2527	-0.1842	-3.0308	0.233
C	7.2951	6.2894	1.1972	-0.208
H	6.2713	6.1135	0.8307	0.245
C	5.8812	-5.6500	3.3832	-0.208
H	6.4131	-5.6117	2.4194	0.239
F	5.1751	6.9195	-7.7859	-0.341

C	6.8326	-1.6446	4.1949	-0.202
H	5.8941	-2.1303	4.5045	0.243
C	5.6361	-6.5685	5.6056	0.395
C	4.5171	-5.7594	5.8376	-0.290
H	3.9938	-5.8193	6.8047	0.232
C	6.3244	-6.5259	4.3868	-0.295
H	7.1961	-7.1805	4.2295	0.230
C	5.0571	1.7625	-5.7401	-0.205
H	4.1799	2.3916	-5.5192	0.242
C	4.2291	6.2285	-1.2867	-0.165
C	-4.2843	-7.8983	-4.3468	-0.303
H	-4.7829	-8.3615	-5.2132	0.229
F	9.5050	9.1049	1.9728	-0.344
F	10.4346	-2.2688	4.2998	-0.343
F	8.4449	2.1130	-7.0727	-0.340
C	9.0546	7.8307	1.8192	0.386
C	3.5983	8.4779	-0.5515	-0.289
H	2.9181	9.1585	-0.0161	0.238
C	5.6381	8.1544	-1.8548	-0.298
H	6.5339	8.5859	-2.3287	0.233
C	7.7521	7.6079	1.3564	-0.287
H	7.1000	8.4630	1.1208	0.240
C	7.3274	1.5498	-6.5458	0.393
C	6.2098	2.3525	-6.2851	-0.290
H	6.2447	3.4318	-6.4993	0.241
C	9.4416	5.4490	1.9627	-0.220
H	10.1043	4.5999	2.1973	0.230
C	8.0569	-2.2838	4.4484	-0.293
H	8.0901	-3.2660	4.9446	0.237
C	6.1622	-0.4069	-5.7331	-0.203
H	6.1448	-1.4849	-5.5075	0.244
C	9.2458	-1.6559	4.0576	0.391
C	9.9071	6.7632	2.1277	-0.303
H	10.9273	6.9691	2.4907	0.223
C	-7.8135	-7.4580	-2.4227	-0.292
H	-7.2278	-8.1440	-3.0550	0.239
C	-7.3814	-6.1399	-2.2016	-0.214
H	-6.4416	-5.7947	-2.6633	0.240
C	-8.1235	-5.2529	-1.3862	-0.170
C	-9.3147	-5.7358	-0.7875	-0.216
H	-9.9032	-5.0596	-0.1461	0.234
C	-9.7562	-7.0506	-1.0035	-0.300
H	-10.6817	-7.4279	-0.5390	0.226
C	-9.0006	-7.8982	-1.8245	0.386
F	4.9959	10.3221	-1.1155	-0.338
F	-5.0383	11.6979	-3.2962	-0.343
F	-9.4301	-9.1695	-2.0407	-0.342
C	4.7429	8.9902	-1.1751	0.394
C	-4.7305	-9.0475	1.4677	0.393
C	-5.6044	-8.1921	0.7849	-0.289

H	-6.4668	-8.6067	0.2400	0.237
C	-5.3576	-6.8105	0.7994	-0.208
H	-6.0376	-6.1318	0.2592	0.236
C	-4.2467	-6.2808	1.4926	-0.159
C	-3.3791	-7.1689	2.1701	-0.206
H	-2.5027	-6.7746	2.7077	0.243
C	-3.6180	-8.5527	2.1593	-0.292
H	-2.9442	-9.2463	2.6860	0.238

Table S2. $Ag_{32}Au_{12}(FTP)_{30}^{4-}$ I isomer: all Au atoms in the inner shell

atom	x	y	z	charge
Au	-0.1046	0.3495	-2.7301	-0.262
Au	1.1826	2.2893	-0.9803	-0.257
Au	-1.7397	1.9607	-0.8734	-0.264
Au	2.3886	-0.3378	-1.3745	-0.261
Au	-2.3003	-0.8892	-1.2609	-0.261
Au	0.2339	-2.3345	-1.5494	-0.257
Au	-2.3542	0.2763	1.4204	-0.265
Au	-0.1901	2.2766	1.6099	-0.256
Au	-1.1366	-2.3517	1.0342	-0.260
Au	2.3558	0.8460	1.3076	-0.262
Au	1.7672	-2.0277	0.9301	-0.261
Au	0.1684	-0.3760	2.7774	-0.258
Ag	-0.4959	3.2712	-3.1485	0.428
Ag	-2.8498	1.0011	-3.4194	0.457
Ag	2.3980	1.6027	-3.5492	0.587
Ag	1.6590	-1.6004	-3.9629	0.427
Ag	-1.5288	-1.9592	-3.8751	0.557
Ag	-0.5356	4.5421	-0.2189	0.561
Ag	-2.2505	-3.8028	-1.2358	0.440
Ag	-3.0005	3.1223	1.4814	0.434
Ag	4.1197	1.9241	-0.7299	0.440
Ag	-4.4692	0.9426	-0.5111	0.561
Ag	2.2763	3.7795	1.2614	0.449
Ag	-4.0647	-2.0076	0.7705	0.438
Ag	3.0436	-3.1796	-1.4305	0.466
Ag	-1.6852	1.5084	3.9981	0.439
Ag	-2.3347	-1.6388	3.6142	0.584
Ag	4.5044	-1.0121	0.5652	0.563
Ag	2.9467	-1.0818	3.4155	0.446
Ag	0.5747	-4.6208	0.2680	0.565
Ag	0.4858	-3.2357	3.2929	0.440
Ag	1.6173	1.9345	3.9134	0.562
S	0.8069	2.7993	-5.3463	-0.421
S	4.1746	3.4381	-2.8170	-0.432
S	-2.2193	-0.0878	-5.7032	-0.428
S	5.4573	-2.2700	-1.6522	-0.424
S	-4.8809	2.4332	-2.7478	-0.442
S	-4.0511	-3.5409	2.8454	-0.429
S	-1.9735	5.4808	1.8876	-0.426
S	3.7057	-0.3036	-4.9083	-0.420
S	2.0412	-5.5307	-1.8113	-0.436
S	1.8634	5.8553	-0.2656	-0.414
S	-5.9585	-1.2549	-0.8734	-0.426
S	-3.7587	0.2450	4.8732	-0.428
S	-3.6832	-3.6302	-3.3952	-0.425
S	-0.2771	3.4098	5.1229	-0.439
S	-5.4798	2.2718	1.6589	-0.404

S	0.2665	-3.5855	-5.0542	-0.402
S	6.0049	1.1715	0.9265	-0.421
S	-0.7199	-2.6352	5.5240	-0.416
S	-1.7971	-5.9365	0.2122	-0.424
S	2.4599	0.0744	5.6858	-0.429
S	-1.9566	5.3645	-2.3546	-0.396
S	4.9368	-2.5892	2.7247	-0.437
S	3.7371	3.6534	3.4017	-0.424
S	1.7930	-5.3892	2.5932	-0.422
Ag	-1.6530	2.4682	-5.9356	0.546
Ag	4.6141	-2.5528	-4.1118	0.542
Ag	-3.3393	4.0991	-4.0622	0.547
Ag	4.2495	5.1117	-0.8058	0.555
Ag	-2.4489	4.5424	4.2304	0.555
Ag	2.4438	-4.6022	-4.2346	0.548
Ag	-4.1553	-5.2041	0.8273	0.560
Ag	-5.3972	-3.7272	-1.4814	0.547
Ag	5.4555	3.6513	1.5119	0.550
Ag	-4.6865	2.5580	4.0706	0.553
Ag	3.3828	-4.1260	4.1289	0.550
Ag	1.7848	-2.4354	6.0291	0.547
H	1.3831	-0.4513	-6.7666	0.248
H	-1.6849	-5.8261	-3.5130	0.249
H	6.1510	1.2205	-2.9792	0.248
H	-4.4977	5.4955	0.3129	0.244
H	-6.2451	-1.5307	2.8274	0.245
H	-1.5482	0.5754	6.8502	0.245
H	-5.8491	-0.1396	-3.8657	0.248
H	0.9796	6.5340	2.4856	0.251
H	5.8886	-0.0815	4.0115	0.247
H	5.9033	-4.1697	0.5760	0.248
H	3.4109	-6.3800	0.6626	0.248
H	-6.4104	3.5387	-0.8299	0.247
H	-4.2951	-2.1640	-5.5237	0.244
H	-1.0359	-5.4845	4.6854	0.241
H	1.7553	5.0450	5.0604	0.246
H	0.4979	5.6845	-4.6484	0.241
H	4.3533	2.3144	5.5440	0.244
H	-0.5764	-7.0652	2.1606	0.245
C	1.5249	4.3099	-5.9936	-0.159
C	5.7682	3.2703	-3.6215	-0.155
C	3.5408	-0.1338	-6.6851	-0.163
C	-5.6182	-3.4238	3.7091	-0.154
C	-3.6002	-5.1653	-4.3191	-0.161
C	-3.1470	6.7675	1.4572	-0.159
C	-3.6659	0.0924	6.6564	-0.154
C	-6.3098	1.9865	-3.7336	-0.154
H	-0.3247	7.5090	-1.2483	0.241
C	-3.6451	-0.4642	-6.7280	-0.157
C	6.6517	-3.5825	-1.3858	-0.158

