

## Supporting Information

# Linker Driven Site-specific Catalysis in Atomically Precise Silver Cluster-Assemblies

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## 1. Experimental Section

### Materials

Silver nitrate ( $\text{AgNO}_3$ ), cyclohexane thiol (HSCy), silver trifluoroacetate ( $\text{AgCF}_3\text{COO}$ ) (98%), pyrazine (99%), 4,4'-Bipyridine (98%), 1,2-Bis(4-pyridyl)ethane (99%), 4,4'-Azopyridine, trifluoroacetic acid ( $\text{CF}_3\text{COOH}$ ) were purchased from Sigma-Aldrich. The HPLC-grade solvents dimethylformamide (DMF), acetonitrile ( $\text{CH}_3\text{CN}$ ), chloroform ( $\text{CH}_2\text{Cl}_2$ ), pyridine, and triethyl amine ( $\text{Et}_3\text{N}$ ) were purchased from Spectrochem Pvt. Ltd. All the chemicals and solvents procured were utilized without further purification.

### Methods

Optical microscope images were captured on a Leica microscope with an MC170 HD camera. Powder XRD for the crystal samples were recorded on a Bruker D8 Advance X-ray diffractometer ( $2\theta$  from  $5^\circ$  to  $50^\circ$ ) with  $\text{Cu-K}\alpha$  X-ray source ( $\lambda = 1.5418 \text{ \AA}$ ). The temperature dependent PXRD was done using PANalytical ( $\text{Cu K}\alpha$  radiation,  $\lambda_{\text{avg}} \approx 1.54060 \text{ \AA}$ ) diffractometer, the material was mounted on a glass slide, except for  $\text{Ag}_{12}$ -azopy which was done using Bruker D8. The samples were subjected to a temperature ramp from room temperature (RT) to the target temperature over a duration of 3 hours, followed by heating at the target temperature for 2 hours. Subsequently, the samples were allowed to cool down over a period of 3 hours. Scanning electron microscopic (SEM) images and Energy Dispersive X-ray Spectra (EDS) were obtained using Nova NANOSEM 450 scanning electron microscope for surface morphology and elemental analysis, respectively. The crystals were handpicked and mounted on a carbon tape for the analysis. X-ray photoelectron spectroscopy (XPS) measurements were performed using the Omicron Nanotech instrument with a  $\text{Mg K}\alpha$  X-ray source, and casaXPS software was used for data deconvolution. The carbon correction with respect to 284.8 eV was done before plotting. Thermogravimetric analysis were done using an SDT Q600 analyzer by Shimadzu. The samples were heated at a rate of  $10^\circ\text{C}/\text{min}$  up to  $500^\circ\text{C}$  under a constant flow of nitrogen ( $\text{N}_2$ ).

### Single-Crystal X-ray Diffraction:

**$\text{Ag}_{12}$ -pyz:** The Bruker D8 Quest - Microfocus SCXRD (single crystal X-ray diffractometer) with Bruker PHOTON III C14, CPAD detector was used to collect the single crystal data.  $\text{MoK}\alpha$  ( $\lambda = 0.71073 \text{ \AA}$ ) was the radiation source for the experiment. The frames were integrated with the Bruker SAINTS software package using a narrow-frame algorithm. The crystal structure was solved and refined by SHELXTL software package.<sup>1,2,3,4</sup>

A solvent mask was calculated and 298 electrons were found in a volume of  $1048 \text{ \AA}^3$  in one void per unit cell. This is consistent with  $7.5[\text{H}_2\text{O}]$  per formula unit, which accounts for 75 electrons per unit cell.

### **$\text{Ag}_{12}$ -bpy, $\text{Ag}_{12}$ -bpa, $\text{Ag}_{12}$ -azopy:**

Data collection was conducted at the X-ray diffraction beamline (XRD1) of the Elettra Synchrotron (Trieste, Italy).<sup>5</sup> The crystals were immersed in NHV oil (Jena Bioscience, Jena, Germany) and mounted on the goniometer head using nylon loops (MiTeGen, Ithaca, USA). Complete datasets were obtained at 100 K using a nitrogen stream supplied by an Oxford Cryostream 700. Data acquisition employed a monochromatic wavelength of 0.70 Å, utilizing the rotating crystal method on a Pilatus 2M hybrid-pixel area detector (DECTRIS Ltd., Baden-Daettwil, Switzerland). The diffraction data were indexed and integrated with XDS.<sup>6</sup> The structure was solved with the SHELXT<sup>7</sup> structure solution program using Intrinsic Phasing and refined using the SHELXL<sup>8</sup> refinement package through Least Squares minimization, all within the Olex2 software environment.<sup>9</sup> PLATON SQUEEZE<sup>10</sup> was applied during the final refinements to remove density mess from randomly oriented solvent molecules. All non-hydrogen atoms were refined anisotropically and hydrogen atoms were (positioned geometrically) refined isotropically using an olex2.<sup>9</sup>

### **Density functional theory (DFT) calculations:**

All DFT calculations of the studied cluster model were carried out in the Gaussian 16 package.<sup>11</sup> The PBE exchange-correlation (XC) functional was applied under the generalized gradient approximation (GGA).<sup>12</sup> A standard 6-31G(d) basis set was employed for C, N, O, F, S, and H, while the effective core potential SDD basis set was used for Ag.<sup>13</sup> The atom positions in all systems underwent complete optimization without constraints, and subsequently, frequency calculations were conducted to confirm the absence of imaginary frequencies.

### **Electrochemical Studies:**

All the electrochemical experiments were conducted using the electrochemical analyzer AURT-M204. Three electrode systems with graphite rods, saturated calomel electrode (SCE), and the catalyst coated on carbon cloth were used for all the electrocatalytic experiments. 0.5 M H<sub>2</sub>SO<sub>4</sub> prepared with DI water was used as the electrolyte. 3 mg of catalyst, 750 μL of DI water, 200 μL of ethanol, and 50 μL of Nafion binder solution were mixed for the preparation of catalyst ink, which was then drop-casted on carbon cloth (Catalyst loading = 0.1045 mg). LSV polarization analysis was done at a scan rate of 5 mV s<sup>-1</sup> and all the polarization curves were 100 % iR corrected. EIS studies were done in the frequency window of 0.1 Hz to 100 Hz with an applied potential of 350 mV. Inductively coupled plasma-mass spectrometry (ICP-MS) data were collected using iCAP RQ instrument from ThermoScientific.

## Synthesis:

**Synthesis of Ag<sub>12</sub>-py cluster:** The synthesis procedure is similar to the earlier reported NC-1 from our group.<sup>14</sup>

To the solution containing 0.1 mmol of the (Ag-SCy)<sub>n</sub> complex in 4 mL CH<sub>3</sub>CN, 0.2 mmol of AgCF<sub>3</sub>COO was added and sonicated until fully soluble. Subsequent dropwise addition of 0.6 mmol of pyridine in 2 mL CHCl<sub>3</sub> to the previous mixture. The resulting solution was allowed to slowly evaporate under ambient conditions, yielding bulk transparent block-shaped crystals after a 4-day. These crystals were then washed with CHCl<sub>3</sub> and vacuum-dried and used in subsequent experiments. Yield = 37 % based on Ag.

**Synthesis of Ag<sub>12</sub>-pyz CAM:** 0.06 mmol of (Ag-SCy)<sub>n</sub> complex and 0.1 mmol of AgCF<sub>3</sub>COO were added to a vial containing 3 mL DMF solvent and sonicated until soluble and to the resultant clear solution was added dropwise 0.12 mmol pyrazine in 1 mL CH<sub>3</sub>CN solution. The resulting mixture was allowed to slowly evaporate in the dark to give bulk transparent crystals after 24 h. These crystals were then washed with DMF solvent and subjected to vacuum drying for further characterization. Yield = 95 % based on Ag.

**Synthesis of Ag<sub>12</sub>-bpy CAM:** 0.06 mmol of (Ag-SCy)<sub>n</sub> complex and 0.1 mmol of AgCF<sub>3</sub>COO were added to a vial containing 3 mL DMF solvent and kept for stirring, 0.038 mmol (6 mg) 4,4'-Bipyridine in 1.5 mL CH<sub>3</sub>CN solution was added to it. The resulting mixture was filtered after 1 h stirring at 250 rpm. The filtrate was allowed to slowly evaporate in the dark to give bulk transparent hexagonal crystals after 2 days. The crystals were washed with DMF solvent and the solvent was removed from the vial. The crystals were slowly dried for a day in ambient conditions and then vacuum-dried before further characterization. Yield = 20 % based on Ag.

**Synthesis of Ag<sub>12</sub>-bpa CAM:** 0.06 mmol of (Ag-SCy)<sub>n</sub> complex and 0.1 mmol of AgCF<sub>3</sub>COO were added to a vial containing 3 mL DMF solvent and sonicated until soluble and to the resultant clear solution was added dropwise 0.05 mmol 1,2-Bis(4-pyridyl)ethane in 1 mL CH<sub>3</sub>CN solution. The resulting mixture was allowed to slowly evaporate in the dark to give bulk transparent crystals after 24 h. The crystals were washed with DMF solvent before vacuum drying and used for further characterization. Yield = 98 % based on Ag.

**Synthesis of Ag<sub>12</sub>-azopy CAM:** 0.06 mmol of (Ag-SCy)<sub>n</sub> complex and 0.1 mmol of AgCF<sub>3</sub>COO were added to a vial containing 3 mL DMF solvent and sonicated until soluble and to the resultant clear solution was added dropwise 0.05 mmol 4,4'-Azopyridine in 1 mL DMF solution. The resulting mixture was allowed to slowly evaporate in the dark to give bulk orange crystals after 24 h. The crystals were washed with DMF solvent and subjected to vacuum drying for further characterization. Yield = 34 % based on Ag.

## 2. Crystallographic details

### 2.1. Table S1. Crystallographic parameters for Ag<sub>12</sub>-pyz.

Parameters	Ag <sub>12</sub> -pyz
CCDC number	2342609
Empirical formula	C <sub>10</sub> H <sub>15.5</sub> Ag <sub>2</sub> F <sub>3</sub> NO <sub>3.25</sub> S
Formula weight	506.53
Crystal System	cubic
Space Group	<i>Pn-3</i> (No. 201)
a (Å)	20.9199(3)
b (Å)	20.9199(3)
c (Å)	20.9199(3)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å <sup>3</sup> )	9155.4(4)
Z	24
Temperature (K)	100
Calculated density (g/cm <sup>3</sup> )	2.205
Absorption coefficient (mm <sup>-1</sup> )	2.714
2θ range (°)	5.806 to 54.964
Reflections collected	62054
Unique reflections	3516
Number of parameters	172
Goodness-of-fit on F <sup>2</sup>	1.032
Final R indices [I ≥ 2σ(I)]	R <sub>1</sub> = 0.0313, wR <sub>2</sub> = 0.0694
Final R indices (all data)	R <sub>1</sub> = 0.0341, wR <sub>2</sub> = 0.0716
$R_1 = \sum  F_o  -  F_c  / \sum  F_o ; wR_2 = \{ [w(F_o^2 - F_c^2)^2] / [w(F_o^2)] \}^{1/2}; w = 1 / [\sigma^2 (F_o)^2 + (aP)^2 + bP]; P = [\max(F_o^2, 0) + 2(F_c)^2] / 3, \text{ where } a = 0.0221 \text{ and } b = 23.72$	

2.2. Table S2. Crystallographic parameters for Ag<sub>12</sub>-bpy.

Parameters	Ag <sub>12</sub> -bpy
CCDC number	2379538
Empirical formula	C <sub>39</sub> H <sub>45</sub> Ag <sub>6</sub> F <sub>9</sub> N <sub>3</sub> O <sub>6</sub> S <sub>3</sub>
Formula weight	1566.18
Crystal System	orthorhombic
Space Group	<i>P n n m</i> (No. 58)
a (Å)	22.946(5)
b (Å)	27.850(6)
c (Å)	18.982(4)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å <sup>3</sup> )	12130(4)
Z	8
Temperature (K)	100
Calculated density (g/cm <sup>3</sup> )	1.715
Absorption coefficient (mm <sup>-1</sup> )	1.992
2θ range (°)	2.264 to 51.888
Reflections collected	157382
Unique reflections	12774
Number of parameters	632
Goodness-of-fit on F <sup>2</sup>	1.127
Final R indices [I ≥ 2σ(I)]	R <sub>1</sub> = 0.0920, wR <sub>2</sub> = 0.2806
Final R indices (all data)	R <sub>1</sub> = 0.1071, wR <sub>2</sub> = 0.2955
$R_1 = \sum   F_0  -  F_c   / \sum  F_0 ; wR_2 = \{ [\sum w(F_0^2 - F_c^2)^2] / [\sum w(F_0^2)^2] \}^{1/2}; w = 1/[\sigma^2 (F_0)^2 + (aP)^2 + bP]; P = [\max(F_0^2, 0) + 2(F_c)^2] / 3, \text{ where } a = 0.1364 \text{ and } b = 41.42$	

2.3. Table S3. Crystallographic parameters for Ag<sub>12</sub>-bpa.

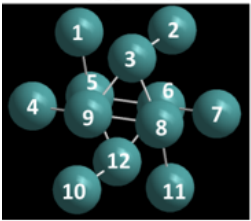
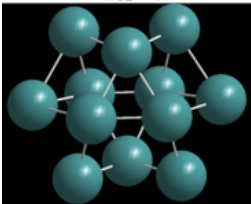
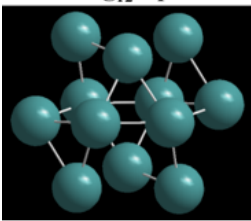
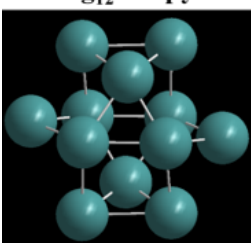
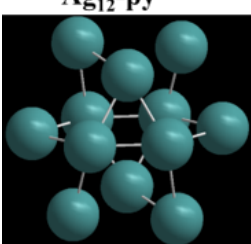
Parameters	Ag <sub>12</sub> -bpa
CCDC number	2379540
Empirical formula	C <sub>45</sub> H <sub>58</sub> Ag <sub>6</sub> F <sub>9</sub> N <sub>4</sub> O <sub>7</sub> S <sub>3</sub>
Formula weight	1681.35
Crystal System	monoclinic
Space Group	C 2/c (No. 15)
a (Å)	25.337(5)
b (Å)	24.666(5)
c (Å)	19.661(4)
α (°)	90
β (°)	109.96(3)
γ (°)	90
Volume (Å <sup>3</sup> )	11549(4)
Z	8
Temperature (K)	100
Calculated density (g/cm <sup>3</sup> )	1.934
Absorption coefficient (mm <sup>-1</sup> )	2.101
2θ range (°)	2.342 to 59.81
Reflections collected	92731
Unique reflections	17230
Number of parameters	733
Goodness-of-fit on F <sup>2</sup>	1.005
Final R indices [I ≥ 2σ(I)]	R <sub>1</sub> = 0.0399, wR <sub>2</sub> = 0.1114
Final R indices (all data)	R <sub>1</sub> = 0.0439, wR <sub>2</sub> = 0.1144
$R_1 = \frac{\sum   F_o  -  F_c  }{\sum  F_o }; wR_2 = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)]} \right\}^{1/2}; w = 1/[\sigma^2(F_o)^2 + (aP)^2 + bP]; P = [\max(F_o^2, 0) + 2(F_c)^2]/3, \text{ where } a = 0.0532 \text{ and } b = 32.72$	



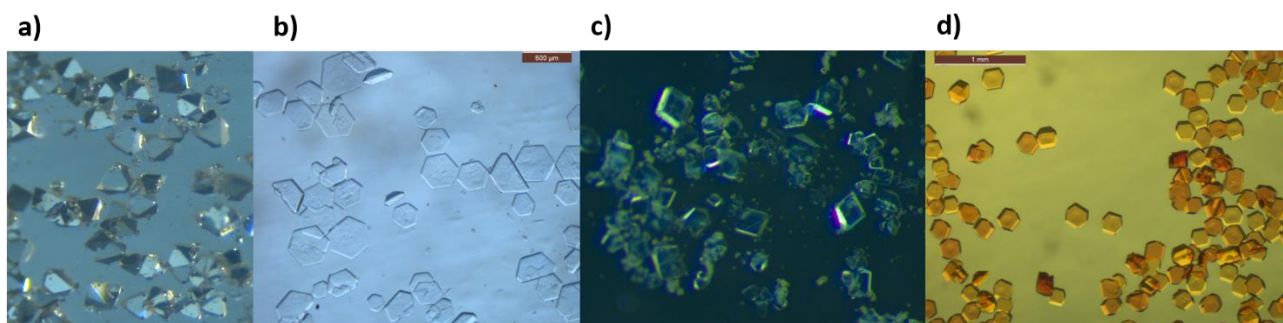
2.4. Table S4. Crystallographic parameters for Ag<sub>12</sub>-azopy.

