Supporting Information

Isomerism in Monolayer Protected Silver Cluster Ions: An Ion Mobility-Mass Spectrometry Approach

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Contents:

Materials and Methods:

Synthesis of $Au_{25}(PET)_{18}^-$:

About 40 mg of $HAuCl_4.3H_2O$ was taken in 7.5 ml THF and mixed with 65 mg of TAOBr and stirred for around 15 min to get an orange red solution. To the solution, PET was added in 1:5 molar ratio (68 μL) and stirred for another hour. This resulted in Au-thiolate formation. The as-formed thiolate was then reduced by adding about 39 mg of $NaBH_4$ in ice-cold water. The color changed from yellow to brown. The solution was allowed to stir for another 5 hours for complete conversion and size focusing synthesis of $Au_{25}(PET)_{18}^-$. The as-synthesized cluster was then vacuum dried by rotavapor and precipitated using excess MeOH to get rid of free thiol and excess thiolate. The process was repeated a few times. Then the Au_{25} cluster was extracted into acetone and centrifuged and the supernatant solution was collected leaving behind a precipitate consisting of larger clusters. The acetone solution was vacuum dried. Finally the cluster was dissolved in dichloromethane (DCM) and centrifuged and the supernatant solution was collected which consisted of the pure cluster. The resulting cluster was characterized by UV-vis absorption spectroscopy, where characteristic peaks at 675 and 450 nm confirmed the formation of Au_{25} clusters. Detailed characterization was by done by electrospray ionization (ESI) mass spectrometry (MS).

Computational details

$[Ag_{44}(4\text{-FTP})_{30}]^{4-}$ was modelled based on the crystal structure of $[Ag_{44}(SR)_{30}]^{4-}$. In the structure of $[Ag_{44}(4\text{-FTP})30]^{4-}$, FTP ligands bonded to core of the cluster were replaced with methyl groups to reduce the computational cost. First, Ag_{44} with six 4-FTP ligands in the axial positions was optimized without any geometrical constrains. In $[Ag_{44}(4\text{-FTP})\ (CH_3)_{24}]$, 4-FTP ligands were act as bridge by connecting two S-Ag-S through the formation S-Ag bond. In optimized geometry, one Ag-S-Ag staple was opened and FTP ligand was kept away from S-Ag-S unit and the same structure was optimized by fixing the distance between sulphur (from 4-FTP) and Ag (from S-Ag-S). The same approach was followed for the other geometries with two and three opened staples. All the geometries were optimized using Gaussian09 package with the help of density functional theory. The meta-generalized gradient approximation of Tao, Perdew, Staroverov, and Scuseria (TPSS) was employed for exchange-correlation functional. LANL2DZ basis set was used for the silver atoms and the remaining atoms were treated with 6-31G*. All the geometries were constructed and visualized using gassview-5.0 package. The relative energies for all staple-opened-geometries were calculated with respect to closed geometry. The isomeric structures are not checked for real local minimum on the potential energy surface using vibrational frequencies. The frequency calculations for this type of large clusters are difficult with the current computational facilities.

Supporting Information 1:

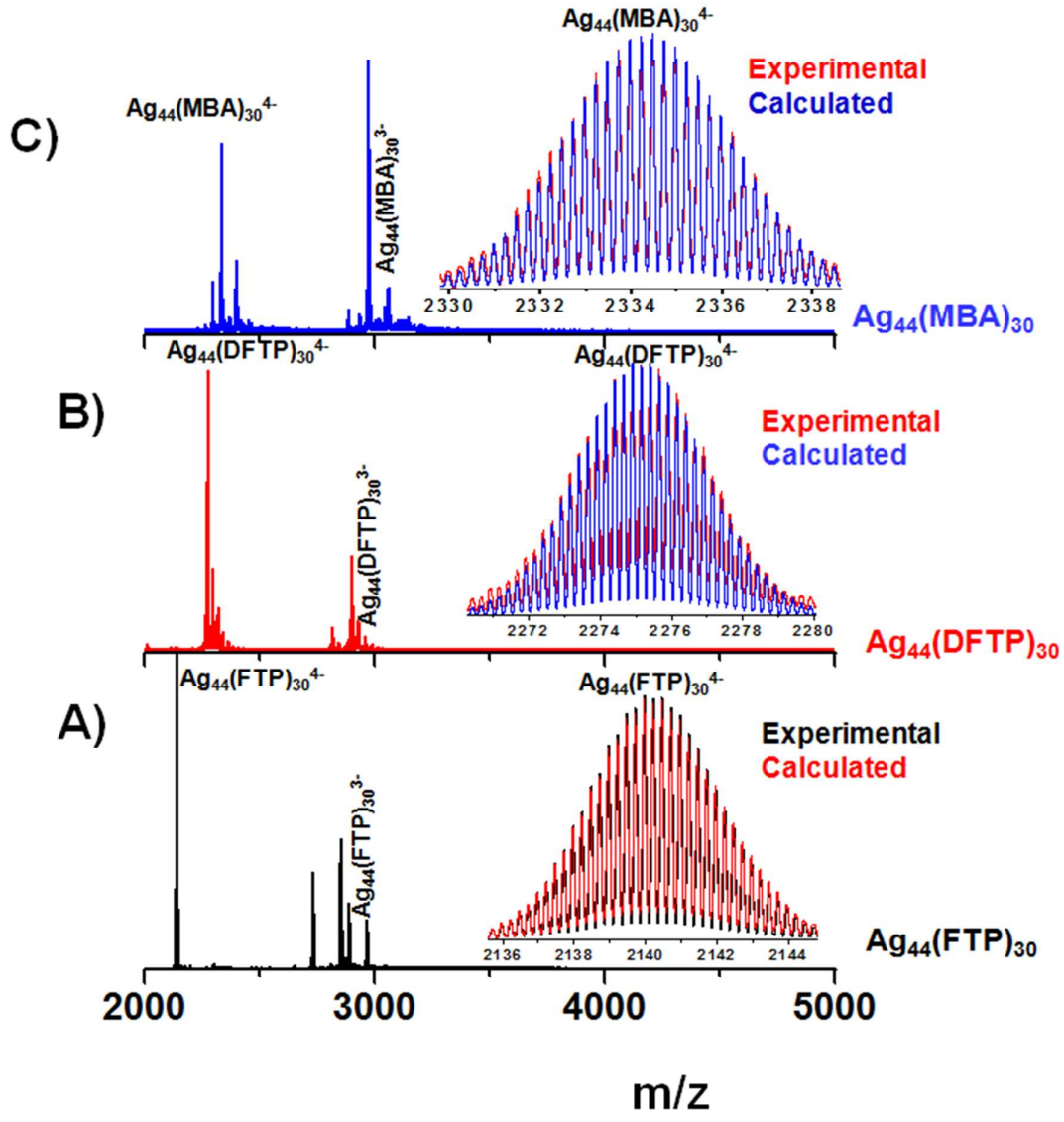

Figure S1: ESI MS of A) $Ag_{44}(FTP)_{30,}$ B) $Ag_{44}(DFTP)_{30,}$ C) $Ag_{44}(p\text{-}MBA)_{30}$ showing 4- charged species as the major peak. Each 4- charged ion is expanded in the respective insets which are matching exactly with their calculated isotope pattern.

Supporting Information 2:

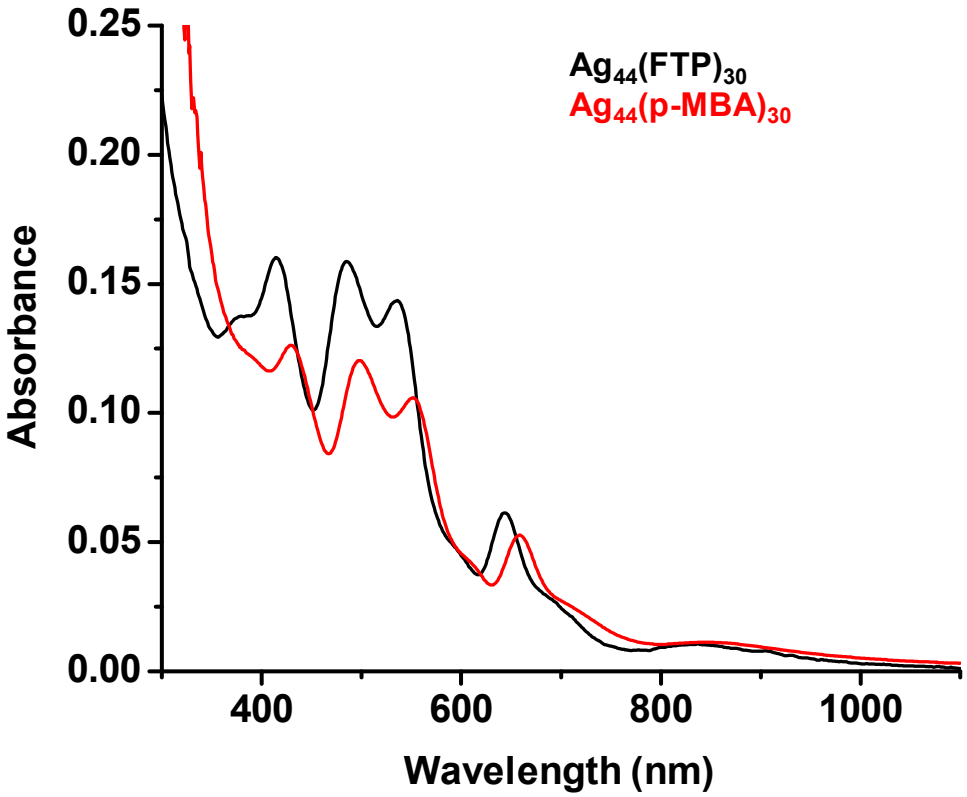

Figure S2: UV-Vis absorption spectra of $Ag_{44}(FTP)_{30}$ and $Ag_{44}(p\text{-}MBA)_{30}$ are showing well defined peaks.