C	1.9040	7.3687	0.6959	-0.166
C	2.2943	-0.2296	-7.3443	-0.195
C	7.6073	0.9999	0.1366	-0.157
C	-7.5824	-1.1166	-0.1206	-0.157
C	-1.4622	-4.0746	6.2929	-0.162
C	0.2486	-3.5251	-6.8459	-0.160
C	3.1799	-6.8700	-1.4511	-0.158
H	0.3866	-7.6491	-0.6625	0.243
H	-1.8211	-2.8425	-6.9392	0.240
H	-7.6144	1.0546	-0.3211	0.239
H	7.6100	-1.1700	0.3550	0.242
C	-2.5071	-6.0546	-4.2089	-0.193
H	1.8507	2.6709	6.9606	0.241
C	-0.2107	3.3842	6.9185	-0.160
C	3.9593	0.4459	6.6039	-0.160
C	-1.7893	-7.4864	-0.6922	-0.160
C	-6.7324	3.5123	1.3303	-0.160
C	6.5233	2.0773	-3.5633	-0.198
C	6.3976	-2.1749	3.6790	-0.155
C	-1.4618	6.9511	-3.0232	-0.165
C	3.8184	5.1705	4.3575	-0.157
C	1.2178	-6.8919	3.3907	-0.159
C	-6.5016	-2.3353	3.5350	-0.196
C	-2.4694	0.2882	7.3811	-0.197
C	-4.2957	6.5160	0.6748	-0.202
C	-6.5606	0.6556	-4.1359	-0.196
C	1.3939	7.4380	2.0126	-0.201
C	1.2113	5.5883	-5.4830	-0.203
C	6.6312	-0.8760	4.1823	-0.196
C	6.6623	-4.3537	-0.2018	-0.207
C	-4.4794	-1.5674	-6.4335	-0.217
C	3.6803	-7.0796	-0.1458	-0.205
C	-1.5013	-5.3431	5.6739	-0.194
C	-7.0154	3.9277	0.0076	-0.223
C	4.6716	1.6430	6.3596	-0.217
C	2.7053	5.6040	5.1149	-0.210
C	0.0334	-7.5283	2.9549	-0.214
C	8.1756	-0.2894	0.0125	-0.201
C	-8.1740	0.1623	0.0003	-0.200
C	-0.9374	-3.1512	-7.5187	-0.201
C	-0.6804	7.8317	-2.2388	-0.198
C	-0.5588	-8.1331	-0.9530	-0.206
C	0.9933	3.0125	7.5612	-0.205
S	-3.6782	3.8459	-6.5620	-0.369
H	2.7223	3.2135	-7.4467	0.244
S	4.8674	-4.9188	-4.9616	-0.369
C	2.4595	4.2073	-7.0508	-0.204
H	7.9254	3.1313	-0.2228	0.243
S	6.5965	5.4257	0.0738	-0.386
H	-7.8793	-3.2557	0.2119	0.242

S	-6.5101	-5.5228	-0.0839	-0.382
S	-4.4536	4.4040	5.7889	-0.388
H	2.3062	-4.1970	-7.1034	0.235
S	3.6975	-3.9768	6.6446	-0.380
H	-2.2592	4.0778	7.2336	0.244
H	-3.9543	-7.6226	-0.9035	0.236
C	8.3493	2.1172	-0.3074	-0.209
H	-5.2375	6.0837	3.4007	0.245
C	-8.3190	-2.2482	0.2959	-0.211
C	1.3708	-3.9113	-7.6123	-0.208
C	-1.3061	3.7959	7.7115	-0.210
C	-2.9879	-8.1185	-1.0904	-0.207
H	-2.5028	6.7101	-4.9251	0.237
C	6.2655	4.3563	-4.3790	-0.207
C	-5.9598	-4.4400	4.6316	-0.206
C	-1.8999	7.3867	-4.2952	-0.216
C	4.6951	0.1633	-7.4479	-0.219
C	-3.9063	0.2912	-7.8948	-0.206
C	-2.9007	8.0876	1.9015	-0.207
C	-4.8347	-0.2849	7.3586	-0.206
C	-2.0673	-3.9145	7.5619	-0.207
H	-3.2759	1.1641	-8.1289	0.240
C	7.6451	-3.8223	-2.3637	-0.208
C	-7.2400	2.9916	-4.0876	-0.216
C	-4.6408	-5.4763	-5.2261	-0.226
C	4.4064	-0.4127	7.6342	-0.207
H	4.7082	7.3301	1.4435	0.244
H	-2.0590	-2.9239	8.0446	0.243
H	3.8789	-1.3626	7.8208	0.240
H	7.6440	-3.2313	-3.2931	0.238
C	3.5242	-7.7907	-2.4681	-0.210
H	-5.2690	-5.2838	4.7862	0.240
C	2.4220	8.5454	0.1047	-0.222
C	-7.5155	4.0340	2.3864	-0.212
H	-1.0260	5.1193	-7.1750	0.241
H	4.7575	-2.7565	-7.0479	0.240
H	5.6797	5.2873	-4.4370	0.239
H	-2.0011	8.2973	2.5015	0.238
H	-5.7685	-0.4544	6.7995	0.240
H	3.1487	-7.6322	-3.4918	0.238
H	-7.0485	4.0349	-3.7880	0.232
C	1.9747	-7.4956	4.4211	-0.210
C	7.3680	-3.1784	3.9049	-0.212
H	5.6677	0.2602	-6.9395	0.242
C	5.0251	5.9019	4.4427	-0.215
H	-7.3003	3.7252	3.4231	0.238
H	2.8904	-7.0017	4.7860	0.236
C	2.2014	-0.0458	-8.7333	-0.285
H	5.8981	5.5809	3.8503	0.238
H	2.8242	8.5027	-0.9202	0.242

H	-5.4965	-4.7892	-5.3259	0.233
C	-2.4566	-7.2286	-4.9765	-0.278
H	7.1965	-4.1945	3.5147	0.232
C	7.7490	1.9705	-4.2404	-0.289
H	-5.7988	-6.3916	-2.8631	0.240
H	0.9999	-4.9113	7.5565	0.240
C	-2.4396	0.1226	8.7758	-0.292
C	-5.1906	7.5516	0.3600	-0.287
C	-7.7065	-2.2670	4.2538	-0.289
C	-7.7116	0.3348	-4.8720	-0.282
C	1.7975	6.7435	-6.0260	-0.290
C	1.4074	8.6482	2.7245	-0.288
C	7.8020	-0.5860	4.9003	-0.281
H	1.2332	-0.1271	-9.2509	0.244
C	-2.1188	-6.4332	6.3081	-0.289
C	7.6401	-5.3413	0.0002	-0.290
H	-1.6093	-7.9253	-4.8877	0.243
C	4.4961	-8.1860	0.1399	-0.289
C	-5.5415	-1.9113	-7.2855	-0.294
C	-8.0570	4.8345	-0.2516	-0.296
C	5.7954	1.9804	7.1315	-0.295
H	8.3454	1.0467	-4.1885	0.240
C	2.7968	6.7348	5.9418	-0.291
C	-0.3799	-8.7433	3.5252	-0.295
H	-1.5108	0.2831	9.3447	0.242
C	9.4548	-0.4623	-0.5390	-0.292
H	-6.0924	7.3565	-0.2408	0.240
H	-8.4014	-1.4249	4.1137	0.241
C	-9.4685	0.3122	0.5214	-0.291
C	-1.0047	-3.1699	-8.9211	-0.293
C	-0.5265	-9.3853	-1.5879	-0.292
C	-0.3525	9.1137	-2.7074	-0.293
C	1.1094	3.0640	8.9598	-0.292
H	-7.9100	-0.6997	-5.1919	0.237
C	-5.7517	6.4511	4.3031	-0.208
H	1.0263	8.7035	3.7558	0.240
H	7.9839	0.4225	5.3020	0.239
C	-3.1798	5.3174	-7.4479	-0.171
H	1.5498	7.7414	-5.6323	0.242
C	3.0552	5.3557	-7.5951	-0.295
C	5.0879	-4.8901	-6.7362	-0.170
C	3.1032	-5.4686	7.4326	-0.167
C	-5.5414	5.8054	5.5433	-0.163
C	-1.8339	5.7125	-7.6339	-0.213
C	5.7326	7.7326	1.4822	-0.209
C	5.0199	-3.7159	-7.5241	-0.218
H	-2.1417	-7.4251	5.8304	0.241
H	4.8800	-8.3588	1.1576	0.235
C	-6.7100	-7.0479	-0.9934	-0.169
H	7.6514	-5.9502	0.9177	0.233