Parameters	Ag <sub>12</sub> -azopy
CCDC number	2379541
Empirical formula	C <sub>42</sub> H <sub>52</sub> Ag <sub>6</sub> F <sub>9</sub> N <sub>7</sub> O <sub>7</sub> S <sub>3</sub>
Formula weight	1681.30
Crystal System	monoclinic
Space Group	C 2/c (No. 15)
a (Å)	26.994(5)
b (Å)	14.021(3)
c (Å)	29.259(6)
α (°)	90
β (°)	92.57(3)
γ (°)	90
Volume (Å <sup>3</sup> )	11063(4)
Z	8
Temperature (K)	90
Calculated density (g/cm <sup>3</sup> )	2.019
Absorption coefficient (mm <sup>-1</sup> )	2.195
2θ range (°)	3.224 to 49.996
Reflections collected	61389
Unique reflections	9951
Number of parameters	686
Goodness-of-fit on F <sup>2</sup>	1.068
Final R indices [I >= 2sigma(I)]	R <sub>1</sub> = 0.0626, wR <sub>2</sub> = 0.1860
Final R indices (all data)	R <sub>1</sub> = 0.0680, wR <sub>2</sub> = 0.1931
$R_1 = \sum   F_o  -  F_c   / \sum  F_o ; wR_2 = \{ [\sum w(F_o^2 - F_c^2)^2] / [\sum w(F_o^2)^2] \}^{1/2}; w = 1/[\sigma^2 (F_o)^2 + (aP)^2 + bP]; P = [\max(F_o^2, 0) + 2(F_c)^2] / 3, \text{ where } a = 0.1172 \text{ and } b = 71.45$	

2.5. Table S5. Table showing all possible Ag...Ag interactions in the 5 assemblies.

	Ag <sub>12</sub> -pyz (Å)	Ag <sub>12</sub> -bpy (Å)	Ag <sub>12</sub> -bpa (Å)	Ag <sub>12</sub> -azopy (Å)	Ag <sub>12</sub> -py (Å)
			1-2: 3.19		
	1-3: 2.92	1-3: 3.40	1-3: 3.16	1-3 : 3.03	1-3: 3.21
		1-4: 3.35			
		1-5: 3.32	1-5: 3.28	1-5: 3.30	1-5: 3.38
	2-6: 2.92	2-6: 3.18		2-6: 3.19	2-6: 3.08
				2-7 :3.38	
		3-2: 2.96	3-2:3.04	3-2: 3.18	
	3-9: 2.95	3-9: 3.03	3-9: 3.00	3-9: 2.94	3-9: 3.03
	3-8: 2.95	3-8: 2.97	3-8: 2.99	3-8: 3.14	3-8: 2.98
	4-5: 2.92	4-5: 3.07	4-5: 3.06	4-5: 3.35	4-5: 3.21
		4-9: 3.27	4-9: 3.15	4-9: 3.04	4-9: 3.10
				4-10: 3.38	
	5-6: 2.95	5-6: 3.09	5-6: 3.06	5-6: 3.03	5-6: 2.91
	5-12: 2.95	5-12: 2.74	5-12:2.99	5-12: 3.14	5-12: 2.98
	6-12: 2.95	6-12: 3.09	6-12: 3.00	6-12: 2.94	6-12: 3.03
		7-6: 3.18	7-6: 3.15	7-6: 3.04	7-6: 3.10
	7-8: 2.92	8-7: 2.96	7-8: 3.06	7-8: 3.35	7-8: 3.21
	8-9: 2.95	8-9: 3.03	8-9: 3.06	8-9: 3.03	8-9: 2.91
		8-11: 3.40	8-11: 3.28	8-11: 3.30	8-11: 3.39
	9-10: 2.92	9-10: 3.27		9-10: 3.19	9-10: 3.08
		10-11: 3.35	10-11: 3.19		
		10-12: 3.07	10-12: 3.04	10-12: 3.18	
	11-12: 2.92	11-12:3.32	11-12: 3.16	11-12: 3.03	11-12: 3.21
<b>Argentophilic Interactions</b>	<b>12</b>	<b>20</b>	<b>18</b>	<b>20</b>	<b>16</b>
~Ag...Ag distance	<b>2.93</b>	<b>3.15</b>	<b>3.10</b>	<b>3.15</b>	<b>3.11</b>
~ Ag-S distance	<b>2.51</b>	<b>2.47</b>	<b>2.49</b>	<b>2.48</b>	<b>2.49</b>

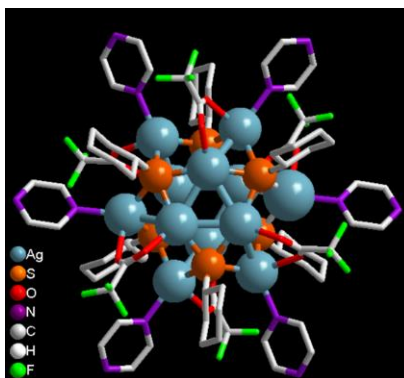
### 3. Optical microscopic images



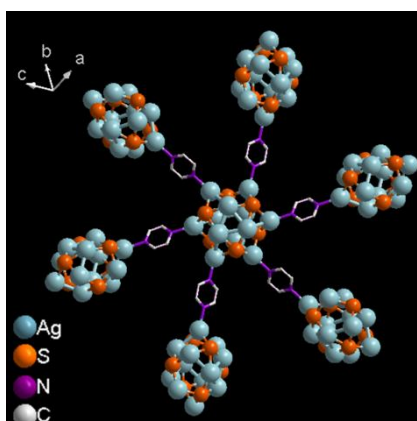
**Figure S1.** Optical microscopic image of a) Ag<sub>12</sub>-pyz, b) Ag<sub>12</sub>-bpy, c) Ag<sub>12</sub>-bpa, d) Ag<sub>12</sub>-azopy crystals.

## 4. Crystal structure

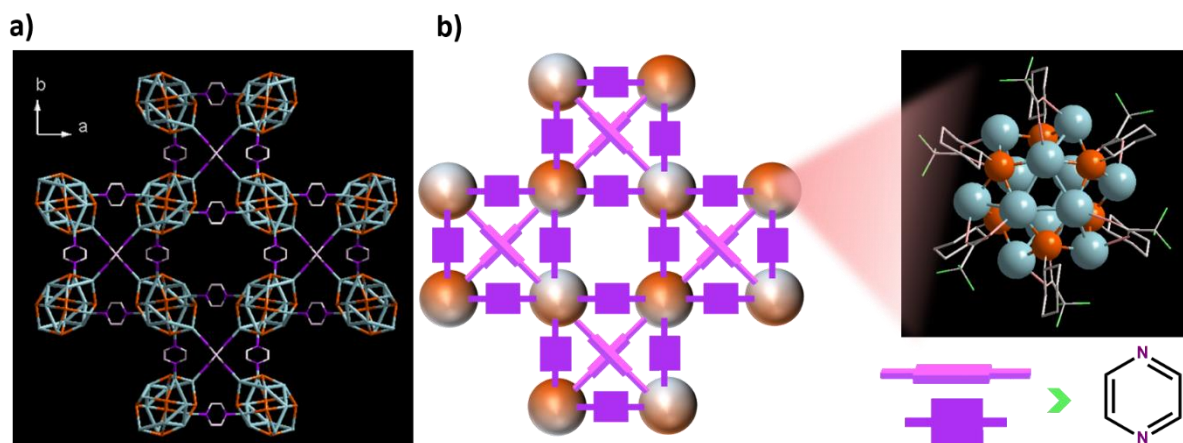
### 4.1. Crystal structure of Ag<sub>12</sub>-pyz



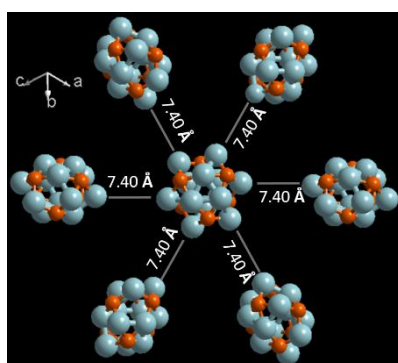
**Figure S2.** Schematic representation of the Ag<sub>12</sub> cluster surrounded by SCy<sup>-</sup> & CF<sub>3</sub>COO<sup>-</sup> ligands and pyrazine linker in Ag<sub>12</sub>-pyz CAM. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey. H atoms and disorder atoms are omitted for clarity.



**Figure S3.** a) Each cluster connects to six other clusters with the bidentate pyrazine linker. Color code: Ag: blue, S: orange, N: violet, C: grey.

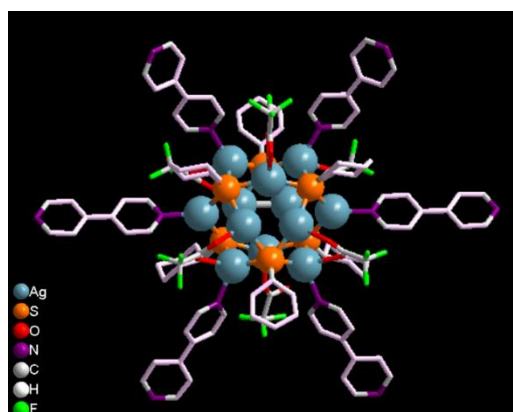


**Figure S4.** (a) Small unit of three-dimensionally extended Ag<sub>12</sub>-pyz CAM (along *c* direction), (b) Topology view of the same. Color code: Ag: blue, S: orange, N: violet, O: red, F: green C: grey.

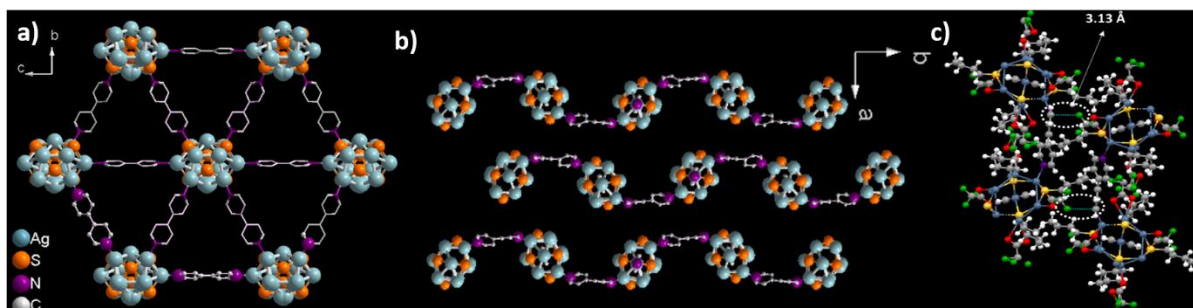


**Figure S5.** The shortest Ag ... Ag distance between two clusters in 7.40 Å. Color code: Ag: blue, S: orange.

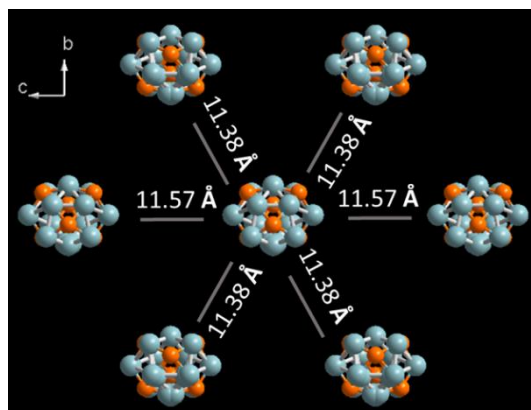
## 4.2. Crystal structure of Ag<sub>12</sub>-bpy



**Figure S6.** Schematic representation of the Ag<sub>12</sub> cluster surrounded by SCy<sup>-</sup> & CF<sub>3</sub>COO<sup>-</sup> ligands and 4,4'-Bipyridine linker. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey.

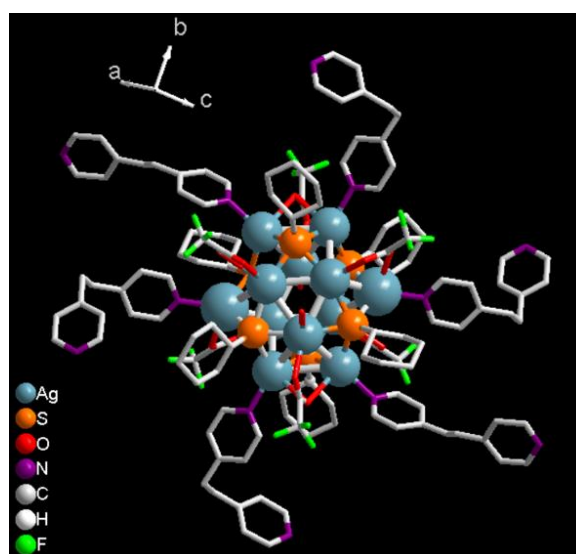


**Figure S7.** Each cluster connects to six other clusters with the bidentate 4,4'-Bipyridine linker and extends in two-dimension, b) the stacked 2D layers viewed along *ab* plane, c) These layers are connected by F...C interactions (3.13 Å). These interactions are studied using mercury software. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey.

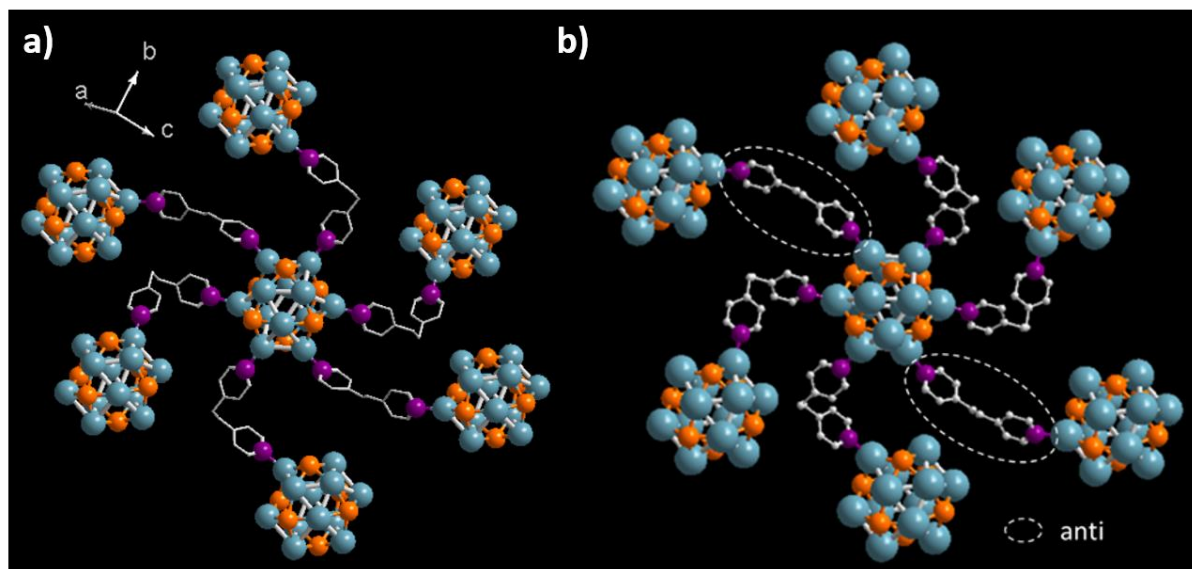


**Figure S8.** The shortest Ag ... Ag distance between two clusters in *bc* plane 11.38 & 11.57 Å. Color code: Ag: blue, S: orange.

#### 4.3. Crystal structure of Ag<sub>12</sub>-bpa

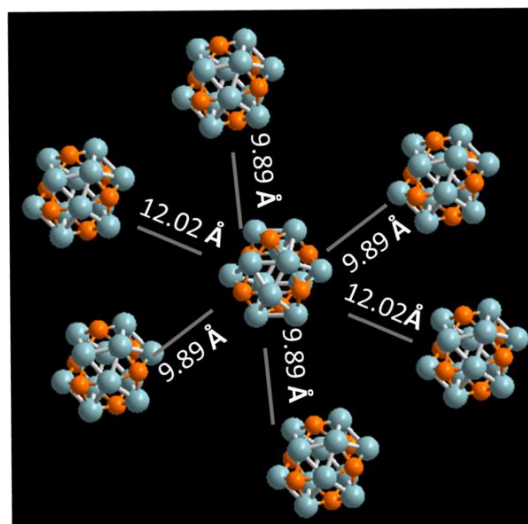


**Figure S9.** Schematic representation of the Ag<sub>12</sub> cluster surrounded by SCy<sup>-</sup> & CF<sub>3</sub>COO<sup>-</sup> ligands and 1,2-Bis(4-pyridyl)ethane linker. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey.



**Figure S10.** a) Each cluster connects to six other clusters with the bidentate bpa linker, b) Schematic representation of  $\text{Ag}_{12}$ -bpa CAM showing the anti-gauche conformations of bpa linker. The white dotted circle represents the anti-conformation of the bpa linker, the remaining four linkers are in gauche conformation. Color code: Ag: blue, S: orange, N: violet, C: grey.

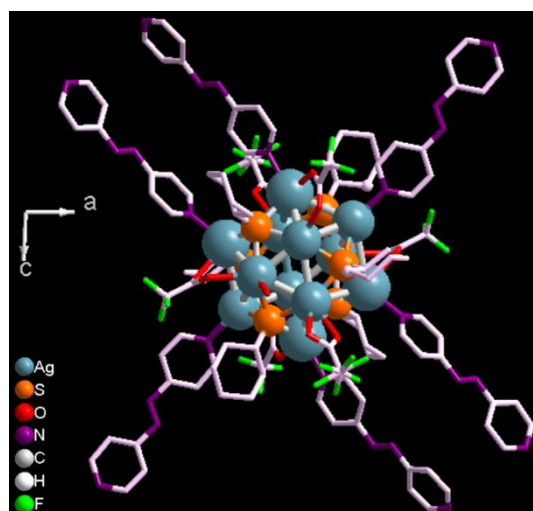
Bpa linker with its flexibility (conferred by its  $-\text{CH}_2-\text{CH}_2-$  backbone) can adopt anti and gauche conformations, here out of six linkers, four are in gauche and two are in anti-conformations. This flexibility in bpa linker has led to its 3D structure.



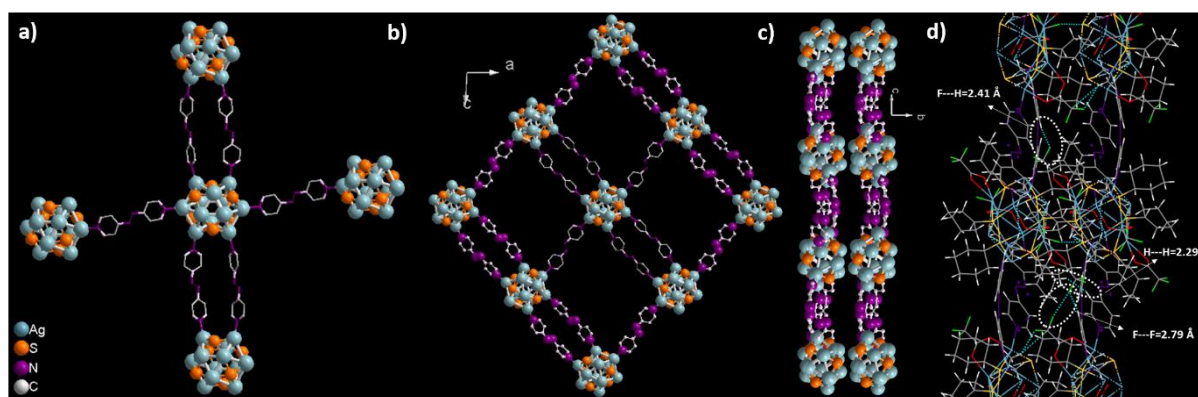
**Figure S11.** The shortest Ag ... Ag distance between two clusters is 9.89 & 12.02 Å. Color code: Ag: blue, S: orange.