Supporting Information 3:

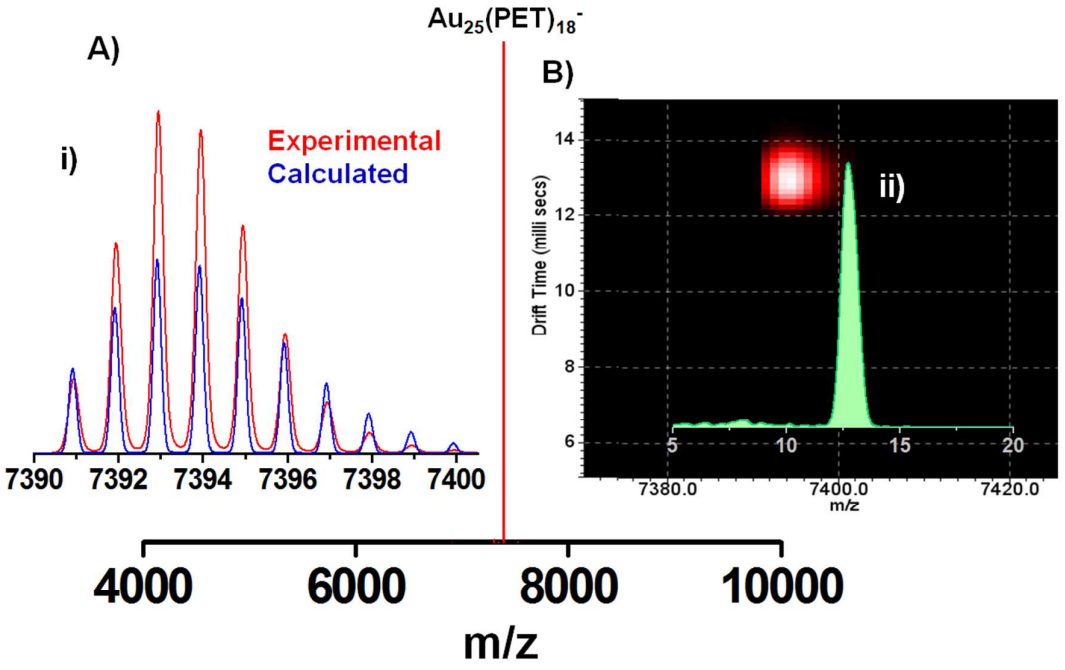

Figure S3: A) ESI MS of $Au_{25}(PET)_{18}$ showing the molecular ion peak. Experimental data are matching well with the calculated spectrum as shown in inset i). B) Plot of m/z vs. drift time for $Au_{25}(PET)_{18}$ is shown. Drift time profile is shown in the inset ii).

Supporting Information 4:

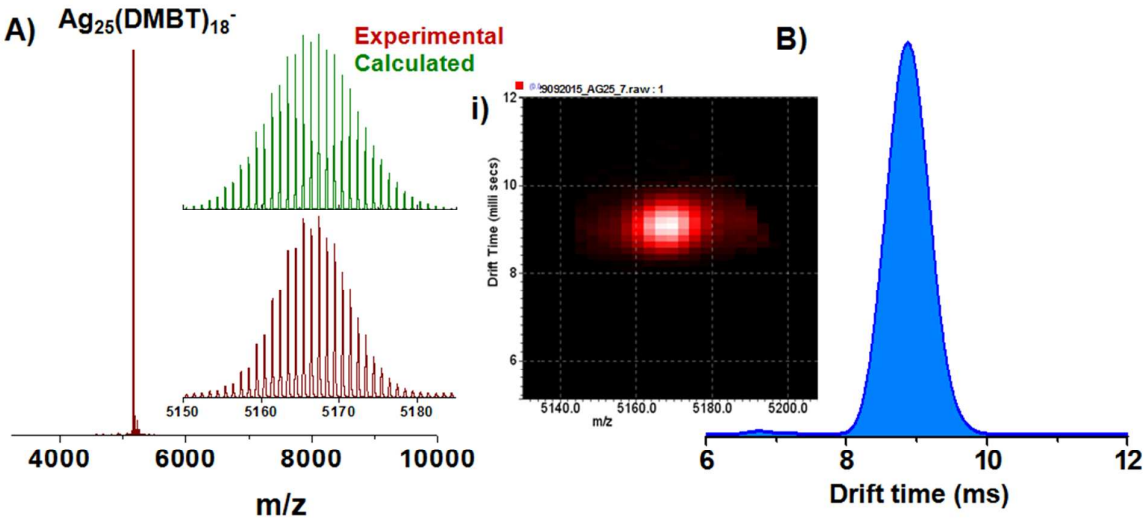

Figure S4: A) ESI MS of $Ag_{25}(DMBT)_{18}$ showing the molecular ion peak. Experimental data are matching well with the calculated spectrum as shown in inset i). B) Drift time profile of the same cluster is showing peak at 8.8 ms.

Supporting Information 5:

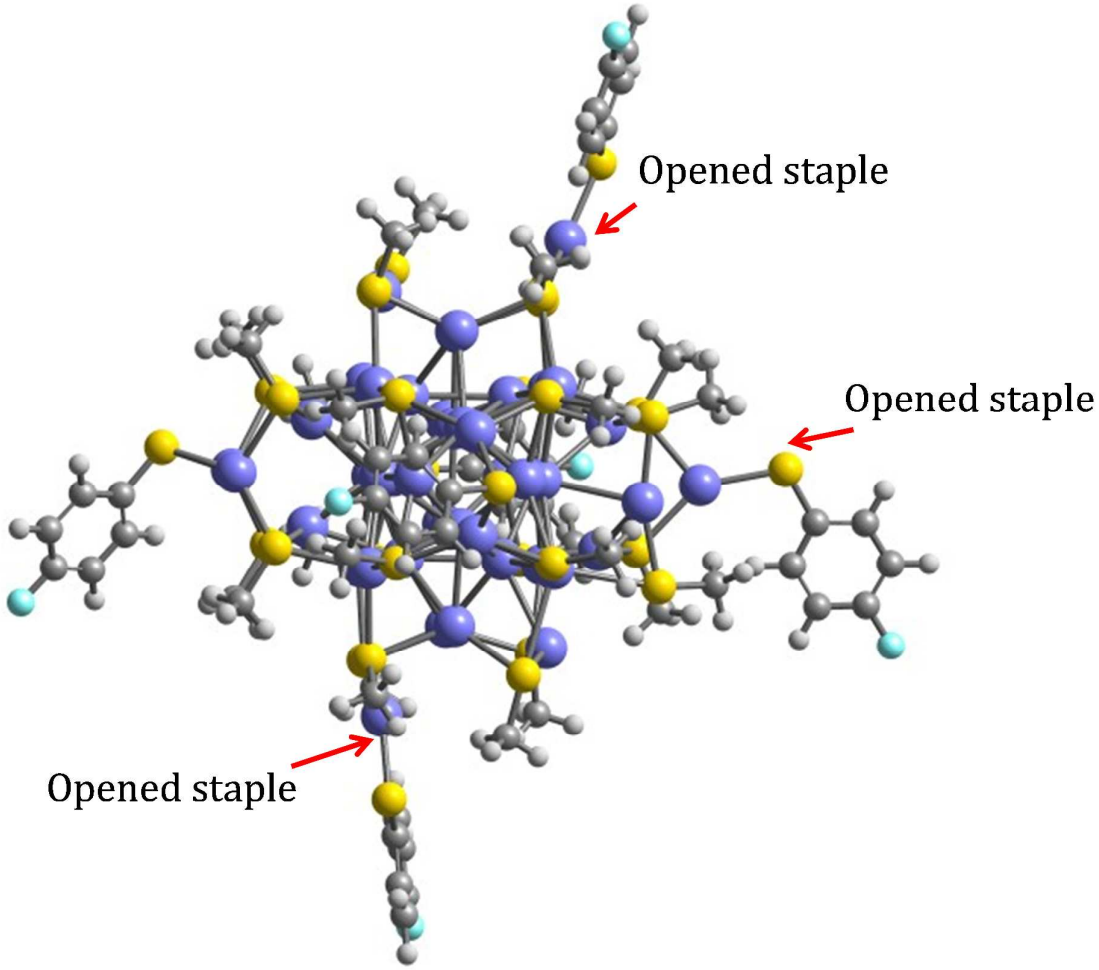

Figure S5: Optimized geometries of three staples opened structures. Six axial ligands were optimized without any geometrical constrains. Other 24 positions were replaced with -SMe. Color code used are; Ag: purple, S: yellow, C: grey, H: light grey, F: cyan.

Supporting Information 6:

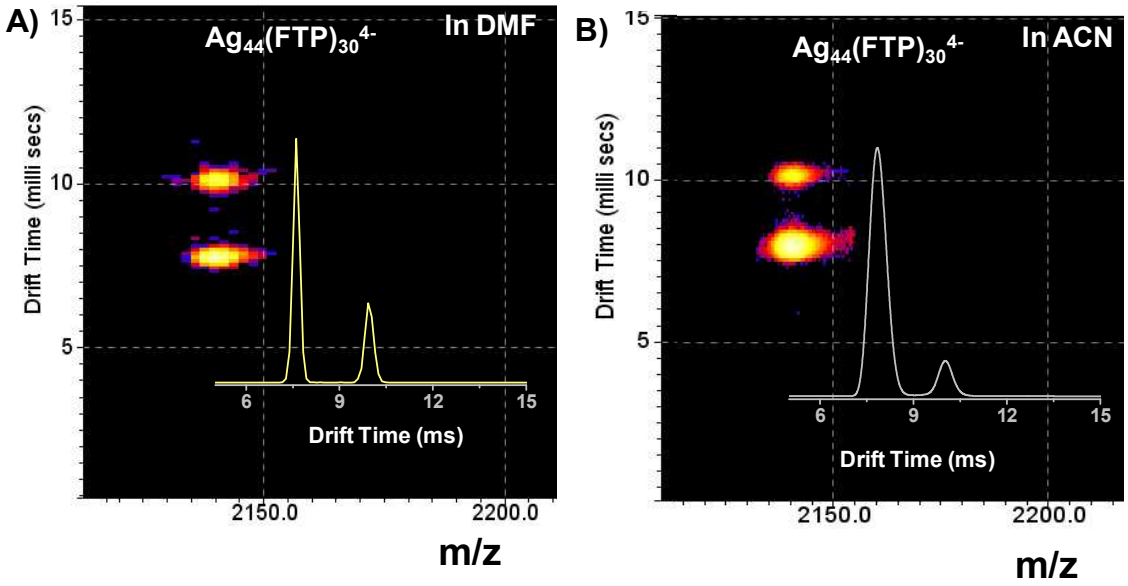

Figure S6: Gas phase isomerism is highly dependent on the solvent used which was proven by measuring the spectra in DMF and ACN along with DCM. A) and B) Drift time vs. m/z plot of $Ag_{44}(FTP)_{30}^{4-}$ showing two isomeric peaks when measured in DMF (A) and ACN (B). Corresponding drift profile is shown in the insets of A and B.