H	-8.2860	5.1558	-1.2800	0.235
C	6.7957	6.9919	0.9160	-0.164
H	-6.1929	-2.7714	-7.0644	0.230
C	1.7560	-5.6711	7.8134	-0.204
H	6.3512	2.9129	6.9447	0.236
C	-6.3161	-7.2141	-2.3420	-0.214
H	1.9344	7.0705	6.5393	0.237
C	9.6305	1.9519	-0.8573	-0.293
H	-1.2988	-9.2446	3.1821	0.238
C	-9.6158	-2.1064	0.8157	-0.294
C	1.3127	-3.9337	-9.0143	-0.290
C	-2.9645	-9.3697	-1.7263	-0.290
C	4.6108	0.3471	-8.8380	-0.305
C	-1.1964	3.8502	9.1101	-0.293
C	7.4904	4.2579	-5.0577	-0.299
C	-7.1614	-4.3790	5.3547	-0.298
C	-4.8136	-0.4530	8.7519	-0.299
C	-3.7886	9.1288	1.5903	-0.293
C	-4.5982	-6.6486	-5.9986	-0.304
C	2.7124	6.6122	-7.0780	0.393
C	3.3615	0.2392	-9.4640	0.395
H	9.8967	-1.4655	-0.6410	0.237
C	-2.6868	-4.9987	8.2030	-0.298
H	-9.9282	1.3080	0.6189	0.237
C	-1.5770	8.6677	-4.7718	-0.294
H	0.2525	9.8005	-2.0952	0.236
C	-4.9678	-0.0459	-8.7491	-0.292
H	0.4306	-9.8905	-1.7912	0.237
H	-1.9277	-2.8794	-9.4465	0.237
C	-8.3945	2.6786	-4.8225	-0.296
C	-3.5031	-7.5118	-5.8626	0.399
C	5.5296	-0.0824	8.4078	-0.291
C	8.2177	3.0630	-4.9798	0.394
C	8.6255	-4.8074	-2.1684	-0.295
H	2.0470	2.7759	9.4600	0.238
C	-3.6135	-0.2451	9.4444	0.392
C	2.4388	9.7597	0.8099	-0.301
C	-8.0218	-3.2915	5.1545	0.394
C	4.3403	-8.8988	-2.1893	-0.296
C	-8.5563	4.9415	2.1351	-0.291
C	-4.9274	8.8455	0.8253	0.394
C	8.5422	-2.8963	4.6203	-0.297
C	1.5681	-8.7102	4.9959	-0.289
C	5.1239	7.0340	5.2682	-0.293
C	-8.6155	1.3499	-5.2058	0.399
C	10.1681	0.6638	-0.9670	0.391
C	1.9310	9.7951	2.1150	0.394
C	-2.7042	-6.2468	7.5664	0.391
C	-10.1755	-0.8274	0.9232	0.391
C	-5.7735	-1.1472	-8.4351	0.396

C	0.1222	-3.5645	-9.6530	0.393
C	8.6103	-5.5570	-0.9859	0.396
C	6.2095	1.1143	8.1502	0.393
C	8.7436	-1.5998	5.1104	0.398
C	-1.7317	-9.9910	-1.9643	0.393
C	4.8149	-9.0846	-0.8848	0.396
C	-8.8172	5.3305	0.8155	0.393
C	0.0119	3.4876	9.7187	0.391
C	-0.8077	9.5189	-3.9687	0.390
C	0.3954	-9.3230	4.5368	0.394
C	4.0069	7.4362	6.0110	0.395
H	3.7856	5.2847	-8.4166	0.231
H	10.2105	2.8186	-1.2112	0.231
H	-10.1918	-2.9854	1.1453	0.232
H	2.1893	-4.2295	-9.6116	0.237
H	-3.8984	-9.8595	-2.0428	0.237
H	-2.0481	4.1676	9.7323	0.231
C	-6.6010	7.5651	4.2020	-0.286
C	4.0479	-6.4746	7.7565	-0.223
H	-6.7593	8.0668	3.2347	0.240
H	-1.9172	9.0046	-5.7633	0.237
H	5.5036	0.5809	-9.4398	0.230
H	-5.7191	-0.7472	9.3063	0.228
H	-7.4364	-5.1654	6.0755	0.228
H	7.8874	5.0998	-5.6471	0.227
H	-3.1630	-4.8828	9.1895	0.231
H	-3.6089	10.1581	1.9388	0.230
C	-4.1953	6.1036	-8.0483	-0.219
C	-7.3568	-8.1322	-0.3485	-0.216
H	-5.1783	0.5452	-9.6545	0.230
H	5.8864	-0.7533	9.2054	0.231
C	1.3626	-6.8310	8.5006	-0.286
C	-1.5084	6.8510	-8.3889	-0.290
C	5.4236	-6.1064	-7.3833	-0.217
H	-5.4016	-6.8966	-6.7104	0.230
C	5.2831	-3.7488	-8.9038	-0.293
C	5.9602	8.9780	2.0894	-0.288
H	5.1018	-6.3323	7.4666	0.233
H	9.3971	-5.0047	-2.9294	0.229
H	-9.1226	3.4555	-5.1050	0.227
H	-9.1616	5.3543	2.9570	0.236
H	4.6139	-9.6188	-2.9768	0.228
H	2.8512	10.6769	0.3601	0.233
C	-6.5622	-8.4145	-3.0283	-0.292
C	-6.2125	6.3112	6.6843	-0.221
H	2.1495	-9.1778	5.8054	0.235
C	8.1023	7.5367	0.9849	-0.220
H	6.0605	7.6095	5.3337	0.234
H	-7.6677	-8.0207	0.7031	0.234
H	9.3028	-3.6722	4.8026	0.226

H	-5.2488	5.8080	-7.9145	0.233
H	5.1289	9.5528	2.5261	0.240
H	5.4822	-7.0307	-6.7856	0.232
H	-0.4595	7.1583	-8.5231	0.241
H	5.2270	-2.8307	-9.5097	0.240
H	0.3110	-6.9892	8.7863	0.240
F	3.2790	0.4155	-10.8067	-0.338
F	3.2815	7.7247	-7.6091	-0.340
H	-6.2470	-8.5389	-4.0765	0.239
H	8.9411	6.9707	0.5474	0.231
F	-3.4631	-8.6460	-6.6049	-0.337
F	9.4041	2.9661	-5.6349	-0.342
F	-3.5918	-0.4052	10.7933	-0.341
H	-6.0558	5.8189	7.6581	0.230
F	-9.1861	-3.2330	5.8521	-0.341
F	-5.7978	9.8469	0.5386	-0.339
F	-9.7286	1.0429	-5.9191	-0.340
F	11.4077	0.5038	-1.5008	-0.343
F	1.9581	10.9632	2.8049	-0.338
F	-3.3023	-7.2964	8.1866	-0.340
F	-11.4297	-0.6899	1.4277	-0.342
F	0.0592	-3.5906	-11.0096	-0.341
F	-6.7986	-1.4809	-9.2613	-0.341
F	7.2947	1.4377	8.8999	-0.341
F	9.8767	-1.3242	5.8055	-0.341
F	-1.7044	-11.2048	-2.5729	-0.340
F	9.5575	-6.5106	-0.7935	-0.341
F	-9.8239	6.2069	0.5672	-0.340
F	5.5961	-10.1606	-0.6087	-0.341
F	0.1196	3.5473	11.0719	-0.342
F	-0.4970	10.7616	-4.4209	-0.341
F	-0.0002	-10.5000	5.0863	-0.340
F	4.0991	8.5274	6.8135	-0.340
C	3.6649	-7.6385	8.4427	-0.305
C	2.3231	-7.8009	8.8120	0.387
C	-7.2454	8.0420	5.3502	0.387
C	-2.5365	7.6007	-8.9733	0.385
C	-7.6102	-9.3348	-1.0262	-0.300
C	-3.8806	7.2397	-8.8105	-0.302
C	5.6233	-4.9659	-9.5068	0.386
C	5.6938	-6.1494	-8.7601	-0.301
C	-7.2113	-9.4617	-2.3633	0.386
C	7.2622	9.4902	2.1348	0.386
C	-7.0609	7.4263	6.5944	-0.303
C	8.3404	8.7813	1.5896	-0.303
H	4.3973	-8.4219	8.6968	0.225
H	-8.1136	-10.1788	-0.5273	0.226
H	-4.6684	7.8511	-9.2798	0.225
H	5.9598	-7.0937	-9.2624	0.225
F	1.9521	-8.9230	9.4831	-0.342

F	-8.0643	9.1239	5.2615	-0.343
H	-7.5803	7.8252	7.4810	0.223
H	9.3548	9.2095	1.6408	0.224
F	-2.2283	8.6986	-9.7128	-0.343
F	5.8937	-5.0028	-10.8385	-0.343
F	-7.4595	-10.6239	-3.0233	-0.342
F	7.4867	10.6992	2.7154	-0.344

Table S3. $Ag_{32}Au_{12}(FTP)_{30}^{4-}$ M isomer: all Au atoms in the outer shell