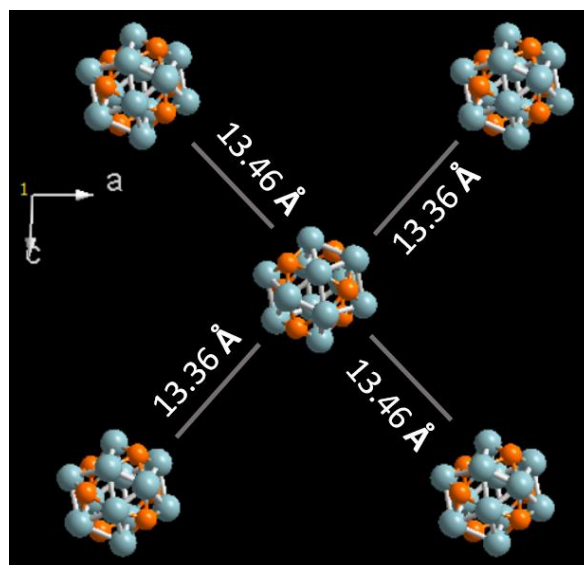
#### 4.4. Crystal structure of Ag<sub>12</sub>-azopy



**Figure S12.** Schematic representation of the Ag<sub>12</sub> cluster surrounded by SCy<sup>-</sup> & CF<sub>3</sub>COO<sup>-</sup> ligands and 4,4'-Azopyridine linker. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey.

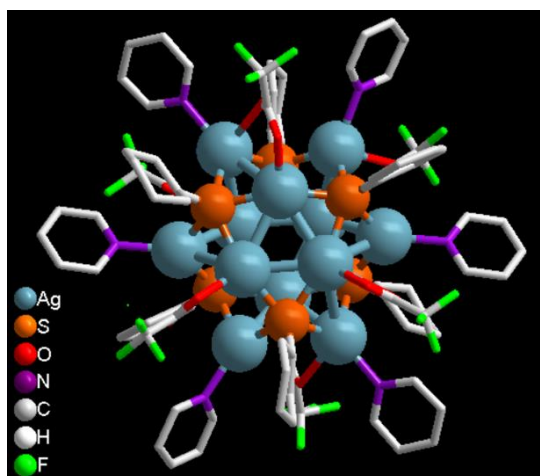


**Figure S13.** a) Each cluster connects to six other clusters with the bidentate azo-py linker and, b) extends in two-dimension, c) The 2D stacked layers are viewed along *bc* plane, d) These layers are connected by F---F (2.79 Å), F---H (2.41 Å), and H---H (2.29 Å) interactions. Two DMF molecules also show H---H (2.26 Å) interactions between them. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey.



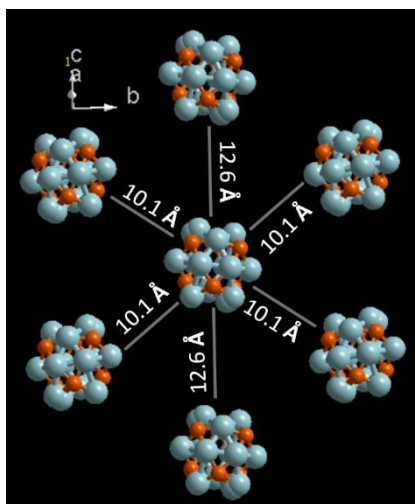
**Figure S14.** The shortest Ag ... Ag distance between two clusters in *ac* plane 13.36 & 13.46 Å. Color code: Ag: blue, S: orange.

#### 4.5. Crystal structure of Ag<sub>12</sub>-py



**Figure S15.** a) Schematic representation of the Ag<sub>12</sub> cluster surrounded by SCy- & CF<sub>3</sub>COO- ligands and pyridine ligand. Color code: Ag: blue, S: orange, O: red, F: green, N: violet, C: grey.

Note: This crystal structure was earlier reported by us<sup>14</sup>. We have redrawn using the same crystal structure.



**Figure S16.** The shortest Ag ... Ag distance between two clusters in *bc* plane is 10.1 & 12.6 Å. Color code: Ag: blue, S: orange.

**Table S6.** Table showing Ag...Ag inter/intra cluster distance in the five cluster assemblies

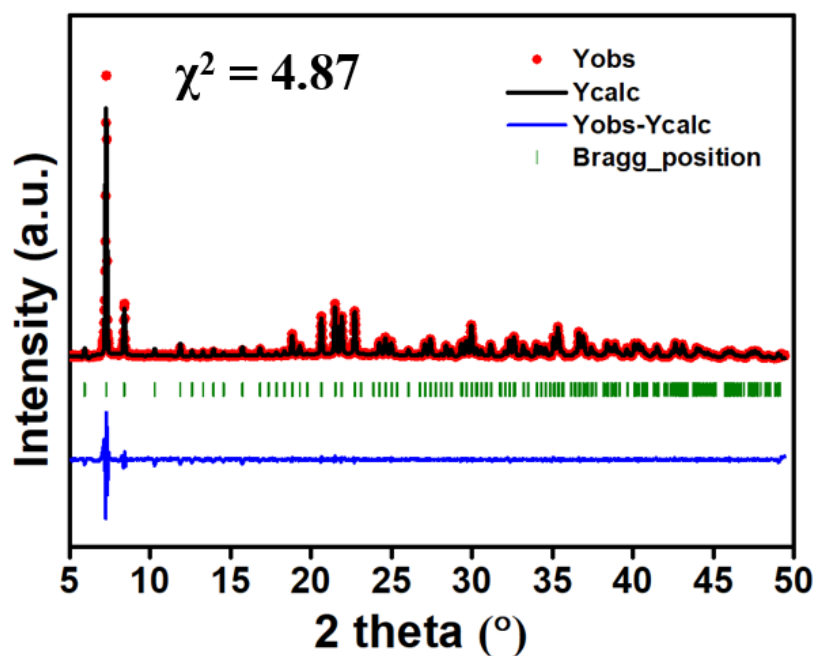
Ag—Ag distance	Ag <sub>12</sub> -pyz	Ag <sub>12</sub> -bpa	Ag <sub>12</sub> -py	Ag <sub>12</sub> -bpy	Ag <sub>12</sub> -azopy
Intra-cluster (Å)	2.93	3.10	3.11	3.15	3.15
Inter-cluster (Å)	7.40	9.89	10.1	11.38	13.36

## 5. Characterizations

### 5.1. Powder XRD

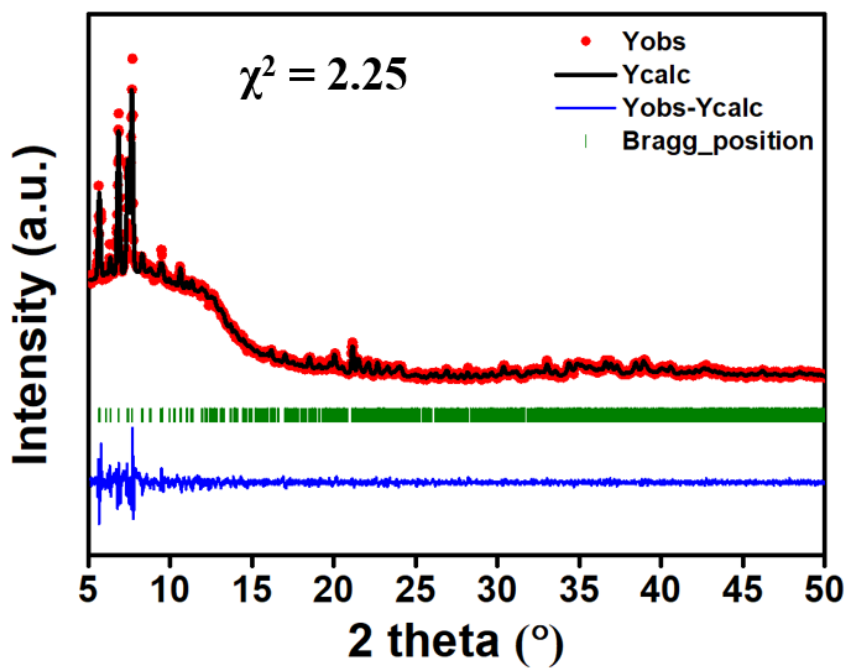
Le Bail analysis of the XRD patterns is performed for all the samples using the FullProf package taking the initial structural parameters from the single-crystal data, the data produced well fits the experimental analysis.

For Ag<sub>12</sub>-pyz, all the peaks were fitted using a cubic (*Pn-3*) crystal system. The best-fit parameters were obtained to be [*a* = 21.0822 Å, *b* = 21.0822 Å, *c* = 21.0822 Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\delta = 90^\circ$ , and  $\chi^2 = 4.87$ ], which are in good agreement with the single crystal XRD data.



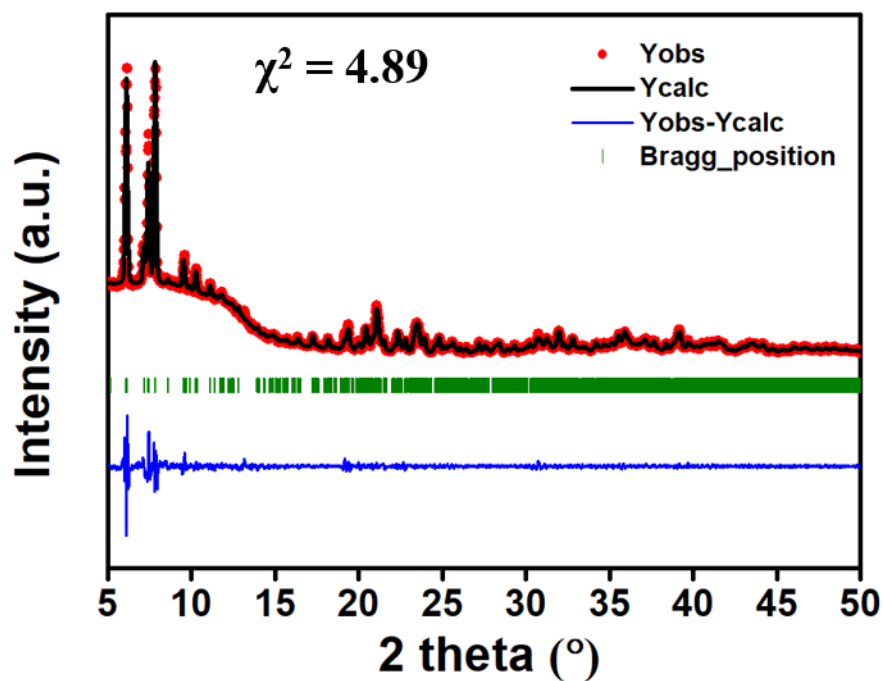
**Figure S17.** Powder XRD pattern of Ag<sub>12</sub>-pyz. As synthesized (red line), the solid black line represents the Le-Bail fit, with vertical bars showing the expected Bragg peak positions. The solid blue line indicates the difference between experimental and calculated intensities.

For Ag<sub>12</sub>-bpy, all the peaks were fitted using an orthorhombic (*Pnmm*) crystal system. The best-fit parameters were obtained to be [*a* = 23.1032 Å, *b* = 27.8838 Å, *c* = 18.8240 Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\delta = 90^\circ$ , and  $\chi^2 = 2.25$ ], which are in good agreement with the single crystal XRD data.



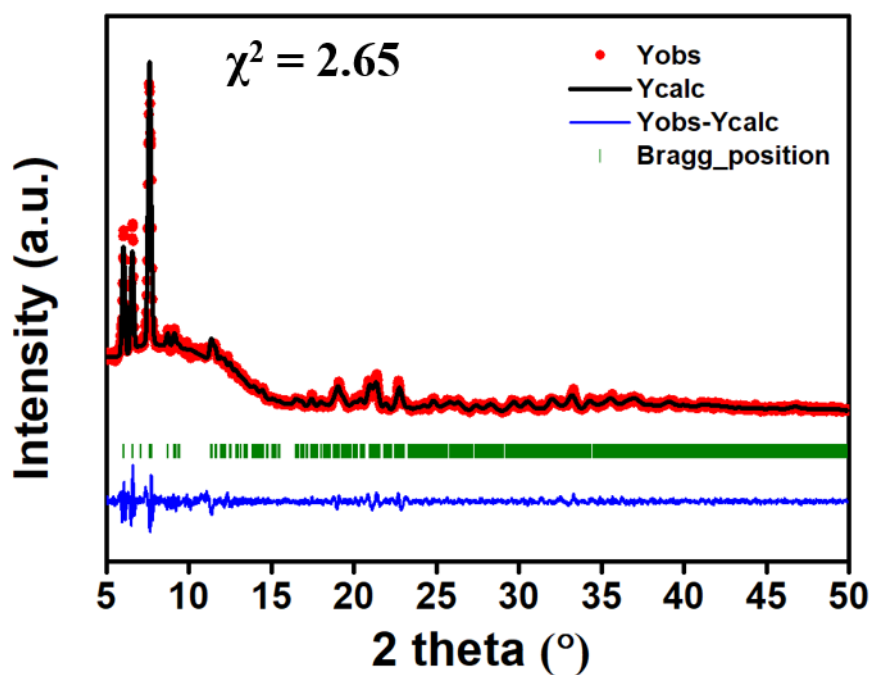
**Figure S18.** Powder XRD pattern of Ag<sub>12</sub>-bpy. As synthesized (red line), the solid black line represents the Le-Bail fit, vertical bars showing the expected Bragg peak positions. The solid blue line indicates the difference between experimental and calculated intensities.

For Ag<sub>12</sub>-bpa, all the peaks were fitted using monoclinic (*C2/c*) crystal system. The best-fit parameters were obtained to be [*a* = 25.3355 Å, *b* = 24.7027 Å, *c* = 19.7430 Å,  $\alpha$  = 90 °,  $\beta$  = 109.816 °,  $\delta$  = 90 °, and  $\chi^2$  = 4.89], which are in good agreement with the single crystal XRD data.



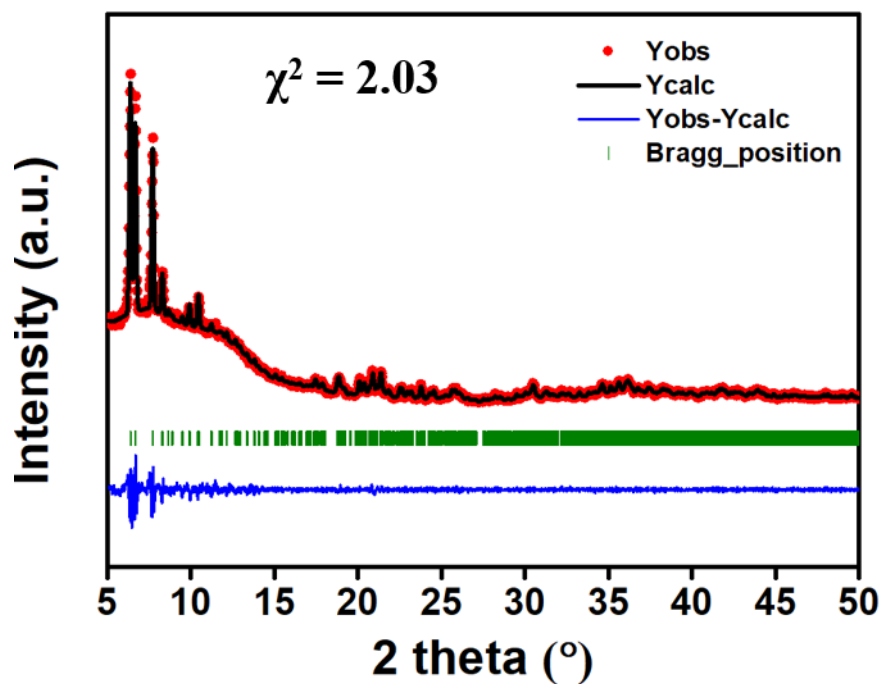
**Figure S19.** Powder XRD pattern of Ag<sub>12</sub>-bpa. As synthesized (red line), the solid black line represents the Le-Bail fit, vertical bars showing the expected Bragg peak positions. The solid blue line indicates the difference between experimental and calculated intensities.

For Ag<sub>12</sub>-azopy, all the peaks were fitted using monoclinic (*C2/c*) crystal system. The best-fit parameters were obtained to be [*a* = 27.0063 Å, *b* = 14.1917 Å, *c* = 29.3766 Å,  $\alpha$  = 90 °,  $\beta$  = 92.656 °,  $\delta$  = 90 °, and  $\chi^2$  = 2.65], which are in good agreement with the single crystal XRD data.



**Figure S20.** Powder XRD pattern of Ag<sub>12</sub>-azopy. As synthesized (red line), the solid black line represents the Le-Bail fit, vertical bars showing the expected Bragg peak positions. The solid blue line indicates the difference between experimental and calculated intensities.