Supporting Information 7:

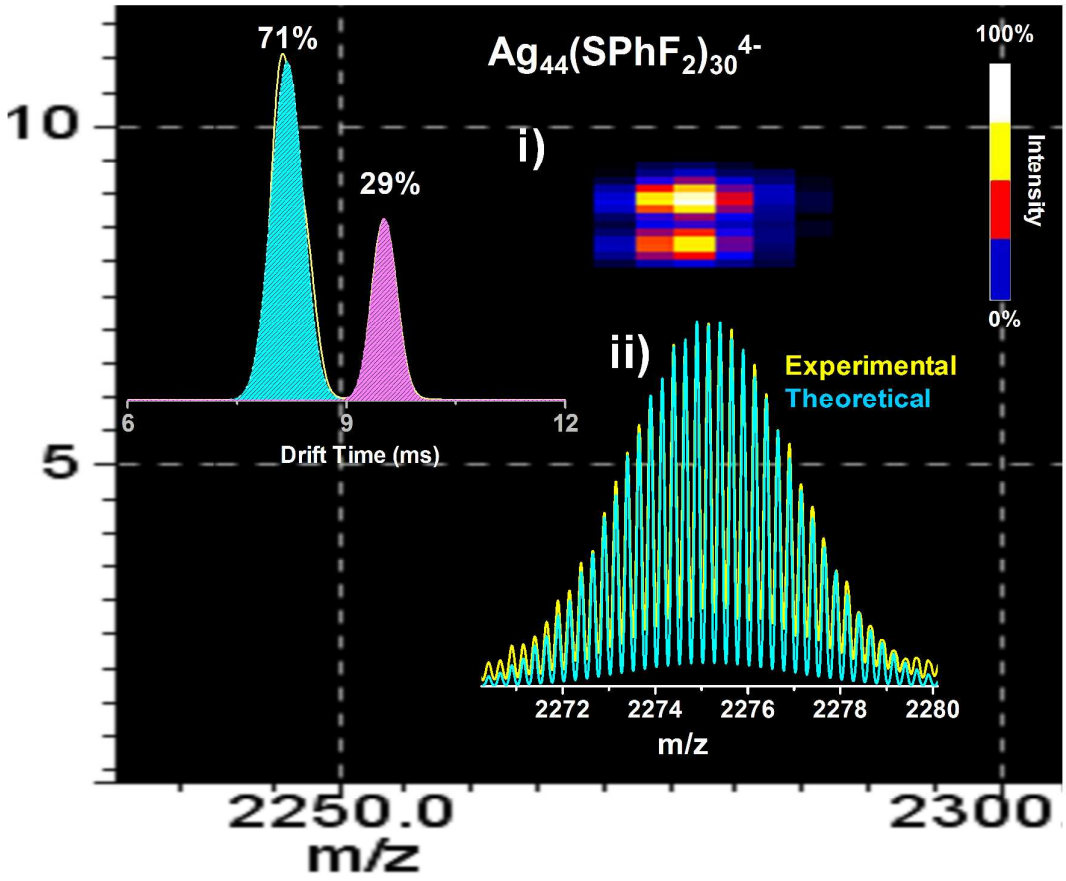

Figure S7: Drift time vs. m/z plot of $Ag_{44}(DFTP)_{30}^{4-}$ showing presence of two isomeric structures. Corresponding mass spectrum and drift profile are shown in insets i) and ii), respectively.

Supporting Information 8:

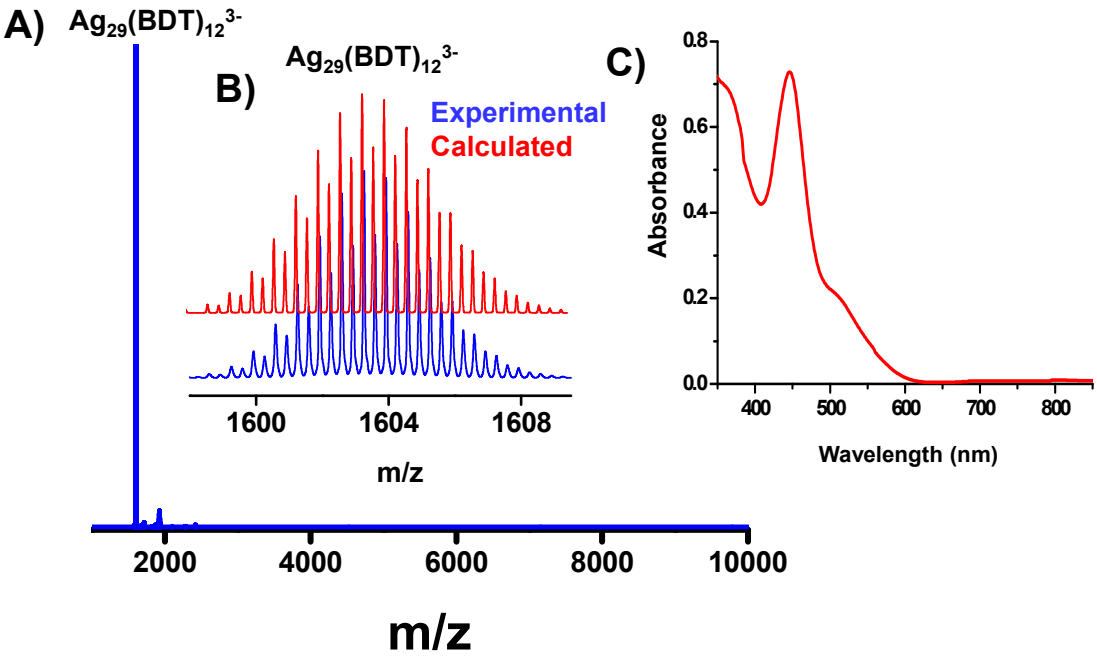

Figure S8: A) ESI MS of $Ag_{29}(BDT)_{12}$ showing maximum intense peak at m/z 1603 due to $Ag_{29}(BDT)_{12}^{3-}$. The peak is expanded in B. Experimental data is matching well with calculated spectrum. C) UV-vis absorption spectrum of $Ag_{29}(BDT)_{12}$ showing characteristic peak confirming the purity of the sample.

Table S1: *Collision cross section values for four different isomers of* $Ag_{44}(FTP)_{30}^{4-}$.

$[Ag_{44}(FTP)_{30}]^{4-}$	CCS value (Å^2)
Isomer 1	829.8
Isomer 2	858.4
Isomer 3	872.2
Isomer 4	896.7

Table S2:*Collision cross section values for four different isomers of* $Ag_{44}(p\text{-}MBA)_{30}^{4-}$.

$[Ag_{44}(MBA)_{30}]^{4-}$	CCS value (Å^2)
Isomer 1	819.1
Isomer 2	854.2
Isomer 3	882.7

Table S3: *Collision cross section values for four different isomers of* $Ag_{44}(DFTP)_{30}^{4-}$.

$[Ag_{44}(DFTP)_{30}]^{4-}$	CCS value (Å^2)
Isomer 1	862.4
Isomer 2	889.7

Table S4: *Calculated HOMO-LUMO gap for different isomers of* $Ag_{44}(FTP)_{30}^{4-}$.

System	HOMO-LUMO gap (in eV)
Closed structure	0.85
One staple opened structure	0.81
Two staple opened structure(Cis)	0.74
Two staple opened structure (Trans)	0.76
Three staple opened structure	0.72

Coordinates for $Ag_{44}(4\text{-}FTP)_6(SMe)_{24}^{4-}$

Ag	0.14800	1.52800	-2.25800
Ag	1.96900	-0.65500	-1.89200
Ag	0.56600	-2.70800	-0.40800
Ag	-2.08400	-1.75900	0.10900
Ag	-2.33700	0.87000	-1.00300
Ag	-0.80800	-1.16400	-2.38300
Ag	-2.14500	0.87500	-3.84200
Ag	0.84700	-0.14600	-4.46600
Ag	1.18500	-3.07700	-3.15800
Ag	-1.64600	-3.81500	-1.81900
Ag	-3.64900	-1.33200	-2.23900
Ag	2.78400	-5.58900	-2.34800
Ag	4.16900	-3.48100	-3.82300
Ag	-3.72700	-1.36000	-5.28700
Ag	-5.21400	0.73500	-3.88800
Ag	-1.86600	3.51600	-1.95500
Ag	-3.26100	2.82700	0.85700
Ag	-4.38500	-0.17600	0.67400
Ag	-2.81900	-1.94500	2.85300
Ag	-2.08300	-4.54000	4.28700
Ag	-4.09700	-4.64400	2.16400
Ag	-1.17400	-4.13200	1.37100
C	-7.05900	-2.55200	-6.11400

H	-6.07100	-2.98900	-5.96500
C	5.80100	-6.73400	-3.91200
C	-7.16800	-1.15100	-6.27100
C	-5.18200	-6.02100	5.31400
C	-4.94900	-5.18700	6.43100
H	-3.97700	-4.70500	6.53400
C	5.98400	-7.27200	-2.61700
H	5.16400	-7.21000	-1.90100
C	-8.46200	-0.60900	-6.45300
H	-8.57000	0.46800	-6.57200
C	-5.94200	-4.96200	7.39500
H	-5.76000	-4.31200	8.24900
C	-9.60000	-1.42600	-6.48100
C	-6.45600	-6.62500	5.19800
H	-6.65900	-7.26600	4.34200
C	-9.44500	-2.80300	-6.32200
C	-7.18200	-5.58300	7.24400
C	-8.18900	-3.38100	-6.13500
H	-8.10000	-4.45800	-6.00600
C	6.88400	-6.82000	-4.81900
H	6.76600	-6.40900	-5.82000
C	8.23300	-7.93900	-3.16700
C	8.09700	-7.42000	-4.45500
C	7.19300	-7.87200	-2.23800
C	-7.45600	-6.41300	6.15600
F	9.41900	-8.53200	-2.80700
F	-10.55800	-3.60800	-6.35300
F	-8.15800	-5.37400	8.18800
S	-5.39500	1.87100	2.17500
S	-3.10000	5.27100	-0.25000
S	-5.93300	-0.09600	-1.57300
S	-3.83200	2.93400	-3.73200