Ag	-0.0958	-2.8535	-0.2800	-0.149
Ag	0.3778	-1.5968	2.3620	-0.192
Ag	2.3699	-1.3614	0.2924	-0.159
Ag	0.1097	2.7141	0.1736	-0.145
Ag	-0.3692	1.3595	-2.3162	-0.144
Ag	-2.3707	1.2477	-0.2286	-0.150
Ag	-1.7664	-1.1087	-1.8540	-0.141
Ag	-2.1868	-1.3208	1.0311	-0.181
Ag	-3.7950	0.7986	2.2823	0.513
Ag	-0.9368	1.0044	2.3048	-0.159
Ag	-4.4954	-0.7168	-0.7146	0.450
Ag	4.5209	0.5487	0.7726	0.428
Ag	2.3832	-3.5645	-1.4781	0.226
Ag	2.2841	1.2023	-1.0329	-0.111
Ag	-2.2148	3.5372	1.6810	0.446
Ag	-0.6105	-0.5966	-4.4991	0.474
Ag	0.6972	3.3687	2.9725	0.509
Ag	1.9910	1.0085	-3.8340	0.214
Ag	1.8570	0.9893	1.8197	-0.189
Ag	-3.1736	1.2184	-3.0305	0.518
Ag	-2.1202	-1.1004	3.8851	0.404
Ag	1.3675	3.6174	-2.3736	0.464
Ag	-2.8860	-3.5062	-0.6714	0.350
Ag	1.1101	-1.1646	-2.2615	-0.154
Ag	-1.9588	3.6699	-1.6764	0.350
Ag	4.0171	-0.9248	-2.0410	0.485
Ag	2.8034	3.4835	0.6092	0.374
Au	-2.0240	-0.1939	6.8159	0.237
Au	0.1814	-2.5208	5.5296	0.297
Ag	3.2677	-1.2848	2.9864	0.518
Ag	-1.4545	-3.9589	1.9476	0.488
Ag	-0.3927	-3.4645	-3.0973	0.470
Ag	0.9592	0.2870	4.4719	0.466
Ag	1.8791	-3.9776	1.5689	0.482
Au	5.6664	4.0706	-0.3082	0.274
Au	1.7830	-6.5093	-1.1278	0.279
Au	-5.4453	-3.2928	-2.4377	0.316
Au	-1.8523	6.2640	0.2886	0.370
Au	5.2250	2.8823	2.6062	0.369
Au	2.4762	-0.3883	-6.2933	0.287
Au	0.9773	2.3795	-6.3357	0.271
Au	-4.4778	5.2977	-0.8917	0.274
Au	-5.8115	-4.0080	0.4528	0.285
Au	4.5973	-5.2387	-0.6666	0.274
S	0.0558	2.4756	5.3285	-0.412
S	-4.6569	3.6179	-2.5729	-0.252

S	5.9072	0.7540	-1.3369	-0.417
S	-4.0354	-4.9380	1.7252	-0.257
S	3.7993	4.7986	-1.6171	-0.300
S	-4.7046	3.2044	1.9154	-0.406
S	5.3881	-3.3355	-1.8330	-0.250
S	-5.5162	-1.0414	1.5873	-0.407
S	-3.3427	-4.1674	-3.2381	-0.312
S	-0.6770	5.6022	2.4584	-0.388
S	5.2474	0.5046	3.3598	-0.356
S	-1.9280	1.4043	-5.3510	-0.433
S	0.2129	-5.9121	1.5139	-0.432
S	-0.4366	5.8012	-1.7307	-0.370
S	4.2095	-0.9370	-4.7708	-0.257
S	-4.2882	7.1386	0.6433	-0.220
S	-5.2033	-0.4430	-3.1439	-0.422
S	0.1081	-6.0608	-2.7459	-0.231
S	2.3892	-1.6153	5.6239	-0.325
S	3.6216	-7.1780	0.3649	-0.148
S	-7.5282	-3.2568	-1.1063	-0.183
S	-3.5701	0.6981	5.2086	-0.275
S	7.4960	3.4616	1.0925	-0.206
S	-1.7582	-3.6200	4.6877	-0.316
S	1.0712	4.2947	-4.9469	-0.225
S	4.3047	-3.5479	2.1580	-0.423
S	3.3453	4.4165	3.0223	-0.351
S	0.3914	-2.7157	-5.5085	-0.421
S	-0.5324	-1.0139	8.4602	-0.220
S	0.9246	0.5174	-7.9122	-0.153
F	3.3633	4.1918	9.9832	-0.344
F	1.6615	-8.5829	-7.9166	-0.342
F	-2.7710	-4.3535	-10.2910	-0.343
F	5.9039	-12.1671	-1.9668	-0.339
C	-1.2967	6.4477	3.9154	-0.162
F	-5.5291	-5.8008	8.7405	-0.340
C	0.6261	2.7797	8.0119	-0.203
H	-0.3314	2.2569	8.1643	0.247
F	-6.0398	6.6107	-7.5454	-0.340
C	1.7516	-7.6769	-4.3739	-0.219
H	2.3409	-7.8978	-3.4680	0.236
F	4.7146	10.1822	3.5772	-0.341
C	0.6588	-6.7840	-4.2878	-0.163
F	-6.7811	5.4661	7.0243	-0.343
C	-6.7638	0.4136	-3.3412	-0.153
C	-0.5961	-3.1977	-6.9191	-0.156
C	-5.0237	4.5667	-4.0552	-0.164
C	-2.9495	0.9362	-6.7474	-0.157
C	4.9970	-4.5286	-4.3706	-0.189
H	3.9193	-4.5580	-4.1434	0.243
C	5.9009	-3.9957	-3.4250	-0.166
C	7.7201	-1.1002	-0.2156	-0.200

H	6.9058	-1.4336	0.4463	0.245
F	7.2801	-5.4407	-7.0748	-0.339
C	-3.6965	-5.9226	-3.4323	-0.165
C	-5.2689	3.8621	3.4795	-0.160
C	7.4814	-0.0741	-1.1601	-0.157
F	1.0114	-10.0000	5.7782	-0.342
C	2.0905	-8.2845	-5.5935	-0.298
H	2.9397	-8.9829	-5.6636	0.230
F	4.0639	2.1949	-12.6991	-0.339
F	-8.8941	-1.3602	6.9261	-0.342
C	-4.4003	4.2427	4.5286	-0.200
H	-3.3128	4.1123	4.4123	0.244
C	1.3837	3.1853	9.1209	-0.293
H	1.0353	2.9942	10.1481	0.233
C	3.7812	6.1536	3.0806	-0.157
C	-7.1297	-0.2766	1.7192	-0.155
C	6.8631	-0.2462	3.5672	-0.157
C	-0.6956	-3.7001	-9.3205	-0.298
H	-0.2121	-3.7833	-10.3073	0.227
C	-0.9494	6.9548	-3.0047	-0.165
C	-5.1549	0.0079	5.7151	-0.160
F	11.2525	-1.8379	-0.8308	-0.345
C	4.0625	-9.8820	0.2087	-0.210
H	3.4354	-9.9087	1.1146	0.241
C	8.9862	-1.6972	-0.1029	-0.293
H	9.1752	-2.4875	0.6397	0.237
C	6.8271	-4.9629	-5.8886	0.397
C	1.0911	3.0061	6.6930	-0.168
F	-10.9172	1.4045	2.1923	-0.344
C	4.8606	-4.6692	3.4360	-0.157
C	0.4718	-7.1010	2.8246	-0.160
C	2.6141	3.8202	8.9098	0.384
F	-4.4195	-9.9746	-4.0512	-0.338
C	-5.8948	5.6814	-4.0135	-0.210
H	-6.3050	6.0122	-3.0456	0.242
C	8.5478	0.3292	-2.0008	-0.209
H	8.3739	1.1239	-2.7431	0.237
C	8.3584	4.9491	1.5674	-0.177
C	4.4089	8.8698	3.4053	0.394
C	2.9847	-1.2521	7.2801	-0.149
C	4.3266	-8.6408	-0.4137	-0.169
C	-1.9777	-3.4891	-6.8245	-0.218
H	-2.4851	-3.4079	-5.8487	0.246
C	-0.0771	-6.5008	-5.4627	-0.202
H	-0.9236	-5.7976	-5.4232	0.244
C	-7.5056	0.8694	0.9813	-0.208
H	-6.7886	1.3333	0.2861	0.250
C	-6.6633	4.0279	3.6644	-0.209
H	-7.3525	3.7233	2.8609	0.238
C	-4.9149	-5.4802	6.4648	-0.298