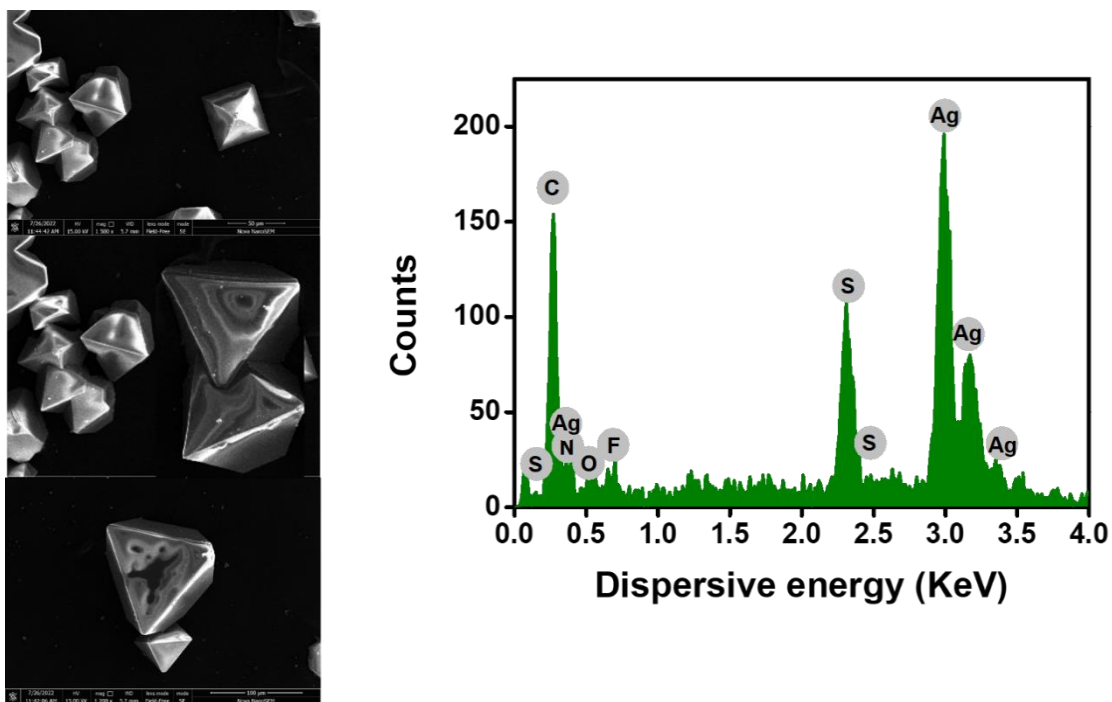
For Ag<sub>12</sub>-py, all the peaks were fitted using monoclinic (*P2/n*) crystal system. The best-fit parameters were obtained to be [ $a = 12.8170 \text{ \AA}$ ,  $b = 27.7169 \text{ \AA}$ ,  $c = 15.3524 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 100.421^\circ$ ,  $\delta = 90^\circ$ , and  $\chi^2 = 2.03$ ], which are in good agreement with the single crystal XRD data.



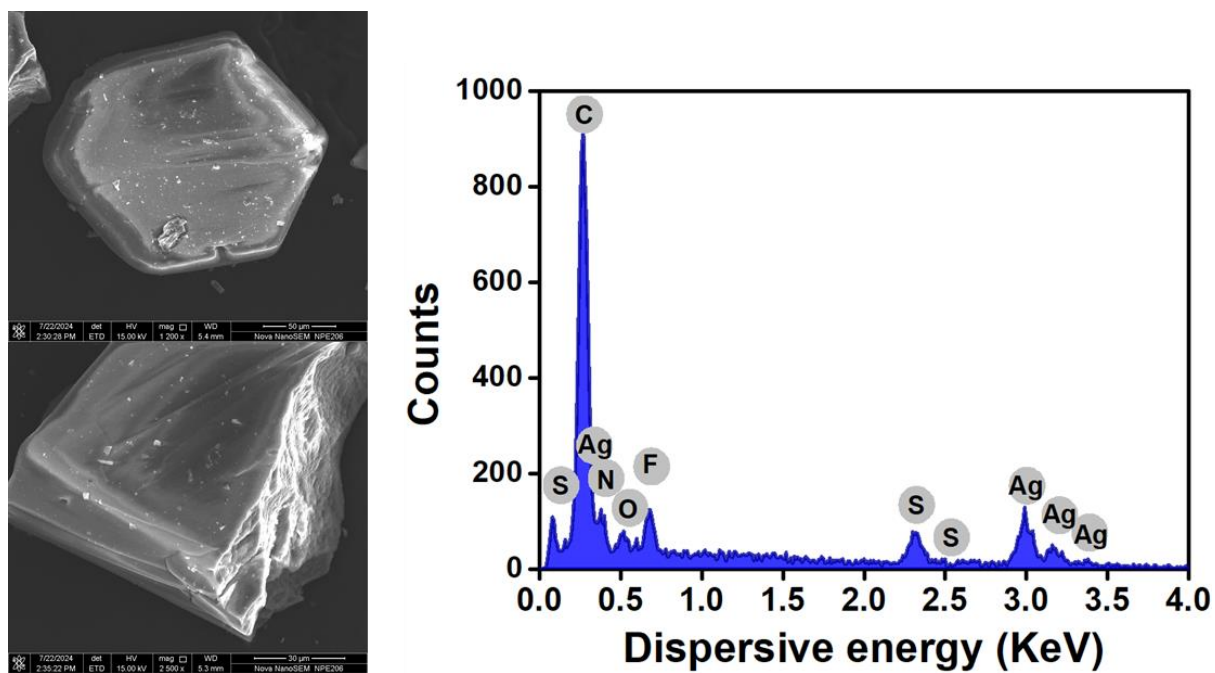
**Figure S21.** Powder XRD pattern of Ag<sub>12</sub>-py. As synthesized (red line), the solid black line represents the Le-Bail fit, vertical bars showing the expected Bragg peak positions. The solid blue line indicates the difference between experimental and calculated intensities.



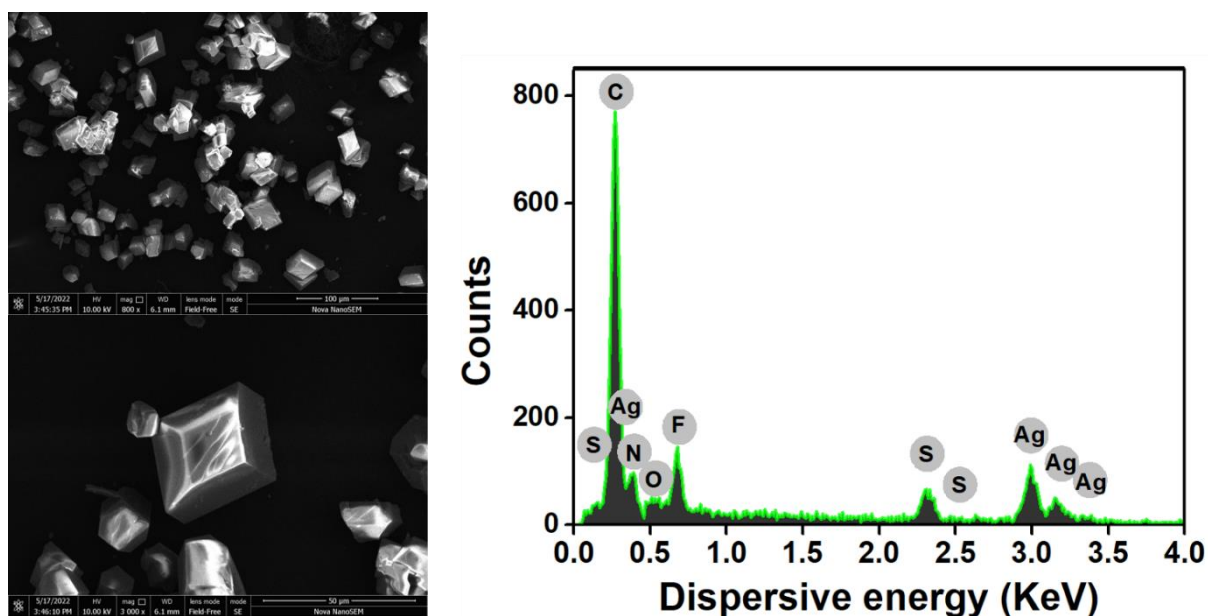
## 5.2. Scanning Electron Microscope (SEM) and Energy Dispersive X-ray Spectroscopy (EDS)



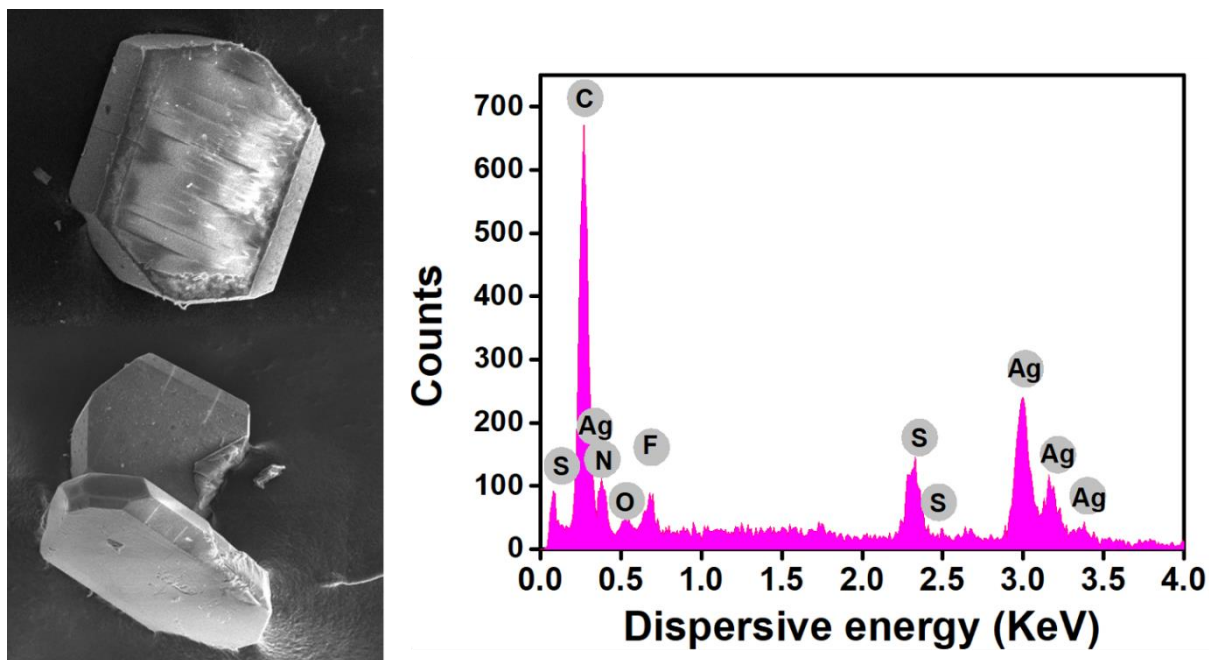
**Figure S22.** (Left) Morphology (3D- octahedral like) of  $\text{Ag}_{12}\text{-pyz}$  by SEM, (right) EDS elemental mapping showing the presence of all the desired elements.



**Figure S23.** (Left) Morphology (hexagonal) of Ag<sub>12</sub>-bpy by SEM, (right) EDS elemental mapping showing the presence of all the desired elements.

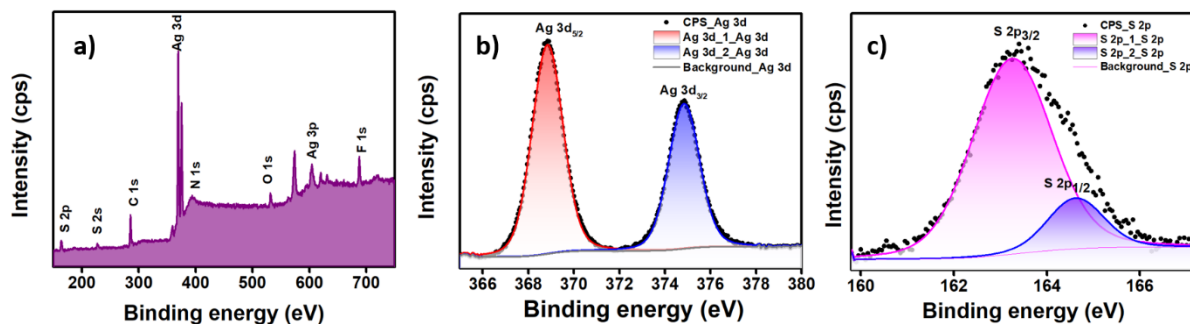


**Figure S24.** (Left) Morphology (block like) of Ag<sub>12</sub>-bpa by SEM, (right) EDS elemental mapping showing the presence of all the desired elements.

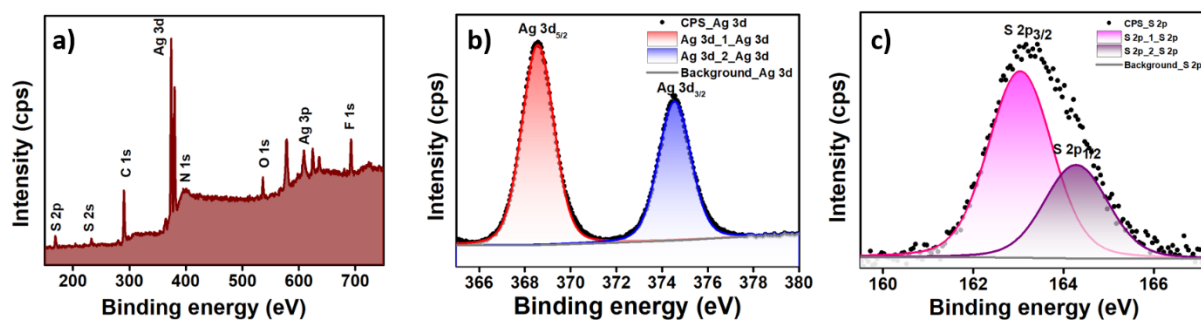


**Figure S25.** (Left) Morphology (hexagonal) of Ag<sub>12</sub>-azopy by SEM, (right) EDS elemental mapping showing the presence of all the desired elements.

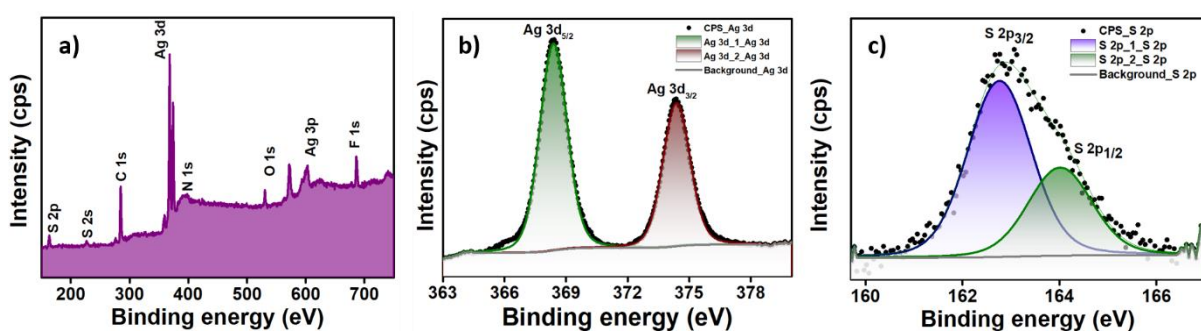
### 5.3. X-ray Photoelectron Spectroscopy (XPS)



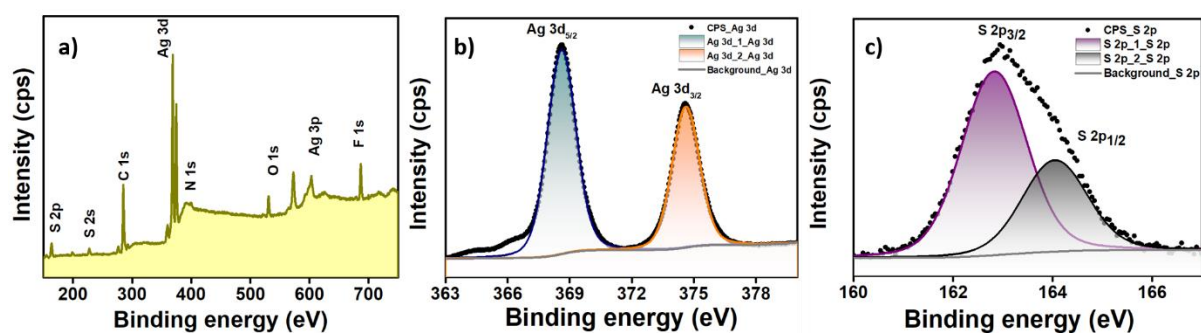
**Figure S26.** (a) XPS survey spectrum, (b) and (c) deconvoluted spectra of Ag and S elements present in Ag<sub>12</sub>-pyz.



**Figure S27.** (a) XPS survey spectrum, (b) and (c) deconvoluted spectra of Ag and S elements present in Ag<sub>12</sub>-bpy.

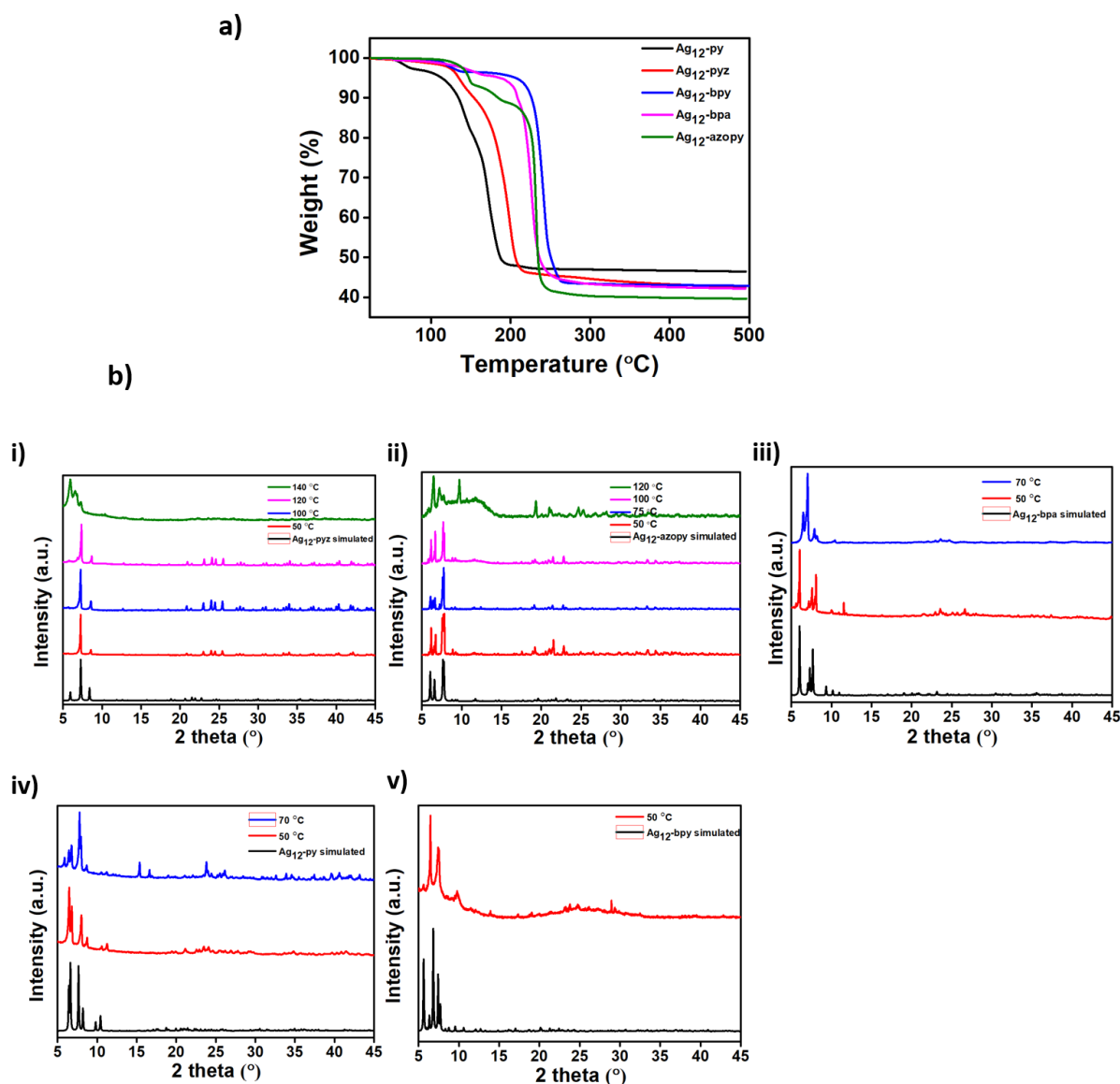


**Figure S28.** (a) XPS survey spectrum, (b) and (c) deconvoluted spectra of Ag and S elements present in Ag<sub>12</sub>-bpa.