S	-0.20200	5.12300	-3.40800
S	2.04300	2.08500	-5.44900
S	2.47700	-2.16400	-5.29200
S	4.25000	-6.03700	-4.45500
S	0.21600	-5.53000	-2.80800
S	-3.02600	-5.38700	-0.08400
S	-3.91300	-6.39300	4.11500
S	-5.30900	-2.39600	1.96700
S	-5.74300	-0.07700	-6.33000
S	-3.44800	-3.47800	-3.84100
S	-1.37700	-0.47900	-5.99700
Ag	-0.06300	-1.64800	2.18300
Ag	-1.87100	0.53300	1.80800
Ag	-0.47400	2.58800	0.33800
Ag	2.17300	1.63500	-0.19500
Ag	2.42300	-0.99100	0.92500
Ag	0.90900	1.04300	2.30400
Ag	2.23900	-1.00200	3.76200
Ag	-0.74500	0.02100	4.38300
Ag	-1.09000	2.93600	3.09800
Ag	1.76400	3.68800	1.72400
Ag	3.74900	1.20800	2.14900
Ag	-2.67800	5.46200	2.28300
Ag	-4.06100	3.35500	3.76900
Ag	3.82200	1.25500	5.19300
Ag	5.30600	-0.85900	3.82400
Ag	1.95600	-3.63100	1.89200
Ag	3.35900	-2.94400	-0.92500
Ag	4.48000	0.05300	-0.73700
Ag	2.89000	1.84600	-2.93900
Ag	2.07900	4.43900	-4.34800
Ag	4.12100	4.61600	-2.26100

Ag	1.24600	4.02100	-1.43400
C	7.15600	2.43800	6.03800
H	6.17100	2.87900	5.88600
C	-5.68300	6.60600	3.86400
C	7.25800	1.03700	6.20100
C	4.04700	7.45300	-4.45800
C	3.80100	8.22800	-5.61600
H	3.76000	7.73000	-6.58400
C	-5.86800	7.16100	2.57700
H	-5.04700	7.11300	1.86100
C	8.54900	0.48900	6.38700
H	8.65200	-0.58800	6.51000
C	3.60800	9.61400	-5.54100
H	3.41600	10.20800	-6.43400
C	9.69100	1.30100	6.41300
C	4.09000	8.12500	-3.21400
H	4.27200	7.54500	-2.31000
C	9.54300	2.67800	6.24900
C	3.65900	10.23500	-4.29300
C	8.29000	3.26100	6.05800
H	8.20700	4.33800	5.92400
C	-6.76700	6.67300	4.77100
H	-6.64800	6.24900	5.76700
C	-8.12000	7.80700	3.13300
C	-7.98300	7.27100	4.41400
C	-7.08000	7.75800	2.20500
H	-7.21900	8.17800	1.21000
C	3.89500	9.51000	-3.12500
F	-9.31000	8.39800	2.78000
F	10.66000	3.47800	6.27700
F	3.47400	11.59500	-4.21600
S	5.50000	-1.98300	-2.23800

S	3.19400	-5.38300	0.18600
S	6.03600	-0.03800	1.51000
S	3.92900	-3.05900	3.66700
S	0.26500	-5.18400	3.35100
S	-1.97700	-2.20500	5.38400
S	-2.37800	2.02300	5.24200
S	-4.12800	5.91000	4.39900
S	-0.10900	5.37700	2.73900
S	3.10800	5.33100	0.00000
S	4.36700	5.70400	-4.61600
S	5.32700	2.31500	-1.98900
S	5.82700	-0.02900	6.26200
S	3.56300	3.36900	3.74300
S	1.48000	0.36400	5.91300
H	-8.43700	-6.87600	6.06400
H	-10.59600	-1.00500	-6.61800
H	-8.81700	7.32000	5.11300
H	8.93000	-7.48300	-5.15400
H	7.33100	-8.27800	-1.23800
H	10.68500	0.87600	6.55300
H	3.92100	10.02100	-2.16400
C	6.44100	1.91700	-3.41600
H	6.16000	2.50600	-4.29500
H	7.47400	2.15900	-3.13400
H	6.36600	0.84600	-3.63900
C	3.55600	1.70200	-6.44800
H	3.29100	1.74000	-7.51300
H	4.33900	2.43800	-6.24300
H	3.90800	0.69400	-6.20100
C	-0.34100	6.90900	-2.93400
H	0.65000	7.37300	-2.90100
H	-0.95600	7.42300	-3.68400

H	-0.82700	6.98400	-1.95400
C	2.37800	7.03200	0.10300
H	3.13000	7.72000	0.51200
H	2.06300	7.38100	-0.88400
H	1.51300	6.99500	0.77600
C	6.96200	-2.79400	-1.43800
H	7.05100	-2.42200	-0.41000
H	6.84700	-3.88200	-1.43700
H	7.86400	-2.52700	-2.00300
C	4.92800	-5.66200	0.77900
H	5.02900	-6.70500	1.10900
H	5.65000	-5.46100	-0.01800
H	5.11500	-4.99300	1.62700
C	-0.20900	-6.09200	-4.52300
H	0.69900	-6.17200	-5.12900
H	-0.68900	-7.07800	-4.45800
H	-0.90800	-5.38200	-4.97800
C	1.73800	-3.16200	-6.66700
H	2.21800	-2.86900	-7.61100
H	1.90500	-4.22900	-6.49300
H	0.66400	-2.95100	-6.72600
C	-4.98300	-4.42900	-3.41500
H	-4.86100	-4.84600	-2.40800
H	-5.86500	-3.78200	-3.44400
H	-5.10600	-5.24700	-4.13700
C	-7.21900	-1.43100	-1.59300
H	-7.22900	-1.93900	-2.56200
H	-6.99700	-2.14600	-0.79200
H	-8.20200	-0.97600	-1.41500
C	-1.47600	0.77200	-7.36100
H	-1.18500	0.28800	-8.30300
H	-2.49900	1.15100	-7.45200

H	-0.78500	1.59500	-7.14800
C	-3.58700	3.80400	-5.35000
H	-2.58000	4.23600	-5.37200
H	-3.71500	3.10300	-6.18100
H	-4.33100	4.60700	-5.43600
C	0.32700	5.95600	4.44500
H	0.78900	6.95000	4.37100
H	-0.57500	6.02300	5.06200
H	1.04400	5.26000	4.89400
C	-4.83600	5.55000	-0.83500
H	-5.55400	5.35300	-0.03400
H	-4.93700	6.59200	-1.16800
H	-5.02900	4.87700	-1.68000
C	-6.86100	2.68800	1.38900
H	-6.74500	3.77600	1.39300
H	-6.95700	2.32300	0.36000
H	-7.76000	2.41900	1.95800
C	-1.62400	3.00800	6.61800
H	-0.55400	2.77800	6.67800
H	-1.77200	4.07900	6.44300
H	-2.11100	2.72500	7.56100
C	0.38700	-6.96900	2.86900
H	0.99000	-7.49500	3.62200
H	-0.61000	-7.41900	2.82700
H	0.87900	-7.04800	1.89300
C	-2.43600	-7.14200	-0.11700
H	-1.46300	-7.18300	-0.62100
H	-2.35000	-7.53300	0.90200
H	-3.16100	-7.74700	-0.67700
C	-6.40300	-1.97900	3.40400
H	-7.44200	-2.20800	3.13300
H	-6.12200	-2.56700	4.28300

H	-6.31000	-0.90800	3.62000
C	-3.46400	-1.66100	6.34800
H	-4.37200	-2.13900	5.97000
H	-3.32300	-1.92800	7.40400
H	-3.55400	-0.57200	6.25700
C	1.60000	-0.87300	7.28800
H	2.62800	-1.23800	7.37900
H	1.30700	-0.38300	8.22700
H	0.91800	-1.70600	7.08700
C	3.66600	-3.92200	5.28600
H	4.40200	-4.73100	5.37800
H	3.79500	-3.22100	6.11600
H	2.65500	-4.34600	5.30200
C	5.10700	4.30100	3.30900
H	5.25700	5.10300	4.04400
H	5.97700	3.63900	3.30800
H	4.97400	4.74100	2.31300
C	7.32400	1.29400	1.53300
H	7.08900	2.02800	0.75400
H	7.35500	1.78000	2.51300
H	8.30200	0.84100	1.32500

Coordinates for $Ag_{44}(4\text{-FTP})_6(SMe)_{24}^{4-}$: one staple opened

Ag	0.41100	0.94900	-2.52800
Ag	1.46800	-1.62900	-1.71900
Ag	-0.40700	-2.75200	0.13900
Ag	-2.60800	-0.97000	0.37600
Ag	-2.09500	1.34100	-1.20500
Ag	-1.33200	-1.28500	-2.17200
Ag	-1.99600	0.83100	-4.00500
Ag	0.50000	-1.13500	-4.37300

Ag	-0.14500	-3.89000	-2.42800
Ag	-2.87900	-3.41400	-1.10100
Ag	-4.05600	-0.52200	-2.05800
Ag	0.71700	-6.53000	-1.15700
Ag	2.56300	-5.21100	-3.02300
Ag	-4.13400	-1.05800	-5.03600
Ag	-4.96300	1.58300	-4.05100
Ag	-0.93200	3.49900	-2.62700
Ag	-2.32600	3.79500	0.26000
Ag	-4.27600	1.33400	0.62100
Ag	-3.23700	-0.40300	3.08100
Ag	-3.25400	-2.71600	5.04400
Ag	-5.30700	-2.63100	2.93900
Ag	-2.42100	-3.19300	2.12200
C	-7.67600	-1.27600	-5.79500
H	-6.87700	-1.92600	-5.43900
C	3.18400	-8.73200	-2.51800
C	-7.34300	0.01300	-6.26900
C	-6.62400	-3.10200	6.24200
C	-6.18900	-2.08000	7.11600
H	-5.13900	-1.78800	7.10300
C	3.26700	-9.09000	-1.15200
H	2.52400	-8.69400	-0.45900
C	-8.39800	0.84000	-6.72400
H	-8.16500	1.83800	-7.09200
C	-7.08000	-1.43600	7.98700
H	-6.74200	-0.64400	8.65300
C	-9.72900	0.40100	-6.70800
C	-7.99300	-3.45800	6.27400
H	-8.34900	-4.24100	5.60600