H	-5.8054	-6.0446	6.1460	0.234
C	-6.2352	6.3731	-5.1856	-0.294
H	-6.9044	7.2476	-5.1570	0.232
C	7.2759	-3.9397	-3.7444	-0.211
H	7.9820	-3.5123	-3.0151	0.247
C	7.7444	-4.4236	-4.9777	-0.306
H	8.8148	-4.3914	-5.2367	0.230
F	-5.2854	-0.0140	-10.0713	-0.342
C	-6.2868	4.9420	5.8714	0.386
C	1.3358	-7.9923	-6.7366	0.391
C	-4.9037	4.7842	5.7224	-0.289
H	-4.2256	5.0824	6.5366	0.241
C	2.7576	7.1051	3.2995	-0.207
H	1.7055	6.7787	3.3308	0.243
C	0.2560	-7.1027	-6.6856	-0.286
H	-0.3124	-6.8729	-7.5999	0.239
C	0.0315	-3.3117	-8.1837	-0.211
H	1.1073	-3.0909	-8.2712	0.238
F	-3.4642	-2.3797	13.4737	-0.348
C	5.4568	-5.0196	-5.6023	-0.286
H	4.7570	-5.4366	-6.3426	0.243
C	-2.8207	1.6643	-7.9553	-0.223
H	-2.0883	2.4858	-8.0118	0.238
C	-5.4100	-1.3762	5.8167	-0.196
H	-4.6161	-2.1017	5.5795	0.241
C	-8.7809	1.4372	1.1376	-0.300
H	-9.0771	2.3292	0.5632	0.238
C	-8.0625	-0.8377	2.6240	-0.206
H	-7.7747	-1.7221	3.2141	0.240
C	1.2596	1.3327	-10.5195	-0.212
H	0.1628	1.2332	-10.5639	0.240
C	-1.4787	-1.3937	9.9151	-0.181
C	-4.0210	-4.9483	5.5223	-0.215
H	-4.2133	-5.0803	4.4440	0.248
C	5.5712	0.1374	-5.2460	-0.163
C	-2.6475	-4.0439	7.3283	-0.214
H	-1.7717	-3.4650	7.6670	0.249
C	-4.5035	4.1585	-5.3044	-0.218
H	-3.8043	3.3066	-5.3548	0.247
C	-7.1756	4.5685	4.8545	-0.306
H	-8.2597	4.7009	5.0018	0.227
C	3.1217	-2.2964	8.2205	-0.200
H	2.7823	-3.3111	7.9599	0.237
C	3.4177	0.0468	7.6188	-0.188
H	3.3017	0.8711	6.8972	0.249
C	0.4852	-6.7442	4.1941	-0.205
H	0.3343	-5.6913	4.4823	0.246
C	5.4386	7.9502	3.1732	-0.289
H	6.4826	8.2967	3.1201	0.234
F	-2.2016	9.7557	-5.8195	-0.340

C	3.3677	1.8323	-11.5923	0.396
C	4.5902	-11.0736	-0.3128	-0.294
H	4.3884	-12.0462	0.1635	0.230
C	-6.0300	10.5879	-0.6527	-0.300
H	-6.8424	11.2544	-0.3204	0.225
C	-5.3261	10.8869	-1.8250	0.392
C	-4.2898	10.0640	-2.2837	-0.285
H	-3.7546	10.3201	-3.2114	0.238
C	-3.9504	8.9168	-1.5503	-0.199
H	-3.1352	8.2660	-1.9049	0.246
C	-4.6488	8.5817	-0.3691	-0.167
C	-5.6881	9.4337	0.0711	-0.218
H	-6.2409	9.1790	0.9903	0.234
C	-2.0617	-3.9799	-9.1934	0.390
C	5.1213	6.5921	3.0099	-0.210
H	5.9241	5.8587	2.8317	0.240
C	9.8160	-0.2636	-1.8964	-0.304
H	10.6506	0.0534	-2.5424	0.225
C	-2.8780	-4.2315	5.9482	-0.163
C	-6.6686	-1.8415	6.2297	-0.292
H	-6.8709	-2.9203	6.3189	0.238
C	-3.3648	-6.8685	-2.4379	-0.191
H	-2.9164	-6.5327	-1.4899	0.248
C	-6.1902	0.9219	6.0120	-0.200
H	-6.0041	2.0037	5.9218	0.243
C	-1.4413	-2.2907	12.2092	-0.303
H	-0.8954	-2.7298	13.0604	0.223
C	5.3896	-11.0177	-1.4610	0.396
C	1.9316	1.0633	-9.3061	-0.169
C	-7.6744	-0.9135	6.5272	0.396
C	-7.4535	0.4641	6.4188	-0.291
H	-8.2673	1.1697	6.6479	0.232
C	0.6651	-7.7166	5.1905	-0.290
H	0.6657	-7.4433	6.2575	0.235
C	-1.7717	8.8322	-4.9206	0.393
C	-5.7102	5.9410	-6.4109	0.390
C	2.3339	3.6564	6.5119	-0.220
H	2.7141	3.8404	5.4929	0.246
C	3.3380	1.1876	-9.2617	-0.209
H	3.8711	0.9747	-8.3197	0.249
F	4.6791	-0.5170	11.0023	-0.340
C	-3.5430	-4.5736	8.2725	-0.286
H	-3.3804	-4.4220	9.3509	0.241
C	1.9738	1.7194	-11.6654	-0.296
H	1.4598	1.9295	-12.6170	0.230
C	-2.7103	-3.8807	-7.9564	-0.294
H	-3.7874	-4.1015	-7.8890	0.230
C	-3.6052	-8.2365	-2.6431	-0.281
H	-3.3491	-8.9775	-1.8708	0.243
C	4.1210	-0.7524	9.7879	0.402

C	5.1392	-8.6135	-1.5682	-0.210
H	5.3531	-7.6480	-2.0564	0.247
C	3.0985	4.0632	7.6190	-0.298
H	4.0696	4.5652	7.4830	0.235
C	-4.6634	-5.2869	7.8297	0.394
C	-4.1806	-8.6547	-3.8487	0.400
C	10.0208	-1.2701	-0.9436	0.385
C	-2.8191	-2.0576	12.3172	0.375
C	3.0697	8.4635	3.4654	-0.294
H	2.2786	9.2091	3.6436	0.235
C	4.0592	1.5735	-10.4020	-0.289
H	5.1559	1.6705	-10.3749	0.237
C	0.6423	-8.4646	2.4806	-0.219
H	0.6227	-8.7549	1.4182	0.239
C	-3.6067	1.3491	-9.0764	-0.302
H	-3.5094	1.9080	-10.0212	0.226
C	5.6716	-9.8009	-2.0954	-0.291
H	6.3060	-9.7897	-2.9958	0.235
C	-0.7808	-1.9580	11.0174	-0.222
H	0.3034	-2.1368	10.9264	0.232
C	4.0924	-4.9933	4.5781	-0.203
H	3.1006	-4.5340	4.7123	0.244
C	-3.8928	-0.1162	-6.6897	-0.205
H	-4.0229	-0.6793	-5.7519	0.250
C	-4.8483	4.8408	-6.4841	-0.292
H	-4.4450	4.5207	-7.4575	0.240
C	-9.3380	-0.2756	2.7873	-0.298
H	-10.0628	-0.7025	3.4986	0.229
C	-3.5399	-1.4990	11.2552	-0.296
H	-4.6229	-1.3266	11.3634	0.231
C	-2.8724	-1.1716	10.0634	-0.225
H	-3.4384	-0.7388	9.2219	0.243
C	-2.2729	7.5269	-4.9839	-0.281
H	-2.9953	7.2506	-5.7674	0.242
C	-0.4386	8.2742	-2.9834	-0.216
H	0.2769	8.5646	-2.1974	0.241
C	0.8281	-9.4427	3.4716	-0.306
H	0.9624	-10.5052	3.2116	0.227
C	-9.6820	0.8568	2.0386	0.391
C	7.9128	0.3093	-5.9381	-0.297
H	8.8773	-0.1550	-6.1982	0.230
C	3.6890	-2.0493	9.4796	-0.298
H	3.8055	-2.8524	10.2249	0.228
C	3.9912	0.3004	8.8753	-0.283
H	4.3225	1.3124	9.1543	0.239
C	-1.8534	6.5895	-4.0270	-0.191
H	-2.2511	5.5634	-4.0628	0.243
C	-4.2708	-6.3745	-4.6429	-0.215
H	-4.5261	-5.6437	-5.4264	0.236
C	-4.6837	-0.4345	-7.8049	-0.288

H	-5.4216	-1.2509	-7.7619	0.235
C	-0.8501	9.2178	-3.9382	-0.300
H	-0.4715	10.2523	-3.9215	0.231
C	0.8381	-9.0554	4.8177	0.392
C	-4.5277	0.2980	-8.9879	0.394
C	3.5721	7.4770	-5.3873	-0.290
H	3.7556	8.4318	-4.8706	0.236
C	4.2998	7.1559	-6.5396	0.390
C	4.0982	5.9443	-7.2113	-0.296
H	4.6885	5.7151	-8.1127	0.231
C	3.1410	5.0408	-6.7223	-0.220
H	2.9695	4.0861	-7.2473	0.237
C	2.3827	5.3416	-5.5672	-0.165
C	2.6199	6.5685	-4.9025	-0.203
H	2.0408	6.8208	-3.9997	0.244
F	-2.4404	8.6146	7.2860	-0.341
F	-10.4257	2.2875	-4.0308	-0.343
C	-0.6741	6.2159	5.1651	-0.210
H	0.1172	5.4542	5.2512	0.244
C	-2.3344	7.4037	3.8371	-0.208
H	-2.8480	7.5732	2.8768	0.242
F	6.3201	-7.3341	6.2966	-0.343
C	-1.0586	6.9418	6.3042	-0.292
H	-0.5741	6.7653	7.2770	0.239
C	-2.0746	7.8985	6.1914	0.392
C	2.7996	7.1805	-0.4971	-0.195
H	2.0309	6.5632	-0.0085	0.252
C	8.0503	0.3515	3.0920	-0.210
H	7.9976	1.2890	2.5148	0.245
F	-4.3474	-10.8856	1.5413	-0.341
C	-2.7240	8.1310	4.9723	-0.292
H	-3.5341	8.8754	4.9186	0.230
C	-7.8622	0.1891	-2.4809	-0.206
H	-7.7551	-0.4895	-1.6214	0.243
C	-6.9313	1.2918	-4.4386	-0.206
H	-6.0851	1.4798	-5.1182	0.242
C	-8.1617	1.9236	-4.6763	-0.292
H	-8.2923	2.6137	-5.5245	0.233
C	4.7636	7.3863	-1.9221	-0.215
H	5.5301	6.9176	-2.5594	0.243
C	-9.2319	1.6772	-3.8074	0.394
C	9.2966	-0.2465	3.3378	-0.293
H	10.2273	0.2064	2.9611	0.232
C	-9.0969	0.8166	-2.7119	-0.294
H	-9.9529	0.6449	-2.0405	0.234
C	8.1366	6.2181	0.9797	-0.221
H	7.3446	6.3274	0.2204	0.244
C	6.1372	-5.2642	3.2889	-0.214
H	6.7445	-5.0201	2.4028	0.239
F	5.2181	8.0367	-7.0162	-0.342