**Figure S29.** (a) XPS survey spectrum, (b) and (c) deconvoluted spectra of Ag and S elements present in Ag<sub>12</sub>-azopy.

## 5.4. Thermal stability



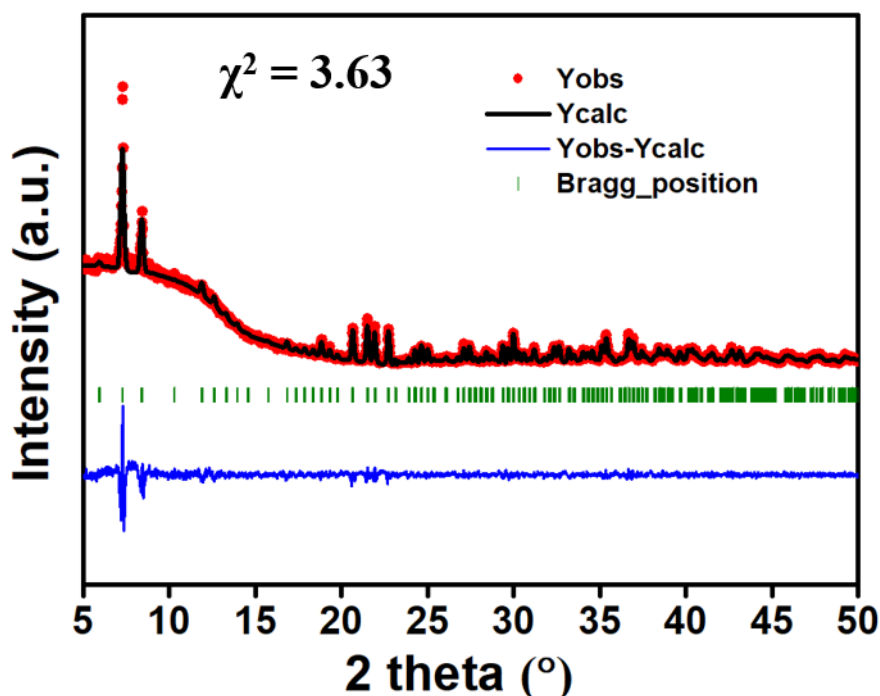
**Figure S30.** a) Thermogravimetric analysis of Ag<sub>12</sub>-pyz, Ag<sub>12</sub>-bpy, Ag<sub>12</sub>-bpa, Ag<sub>12</sub>-azopy which is thermally stable up to ~ 130 °C and the Ag<sub>12</sub>-py is stable up to ~ 60 °C. Whereas the retention of structural integrity at elevated temperatures is confirmed by, b) PXRD, i) Ag<sub>12</sub>-pyz stable up to 120 °C, ii) Ag<sub>12</sub>-azopy up to 100 °C, iii) Ag<sub>12</sub>-bpa and iv) Ag<sub>12</sub>-py up to 50 °C, v) whereas, Ag<sub>12</sub>-bpy is not stable at 50 °C.

Discussion: The 2D Ag<sub>12</sub>-bpy assembly demonstrates lower stability compared to Ag<sub>12</sub>-azopy. This reduced stability may be due to the layer-sliding in the 2D structure of Ag<sub>12</sub>-bpy, which is only stabilized by C---F interactions. Whereas, in Ag<sub>12</sub>-azopy, the layers are stabilized by multiple interactions, including F---F, F---H, and H---H.

## 6. Water stability of Ag<sub>12</sub>-pyz

Le Bail analysis of the XRD patterns is performed for the samples using the FullProf package taking the initial structural parameters from the single-crystal data, the data produced well fits the experimental analysis.

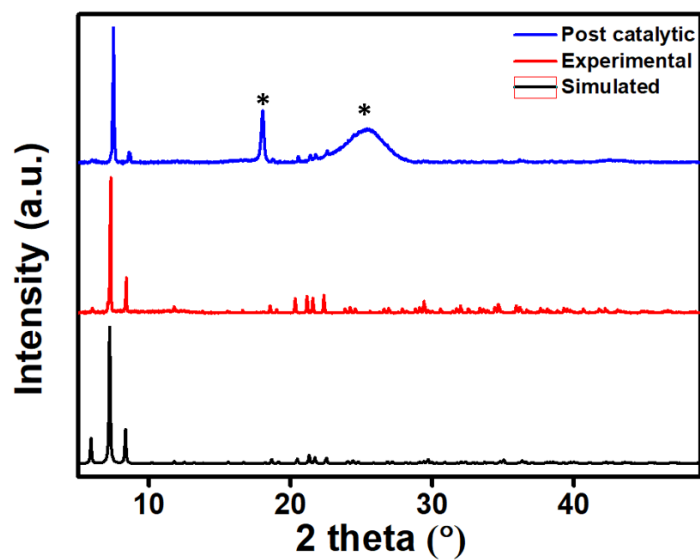
For the stability test for Ag<sub>12</sub>-pyz in water, the best-fit parameters were obtained to be [ $a = 21.0650 \text{ \AA}$ ,  $b = 21.0650 \text{ \AA}$ ,  $c = 21.0650 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\delta = 90^\circ$ , and  $\chi^2 = 3.63$ ], which are in good agreement with the single crystal XRD data.



**Figure S31.** The water stability of Ag<sub>12</sub>-pyz CAM was determined by dipping the crystals in distilled water for 24 h and the PXRD pattern of the dried samples matched with the simulated pattern. The solid black line represents the Le-Bail fit, vertical bars showing the expected Bragg peak positions. The solid blue line indicates the differences between experimental and calculated intensities.

## 7. Post-catalytic studies

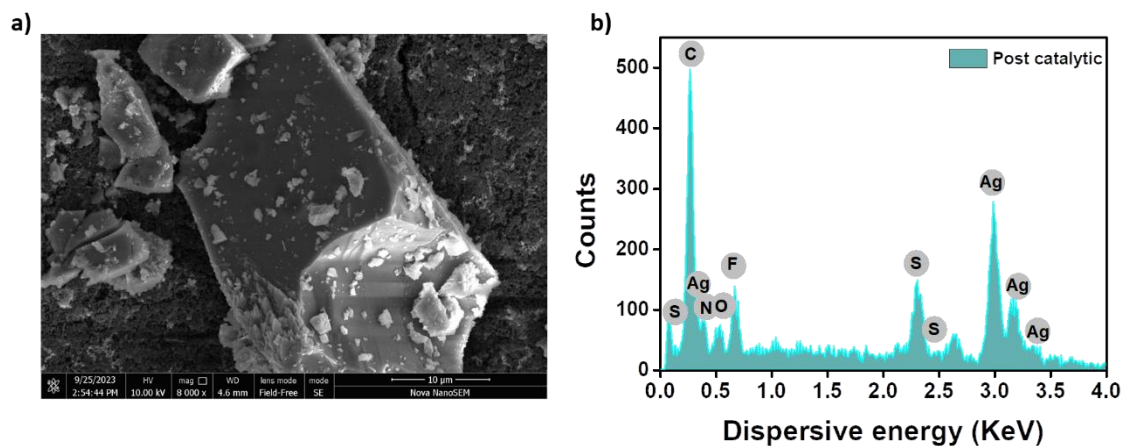
### 7.1. PXRD



**Figure S32.** The powder pattern of Ag<sub>12</sub>-pyz CAM (blue solid line) on the carbon cloth (post-catalysis) matches well with the simulated (black) and experimental pattern (red). (\*) The broad peak corresponds to the diffraction peaks from the sample holder (Bruker D8 advance) made of polymethyl methacrylate (PMMA) and the carbon cloth coated with PTFE.

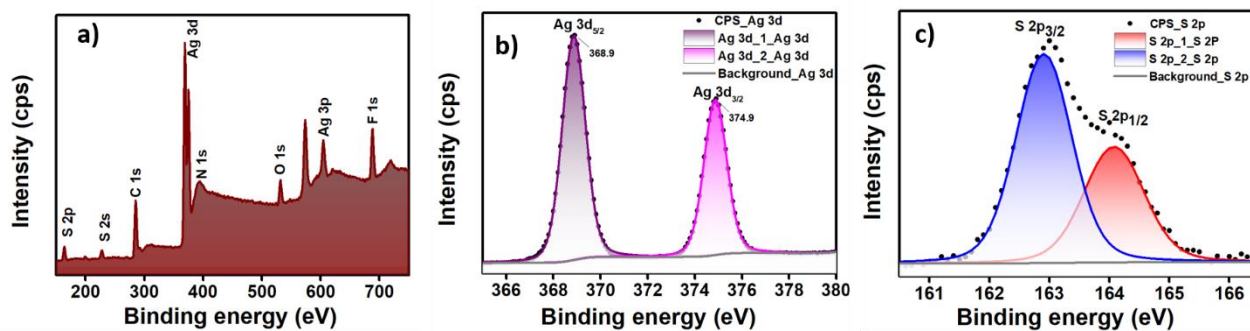


## 7.2. Scanning Electron Microscope (SEM) and Energy Dispersive X-ray Spectroscopy (EDS)



**Figure S33.** a) The post-catalysis morphology of Ag<sub>12</sub>-pyz by SEM (broken block-like morphology), b) EDS elemental mapping affirming the presence of all the elements intact.

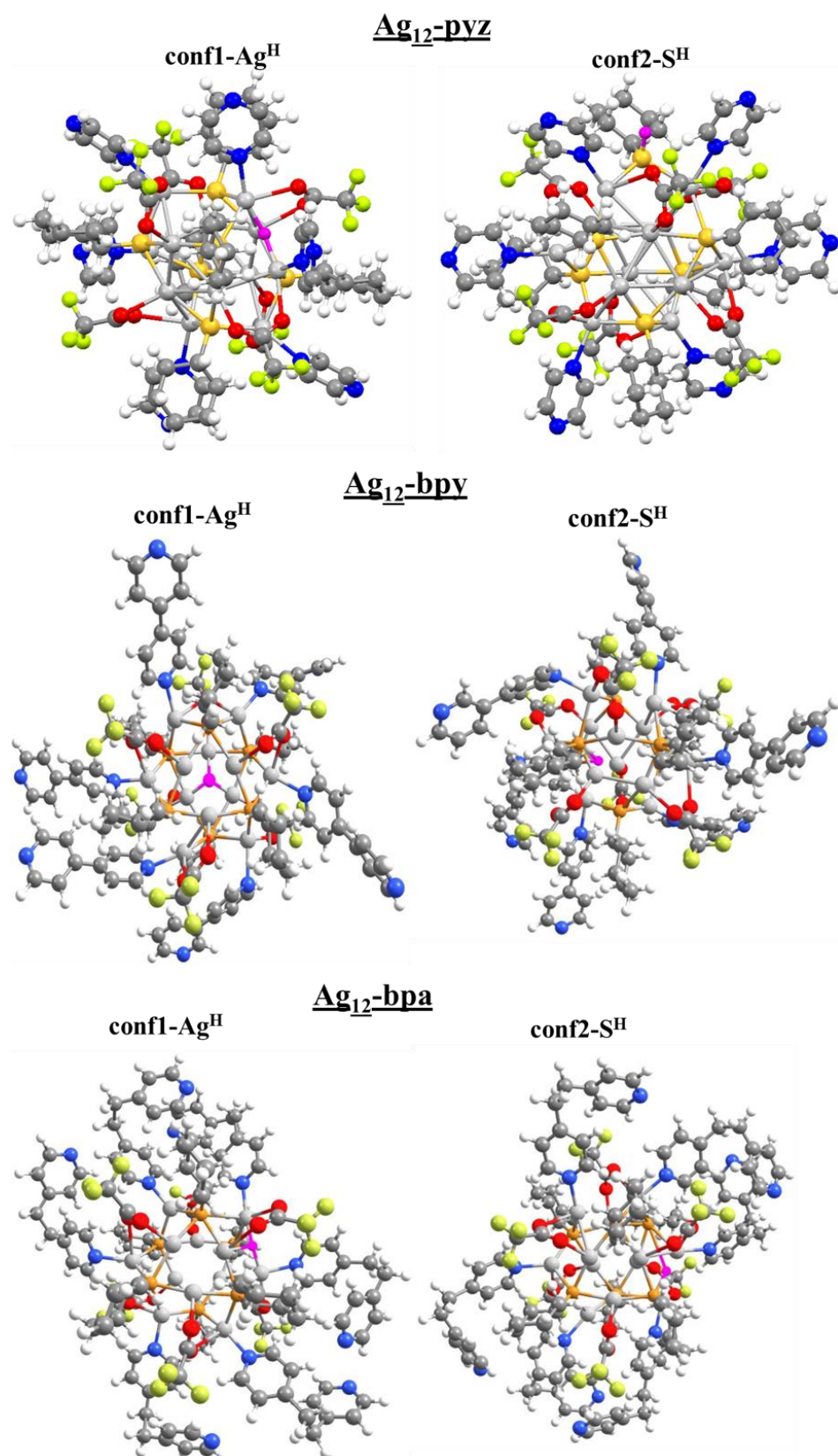
## 7.3. X-ray Photoelectron Spectroscopy (XPS)

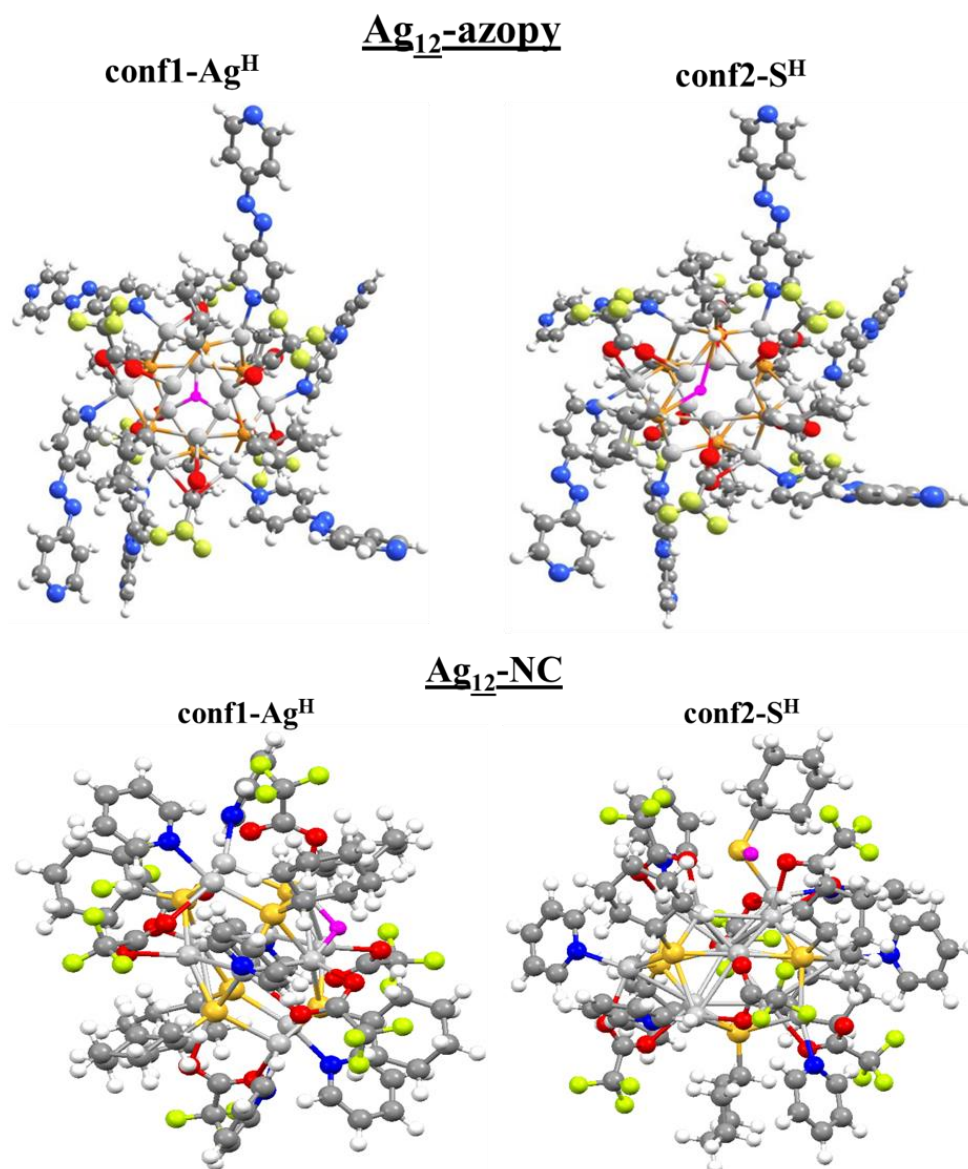


**Figure S34.** a) XPS survey spectrum, (b) deconvolution spectra of Ag, and (c) S elements, after the catalytic experiments.