C	-10.01200	-0.87800	-6.23000
C	-8.42000	-1.82200	7.98800
C	-9.00300	-1.72600	-5.77000
H	-9.25500	-2.71800	-5.39800
C	4.16400	-9.25300	-3.39500
H	4.12100	-8.98600	-4.45000
C	5.22500	-10.42600	-1.57900
C	5.18200	-10.09800	-2.93500
C	4.28300	-9.93100	-0.67700
C	-8.89300	-2.82500	7.14200
F	6.21900	-11.25700	-1.12400
F	-11.31500	-1.31400	-6.21500
F	-9.29800	-1.20100	8.84200
S	-4.57300	3.82500	1.73500
S	-1.48200	5.79700	-1.29700
S	-5.81300	1.44600	-1.64100
S	-3.00200	3.28700	-4.33100
S	1.05500	4.10100	-4.63900
S	3.17000	-0.04700	-5.98700
S	1.23100	-3.67900	-4.66600
S	1.85600	-7.73200	-3.16900
S	-1.76400	-5.84600	-1.66200
S	-4.60800	-4.06000	0.87100
S	-5.51000	-3.99600	5.17100
S	-5.78600	-0.19600	2.29700
S	-5.65900	0.59500	-6.38000
S	-4.51200	-2.87600	-3.24500
S	-1.67200	-0.94000	-5.97000
Ag	-0.52700	-1.07900	2.44600
Ag	-1.60000	1.41100	1.60900

Ag	0.26600	2.65200	-0.21700
Ag	2.47000	0.83200	-0.60700
Ag	1.96400	-1.46300	1.08100
Ag	1.24500	1.16200	1.97900
Ag	1.96400	-0.85500	3.85200
Ag	-0.49300	1.14600	4.23400
Ag	-0.09300	3.65100	2.43100
Ag	2.87300	3.22400	0.82700
Ag	3.98600	0.40000	1.79900
Ag	-0.86300	6.33400	1.14500
Ag	-2.74900	5.08100	3.00200
Ag	4.27800	1.05800	4.75500
Ag	4.90100	-1.67000	3.94300
Ag	0.79700	-3.60700	2.56700
Ag	2.13300	-3.97700	-0.25700
Ag	4.17500	-1.42600	-0.71300
Ag	3.10500	-0.00000	-3.30600
Ag	1.68400	1.74400	-5.08800
Ag	6.38200	2.81900	-2.52100
Ag	2.10200	3.16000	-2.33800
C	7.88000	0.96200	5.33700
H	7.14800	1.61600	4.86200
C	-3.29400	8.61700	2.41900
C	7.42300	-0.18800	6.02000
C	8.95400	4.84000	-3.82100
C	10.19500	5.23500	-4.38700
H	10.91300	4.46300	-4.65900
C	-3.33900	8.97400	1.05200
H	-2.58300	8.57200	0.37800
C	8.39100	-1.02100	6.62800

H	8.06100	-1.91300	7.15800
C	10.51600	6.58100	-4.60300
H	11.47300	6.87100	-5.03800
C	9.75900	-0.72100	6.56200
C	8.04800	5.87800	-3.48100
H	7.08700	5.60600	-3.04400
C	10.16500	0.42300	5.87600
C	9.59000	7.56300	-4.25100
C	9.24500	1.27100	5.25800
H	9.59200	2.15400	4.72500
C	-4.29200	9.14600	3.27100
H	-4.27800	8.88000	4.32700
C	-5.29900	10.32400	1.42800
C	-5.29200	9.99700	2.78500
C	-4.33700	9.82200	0.55100
H	-4.37200	10.08900	-0.50400
C	8.35700	7.22800	-3.69100
F	-6.27600	11.16100	0.94800
F	11.50400	0.72100	5.81000
F	9.90300	8.88900	-4.46100
S	4.35900	-3.92600	-1.74400
S	1.29300	-5.99100	1.29200
S	5.71300	-1.63300	1.52500
S	2.90400	-3.32300	4.23600
S	-1.25000	-4.21400	4.25200
S	-2.32600	-0.37200	5.58500
S	-1.44700	3.64600	4.73400
S	-1.99300	7.60500	3.10500
S	1.58700	5.49900	1.54800
S	4.37600	3.92800	-1.34700

S	8.61800	3.11900	-3.58500
S	5.51400	0.28000	-2.31500
S	5.69300	-0.59100	6.19800
S	4.60000	2.77600	2.88000
S	1.81700	1.07200	5.66100
H	-9.94700	-3.09900	7.16300
H	-10.54000	1.04000	-7.05600
H	-6.06100	10.40200	3.44200
H	5.93700	-10.49600	-3.61200
H	4.34700	-10.19800	0.37600
H	10.50300	-1.36400	7.02900
H	7.65100	8.01400	-3.42500
C	6.58900	-0.81200	-3.35800
H	6.68300	-0.39400	-4.36600
H	7.58200	-0.87200	-2.89600
H	6.14400	-1.81200	-3.40800
C	4.71300	0.94400	-6.31000
H	4.51400	1.73100	-7.04700
H	5.09700	1.39500	-5.38800
H	5.47100	0.25900	-6.71200
C	2.44900	5.19300	-5.20800
H	3.41600	4.77300	-4.91600
H	2.40600	5.29900	-6.29900
H	2.32500	6.17800	-4.74100
C	4.41000	5.77900	-1.39700
H	5.32800	6.13600	-0.91200
H	4.38300	6.13400	-2.43400
H	3.53900	6.15800	-0.85100
C	5.55300	-4.99300	-0.81200
H	5.76500	-4.52500	0.15600

H	5.13700	-5.99500	-0.66700
H	6.48200	-5.06800	-1.39200
C	2.87600	-6.69800	1.94800
H	2.66700	-7.67200	2.40900
H	3.61200	-6.82500	1.14800
H	3.27100	-6.01200	2.70700
C	-2.34400	-6.51900	-3.28800
H	-1.50000	-6.93700	-3.84700
H	-3.07900	-7.31200	-3.09600
H	-2.82000	-5.71800	-3.86500
C	0.23800	-4.57700	-5.94700
H	0.79500	-4.55800	-6.89200
H	0.08000	-5.61600	-5.63800
H	-0.72300	-4.06900	-6.08200
C	-6.26700	-3.21800	-2.75200
H	-6.27900	-3.47200	-1.68600
H	-6.90200	-2.34500	-2.92900
H	-6.64300	-4.06900	-3.33500
C	-7.45100	0.60000	-1.44600
H	-7.67100	-0.01300	-2.32600
H	-7.42400	-0.02400	-0.54500
H	-8.23000	1.36500	-1.33500
C	-1.54200	0.08900	-7.50700
H	-1.12200	-0.53200	-8.30700
H	-2.53900	0.43700	-7.79800
H	-0.88200	0.94600	-7.33600
C	-2.64200	3.70600	-6.09800
H	-1.55800	3.78300	-6.23600
H	-3.05700	2.93600	-6.75700
H	-3.10800	4.67300	-6.33200

C	2.33100	6.20200	3.09300
H	3.02800	7.00200	2.81000
H	1.54600	6.61600	3.73400
H	2.88000	5.41600	3.62300
C	-3.05300	6.52600	-1.95900
H	-3.77300	6.70400	-1.15500
H	-2.81800	7.47700	-2.45700
H	-3.47600	5.82800	-2.69000
C	-5.71000	4.92700	0.77100
H	-5.27200	5.92400	0.66400
H	-5.88500	4.48400	-0.21600
H	-6.66300	5.00600	1.30900
C	-0.34700	4.62400	5.85700
H	0.60600	4.09700	5.97400
H	-0.17800	5.62300	5.44300
H	-0.83500	4.71700	6.83700
C	-1.68200	-6.01600	4.20000
H	-1.16900	-6.52100	5.02800
H	-2.76400	-6.14700	4.31000
H	-1.34200	-6.44500	3.25100
C	-4.60100	-5.88400	1.20200
H	-3.74300	-6.33600	0.69300
H	-4.54600	-6.07100	2.27900
H	-5.52900	-6.31700	0.80600
C	-6.61600	0.80300	3.61900
H	-7.68600	0.87600	3.38300
H	-6.49500	0.32300	4.59400
H	-6.17700	1.80700	3.63200
C	-3.49800	0.77300	6.45300
H	-4.53300	0.56700	6.16200

H	-3.38700	0.64100	7.53800
H	-3.23500	1.80200	6.18100
C	1.67600	0.14000	7.25700
H	2.59500	-0.42600	7.44100
H	1.52500	0.86100	8.07200
H	0.81700	-0.53800	7.21200
C	2.44100	-3.65100	6.00000
H	2.73100	-4.68000	6.25200
H	2.96800	-2.95500	6.66100
H	1.35800	-3.54200	6.11800
C	6.32800	3.02600	2.25400
H	6.77700	3.87700	2.78300
H	6.93700	2.13200	2.41300
H	6.28000	3.24800	1.18200
C	7.34000	-0.78300	1.26400
H	7.25300	-0.09400	0.41700
H	7.63800	-0.24200	2.16700
H	8.09600	-1.54500	1.03500

Coordinates for $Ag_{44}(4\text{-FTP})_6(SMe)_{24}^{4-}$: two *cis*-staple opened

Ag	-0.13100	-0.69900	2.53900
Ag	-0.38500	-2.62300	0.51800
Ag	1.25500	-1.73900	-1.69000
Ag	2.63200	0.65100	-0.95200
Ag	1.78300	1.31600	1.76800
Ag	2.20700	-1.37100	0.99500
Ag	2.32400	-0.59300	3.83900
Ag	1.30900	-3.32200	2.74600
Ag	2.00100	-4.02300	-0.19900
Ag	4.04400	-1.86900	-1.10000
Ag	4.44200	0.46800	1.22100

Ag	1.76200	-5.71600	-2.84000
Ag	0.16500	-6.45800	-0.51800
Ag	6.08400	-2.95800	3.36700
Ag	3.96900	1.88100	3.80500
Ag	0.19800	1.56800	4.13800
Ag	0.88300	3.98300	1.97100
Ag	3.32300	3.14000	0.25500
Ag	2.26000	2.73500	-2.89300
Ag	2.65100	1.95600	-5.79600
Ag	4.96200	1.82800	-3.98200
Ag	2.73600	-0.23700	-3.63600
C	7.26100	-4.51600	6.40100
H	6.30700	-4.16000	6.01300
C	0.52400	-9.08700	-2.93300
C	8.40900	-4.40400	5.57700
C	5.54400	3.70100	-7.01200
C	4.56300	4.68600	-7.27100
H	3.51100	4.42500	-7.15200
C	0.09400	-8.64100	-4.20400
H	0.41100	-7.65700	-4.54800
C	9.63300	-4.87900	6.11700
H	10.53500	-4.80700	5.50900
C	4.91800	5.98300	-7.66900
H	4.16000	6.74000	-7.86100
C	9.71200	-5.43300	7.40000
C	6.90100	4.06600	-7.16700
H	7.67300	3.32300	-6.96900
C	8.55200	-5.52100	8.17100
C	6.26900	6.29800	-7.81400
C	7.32400	-5.06800	7.68700
H	6.43300	-5.14800	8.30900
C	0.09600	-10.36500	-2.50400