C	6.9449	-1.4638	4.2827	-0.206
H	6.0249	-1.9448	4.6527	0.245
C	5.8456	-6.4632	5.3672	0.391
C	4.5805	-5.8890	5.5430	-0.291
H	3.9825	-6.1495	6.4303	0.232
C	6.6331	-6.1596	4.2500	-0.300
H	7.6226	-6.6310	4.1370	0.227
C	5.4793	1.5471	-5.2605	-0.193
H	4.5323	2.0376	-4.9812	0.235
C	3.7862	6.5742	-1.3028	-0.159
C	-4.5200	-7.7399	-4.8544	-0.300
H	-4.9649	-8.1036	-5.7943	0.229
F	10.6598	8.2583	2.6746	-0.343
F	10.5578	-2.0263	4.2925	-0.342
F	8.8563	2.4578	-6.3173	-0.339
C	9.9068	7.1838	2.3191	0.386
C	2.7887	8.5732	-0.3097	-0.289
H	2.0287	9.0516	0.3267	0.244
C	4.7634	8.7775	-1.7341	-0.303
H	5.5233	9.4206	-2.2060	0.230
C	8.9044	7.3333	1.3531	-0.297
H	8.7305	8.3207	0.8964	0.234
C	7.7865	1.7034	-5.9608	0.397
C	6.5823	2.3350	-5.6237	-0.287
H	6.5148	3.4337	-5.6338	0.243
C	9.3732	4.8366	2.5521	-0.213
H	9.5559	3.8597	3.0286	0.235
C	8.1880	-2.0681	4.5279	-0.293
H	8.2564	-3.0185	5.0794	0.237
C	6.8013	-0.4711	-5.5806	-0.204
H	6.8864	-1.5692	-5.5573	0.241
C	9.3511	-1.4479	4.0548	0.391
C	10.1477	5.9444	2.9268	-0.298
H	10.9361	5.8573	3.6917	0.228
C	-8.7218	-6.8950	-2.6684	-0.289
H	-8.3261	-7.7039	-3.3024	0.237
C	-7.9346	-5.7791	-2.3448	-0.207
H	-6.9025	-5.7030	-2.7272	0.248
C	-8.4477	-4.7469	-1.5281	-0.167
C	-9.7710	-4.8534	-1.0433	-0.212
H	-10.1784	-4.0532	-0.4043	0.239
C	-10.5672	-5.9642	-1.3665	-0.297
H	-11.6004	-6.0560	-0.9948	0.229
C	-10.0316	-6.9719	-2.1783	0.395
F	3.7701	10.6971	-0.7451	-0.337
F	-5.6573	11.9987	-2.5322	-0.342
F	-10.7998	-8.0442	-2.4988	-0.340
C	3.7716	9.3538	-0.9285	0.403
C	-4.2758	-9.5289	1.5544	0.390
C	-5.2588	-8.7849	0.8898	-0.297

H	-6.0732	-9.3045	0.3606	0.232
C	-5.1846	-7.3828	0.9044	-0.219
H	-5.9498	-6.7858	0.3808	0.240
C	-4.1376	-6.7210	1.5859	-0.168
C	-3.1553	-7.4996	2.2434	-0.204
H	-2.3245	-7.0048	2.7701	0.246
C	-3.2220	-8.9013	2.2302	-0.288
H	-2.4545	-9.5050	2.7387	0.240

Table S4. $Ag_{32}Au_{12}(FTP)_{30}^{4-}$ S isomer: Au atoms statistically distributed

Au	-0.0736	0.3640	-2.7385	-0.284
Ag	1.2105	2.2678	-0.9226	-0.069
Ag	-1.7047	1.9354	-0.9093	-0.053
Au	2.4095	-0.3432	-1.3204	-0.300
Ag	-2.2384	-0.9497	-1.3415	-0.009
Ag	0.2952	-2.3174	-1.5746	-0.036
Au	-2.3345	0.1878	1.3461	-0.303
Ag	-0.2517	2.2450	1.6038	-0.127
Ag	-1.0918	-2.3918	1.0006	-0.091
Au	2.3157	0.8293	1.3259	-0.343
Ag	1.7667	-2.0510	0.9552	-0.123
Ag	0.1409	-0.3831	2.7210	-0.122
Au	-0.3581	3.2230	-3.0851	0.122
Ag	-2.8377	1.0170	-3.4612	0.483
Ag	2.4928	1.6247	-3.4809	0.576
Au	1.7668	-1.5809	-3.8900	0.149
Ag	-1.4388	-1.8929	-3.9729	0.548
Ag	-0.5035	4.4675	-0.2309	0.504
Au	-2.1023	-3.7670	-1.2555	0.110
Ag	-3.1190	2.9978	1.3530	0.414
Ag	4.1517	1.9107	-0.7025	0.440
Au	-4.3219	0.8516	-0.6115	0.237
Ag	2.1630	3.7717	1.3080	0.410
Ag	-4.0704	-2.1479	0.7556	0.469
Ag	3.0892	-3.1548	-1.3858	0.430
Ag	-1.7708	1.4459	3.9516	0.417
Ag	-2.2832	-1.6581	3.5606	0.526
Ag	4.5196	-1.0293	0.5677	0.564
Ag	2.8824	-1.0738	3.4576	0.436
Ag	0.6292	-4.6157	0.1569	0.523
Ag	0.4050	-3.1702	3.3015	0.373
Ag	1.5548	1.8801	3.9252	0.518
S	0.9108	2.7927	-5.4713	-0.252
S	4.1077	3.4639	-2.7057	-0.408
S	-2.1868	-0.0763	-5.6832	-0.420
S	5.5283	-2.2679	-1.6368	-0.423
S	-4.8632	2.5019	-2.8166	-0.410
S	-3.9137	-3.6459	2.8626	-0.447
S	-2.0474	5.3438	1.7964	-0.434
S	3.7673	-0.2636	-4.9042	-0.369
S	2.2124	-5.5625	-1.8260	-0.442
S	1.8034	6.1032	-0.1249	-0.291
S	-5.8141	-1.2465	-0.8874	-0.361
S	-3.8548	0.1501	4.7637	-0.428
S	-3.7122	-3.7434	-3.4272	-0.262
S	-0.3852	3.3554	5.0765	-0.435

S	-5.6318	2.2569	1.5826	-0.365
S	0.3745	-3.5841	-5.0266	-0.361
S	6.0361	1.1354	0.9632	-0.428
S	-0.8501	-2.6552	5.7195	-0.282
S	-1.7430	-6.0724	0.0294	-0.382
S	2.3086	0.0492	5.6767	-0.421
S	-1.8074	5.4133	-2.4269	-0.357
S	4.9103	-2.5547	2.7425	-0.446
S	3.6702	3.6866	3.4244	-0.424
S	1.6245	-5.4052	2.5924	-0.428
Au	-1.3668	3.1860	-6.0959	0.266
Ag	4.7323	-2.5099	-4.0951	0.552
Ag	-3.2728	4.1065	-4.0216	0.565
Au	4.1620	5.7100	-0.1320	0.272
Ag	-2.5622	4.4485	4.1468	0.551
Ag	2.5846	-4.5872	-4.2122	0.552
Ag	-3.9800	-5.3049	0.8926	0.568
Au	-5.2180	-4.3631	-1.6531	0.272
Ag	5.3866	3.5392	1.5589	0.567
Ag	-4.8053	2.4747	3.9524	0.548
Ag	3.3147	-4.1309	3.9679	0.569
Au	1.4640	-3.1405	6.1341	0.269
H	1.4251	-0.5938	-6.7179	0.249
H	-1.5667	-5.7246	-3.9257	0.253
H	6.1956	1.3342	-3.0253	0.245
H	-4.5858	5.4694	0.2548	0.244
H	-6.2434	-1.7951	2.8635	0.248
H	-1.7551	0.5441	6.8542	0.246
H	-5.8976	-0.0819	-3.8208	0.249
H	0.8870	6.4218	2.6874	0.253
H	5.6978	-0.0913	4.1955	0.247
H	5.9428	-4.1550	0.6065	0.247
H	3.0244	-6.7230	0.7420	0.244
H	-6.5046	3.5027	-0.9168	0.246
H	-4.2602	-2.2164	-5.4850	0.239
H	-1.0903	-5.4881	4.7721	0.243
H	1.8730	4.8094	5.4139	0.243
H	1.1651	5.5491	-4.3519	0.245
H	4.2537	2.3005	5.5170	0.243
H	-0.4797	-7.3241	1.9459	0.247
C	1.7939	4.2699	-5.9996	-0.162
C	5.6096	3.3345	-3.6691	-0.158
C	3.5451	-0.0822	-6.6731	-0.165
C	-5.4565	-3.6121	3.7768	-0.151
C	-3.6420	-5.2576	-4.4005	-0.162
C	-3.1351	6.6928	1.3290	-0.161
C	-3.8490	0.0147	6.5511	-0.155
C	-6.2654	2.0667	-3.8449	-0.156
H	-0.5203	7.7112	-1.2244	0.242
C	-3.6080	-0.5143	-6.6846	-0.163