## 8. TD-DFT of Cluster Mode

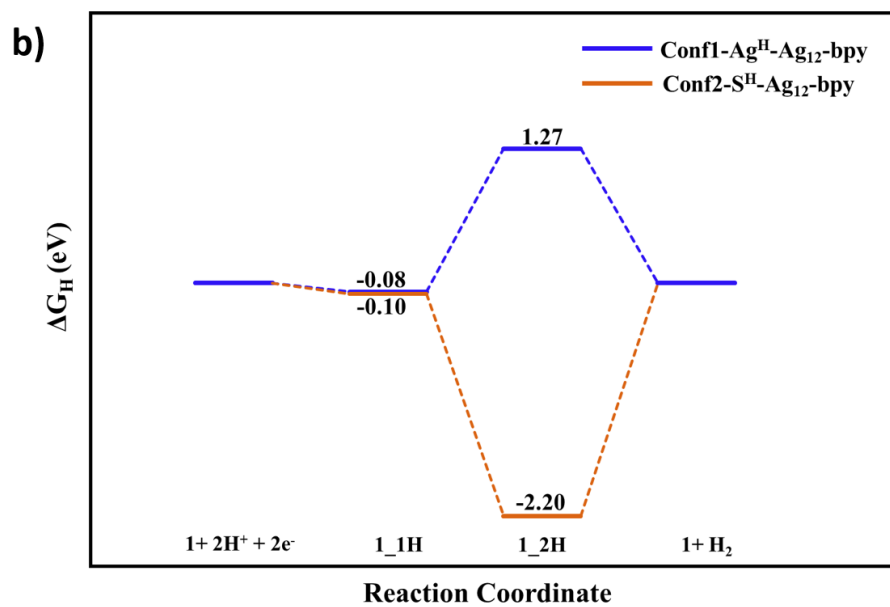
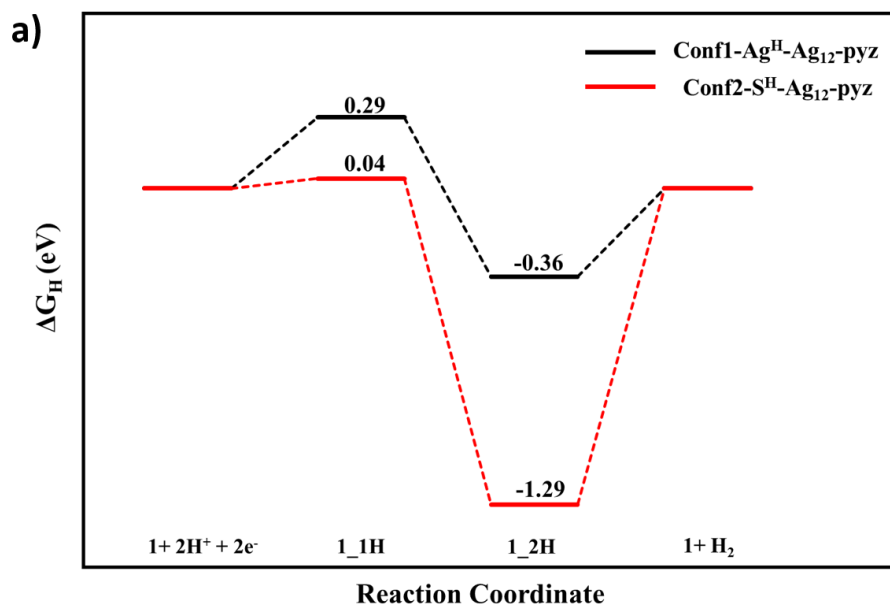


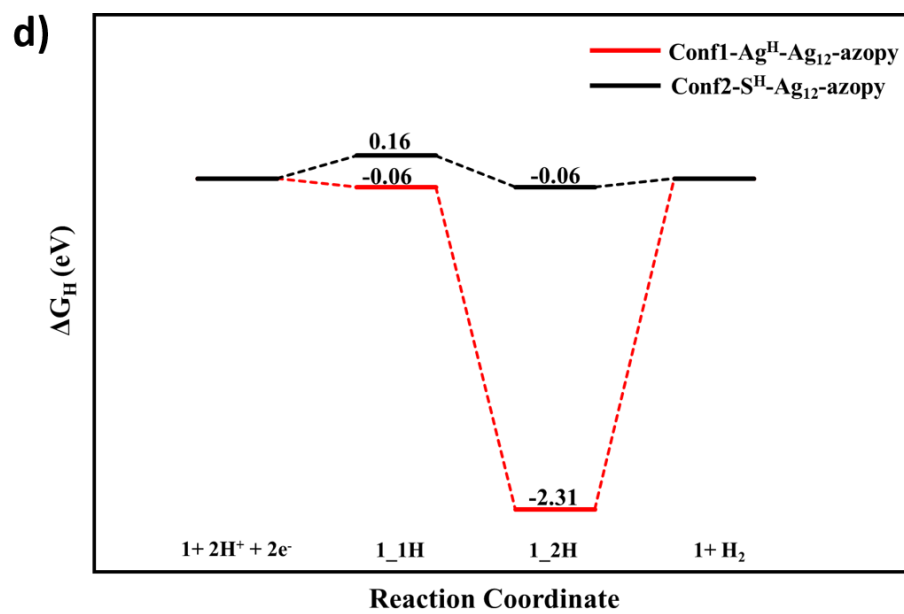
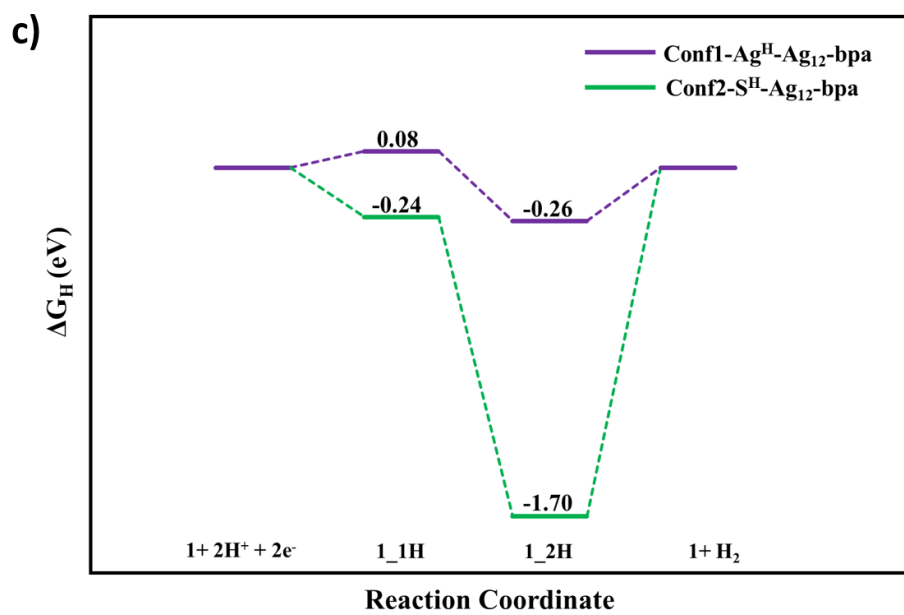


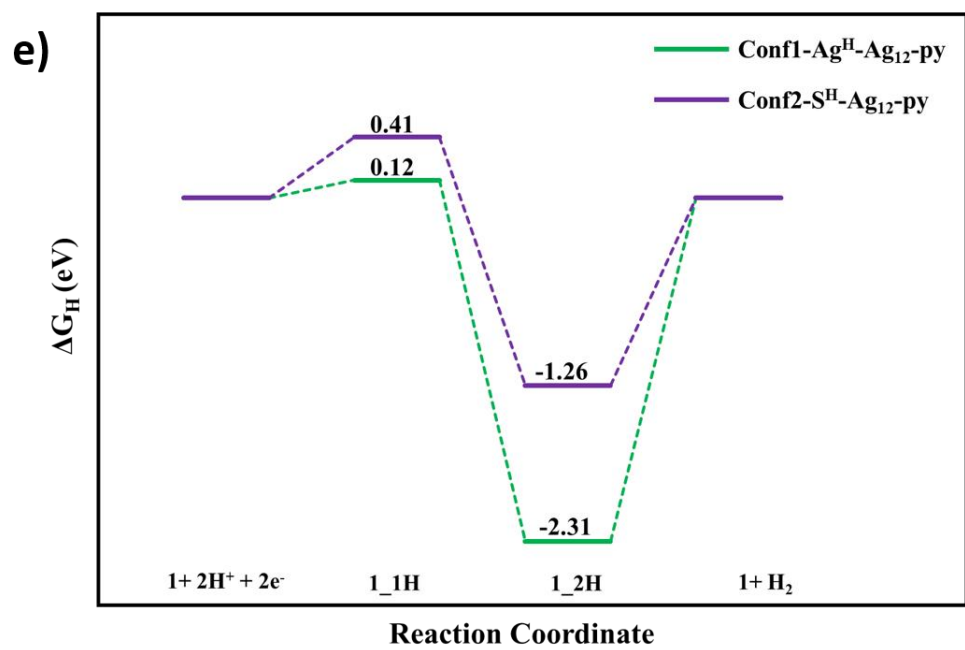
**Figure S35.** Optimized geometries of hydrogen adsorbed conformer structure of, in the order Ag<sub>12</sub>-pyz, Ag<sub>12</sub>-bpy, Ag<sub>12</sub>-bpa, Ag<sub>12</sub>azopy, Ag<sub>12</sub>py, respectively. color code: Ag, light Grey; S, yellow; O, red; N, blue; C, grey; F, greenish yellow.

Theoretical bond lengths: Average Ag-Ag bond lengths are 3.131 Å (py), 3.134 Å (bpy), 3.251 Å (bpa), and 3.383 Å (azopy), whereas it decreases to 2.893 Å in the Pyrazine-based cluster.

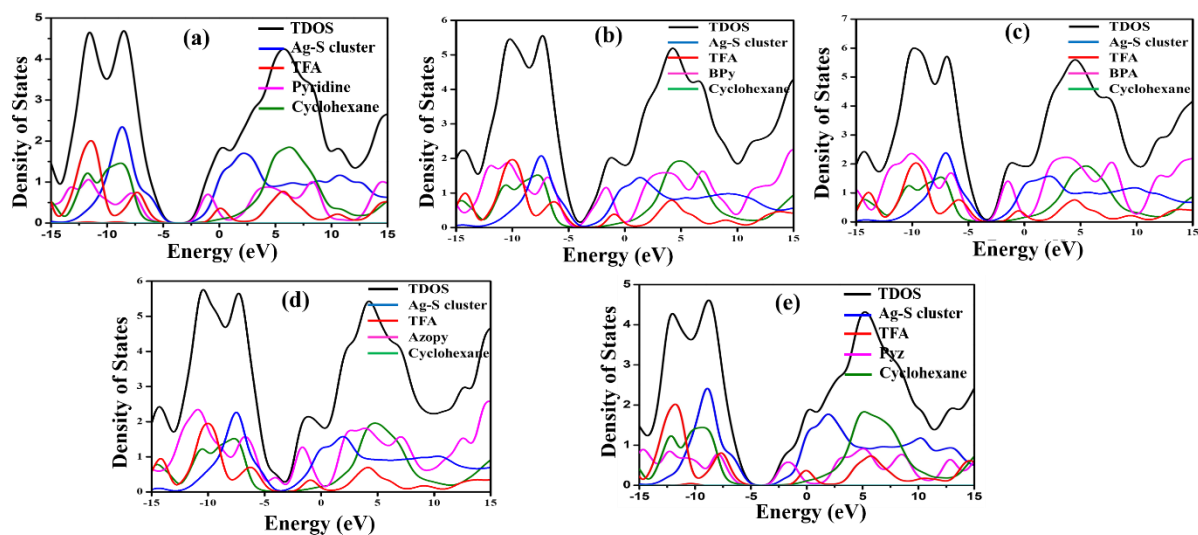
### 8.1. Hydrogen adsorption free energy ( $\Delta G_H$ ) calculations







**Figure S36.** Calculated free energy profile of HER reaction, a) Ag<sub>12</sub>-pyz, b) Ag<sub>12</sub>-bpy, c) Ag<sub>12</sub>-bpa, d) Ag<sub>12</sub>-azopy, e) Ag<sub>12</sub>-py.

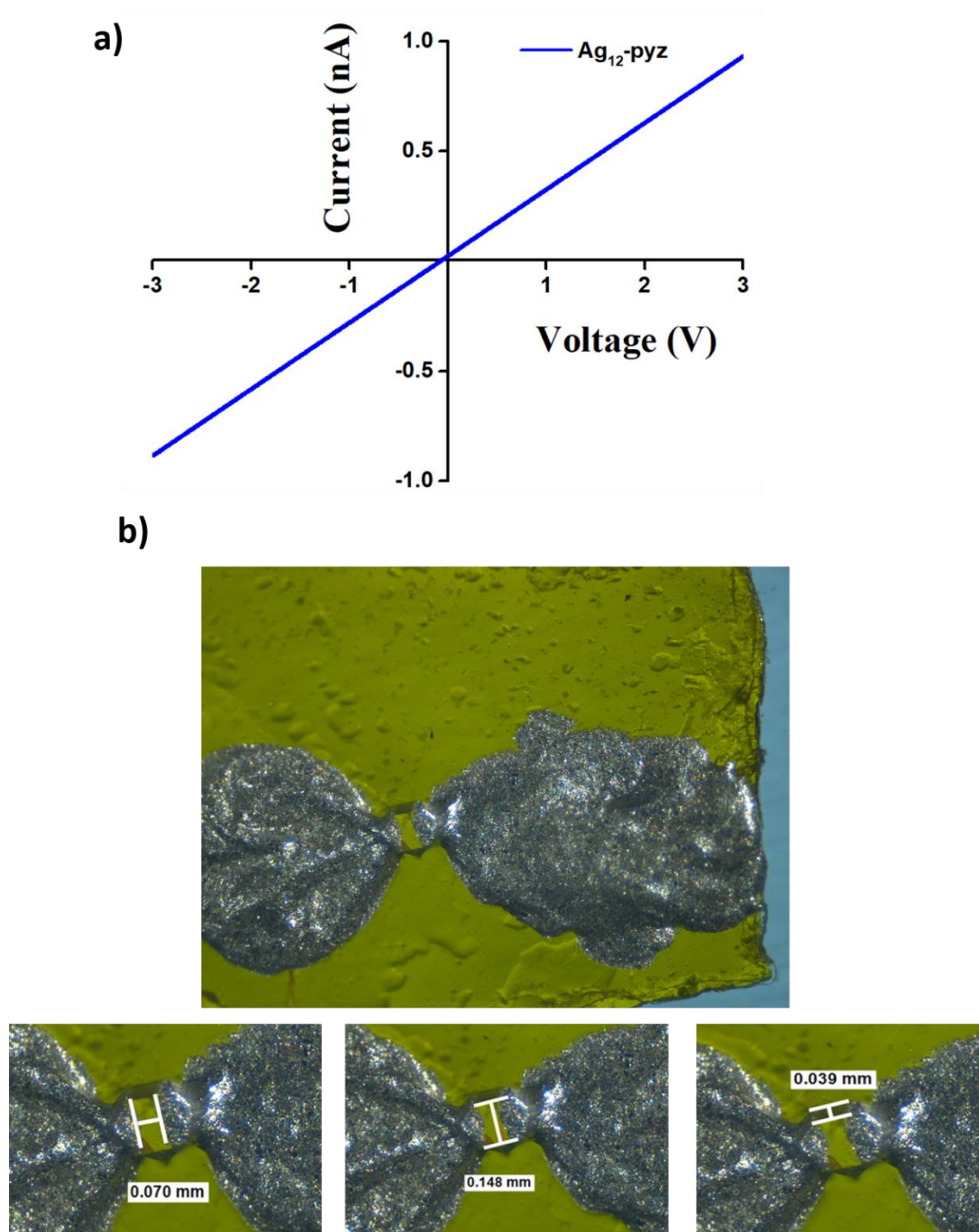


**Figure S37.** Density of states spectra of (a) Ag<sub>12</sub>-py, (b) Ag<sub>12</sub>-bpy (c) Ag<sub>12</sub>-bpa, (d) Ag<sub>12</sub>-azopy, (e) Ag<sub>12</sub>-pyz clusters. Color code: Ag, blue; S, yellow; O, green; N, blue; C, grey; F, pink.

**Table S7.** Calculated band-gap (in eV) of the studied cluster assembly.

Cluster-assembly	Ag <sub>12</sub> -pyz	Ag <sub>12</sub> -azopy	Ag <sub>12</sub> -bpa	Ag <sub>12</sub> -py	Ag <sub>12</sub> -bpy
Band gap (eV)	2.01	2.18	2.23	2.24	2.28

## 9. $I$ - $V$ characteristics of $\text{Ag}_{12}$ -pyz



**Figure S38.** a) Current–voltage ( $I$ - $V$ ) plot of  $\text{Ag}_{12}$ -pyz single crystal.  $R=0.3\text{ G}\Omega$ ,  $\rho=2.4\times 10^5\text{ m}\Omega$ ,  $\sigma=1/\rho=4.1\times 10^{-6}\text{ S m}^{-1}$ . b) Optical microscope image of the single crystal mounted in-between silver paint followed by  $L\times B\times H$  values.