H	0.41400	-10.72800	-1.52800
C	-1.12900	-10.68700	-4.55300
C	-0.72700	-11.16800	-3.30600
C	-0.73200	-9.43100	-5.01500
C	7.27000	5.35700	-7.56800
F	-1.93200	-11.47100	-5.34400
F	8.62400	-6.06500	9.43600
F	6.62500	7.56300	-8.21100
S	2.63800	5.69400	0.88600
S	-0.15500	4.17200	4.43700
S	5.77400	2.52400	2.25300
S	2.56700	1.31800	5.76300
S	-2.34500	0.94200	6.21800
S	-0.51400	-3.31300	4.80000
S	1.33300	-5.77600	1.70100
S	1.63200	-8.13900	-1.90300
S	3.87800	-4.41300	-2.04100
S	5.30600	-0.61000	-3.13000
S	5.12700	2.01800	-6.58700
S	4.66400	3.47200	-2.03100
S	8.38900	-3.71700	3.94600
S	5.72800	-1.78200	1.00100
S	3.61500	-2.84100	4.12600
Ag	0.26000	0.74900	-2.65200
Ag	0.65000	2.63000	-0.53400
Ag	-1.05900	1.88700	1.63000
Ag	-2.41100	-0.54500	0.90500
Ag	-1.57400	-1.25800	-1.71300
Ag	-1.94900	1.54300	-1.03800
Ag	-2.40900	0.62400	-3.68600
Ag	-0.77900	3.39000	-2.88700
Ag	-1.62400	4.18100	0.07700

Ag	-3.88800	1.86100	1.01800
Ag	-4.19200	-0.16900	-1.31900
Ag	-1.49200	5.64200	2.76400
Ag	0.22700	6.53500	0.51200
Ag	-5.28200	1.67300	-3.48100
Ag	-4.86000	-1.14800	-4.13200
Ag	-0.14600	-1.63400	-4.16400
Ag	-0.55300	-3.89500	-2.04300
Ag	-3.14200	-3.07700	-0.12000
Ag	-2.13600	-2.66400	2.81900
Ag	-0.96700	-0.94400	5.35900
Ag	-6.17700	-1.74800	3.68900
Ag	-2.63500	0.55200	3.55700
C	-8.74700	0.72500	-3.95500
H	-8.17400	1.38700	-3.30600
C	-0.17000	8.96400	3.12300
C	-8.10100	0.12900	-5.06200
C	-8.95000	-1.86300	5.84600
C	-9.99000	-2.36400	6.67300
H	-10.10700	-3.44300	6.77100
C	0.00100	8.53500	4.45900
H	-0.49600	7.62200	4.78600
C	-8.86200	-0.73200	-5.88600
H	-8.38100	-1.20500	-6.74100
C	-10.86300	-1.51300	7.36300
H	-11.65700	-1.90900	7.99500
C	-10.21500	-0.98700	-5.62300
C	-8.83400	-0.45300	5.74800
H	-8.04500	-0.04000	5.11900
C	-10.81300	-0.37600	-4.52100
C	-10.70500	-0.13300	7.23300
C	-10.09800	0.47500	-3.67800

H	-10.59100	0.92900	-2.82000
C	0.49400	10.14600	2.71800
H	0.37800	10.49100	1.69200
C	1.43700	10.41400	4.91800
C	1.29600	10.87300	3.60800
C	0.80300	9.25200	5.35800
H	0.93900	8.91400	6.38400
C	-9.69900	0.41000	6.43300
F	2.21900	11.12500	5.79300
F	-12.13900	-0.62000	-4.26200
F	-11.56200	0.70900	7.91000
S	-2.21000	-5.54900	-0.76400
S	0.44700	-4.27000	-4.51400
S	-5.01600	-2.59200	-2.03100
S	-2.57100	-1.42500	-5.35100
S	1.46600	-0.36900	-5.94700
S	0.95300	3.73600	-4.99500
S	-0.81800	5.88400	-1.78900
S	-1.25200	8.11700	1.98100
S	-3.59800	4.41800	1.82900
S	-5.21600	0.55700	3.02800
S	-7.88600	-3.00000	5.00400
S	-4.55600	-3.26100	2.18600
S	-6.40300	0.47900	-5.49200
S	-5.74300	1.99200	-0.96700
S	-3.18000	3.12900	-4.09800
H	8.31600	5.63700	-7.68500
H	10.65800	-5.79500	7.80400
H	1.81000	11.78100	3.29400
H	-1.05800	-12.15000	-2.97300
H	-1.06700	-9.08000	-5.98900
H	-10.80000	-1.65100	-6.25700

H	-9.59600	1.49100	6.34900
C	-4.81300	-5.05500	2.57200
H	-4.69800	-5.22900	3.64700
H	-5.82800	-5.33700	2.26700
H	-4.08200	-5.65200	2.01400
C	-1.33900	-4.52500	5.94200
H	-0.80000	-4.55700	6.89700
H	-2.38100	-4.23600	6.11300
H	-1.30500	-5.51400	5.46900
C	-3.80500	-0.01600	6.86400
H	-4.31600	-0.55500	6.05800
H	-3.48600	-0.72800	7.63400
H	-4.50500	0.70200	7.31000
C	-5.83300	1.91300	4.13000
H	-6.91600	2.02700	3.99100
H	-5.61600	1.68200	5.17700
H	-5.32700	2.84500	3.85000
C	-3.18900	-6.36400	-2.11100
H	-3.73900	-5.59900	-2.67100
H	-2.52500	-6.92100	-2.77900
H	-3.90200	-7.05900	-1.64800
C	-0.97200	-5.08100	-5.39000
H	-0.61000	-5.51200	-6.33300
H	-1.41500	-5.86900	-4.77400
H	-1.72700	-4.31500	-5.60400
C	5.08200	-5.51200	-1.15700
H	4.60900	-6.46800	-0.91100
H	5.93900	-5.69200	-1.81900
H	5.42800	-5.01600	-0.24400
C	2.95100	-6.63300	1.98900
H	2.85000	-7.26800	2.87800
H	3.20200	-7.25600	1.12500

H	3.74000	-5.89300	2.16300
C	7.38100	-1.37800	0.26700
H	7.23300	-0.81600	-0.66300
H	7.97200	-0.78600	0.97400
H	7.90800	-2.31500	0.05000
C	7.27900	1.65500	2.91400
H	7.08400	0.58900	3.06900
H	8.08600	1.77000	2.17900
H	7.58400	2.11500	3.86200
C	3.31400	-3.54000	5.81300
H	3.62300	-4.59300	5.82600
H	3.88200	-2.98300	6.56800
H	2.24200	-3.47500	6.03100
C	3.60300	0.37500	6.98500
H	2.93200	-0.06400	7.73300
H	4.16300	-0.42000	6.48400
H	4.29800	1.06500	7.48000
C	-4.79100	5.57100	1.00100
H	-5.63500	5.74600	1.68000
H	-4.29900	6.52400	0.78100
H	-5.15600	5.11000	0.07700
C	1.13300	5.00800	5.47800
H	1.61900	5.81000	4.91600
H	0.64900	5.42200	6.37200
H	1.87400	4.26000	5.78100
C	3.47400	6.47800	2.34600
H	2.75500	7.07700	2.91300
H	3.90600	5.70200	2.98600
H	4.27800	7.12800	1.97800
C	-2.38000	6.79700	-2.19200
H	-3.11300	6.09200	-2.59900
H	-2.77800	7.27900	-1.29300

H	-2.15500	7.56400	-2.94500
C	2.44500	-1.61500	-6.91000
H	1.99200	-1.72000	-7.90500
H	3.48200	-1.28100	-7.01700
H	2.40700	-2.58000	-6.39300
C	5.82400	-1.79700	-4.45600
H	5.27200	-2.73500	-4.33200
H	5.63100	-1.36700	-5.44400
H	6.90000	-1.99000	-4.34900
C	4.88800	5.26100	-2.46400
H	5.91500	5.55300	-2.20800
H	4.72300	5.41800	-3.53400
H	4.18200	5.85900	-1.87700
C	1.56000	5.48900	-4.98700
H	2.65200	5.52100	-4.94600
H	1.21200	5.98900	-5.90100
H	1.14000	5.99800	-4.11100
C	-3.01100	3.36100	-5.93000
H	-3.66100	2.65700	-6.45900
H	-3.30800	4.38800	-6.17900
H	-1.96600	3.20800	-6.22100
C	-2.50800	-0.61200	-7.01400
H	-2.55800	-1.38900	-7.78700
H	-3.35900	0.06800	-7.13000
H	-1.56600	-0.06200	-7.11200
C	-7.29500	1.21100	-0.32200
H	-8.08400	1.97400	-0.28000
H	-7.61400	0.38800	-0.96800
H	-7.09800	0.83300	0.68800
C	-6.71500	-2.73000	-1.30000
H	-6.64900	-2.59400	-0.21500
H	-7.38200	-1.98100	-1.73800

H	-7.10300	-3.73300	-1.51700

Coordinates for $Ag_{44}(4\text{-FTP})_6(SMe)_{24}^{4-}$: two *trans*-staple opened

Ag	0.61700	1.05600	-2.45900
Ag	0.92600	-1.74600	-1.87900
Ag	-1.12100	-2.47100	0.00300
Ag	-2.67200	-0.16500	0.60700
Ag	-1.58900	2.02200	-0.91800
Ag	-1.70000	-0.59700	-2.07400
Ag	-1.81600	1.74000	-3.74200
Ag	-0.06000	-0.82800	-4.40600
Ag	-1.26300	-3.36900	-2.68300
Ag	-3.77500	-2.23800	-0.99600
Ag	-4.07400	0.90500	-1.68800
Ag	-1.15600	-6.26300	-1.64600
Ag	0.88700	-5.36800	-3.55000
Ag	-4.50200	0.59600	-4.67700
Ag	-4.46500	3.29800	-3.56000
Ag	0.02800	3.90800	-2.25800
Ag	-0.97100	4.35000	0.62900
Ag	-3.62700	2.46500	1.00900
Ag	-2.94300	0.52200	3.39200
Ag	-2.22600	-1.80200	4.99500
Ag	-6.62100	-1.20000	2.96000
Ag	-2.99500	-2.57700	2.15200
C	-7.98000	1.52600	-5.20000
H	-7.40500	0.65600	-4.88300
C	0.40800	-8.93300	-3.44700
C	-7.28700	2.65700	-5.69000
C	-9.25900	-2.73700	4.72100
C	-10.25000	-2.97400	5.71000
H	-10.45900	-2.19100	6.43700