C	6.7088	-3.5889	-1.3553	-0.156
C	1.6854	7.5210	0.9820	-0.163
C	2.3002	-0.2814	-7.3104	-0.193
C	7.6277	0.9730	0.1527	-0.155
C	-7.4274	-0.9809	-0.1541	-0.159
C	-1.6954	-4.1135	6.3534	-0.162
C	0.3478	-3.5515	-6.8187	-0.164
C	3.3875	-6.8537	-1.4068	-0.155
H	0.3016	-7.5227	-1.4328	0.245
H	-1.6939	-2.7866	-6.9179	0.242
H	-7.5325	1.1214	-0.7157	0.240
H	7.7558	-1.1529	0.6237	0.243
C	-2.4593	-6.0208	-4.4978	-0.194
H	1.6575	2.5074	6.9717	0.243
C	-0.3694	3.3102	6.8749	-0.160
C	3.7547	0.4955	6.6394	-0.165
C	-1.8450	-7.5042	-1.0398	-0.162
C	-6.7705	3.5986	1.2486	-0.163
C	6.4539	2.2002	-3.6553	-0.203
C	6.3339	-2.1272	3.7474	-0.153
C	-1.2214	6.9443	-3.1415	-0.164
C	3.6956	5.2502	4.2992	-0.158
C	1.0672	-6.8947	3.4241	-0.162
C	-6.4193	-2.5944	3.6010	-0.196
C	-2.6986	0.2461	7.3374	-0.196
C	-4.3052	6.4888	0.5646	-0.196
C	-6.5603	0.7238	-4.1719	-0.195
C	1.1894	7.4064	2.2981	-0.196
C	1.7674	5.4778	-5.2718	-0.191
C	6.4848	-0.8494	4.3292	-0.192
C	6.7056	-4.3505	-0.1646	-0.207
C	-4.4443	-1.6171	-6.3920	-0.217
C	3.5598	-7.2562	-0.0622	-0.207
C	-1.6620	-5.3669	5.7059	-0.192
C	-7.0572	3.9746	-0.0861	-0.226
C	4.5128	1.6615	6.3782	-0.220
C	2.7011	5.5219	5.2683	-0.207
C	0.0234	-7.6691	2.8653	-0.208
C	8.2628	-0.2911	0.1612	-0.201
C	-8.0635	0.2789	-0.2472	-0.199
C	-0.8273	-3.1467	-7.4940	-0.200
C	-0.6383	7.9203	-2.2987	-0.198
C	-0.6592	-8.0372	-1.5983	-0.204
C	0.7991	2.8845	7.5493	-0.207
S	-3.6184	3.8282	-6.6240	-0.238
H	2.6338	3.2293	-7.7184	0.244
S	4.9834	-4.8283	-5.0771	-0.385
C	2.5929	4.1785	-7.1610	-0.203
H	7.8054	3.0536	-0.4792	0.244
S	6.5212	5.3785	0.0041	-0.243

H	-7.6585	-3.0451	0.5224	0.242
S	-6.4881	-5.4317	0.0930	-0.256
S	-4.5615	4.2928	5.7074	-0.388
H	2.3811	-4.2949	-7.0693	0.235
S	3.7175	-3.8545	6.5611	-0.243
H	-2.4000	4.0753	7.1370	0.244
H	-4.0055	-7.7452	-0.8721	0.235
C	8.2898	2.0644	-0.4515	-0.213
H	-4.9216	6.3676	3.5483	0.243
C	-8.1282	-2.0507	0.4505	-0.213
C	1.4533	-3.9908	-7.5809	-0.205
C	-1.4716	3.7559	7.6395	-0.210
C	-3.0725	-8.1578	-1.2915	-0.209
H	-1.8275	6.4884	-5.1858	0.238
C	5.9657	4.4334	-4.4879	-0.207
C	-5.6941	-4.6210	4.7387	-0.205
C	-1.3745	7.2385	-4.5161	-0.209
C	4.6535	0.3346	-7.4476	-0.218
C	-3.8764	0.2430	-7.8514	-0.206
C	-2.7906	8.0101	1.7130	-0.210
C	-5.0477	-0.3752	7.1942	-0.206
C	-2.4463	-3.9701	7.5416	-0.201
H	-3.2417	1.1116	-8.0879	0.242
C	7.7029	-3.8499	-2.3271	-0.208
C	-7.1367	3.0858	-4.2971	-0.219
C	-4.7784	-5.6483	-5.1457	-0.221
C	4.1198	-0.3112	7.7450	-0.206
H	5.4128	7.9078	1.1968	0.246
H	-2.4918	-2.9879	8.0385	0.245
H	3.5495	-1.2298	7.9551	0.242
H	7.7125	-3.2673	-3.2618	0.238
C	4.0942	-7.5408	-2.4202	-0.210
H	-4.9384	-5.4066	4.8975	0.239
C	2.0664	8.7944	0.4990	-0.220
C	-7.4691	4.2420	2.2969	-0.210
H	-1.3508	5.4363	-7.7681	0.245
H	4.9186	-2.5754	-7.0583	0.240
H	5.3130	5.3203	-4.5109	0.238
H	-1.8733	8.1811	2.2987	0.239
H	-5.9455	-0.5728	6.5873	0.240
H	3.9943	-7.2167	-3.4689	0.239
H	-6.9128	4.1367	-4.0515	0.232
C	1.6844	-7.3427	4.6149	-0.212
C	7.3543	-3.0879	3.9342	-0.213
H	5.6223	0.5146	-6.9545	0.243
C	4.7314	6.1925	4.1063	-0.213
H	-7.2454	3.9712	3.3420	0.237
H	2.4901	-6.7426	5.0696	0.235
C	2.1650	-0.0839	-8.6937	-0.282
H	5.5096	5.9990	3.3495	0.236

H	2.4511	8.8877	-0.5293	0.241
H	-5.7035	-5.0534	-5.0761	0.237
C	-2.4116	-7.1563	-5.3228	-0.279
H	7.2487	-4.0864	3.4806	0.232
C	7.6217	2.1628	-4.4351	-0.295
H	-6.1484	-6.8430	-2.5396	0.246
H	1.4465	-5.4515	7.7110	0.247
C	-2.7441	0.1055	8.7345	-0.291
C	-5.1227	7.5714	0.2022	-0.284
C	-7.6022	-2.5892	4.3587	-0.292
C	-7.6983	0.4053	-4.9288	-0.281
C	2.5051	6.5893	-5.7107	-0.287
C	1.0864	8.5397	3.1225	-0.287
C	7.6248	-0.5365	5.0852	-0.280
H	1.1980	-0.2436	-9.1949	0.245
C	-2.3409	-6.4694	6.2505	-0.293
C	7.6704	-5.3486	0.0497	-0.290
H	-1.4942	-7.7590	-5.4028	0.243
C	4.4015	-8.3322	0.2619	-0.291
C	-5.5129	-1.9570	-7.2378	-0.296
C	-8.0268	4.9533	-0.3640	-0.299
C	5.6000	2.0148	7.1950	-0.300
H	8.2836	1.2830	-4.4202	0.238
C	2.7468	6.6965	6.0352	-0.294
C	-0.3876	-8.8649	3.4766	-0.295
H	-1.8514	0.2938	9.3505	0.242
C	9.5339	-0.4611	-0.4088	-0.291
H	-6.0402	7.4147	-0.3858	0.241
H	-8.3591	-1.8019	4.2185	0.241
C	-9.3627	0.4697	0.2480	-0.290
C	-0.9020	-3.1939	-8.8953	-0.293
C	-0.6975	-9.2039	-2.3774	-0.294
C	-0.2183	9.1560	-2.8146	-0.295
C	0.8741	2.9180	8.9515	-0.292
H	-7.9320	-0.6386	-5.1884	0.238
C	-5.6214	6.5657	4.3763	-0.207
H	0.7180	8.4558	4.1562	0.244
H	7.7394	0.4545	5.5501	0.241
C	-3.5158	5.3572	-7.5460	-0.172
H	2.4875	7.5378	-5.1523	0.242
C	3.3360	5.2843	-7.6040	-0.295
C	5.1244	-4.7369	-6.8569	-0.172
C	3.6118	-5.3754	7.4960	-0.174
C	-5.6534	5.6928	5.4890	-0.165
C	-2.3075	5.9265	-8.0146	-0.224
C	6.5010	7.8662	1.3694	-0.221
C	5.0998	-3.5252	-7.5882	-0.212
H	-2.3088	-7.4531	5.7572	0.242
H	4.5317	-8.6543	1.3071	0.235
C	-6.9928	-7.0274	-0.5399	-0.169