**10.** Table S8: Comparison table of other catalysts reported in the literature.

Sl. No.	Catalyst	Electrolyte	Overpotential (mV)	Tafel slope (mV dec <sup>-1</sup> )	Adsorption site	Reference
01	Ag <sub>29</sub> (BDT) <sub>12</sub> (TPP) <sub>4</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	423	225	Hollow site	<i>Nanoscale</i> , <b>2023</b> , 15, 14941-14948.
02	Pt <sub>1</sub> Ag <sub>28</sub> (BDT) <sub>12</sub> (TPP) <sub>4</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	362	191	Hollow site	<i>Nanoscale</i> , <b>2023</b> , 15, 14941-14948.
03	Pt <sub>1</sub> Ag <sub>28</sub> (BTT) <sub>12</sub> (TPP) <sub>2</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	348	144	Hollow site	<i>Nanoscale</i> , <b>2023</b> , 15, 14941-14948.
04	Ag NCs/MoS <sub>2</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	230	106	-	<i>ACS Appl. Nano Mater.</i> <b>2022</b> , 5, 7132-7141.
05	Ag <sub>25</sub> (SPhMe <sub>2</sub> ) <sub>18</sub>	1.0 M KOH	420	125	-	<i>Bull. Korean Chem. Soc.</i> <b>2021</b> , 42, 1672–1677
06	NiAg <sub>24</sub> (SPhMe <sub>2</sub> ) <sub>18</sub>	1.0 M KOH	270	58	-	<i>Bull. Korean Chem. Soc.</i> <b>2021</b> , 42, 1672–1677
07	Au <sub>36</sub> Ag <sub>2</sub> (SR)	0.5 M H <sub>2</sub> SO <sub>4</sub>	~252	125	kernel's shell Au atom	<i>J. Am. Chem. Soc.</i> <b>2021</b> , 143, 11102-11108
08	Au <sub>15</sub> Ag <sub>23</sub> ( <sup>t</sup> BuC≡C) <sub>18</sub> Br <sub>6</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	125	121	-	<i>Int. J. Hydrogen Energy.</i> <b>2024</b> , 53, 300-307.
09	Au <sub>24</sub> Ag <sub>20</sub> ( <sup>t</sup> BuPh-C≡C) <sub>24</sub> Cl <sub>2</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	262	96	Staple Au atom	<i>Dalton Trans.</i> <b>2022</b> , 51, 7845-7850.
10	Au <sub>22</sub> Ag <sub>22</sub> ( <sup>t</sup> BuC≡C) <sub>16</sub> Br <sub>3.28</sub> Cl <sub>2.72</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	335	117	Staple Au atom	<i>Dalton Trans.</i> <b>2022</b> , 51, 7845-7850.
11	Au <sub>9</sub> Ag <sub>9</sub> (C≡CAr <sup>F</sup> ) <sub>18</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	274	99	-	<i>Eur. J. Inorg. Chem.</i> <b>2022</b> , 2022, e202200176
12	Ag <sub>12</sub> -py: {[Ag <sub>12</sub> (C <sub>6</sub> H <sub>11</sub> S) <sub>6</sub> (CF <sub>3</sub> COO) <sub>6</sub> (C <sub>5</sub> H <sub>5</sub> N) <sub>6</sub> ]. 4H <sub>2</sub> O}	0.5 M H <sub>2</sub> SO <sub>4</sub>	230	178	Ag site	<b>This work</b>



13	Ag <sub>12</sub> -bpy: [Ag <sub>12</sub> (C <sub>6</sub> H <sub>11</sub> S) <sub>6</sub> (CF <sub>3</sub> COO) <sub>6</sub> (C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>3</sub> ]	0.5 M H <sub>2</sub> SO <sub>4</sub>	575	242	Ag site	<b>This work</b>
14	Ag <sub>12</sub> -bpa: [Ag <sub>12</sub> (C <sub>6</sub> H <sub>11</sub> S) <sub>6</sub> (CF <sub>3</sub> COO) <sub>6</sub> (C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> ) <sub>3</sub> (DMF) <sub>2</sub> ]	0.5 M H <sub>2</sub> SO <sub>4</sub>	401	235	Ag site	<b>This work</b>
15	Ag <sub>12</sub> -azopy: [Ag <sub>12</sub> (C <sub>6</sub> H <sub>11</sub> S) <sub>6</sub> (CF <sub>3</sub> COO) <sub>6</sub> (C <sub>10</sub> H <sub>8</sub> N <sub>4</sub> ) <sub>3</sub> (DMF) <sub>2</sub> ]	0.5 M H <sub>2</sub> SO <sub>4</sub>	205	163	Ag site	<b>This work</b>
16	<b>Ag<sub>12</sub>-pyz:</b> <b>[Ag<sub>12</sub>(C<sub>6</sub>H<sub>11</sub>S)<sub>6</sub>(CF<sub>3</sub>COO)<sub>6</sub> (C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>)<sub>3</sub>]</b>	<b>0.5 M H<sub>2</sub>SO<sub>4</sub></b>	<b>122</b>	<b>117</b>	<b>S site</b>	<b>This work</b>

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## 12. Optimized coordinates

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H	2.150422000000	0.862939000000	-4.372935000000
C	3.053040000000	2.430456000000	-5.598132000000
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H	2.463435000000	2.179093000000	-6.498631000000
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C	4.116258000000	4.307824000000	-4.269610000000
H	4.285520000000	5.399172000000	-4.215242000000
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H	5.035164000000	-6.297640000000	3.365990000000
C	6.485293000000	-5.053397000000	2.310577000000
H	7.353336000000	-5.402758000000	2.879032000000
C	6.631884000000	-4.102138000000	1.292240000000
H	7.611389000000	-3.686935000000	1.036972000000
C	5.497004000000	-3.667870000000	0.596198000000
H	5.548487000000	-2.916708000000	-0.200045000000
C	6.582425000000	0.993787000000	-1.603151000000
H	6.398076000000	-0.072711000000	-1.760573000000
C	7.539551000000	1.693368000000	-2.346658000000
H	8.125546000000	1.164569000000	-3.104048000000
C	6.936682000000	3.676743000000	-1.117094000000
H	7.040821000000	4.741511000000	-0.888398000000
C	5.996118000000	2.911266000000	-0.417098000000
H	5.347431000000	3.340538000000	0.354848000000
C	7.717673000000	3.062696000000	-2.105313000000
H	8.452784000000	3.639493000000	-2.675900000000
C	0.882068000000	-3.948201000000	-5.583776000000
H	-0.056267000000	-4.529614000000	-5.690738000000
H	0.974364000000	-3.326237000000	-6.492793000000
C	2.074018000000	-4.912268000000	-5.465300000000
H	2.123426000000	-5.573732000000	-6.349731000000
H	3.014658000000	-4.327752000000	-5.445914000000
C	1.979630000000	-5.748467000000	-4.178796000000
H	2.857934000000	-6.412545000000	-4.078074000000
H	1.085955000000	-6.404135000000	-4.224297000000
Ag	1.651200000000	-0.602175000000	-1.835633000000
Ag	-0.248725000000	1.588135000000	-1.842377000000
Ag	-1.201127000000	-1.137304000000	-1.923870000000
Ag	1.504146000000	3.614539000000	0.011215000000
Ag	3.955516000000	0.553279000000	0.084818000000
F	-5.191731000000	-4.516166000000	-3.461143000000
F	-4.780078000000	-2.907810000000	-4.899665000000

F	-5.865065000000	-2.460844000000	-3.046896000000
N	1.475774000000	5.781181000000	0.688841000000
N	4.256362000000	-4.138592000000	0.869855000000
N	5.814481000000	1.590503000000	-0.660131000000
O	3.437353000000	-1.158342000000	-3.410717000000
O	-0.654360000000	3.349782000000	-3.498052000000
O	-2.564850000000	-2.433004000000	-3.482869000000
O	4.599048000000	-1.512964000000	-1.471911000000
O	-1.001711000000	4.623479000000	-1.629451000000
O	-3.574043000000	-3.202576000000	-1.578675000000
S	2.207282000000	1.801693000000	-1.509628000000
S	-2.635663000000	0.879013000000	-1.629520000000
S	0.581289000000	-2.825452000000	-1.527712000000
Ag	2.423674000000	-3.032050000000	0.106088000000
C	-0.337411000000	5.730783000000	-3.615390000000
C	-2.738873000000	0.796012000000	-4.461996000000
H	-2.741127000000	-0.307704000000	-4.391908000000
H	-1.688270000000	1.136666000000	-4.474395000000
C	-3.450843000000	1.383008000000	-3.238832000000
C	-3.458112000000	1.234119000000	-5.752526000000
H	-3.360445000000	2.332208000000	-5.871993000000
H	-2.955779000000	0.774513000000	-6.623221000000
C	-5.642432000000	1.446663000000	-4.488007000000
H	-6.703693000000	1.138732000000	-4.448886000000
H	-5.633112000000	2.553809000000	-4.554562000000
C	-4.946357000000	0.848900000000	-5.721305000000
H	-5.450656000000	1.183486000000	-6.646446000000
H	-5.035208000000	-0.254916000000	-5.685550000000
C	-4.937466000000	1.011905000000	-3.188913000000
H	-5.416844000000	1.479984000000	-2.310301000000
H	-5.035715000000	-0.083334000000	-3.066276000000
H	-3.334218000000	2.482397000000	-3.242863000000
C	-3.079881000000	-2.319840000000	3.046179000000
H	-4.017452000000	-1.733011000000	3.018285000000
C	-2.305852000000	-1.973315000000	4.322167000000
H	-1.317970000000	-2.469163000000	4.294704000000
H	-2.143638000000	-0.882426000000	4.370922000000
C	-3.092882000000	-2.449186000000	5.558971000000
H	-4.036308000000	-1.871482000000	5.636473000000
H	-2.508927000000	-2.225005000000	6.470244000000
C	-3.412401000000	-3.951104000000	5.478362000000
H	-3.994441000000	-4.269337000000	6.362798000000
H	-2.465309000000	-4.525273000000	5.491050000000
C	-4.179429000000	-4.282421000000	4.187962000000
H	-4.370689000000	-5.369013000000	4.113903000000
H	-5.170170000000	-3.783519000000	4.203535000000
C	-3.398583000000	-3.815975000000	2.944781000000
H	-3.972638000000	-4.022071000000	2.023527000000
H	-2.452595000000	-4.384645000000	2.869719000000
C	-0.673976000000	3.904969000000	3.060445000000
H	0.257043000000	4.502166000000	3.038374000000
C	-0.710761000000	3.066130000000	4.342580000000
H	-1.580432000000	2.383893000000	4.303370000000
H	0.205670000000	2.453690000000	4.410666000000
C	-1.890267000000	4.829794000000	2.932115000000
H	-1.814746000000	5.430724000000	2.007899000000
H	-2.804289000000	4.212461000000	2.846348000000
C	-4.332159000000	1.547038000000	2.772655000000
C	-5.461828000000	2.272708000000	3.562721000000
C	0.680767000000	-4.416952000000	2.840655000000
C	3.545486000000	2.956477000000	2.790733000000



C	4.870048000000	3.263652000000	3.551126000000
C	-0.418650000000	-6.550877000000	-0.409311000000
H	0.245067000000	-6.183905000000	0.381920000000
C	-0.187109000000	-7.756624000000	-1.082820000000
H	0.681889000000	-8.364717000000	-0.814380000000
C	-1.070456000000	-8.153056000000	-2.095778000000
H	-0.907882000000	-9.085115000000	-2.646706000000
C	-2.168980000000	-7.332364000000	-2.387226000000
H	-2.890579000000	-7.598379000000	-3.165227000000
C	-2.335323000000	-6.143457000000	-1.667752000000
H	-3.169808000000	-5.463406000000	-1.863333000000
C	-4.166470000000	5.030121000000	-1.781757000000
H	-3.149077000000	5.364140000000	-2.006936000000
C	-5.274324000000	5.509916000000	-2.490138000000
H	-5.127387000000	6.236911000000	-3.294325000000
C	-6.550834000000	5.040031000000	-2.151700000000
H	-7.436490000000	5.390733000000	-2.691426000000
C	-6.669208000000	4.114819000000	-1.105914000000
H	-7.643614000000	3.722595000000	-0.799797000000
C	-5.512799000000	3.677106000000	-0.448319000000
H	-5.544957000000	2.941319000000	0.363461000000
C	-6.605284000000	-0.950789000000	1.501426000000
H	-6.413052000000	0.116179000000	1.644187000000
C	-7.587671000000	-1.625975000000	2.234354000000
H	-8.183905000000	-1.077419000000	2.969360000000
C	-6.983014000000	-3.636495000000	1.050080000000
H	-7.096413000000	-4.703265000000	0.835766000000
C	-6.017062000000	-2.894580000000	0.359768000000
H	-5.357512000000	-3.341837000000	-0.392436000000
C	-7.777437000000	-2.996753000000	2.011047000000
H	-8.532249000000	-3.555130000000	2.574110000000
C	-0.832830000000	3.986911000000	5.572657000000
H	0.088007000000	4.597851000000	5.666464000000
H	-0.896061000000	3.368028000000	6.486267000000
C	-2.054881000000	4.913383000000	5.461900000000
H	-2.114451000000	5.579307000000	6.342339000000
H	-2.978169000000	4.301287000000	5.456301000000
C	-2.003168000000	5.741892000000	4.168068000000
H	-2.903466000000	6.376921000000	4.074326000000
H	-1.130328000000	6.426001000000	4.196798000000
Ag	-1.625021000000	0.638595000000	1.847875000000
Ag	0.259385000000	-1.564968000000	1.839478000000
Ag	1.234078000000	1.157076000000	1.912100000000
Ag	-1.465635000000	-3.582769000000	-0.018199000000
Ag	-3.943336000000	-0.583706000000	-0.145949000000
F	5.198833000000	4.583444000000	3.428213000000
F	4.820027000000	2.971786000000	4.871326000000
F	5.901433000000	2.538102000000	3.012962000000
N	-1.471743000000	-5.749982000000	-0.701308000000
N	-4.277156000000	4.120672000000	-0.784236000000
N	-5.823404000000	-1.572626000000	0.586878000000
O	-3.372620000000	1.127384000000	3.477377000000
O	0.650929000000	-3.337476000000	3.491005000000
O	2.609547000000	2.447946000000	3.465160000000
O	-4.485220000000	1.505415000000	1.516711000000
O	0.970239000000	-4.620313000000	1.623826000000
O	3.589285000000	3.250546000000	1.558677000000
S	-2.195686000000	-1.765386000000	1.489764000000
S	2.649536000000	-0.866658000000	1.618415000000
S	-0.536989000000	2.852147000000	1.519256000000
Ag	-2.416301000000	3.005170000000	-0.083634000000

F	-5.668484000000	1.738883000000	4.788989000000
F	-6.655097000000	2.241833000000	2.896556000000
F	-5.133362000000	3.591196000000	3.731098000000
C	0.292862000000	-5.712868000000	3.613338000000
F	1.311205000000	-6.622610000000	3.566268000000
F	-0.800690000000	-6.299165000000	3.032065000000
F	-0.008602000000	-5.500539000000	4.915399000000
C	2.748617000000	-0.783249000000	4.452069000000
H	2.719590000000	0.320202000000	4.383501000000
H	1.708952000000	-1.155570000000	4.464058000000
C	3.479317000000	-1.345603000000	3.228356000000
C	3.481243000000	-1.201107000000	5.742092000000
H	3.417932000000	-2.301971000000	5.859542000000
H	2.964373000000	-0.759242000000	6.613464000000
C	5.671741000000	-1.341203000000	4.477609000000
H	6.722424000000	-0.998797000000	4.439578000000
H	5.698280000000	-2.448362000000	4.540320000000
C	4.956762000000	-0.769680000000	5.712591000000
H	5.470841000000	-1.091474000000	6.636903000000
H	5.011769000000	0.336350000000	5.680039000000
C	4.952914000000	-0.925132000000	3.180225000000
H	5.447432000000	-1.373903000000	2.300012000000
H	5.014986000000	0.172891000000	3.061224000000
H	3.400437000000	-2.448435000000	3.230803000000
F	0.753286000000	6.326879000000	-3.038692000000
F	-0.041772000000	5.526901000000	-4.920435000000
F	-1.365706000000	6.628180000000	-3.558698000000
F	5.328474000000	-3.845873000000	-2.870266000000
F	5.109344000000	-2.747732000000	-4.756338000000
F	6.641081000000	-2.132768000000	-3.308406000000

**Conf1-Ag<sup>H</sup> (Ag<sub>12</sub>-pyz):**

Ag	0.111446000000	1.820568000000	2.235418000000
Ag	1.785298000000	3.608934000000	0.359568000000
Ag	-1.301166000000	-0.713204000000	1.929807000000
Ag	1.558998000000	-0.676016000000	1.906399000000
Ag	3.795438000000	0.365931000000	0.078405000000
Ag	-3.637835000000	-0.079570000000	0.203027000000
Ag	-1.912251000000	3.271022000000	-0.223901000000
Ag	2.633124000000	-2.945521000000	0.424867000000
Ag	-1.663519000000	-3.392475000000	-0.194151000000
Ag	-0.063332000000	-1.791566000000	-2.159103000000
Ag	1.594806000000	0.621315000000	-1.855562000000
Ag	-1.288469000000	0.832730000000	-1.898198000000
C	5.443403000000	6.134508000000	1.112451000000
C	3.721962000000	7.314563000000	2.025662000000
C	4.541324000000	5.206376000000	0.573259000000
C	2.797528000000	6.403707000000	1.495950000000
C	-0.423940000000	4.783060000000	2.780655000000
C	-1.117851000000	6.041298000000	3.383234000000
C	3.532732000000	2.082418000000	3.416888000000
C	4.990083000000	2.318088000000	2.997035000000
C	2.938909000000	3.286116000000	4.157397000000
C	5.849675000000	2.681498000000	4.222464000000
C	5.271907000000	3.894443000000	4.968785000000
C	3.811474000000	3.643911000000	5.376737000000
C	-7.849510000000	1.640050000000	0.405624000000
C	-7.964036000000	-0.335301000000	1.533856000000