C	0.55200	-9.41700	-2.12600
H	0.07100	-8.87400	-1.31200
C	-8.05300	3.77600	-6.09300
H	-7.53900	4.65800	-6.47100
C	-10.95800	-4.18000	5.77500
H	-11.71500	-4.35100	6.54000
C	-9.45200	3.77000	-6.01300
C	-9.01700	-3.78400	3.79500
H	-8.26300	-3.63100	3.02300
C	-10.09500	2.63300	-5.52200
C	-10.68100	-5.17900	4.84100
C	-9.37800	1.50800	-5.11100
H	-9.90700	0.63800	-4.72600
C	1.04600	-9.65100	-4.48500
H	0.95100	-9.29300	-5.50900
C	1.90900	-11.24900	-2.90300
C	1.79400	-10.80700	-4.22100
C	1.30000	-10.56900	-1.84800
C	-9.71600	-4.99700	3.85000
F	2.63800	-12.38300	-2.64100
F	-11.46500	2.62200	-5.44500
F	-11.37700	-6.36800	4.90100
S	-3.04900	4.81300	2.24500
S	0.30600	6.20900	-0.83900
S	-5.16400	3.27400	-1.10100
S	-2.10700	4.38900	-3.83600
S	1.95200	3.95500	-4.30500
S	2.80500	-0.48600	-6.09900
S	-0.02100	-3.40500	-5.02300
S	-0.59600	-7.51200	-3.85100
S	-3.32300	-4.78400	-1.84300
S	-5.39900	-2.61000	1.17200

S	-8.41600	-1.18100	4.69500
S	-5.36500	1.12200	2.57100
S	-5.51100	2.69500	-5.87800
S	-5.30000	-1.12300	-2.94300
S	-2.18200	0.09500	-5.80100
Ag	-0.66100	-1.03200	2.46400
Ag	-0.95500	1.77500	1.83100
Ag	1.11200	2.51400	-0.05000
Ag	2.65300	0.18200	-0.64700
Ag	1.54700	-1.99000	0.89000
Ag	1.66600	0.63100	2.01600
Ag	1.79800	-1.67800	3.71200
Ag	0.06700	0.93600	4.34400
Ag	1.22600	3.40400	2.64400
Ag	3.77000	2.24200	0.95300
Ag	4.03900	-0.88900	1.65900
Ag	1.16200	6.29300	1.58700
Ag	-0.90500	5.44500	3.48200
Ag	4.49700	-0.57900	4.64500
Ag	4.37600	-3.29200	3.55700
Ag	-0.09600	-3.86400	2.22800
Ag	0.96400	-4.31100	-0.68200
Ag	3.59400	-2.45800	-1.02700
Ag	2.93100	-0.52400	-3.42400
Ag	1.96000	1.60500	-5.07300
Ag	6.89500	1.09800	-2.64200
Ag	2.96300	2.56300	-2.25500
C	7.93500	-1.61300	5.17400
H	7.38800	-0.73500	4.83100
C	-0.41700	9.01100	3.30000
C	7.20700	-2.70800	5.69200
C	9.89300	2.42100	-3.92000

C	11.11100	2.52700	-4.64100
H	11.49500	1.64400	-5.15100
C	-0.47300	9.50800	1.97700
H	0.06500	8.97500	1.19300
C	7.93800	-3.83800	6.13000
H	7.39600	-4.69300	6.53100
C	11.82500	3.73000	-4.71600
H	12.75900	3.79900	-5.27400
C	9.33700	-3.87600	6.05600
C	9.42900	3.59400	-3.27100
H	8.49800	3.54200	-2.70700
C	10.01500	-2.77300	5.53600
C	11.32400	4.85600	-4.06200
C	9.33400	-1.63900	5.09000
H	9.89000	-0.79700	4.68300
C	-1.12900	9.71500	4.29900
H	-1.10300	9.34700	5.32300
C	-1.89100	11.32500	2.67800
C	-1.86400	10.86900	3.99600
C	-1.20700	10.65900	1.66000
H	-1.25200	11.03400	0.63900
C	10.13300	4.80300	-3.33800
F	-2.60700	12.45700	2.37700
F	11.38500	-2.80600	5.46500
F	12.02400	6.04200	-4.13400
S	3.04100	-4.78300	-2.30900
S	-0.31000	-6.16100	0.77900
S	5.08800	-3.28700	1.10700
S	1.99000	-4.33200	3.85700
S	-2.17300	-4.11700	4.18900
S	-2.68700	0.37400	6.03400
S	-0.00300	3.51400	4.99200

S	0.57100	7.59500	3.75600
S	3.30300	4.78900	1.78900
S	5.34400	2.61500	-1.24400
S	9.04800	0.86600	-3.87500
S	5.33800	-1.08900	-2.55800
S	5.43000	-2.68900	5.87400
S	5.30200	1.12200	2.89800
S	2.17400	0.00300	5.73600
H	-9.51700	-5.79300	3.13300
H	-10.04100	4.63300	-6.32100
H	-2.41400	11.40800	4.76600
H	2.28600	-11.35700	-5.02200
H	1.41300	-10.93500	-0.82900
H	9.89800	-4.74700	6.39100
H	9.76400	5.69700	-2.83600
C	6.01700	-2.34200	-3.74400
H	6.16800	-1.88500	-4.72700
H	6.97900	-2.70300	-3.36100
H	5.31300	-3.17900	-3.82500
C	4.54500	0.03700	-6.51000
H	4.53300	0.83800	-7.25900
H	5.08200	0.37800	-5.61800
H	5.06400	-0.83600	-6.92500
C	3.40400	4.90500	-4.97000
H	4.31200	4.29400	-4.93900
H	3.19800	5.21000	-6.00300
H	3.54200	5.79600	-4.34600
C	5.89900	4.38200	-1.20800
H	6.89500	4.43500	-0.75200
H	5.93800	4.78800	-2.22500
H	5.19000	4.95700	-0.60100
C	3.92000	-6.23200	-1.55700

H	4.29700	-5.94300	-0.56900
H	3.24300	-7.08700	-1.47000
H	4.76300	-6.50200	-2.20500
C	1.07500	-7.30800	1.23100
H	0.64800	-8.22300	1.66200
H	1.67700	-7.56200	0.35400
H	1.70300	-6.81200	1.98000
C	-4.25400	-5.14200	-3.40600
H	-3.62500	-5.71200	-4.09700
H	-5.14300	-5.73400	-3.15300
H	-4.56700	-4.19900	-3.86800
C	-1.34000	-3.87400	-6.23500
H	-0.88800	-3.93500	-7.23400
H	-1.76300	-4.84800	-5.96700
H	-2.12100	-3.10600	-6.23600
C	-7.03300	-0.94800	-2.30500
H	-7.04400	-1.26100	-1.25400
H	-7.37600	0.08800	-2.38300
H	-7.69500	-1.60100	-2.88900
C	-6.94500	2.85400	-0.80800
H	-7.41100	2.50600	-1.73500
H	-7.01100	2.08100	-0.03400
H	-7.46200	3.75900	-0.46200
C	-1.92700	1.14700	-7.30800
H	-1.71400	0.48800	-8.16000
H	-2.83800	1.72100	-7.50700
H	-1.08200	1.82700	-7.16100
C	-1.69100	4.82100	-5.58800
H	-0.63200	4.60200	-5.76800
H	-2.32100	4.24700	-6.27500
H	-1.87300	5.89400	-5.73800
C	4.24800	5.15700	3.34100

H	5.14000	5.74000	3.07500
H	3.62800	5.74000	4.03000
H	4.55700	4.21700	3.81100
C	-1.08200	7.35600	-1.28000
H	-1.64900	7.64700	-0.39100
H	-0.66100	8.25200	-1.75500
H	-1.74200	6.84400	-1.99000
C	-3.94400	6.24300	1.47700
H	-3.27000	7.09500	1.35300
H	-4.34300	5.92900	0.50500
H	-4.77300	6.53000	2.13600
C	1.34300	3.99500	6.17100
H	2.11900	3.22200	6.16900
H	1.76700	4.96200	5.88000
H	0.91200	4.07400	7.17700
C	-3.74500	-4.97100	4.69300
H	-3.68100	-5.25200	5.75100
H	-4.60900	-4.31700	4.53800
H	-3.85300	-5.87400	4.08100
C	-5.92400	-4.38700	1.14700
H	-5.25400	-4.93800	0.47800
H	-5.88000	-4.81400	2.15400
H	-6.95200	-4.44900	0.76700
C	-6.02300	2.37900	3.76400
H	-6.98800	2.74400	3.39200
H	-6.16500	1.92400	4.75000
H	-5.31700	3.21400	3.83400
C	-4.45900	0.18400	6.57300
H	-5.09100	-0.18800	5.76000
H	-4.51400	-0.50800	7.42100
H	-4.81900	1.17200	6.88600
C	1.86100	-0.99900	7.26400

H	2.73200	-1.63100	7.47100
H	1.69900	-0.31100	8.10400
H	0.97000	-1.62100	7.13400
C	1.56600	-4.71700	5.61800
H	1.74500	-5.78500	5.79800
H	2.19500	-4.12600	6.29100
H	0.50700	-4.49400	5.79100
C	7.02500	0.91100	2.24400
H	7.69600	1.58500	2.79000
H	7.36500	-0.12200	2.36300
H	7.02700	1.17700	1.18100
C	6.88500	-2.91600	0.83700
H	6.98200	-2.14200	0.06800
H	7.34800	-2.58400	1.77100
H	7.38000	-3.83300	0.49300

Coordinates for $Ag_{44}(4\text{-FTP})_6(SMe)_{24}^{4-}$: three staple opened

Ag	0.43500	-1.94600	-2.06000
Ag	-1.41600	0.27200	-2.26200
Ag	-0.35100	2.51100	-0.82700
Ag	2.17300	1.63300	0.30400
Ag	2.59900	-1.10300	-0.37200
Ag	1.42200	0.73900	-2.28200
Ag	3.02000	-1.50800	-3.14300
Ag	0.15500	-0.58600	-4.48300
Ag	-0.36900	2.52200	-3.65900
Ag	2.08500	3.49700	-1.86000
Ag	4.19100	0.88600	-1.59800
Ag	-2.14400	5.03300	-3.53300
Ag	-3.15300	2.68300	-4.96300
Ag	4.71500	0.55900	-4.56400