H	7.6677	-5.9523	0.9707	0.233
H	-8.2584	5.2426	-1.4015	0.233
C	7.2312	6.7430	0.9149	-0.171
H	-6.1628	-2.8177	-7.0140	0.229
C	2.4022	-5.9378	7.9675	-0.219
H	6.1866	2.9253	6.9939	0.235
C	-6.7361	-7.4789	-1.8562	-0.222
H	1.9778	6.9064	6.7953	0.237
C	9.5627	1.9018	-1.0219	-0.295
H	-1.1978	-9.4722	3.0425	0.237
C	-9.4296	-1.8687	0.9452	-0.299
C	1.3882	-4.0396	-8.9817	-0.290
C	-3.1177	-9.3242	-2.0708	-0.290
C	4.5256	0.5344	-8.8321	-0.307
C	-1.4027	3.7927	9.0412	-0.294
C	7.1309	4.4047	-5.2693	-0.299
C	-6.8733	-4.6231	5.4999	-0.298
C	-5.1021	-0.5171	8.5895	-0.300
C	-3.6002	9.0982	1.3518	-0.296
C	-4.7393	-6.7846	-5.9684	-0.299
C	3.2781	6.4778	-6.8732	0.397
C	3.2801	0.3199	-9.4385	0.393
H	10.0293	-1.4446	-0.4078	0.236
C	-3.1323	-5.0659	8.0895	-0.295
H	-9.8556	1.4525	0.1835	0.236
C	-0.9563	8.4718	-5.0399	-0.292
H	0.2315	9.9198	-2.1610	0.233
C	-4.9445	-0.0891	-8.6994	-0.295
H	0.2229	-9.6254	-2.8118	0.237
H	-1.8163	-2.8809	-9.4229	0.238
C	-8.2751	2.7748	-5.0579	-0.298
C	-3.5519	-7.5247	-6.0461	0.403
C	5.2061	0.0341	8.5637	-0.296
C	7.9461	3.2664	-5.2337	0.388
C	8.6704	-4.8451	-2.1193	-0.295
H	1.7832	2.5850	9.4758	0.238
C	-3.9468	-0.2720	9.3437	0.391
C	1.9704	9.9305	1.3179	-0.300
C	-7.8141	-3.6049	5.2986	0.394
C	4.9385	-8.6165	-2.1019	-0.294
C	-8.4358	5.2229	2.0269	-0.291
C	-4.7594	8.8635	0.6007	0.395
C	8.4993	-2.7824	4.6872	-0.299
C	1.2781	-8.5370	5.2312	-0.292
C	4.7819	7.3717	4.8679	-0.292
C	-8.5419	1.4343	-5.3635	0.398
C	10.1703	0.6409	-0.9925	0.391
C	1.4825	9.7863	2.6237	0.402
C	-3.0638	-6.3043	7.4393	0.396
C	-10.0307	-0.6086	0.8407	0.392

C	-5.7522	-1.1885	-8.3828	0.391
C	0.2071	-3.6437	-9.6226	0.394
C	8.6421	-5.5842	-0.9305	0.394
C	5.9346	1.1962	8.2797	0.390
C	8.6191	-1.5069	5.2535	0.399
C	-1.9270	-9.8362	-2.6012	0.395
C	5.0769	-9.0046	-0.7634	0.394
C	-8.7086	5.5640	0.6965	0.391
C	-0.2283	3.3775	9.6818	0.391
C	-0.3798	9.4167	-4.1812	0.393
C	0.2473	-9.2872	4.6516	0.391
C	3.7900	7.6077	5.8279	0.394
H	3.9654	5.2256	-8.5059	0.231
H	10.0814	2.7472	-1.5009	0.232
H	-9.9785	-2.7002	1.4148	0.231
H	2.2516	-4.3753	-9.5770	0.237
H	-4.0726	-9.8342	-2.2729	0.234
H	-2.2611	4.1362	9.6401	0.231
C	-6.4651	7.6868	4.3107	-0.287
C	4.8288	-6.0202	7.8320	-0.218
H	-6.4361	8.3635	3.4426	0.240
H	-1.0756	8.7021	-6.1100	0.236
H	5.3810	0.8618	-9.4446	0.230
H	-6.0323	-0.8177	9.0978	0.228
H	-7.0668	-5.4036	6.2528	0.229
H	7.4128	5.2575	-5.9073	0.227
H	-3.7207	-4.9668	9.0152	0.231
H	-3.3402	10.1275	1.6457	0.230
C	-4.7339	6.0004	-7.8806	-0.216
C	-7.7453	-7.8638	0.3219	-0.216
H	-5.1601	0.5044	-9.6023	0.228
H	5.4976	-0.5974	9.4184	0.228
C	2.4044	-7.1008	8.7541	-0.294
C	-2.3129	7.0953	-8.7934	-0.295
C	5.3433	-5.9413	-7.5729	-0.218
H	-5.6166	-7.0998	-6.5554	0.229
C	5.2938	-3.5103	-8.9793	-0.290
C	7.1433	8.9234	2.0347	-0.296
H	5.7805	-5.5950	7.4730	0.237
H	9.4424	-5.0577	-2.8757	0.229
H	-8.9576	3.5614	-5.4177	0.226
H	-8.9740	5.7299	2.8429	0.235
H	5.4960	-9.1537	-2.8856	0.228
H	2.2716	10.9267	0.9563	0.230
C	-7.2197	-8.7196	-2.3026	-0.294
C	-6.5701	5.9727	6.5331	-0.220
H	1.7534	-8.8844	6.1618	0.236
C	8.6290	6.7108	1.1482	-0.216
H	5.5879	8.1073	4.7194	0.233
H	-7.9525	-7.5300	1.3517	0.236

H	9.3017	-3.5223	4.8373	0.226
H	-5.6845	5.5702	-7.5252	0.236
H	6.5757	9.7991	2.3877	0.235
H	5.3653	-6.8949	-7.0204	0.231
H	-1.3726	7.5350	-9.1627	0.235
H	5.2667	-2.5635	-9.5414	0.240
H	1.4624	-7.5367	9.1234	0.237
F	3.1571	0.5100	-10.7765	-0.339
F	3.9937	7.5493	-7.3000	-0.339
H	-7.0214	-9.0672	-3.3288	0.236
H	9.2142	5.8429	0.8021	0.235
F	-3.5135	-8.6225	-6.8400	-0.337
F	9.0756	3.2362	-5.9906	-0.344
F	-3.9987	-0.4045	10.6951	-0.342
H	-6.6074	5.3002	7.4056	0.231
F	-8.9560	-3.6055	6.0344	-0.342
F	-5.5462	9.9139	0.2564	-0.338
F	-9.6432	1.1290	-6.0958	-0.340
F	11.4017	0.4829	-1.5454	-0.343
F	1.3991	10.8809	3.4186	-0.336
F	-3.7153	-7.3680	7.9752	-0.339
F	-11.2877	-0.4300	1.3271	-0.343
F	0.1365	-3.6983	-10.9776	-0.340
F	-6.7865	-1.5157	-9.2022	-0.343
F	6.9879	1.5323	9.0707	-0.343
F	9.7238	-1.2089	5.9835	-0.340
F	-1.9647	-10.9681	-3.3495	-0.340
F	9.5765	-6.5486	-0.7274	-0.342
F	-9.6475	6.5097	0.4320	-0.341
F	5.8809	-10.0556	-0.4552	-0.342
F	-0.1599	3.4199	11.0384	-0.342
F	0.0283	10.6115	-4.6813	-0.341
F	-0.1467	-10.4448	5.2430	-0.340
F	3.8397	8.7423	6.5721	-0.340
C	4.8392	-7.1833	8.6170	-0.298
C	3.6236	-7.7105	9.0729	0.386
C	-7.3505	7.9404	5.3655	0.386
C	-3.5339	7.7028	-9.1096	0.388
C	-8.2327	-9.1046	-0.1170	-0.298
C	-4.7476	7.1672	-8.6594	-0.297
C	5.5171	-4.7179	-9.6520	0.385
C	5.5407	-5.9377	-8.9628	-0.302
C	-7.9664	-9.5189	-1.4289	0.388
C	8.5257	8.8611	2.2484	0.387
C	-7.4162	7.0915	6.4779	-0.303
C	9.2777	7.7629	1.8116	-0.297
H	5.7832	-7.6867	8.8810	0.227
H	-8.8192	-9.7567	0.5502	0.228
H	-5.6932	7.6687	-8.9217	0.227
H	5.7132	-6.8731	-9.5194	0.225

F	3.6302	-8.8326	9.8391	-0.342
F	-8.1610	9.0310	5.3159	-0.343
H	-8.1258	7.3151	7.2911	0.224
H	10.3637	7.7390	1.9959	0.228
F	-3.5443	8.8286	-9.8701	-0.342
F	5.7139	-4.7114	-10.9970	-0.342
F	-8.4454	-10.7148	-1.8601	-0.342
F	9.1510	9.8826	2.8898	-0.342