Ag	6.02900	-1.25800	-2.65400
Ag	2.37500	-3.84800	-1.02500
Ag	3.09700	-2.83600	1.87100
Ag	4.30900	0.22600	1.49700
Ag	2.41100	2.10100	3.13900
Ag	-0.04300	3.25800	4.28400
Ag	4.14100	5.29900	2.19800
Ag	1.14000	4.13800	1.09100
C	8.17000	1.61800	-4.92300
H	7.18300	2.07000	-4.83500
C	-4.79300	5.75500	-5.82000
C	8.27000	0.21200	-5.03300
C	4.69500	8.39700	3.80000
C	5.18400	9.36600	4.71500
H	5.82300	9.03500	5.53400
C	-5.21800	6.56400	-4.74100
H	-4.52600	6.75500	-3.92100
C	9.56200	-0.35000	-5.14600
H	9.66200	-1.43100	-5.23200
C	4.86800	10.72400	4.59500
H	5.24900	11.45900	5.30500
C	10.71100	0.45300	-5.14900
C	3.86600	8.87000	2.75100
H	3.47800	8.14900	2.03100
C	10.56600	1.83600	-5.03500
C	4.04900	11.13800	3.54500
C	9.31100	2.43300	-4.92000
H	9.22900	3.51400	-4.82800
C	-5.71400	5.51400	-6.86600
H	-5.40800	4.88900	-7.70400

C	-7.38200	6.85100	-5.75800
C	-7.00500	6.05800	-6.84200
C	-6.50800	7.11100	-4.70200
C	3.54100	10.22600	2.61900
F	-8.64400	7.38900	-5.73200
F	11.68800	2.62600	-5.04000
F	3.73700	12.47500	3.42100
S	4.81900	-1.56400	3.46300
S	3.19900	-5.37600	1.07900
S	6.28800	-0.17800	-0.33700
S	4.65200	-3.48100	-2.42800
S	1.18200	-5.59500	-2.87700
S	-1.70800	-3.01500	-5.85700
S	-1.16100	1.25700	-5.85200
S	-3.13000	5.11400	-5.93800
S	0.47500	5.02000	-3.44500
S	3.07100	5.36000	-0.14400
S	5.14200	6.69900	4.01600
S	4.84700	2.72400	2.40900
S	6.84000	-0.85700	-5.10400
S	4.19300	2.81200	-3.43300
S	2.60000	-0.62500	-5.60100
Ag	-0.18400	1.72000	1.84600
Ag	1.60400	-0.47400	2.20800
Ag	0.49000	-2.68500	0.72000
Ag	-1.96700	-1.88000	-0.49500
Ag	-2.45600	0.85500	0.33400
Ag	-1.25500	-0.94000	2.13200
Ag	-2.61000	1.57900	3.17900
Ag	-0.13800	0.32300	4.33500

Ag	0.43100	-2.72300	3.55800
Ag	-1.99300	-3.70500	1.66200
Ag	-3.95100	-1.31700	1.53300
Ag	2.20200	-5.22300	3.46100
Ag	3.11600	-2.80800	4.91300
Ag	-3.07400	-0.92400	4.53300
Ag	-6.75800	1.62000	2.38400
Ag	-2.37100	3.59100	0.87700
Ag	-2.99400	2.59500	-1.90900
Ag	-4.16100	-0.39600	-1.53000
Ag	-2.17400	-2.20600	-3.35400
Ag	-0.11700	-4.02600	-4.26600
Ag	-4.80000	-5.42900	-1.85200
Ag	-0.65100	-4.38300	-1.28300
C	-10.47900	2.69300	5.33400
H	-11.14700	1.83500	5.27700
C	4.83200	-5.81600	5.79800
C	-9.31700	2.70800	4.51700
C	-6.46000	-8.46700	-2.45800
C	-7.38800	-9.40700	-2.97800
H	-8.20200	-9.04500	-3.60600
C	5.31100	-6.62700	4.74400
H	4.64000	-6.87200	3.92100
C	-8.47500	3.84300	4.62500
H	-7.57700	3.88300	4.00800
C	-7.28500	-10.77700	-2.70800
H	-8.00400	-11.48900	-3.11300
C	-8.76500	4.90100	5.49600
C	-5.41700	-8.98000	-1.64600
H	-4.69100	-8.28100	-1.23200

C	-9.91800	4.83800	6.27800
C	-6.23900	-11.23100	-1.90400
C	-10.78200	3.74400	6.20800
H	-11.67600	3.72100	6.83100
C	5.72600	-5.50300	6.84900
H	5.37800	-4.87200	7.66600
C	7.47400	-6.77900	5.79400
C	7.04300	-5.98000	6.85300
C	6.62800	-7.10900	4.73500
H	6.99600	-7.72700	3.91800
C	-5.30200	-10.34800	-1.36800
F	8.76200	-7.25200	5.79500
F	-10.21300	5.87400	7.13700
F	-6.13300	-12.57900	-1.63600
S	-4.77000	1.37100	-3.48200
S	-3.13400	5.18000	-1.15700
S	-5.94700	-0.07300	0.49700
S	-4.60400	3.07900	2.34500
S	-0.81600	4.97500	2.62900
S	1.83000	2.41400	5.71900
S	1.05700	-1.45800	5.82600
S	3.13800	-5.25500	5.87900
S	-0.42300	-5.20600	3.29500
S	-2.76700	-5.43100	-0.25100
S	-6.65900	-6.75100	-2.84800
S	-4.58000	-2.84900	-2.54900
S	-9.00100	1.34700	3.42900
S	-3.96600	-3.02600	3.59100
S	-2.78300	1.18900	5.82700
H	2.90200	10.57500	1.80800

H	11.70600	0.01800	-5.23400
H	7.73200	-5.73400	7.66000
H	-7.71400	5.86800	-7.64600
H	-6.83500	7.72600	-3.86500
H	-8.10500	5.76500	5.57000
H	-4.49500	-10.72700	-0.74200
C	-5.70200	-2.53700	-3.99200
H	-5.52600	-3.28600	-4.77100
H	-6.74000	-2.61000	-3.64700
H	-5.51200	-1.53200	-4.38400
C	-2.97600	-4.36700	-6.01500
H	-2.53300	-5.24300	-6.50600
H	-3.37200	-4.65700	-5.03600
H	-3.79700	-3.98400	-6.63300
C	0.47100	-7.31000	-2.94800
H	-0.62200	-7.27900	-2.93600
H	0.81700	-7.81100	-3.86100
H	0.83100	-7.86100	-2.07100
C	-2.33700	-7.11200	0.39600
H	-3.19900	-7.51000	0.94500
H	-2.08500	-7.78400	-0.43200
H	-1.48500	-7.02000	1.07900
C	-6.37100	2.24100	-3.13900
H	-6.59200	2.18300	-2.06800
H	-6.31300	3.28600	-3.46000
H	-7.16500	1.73300	-3.70100
C	-4.97500	5.37300	-1.04000
H	-5.20200	6.42300	-0.81400
H	-5.45600	5.09000	-1.98000
H	-5.34300	4.73800	-0.22600

C	1.24000	5.33300	-5.10400
H	0.50100	5.18300	-5.89800
H	1.59700	6.37000	-5.13300
H	2.08800	4.65300	-5.24500
C	-0.17400	2.02700	-7.21600
H	-0.41000	1.50600	-8.15300
H	-0.43600	3.08600	-7.31200
H	0.89500	1.91800	-7.00100
C	5.65700	3.84900	-2.96100
H	5.37300	4.47400	-2.10700
H	6.50900	3.21900	-2.68900
H	5.92900	4.49100	-3.81000
C	7.49500	1.22700	-0.24700
H	7.77500	1.55900	-1.25200
H	7.03800	2.05000	0.31300
H	8.39200	0.87900	0.28200
C	3.05500	-2.04500	-6.70400
H	2.61700	-1.86900	-7.69400
H	4.14600	-2.10200	-6.78900
H	2.66200	-2.98300	-6.29900
C	4.79100	-4.55400	-3.93200
H	3.83900	-5.07300	-4.08900
H	5.04300	-3.94600	-4.80700
H	5.58600	-5.29200	-3.76300
C	-1.21700	-5.55700	4.93200
H	-1.51600	-6.61300	4.95500
H	-0.50900	-5.36200	5.74400
H	-2.10500	-4.92400	5.04300
C	5.02900	-5.64800	0.95000
H	5.54100	-5.30000	1.85100

H	5.21800	-6.72100	0.81300
H	5.39900	-5.09800	0.07600
C	6.42700	-2.46100	3.24500
H	6.30300	-3.52700	3.45800
H	6.77300	-2.31600	2.21600
H	7.16000	-2.03600	3.94200
C	0.06700	-2.29600	7.14900
H	-0.96900	-2.43400	6.82200
H	0.52000	-3.26800	7.37300
H	0.08300	-1.66500	8.04500
C	-0.65200	6.74500	3.17000
H	-1.37800	6.95300	3.96500
H	0.36300	6.92800	3.53500
H	-0.85900	7.39100	2.30800
C	2.33400	7.00200	-0.58800
H	1.65300	6.85800	-1.43600
H	1.78100	7.42000	0.26000
H	3.14300	7.68600	-0.87300
C	5.79800	2.52800	3.99000
H	6.87000	2.59500	3.76500
H	5.52400	3.32600	4.68700
H	5.57500	1.55000	4.43100
C	2.66900	4.02300	6.14400
H	2.91100	4.61500	5.25600
H	2.02500	4.60900	6.81100
H	3.60100	3.78000	6.66900
C	-4.54500	1.68200	6.16600
H	-5.13300	1.71900	5.24300
H	-4.99900	0.96400	6.85900
H	-4.53300	2.67500	6.63100

C	-4.65300	4.48300	3.55200
H	-5.33400	5.25600	3.17400
H	-4.99700	4.13900	4.53300
H	-3.64300	4.89900	3.64200
C	-5.78500	-3.17400	3.95000
H	-5.92000	-3.52100	4.98200
H	-6.28700	-2.21200	3.81400
H	-6.20900	-3.91000	3.25700
C	-7.23400	-1.37800	0.21200
H	-6.80600	-2.17200	-0.41100
H	-7.57300	-1.79100	1.16800
H	-8.08400	-0.92000	-0.30700