C	-6.513819000000	1.384749000000	0.063660000000
C	-6.631162000000	-0.617782000000	1.204303000000
C	-3.623108000000	-2.501868000000	2.767373000000
C	-4.342576000000	-3.689164000000	3.473893000000
C	-3.304007000000	2.218528000000	3.033955000000
C	-4.287489000000	3.259282000000	2.483901000000
C	-4.014272000000	1.077822000000	3.766261000000
C	-5.179656000000	3.806367000000	3.613647000000
C	-5.910378000000	2.670340000000	4.346965000000
C	-4.911086000000	1.635602000000	4.888143000000
C	2.379415000000	-7.430297000000	-0.271851000000
C	3.971825000000	-7.158238000000	1.334442000000
C	2.196013000000	-6.041635000000	-0.347236000000
C	3.822643000000	-5.765472000000	1.268892000000
C	4.276934000000	-1.940573000000	3.135631000000
C	5.666265000000	-1.578250000000	3.748242000000
C	-0.075006000000	-3.839755000000	2.966570000000
C	-0.318338000000	-5.280819000000	2.498015000000
C	1.152348000000	-3.728140000000	3.873660000000
C	-0.453591000000	-6.221785000000	3.710077000000
C	0.777714000000	-6.128963000000	4.624635000000
C	1.014901000000	-4.679805000000	5.077655000000
C	-5.329506000000	-6.021069000000	-0.388153000000
C	-3.727670000000	-7.176322000000	-1.522425000000
C	-4.390980000000	-5.044939000000	-0.025277000000
C	-2.766921000000	-6.217383000000	-1.172643000000
C	0.091475000000	-4.573349000000	-3.145238000000
C	0.331256000000	-5.913481000000	-3.902864000000
C	-3.611109000000	-1.811689000000	-2.984188000000
C	-5.000936000000	-2.089845000000	-2.396905000000
C	-3.074861000000	-3.005115000000	-3.778624000000
C	-5.986462000000	-2.500587000000	-3.506980000000
C	-5.462140000000	-3.708887000000	-4.298341000000
C	-4.070549000000	-3.416352000000	-4.879979000000
C	7.226630000000	-2.416964000000	-0.927537000000
C	7.694832000000	-0.489966000000	-2.048125000000
C	6.178499000000	-1.784088000000	-0.244101000000
C	6.652359000000	0.166129000000	-1.378022000000
C	4.056673000000	2.566231000000	-2.310076000000
C	4.791505000000	3.796952000000	-2.923906000000
C	3.185708000000	-2.294233000000	-3.441865000000
C	3.869821000000	-3.639958000000	-3.161078000000
C	4.170465000000	-1.250359000000	-3.979210000000
C	4.583555000000	-4.157320000000	-4.424018000000
C	5.578591000000	-3.120410000000	-4.969938000000
C	4.881060000000	-1.777166000000	-5.240191000000
C	-2.464551000000	7.740305000000	-0.715024000000
C	-4.186284000000	6.804426000000	-1.874215000000
C	-2.059021000000	6.475964000000	-0.265133000000
C	-3.807265000000	5.528127000000	-1.435546000000
C	-3.981591000000	1.976245000000	-2.753970000000
C	-5.362359000000	2.078828000000	-3.469199000000
C	0.463629000000	3.830618000000	-2.966164000000
C	0.746066000000	5.265628000000	-2.503834000000
C	-0.788863000000	3.749670000000	-3.841783000000
C	0.861492000000	6.213208000000	-3.712126000000
C	-0.397413000000	6.148115000000	-4.590886000000
C	-0.672640000000	4.706032000000	-5.044229000000
H	6.521226000000	6.012955000000	0.951755000000
H	3.377458000000	8.169122000000	2.620152000000
H	4.866970000000	4.338641000000	-0.009894000000

H	1.718914000000	6.493381000000	1.662334000000
H	3.463140000000	1.165586000000	4.028198000000
H	5.025700000000	3.143082000000	2.259613000000
H	5.391883000000	1.417712000000	2.500646000000
H	1.898802000000	3.080692000000	4.464076000000
H	2.897477000000	4.151156000000	3.465905000000
H	5.893044000000	1.807586000000	4.900071000000
H	6.886860000000	2.879872000000	3.895125000000
H	5.319115000000	4.785902000000	4.309922000000
H	5.884655000000	4.125521000000	5.858853000000
H	3.386319000000	4.530934000000	5.881010000000
H	3.772090000000	2.812718000000	6.108383000000
H	-8.337044000000	2.564282000000	0.073067000000
H	-8.546542000000	-1.043041000000	2.135796000000
H	-5.911796000000	2.074904000000	-0.537466000000
H	-6.120526000000	-1.531314000000	1.528445000000
H	-2.572608000000	2.709970000000	3.699522000000
H	-4.917764000000	2.784061000000	1.708089000000
H	-3.736561000000	4.081313000000	1.994125000000
H	-3.281556000000	0.358108000000	4.168544000000
H	-4.636942000000	0.518221000000	3.040863000000
H	-4.549606000000	4.368653000000	4.330713000000
H	-5.901283000000	4.530383000000	3.192553000000
H	-6.608582000000	2.171873000000	3.643255000000
H	-6.526348000000	3.077563000000	5.169064000000
H	-5.439559000000	0.799753000000	5.381936000000
H	-4.275502000000	2.109977000000	5.662227000000
H	1.788411000000	-8.092521000000	-0.915171000000
H	4.691227000000	-7.604329000000	2.031543000000
H	1.438974000000	-5.592733000000	-1.000888000000
H	4.397508000000	-5.074649000000	1.895015000000
H	-0.968635000000	-3.460862000000	3.491409000000
H	0.530323000000	-5.607217000000	1.866794000000
H	-1.226292000000	-5.328578000000	1.869135000000
H	1.285256000000	-2.687285000000	4.215391000000
H	2.062618000000	-3.982342000000	3.296991000000
H	-1.362874000000	-5.945827000000	4.278692000000
H	-0.602532000000	-7.258211000000	3.355203000000
H	1.669613000000	-6.488992000000	4.071227000000
H	0.657316000000	-6.792345000000	5.500280000000
H	1.922244000000	-4.608173000000	5.704948000000
H	0.165118000000	-4.350202000000	5.708235000000
H	-6.372578000000	-5.930476000000	-0.062158000000
H	-3.446760000000	-8.040337000000	-2.136359000000
H	-4.649556000000	-4.170394000000	0.581263000000
H	-1.724641000000	-6.275417000000	-1.503372000000
H	-3.636834000000	-0.905601000000	-3.614214000000
H	-4.919019000000	-2.905335000000	-1.652215000000
H	-5.372913000000	-1.200247000000	-1.859725000000
H	-2.088981000000	-2.770905000000	-4.213533000000
H	-2.920605000000	-3.856395000000	-3.085871000000
H	-6.135512000000	-1.642593000000	-4.191234000000
H	-6.972385000000	-2.721971000000	-3.057897000000
H	-5.399386000000	-4.587908000000	-3.624100000000
H	-6.168944000000	-3.977030000000	-5.104416000000
H	-3.674315000000	-4.297498000000	-5.416697000000
H	-4.148521000000	-2.599278000000	-5.624648000000
H	7.453315000000	-3.472010000000	-0.732310000000
H	8.306536000000	0.048241000000	-2.781838000000
H	5.574057000000	-2.303819000000	0.508413000000
H	6.410343000000	1.218437000000	-1.557133000000

H	2.352895000000	-2.450243000000	-4.150311000000
H	4.606642000000	-3.505179000000	-2.343060000000
H	3.126023000000	-4.376946000000	-2.811003000000
H	3.651333000000	-0.298026000000	-4.183897000000
H	4.922786000000	-1.034424000000	-3.196094000000
H	3.822985000000	-4.387860000000	-5.195188000000
H	5.097023000000	-5.108786000000	-4.192601000000
H	6.390694000000	-2.966900000000	-4.230624000000
H	6.056642000000	-3.497748000000	-5.892110000000
H	5.608053000000	-1.023467000000	-5.595022000000
H	4.137111000000	-1.905933000000	-6.051580000000
H	-1.910791000000	8.636661000000	-0.411034000000
H	-5.055253000000	6.926237000000	-2.531872000000
H	-1.197593000000	6.328736000000	0.395378000000
H	-4.348944000000	4.620535000000	-1.720618000000
H	1.339535000000	3.426709000000	-3.504008000000
H	-0.081473000000	5.599224000000	-1.848720000000
H	1.670251000000	5.297310000000	-1.899628000000
H	-0.960772000000	2.714907000000	-4.184328000000
H	-1.672036000000	4.026586000000	-3.232400000000
H	1.749510000000	5.929141000000	-4.310499000000
H	1.038027000000	7.243940000000	-3.353470000000
H	-1.266415000000	6.521718000000	-4.010747000000
H	-0.290441000000	6.813620000000	-5.466465000000
H	-1.600388000000	4.651379000000	-5.642293000000
H	0.150738000000	4.365577000000	-5.703285000000
N	5.051241000000	7.191963000000	1.847180000000
N	3.211056000000	5.339828000000	0.771148000000
N	-8.588629000000	0.793475000000	1.146421000000
N	-5.900233000000	0.251759000000	0.471117000000
N	3.260839000000	-8.006115000000	0.566372000000
N	2.928694000000	-5.207167000000	0.422502000000
N	-5.016968000000	-7.091287000000	-1.142411000000
N	-3.103517000000	-5.141475000000	-0.425901000000
N	7.986046000000	-1.788585000000	-1.844651000000
N	5.878917000000	-0.489180000000	-0.485589000000
N	-3.521319000000	7.923287000000	-1.528345000000
N	-2.730604000000	5.361871000000	-0.634526000000
S	2.534142000000	1.707772000000	1.880994000000
S	-2.277670000000	1.570683000000	1.603190000000
S	0.302482000000	2.736105000000	-1.447647000000
S	0.093524000000	-2.739504000000	1.454358000000
S	-2.449468000000	-1.379994000000	-1.576237000000
S	2.387894000000	-1.708785000000	-1.855108000000
O	-0.023886000000	4.928685000000	1.586912000000
O	-0.392820000000	3.767444000000	3.528598000000
O	-4.003377000000	-2.278031000000	1.580036000000
O	-2.710479000000	-1.949320000000	3.441567000000
O	4.330279000000	-2.861399000000	2.261572000000
O	3.307478000000	-1.242049000000	3.531405000000
O	-0.149872000000	-4.676765000000	-1.905030000000
O	0.172125000000	-3.538214000000	-3.860641000000
O	4.351288000000	2.351117000000	-1.088241000000
O	3.253242000000	1.972082000000	-3.068511000000
O	-3.975095000000	2.392663000000	-1.555386000000
O	-3.058419000000	1.447870000000	-3.429208000000
F	-1.093981000000	6.069139000000	4.731012000000
F	-2.432102000000	6.066609000000	2.987301000000
F	-0.543489000000	7.194248000000	2.930037000000
F	-4.386973000000	-3.559800000000	4.816366000000
F	-3.671898000000	-4.854094000000	3.188340000000

F	-5.622271000000	-3.845899000000	3.026807000000
F	5.571188000000	-0.821508000000	4.868615000000
F	6.380605000000	-0.844939000000	2.825810000000
F	6.401698000000	-2.675904000000	4.045387000000
F	-0.603913000000	-6.099955000000	-4.869051000000
F	1.557707000000	-5.930472000000	-4.491019000000
F	0.272160000000	-6.996023000000	-3.067115000000
F	4.874480000000	3.738045000000	-4.268533000000
F	4.112984000000	4.946660000000	-2.599917000000
F	6.055390000000	3.924222000000	-2.429909000000
F	-5.259594000000	2.164327000000	-4.811388000000
F	-6.109595000000	0.964773000000	-3.176976000000
F	-6.076112000000	3.160084000000	-3.035831000000
H	3.001753000000	-1.138345000000	0.707664000000

**Conf2-S<sup>H</sup> (Ag<sub>12</sub>-pyz):**

Ag	0.135706000000	1.672650000000	2.333934000000
Ag	1.827906000000	3.267357000000	0.308718000000
Ag	-1.520834000000	-0.713012000000	2.346041000000
Ag	1.373702000000	-0.953937000000	2.338464000000
Ag	3.833095000000	0.061653000000	-0.162781000000
Ag	-3.745788000000	-0.052565000000	0.309287000000
Ag	-1.965608000000	3.286479000000	-0.161035000000
Ag	1.901772000000	-3.213503000000	0.308154000000
Ag	-1.868700000000	-3.352607000000	-0.166233000000
Ag	-0.101165000000	-1.670277000000	-1.967206000000
Ag	1.498457000000	0.747077000000	-1.972401000000
Ag	-1.395660000000	0.923798000000	-1.969322000000
C	5.426606000000	6.041081000000	0.373315000000
C	3.793032000000	7.191186000000	1.466932000000
C	4.522543000000	5.012040000000	0.073473000000
C	2.866985000000	6.179521000000	1.177358000000
C	-0.286434000000	4.643189000000	2.757091000000
C	-0.909989000000	5.928062000000	3.378037000000
C	3.718902000000	1.786786000000	3.024760000000
C	5.109651000000	2.114056000000	2.464141000000
C	3.121679000000	2.964141000000	3.802241000000
C	6.055982000000	2.566164000000	3.591523000000
C	5.470879000000	3.759368000000	4.363369000000
C	4.078590000000	3.421625000000	4.919552000000
C	-7.949432000000	1.670985000000	0.399676000000
C	-8.122727000000	-0.328136000000	1.477083000000
C	-6.607063000000	1.406492000000	0.092643000000
C	-6.784175000000	-0.620188000000	1.180638000000
C	-3.873534000000	-2.576383000000	2.755223000000
C	-4.663884000000	-3.770625000000	3.367113000000
C	-3.407994000000	2.335272000000	3.026641000000
C	-4.376537000000	3.385262000000	2.465483000000
C	-4.141119000000	1.237035000000	3.804011000000
C	-5.232413000000	3.989851000000	3.593528000000
C	-5.985236000000	2.895918000000	4.367055000000
C	-5.008280000000	1.847171000000	4.921895000000
C	2.554184000000	-7.711806000000	0.363871000000
C	4.356846000000	-6.854167000000	1.460298000000
C	2.097335000000	-6.418674000000	0.071926000000
C	3.926142000000	-5.550370000000	1.178373000000
C	4.149807000000	-2.058403000000	2.776646000000
C	5.576879000000	-2.157099000000	3.392047000000
C	-0.321721000000	-4.117342000000	3.023199000000
C	-0.713685000000	-5.488736000000	2.456437000000

C	0.991553000000	-4.175699000000	3.810102000000
C	-0.790982000000	-6.538053000000	3.580761000000
C	0.530534000000	-6.614781000000	4.361464000000
C	0.914197000000	-5.237040000000	4.924009000000
C	-5.501163000000	-6.019622000000	-0.567739000000
C	-3.841056000000	-7.134795000000	-1.658039000000
C	-4.591195000000	-5.034774000000	-0.158770000000
C	-2.908729000000	-6.166406000000	-1.260587000000
C	0.268786000000	-4.585183000000	-2.728676000000
C	0.856263000000	-5.851623000000	-3.420792000000
C	-3.597246000000	-1.733231000000	-2.963243000000
C	-5.010595000000	-2.025450000000	-2.443833000000
C	-3.008133000000	-2.916477000000	-3.735632000000
C	-5.936539000000	-2.439674000000	-3.602575000000
C	-5.361733000000	-3.638561000000	-4.373291000000
C	-3.945831000000	-3.331279000000	-4.885705000000
C	7.957018000000	-1.757441000000	-0.538884000000
C	8.099509000000	0.231590000000	-1.640089000000
C	6.647884000000	-1.457897000000	-0.136746000000
C	6.793479000000	0.558616000000	-1.249830000000
C	3.830118000000	2.521314000000	-2.739275000000
C	4.630341000000	3.669938000000	-3.423263000000
C	3.303129000000	-2.252267000000	-2.958406000000
C	4.254351000000	-3.336162000000	-2.436081000000
C	4.044516000000	-1.155688000000	-3.727755000000
C	5.073419000000	-3.937813000000	-3.593056000000
C	5.833979000000	-2.847049000000	-4.363492000000
C	4.869075000000	-1.766689000000	-4.877073000000
C	-2.464456000000	7.769624000000	-0.548154000000
C	-4.261539000000	6.889772000000	-1.636648000000
C	-2.062533000000	6.488449000000	-0.145242000000
C	-3.885160000000	5.597483000000	-1.245074000000
C	-4.105252000000	2.054916000000	-2.724602000000
C	-5.500795000000	2.174286000000	-3.407296000000
C	0.296096000000	3.986314000000	-2.961234000000
C	0.743750000000	5.356908000000	-2.438157000000
C	-1.022898000000	4.064979000000	-3.734440000000
C	0.844478000000	6.369596000000	-3.594029000000
C	-0.480753000000	6.467982000000	-4.365899000000
C	-0.916426000000	5.087576000000	-4.881980000000
H	6.468114000000	5.975245000000	0.036600000000
H	3.485321000000	8.075575000000	2.037726000000
H	4.805713000000	4.121067000000	-0.497703000000
H	1.821624000000	6.224750000000	1.500327000000
H	3.776565000000	0.891435000000	3.670087000000
H	5.012114000000	2.921758000000	1.713625000000
H	5.523165000000	1.235307000000	1.939007000000
H	2.136855000000	2.691913000000	4.221539000000
H	2.943406000000	3.802799000000	3.099815000000
H	6.222085000000	1.718484000000	4.285218000000
H	7.042438000000	2.821871000000	3.162664000000
H	5.391224000000	4.630768000000	3.681009000000
H	6.149816000000	4.058742000000	5.182225000000
H	3.641604000000	4.292788000000	5.440886000000
H	4.171208000000	2.614484000000	5.673202000000
H	-8.415313000000	2.608308000000	0.072817000000
H	-8.732069000000	-1.042322000000	2.043898000000
H	-5.979927000000	2.102489000000	-0.475351000000
H	-6.298253000000	-1.549820000000	1.495070000000
H	-2.657854000000	2.826325000000	3.672888000000
H	-5.033807000000	2.902658000000	1.716881000000

H	-3.814942000000	4.176025000000	1.938130000000
H	-3.421017000000	0.511990000000	4.223190000000
H	-4.785103000000	0.670640000000	3.101936000000
H	-4.573555000000	4.550274000000	4.285760000000
H	-5.938990000000	4.724556000000	3.165290000000
H	-6.707328000000	2.399907000000	3.686009000000
H	-6.577153000000	3.341542000000	5.186904000000
H	-5.553395000000	1.039415000000	5.443479000000
H	-4.349460000000	2.323069000000	5.675242000000
H	1.987735000000	-8.586575000000	0.022763000000
H	5.279442000000	-7.020793000000	2.029236000000
H	1.180796000000	-6.227129000000	-0.496900000000
H	4.476621000000	-4.661917000000	1.505097000000
H	-1.135449000000	-3.729839000000	3.662960000000
H	0.043842000000	-5.797435000000	1.710863000000
H	-1.678469000000	-5.417625000000	1.924309000000
H	1.233537000000	-3.184999000000	4.234045000000
H	1.815052000000	-4.428551000000	3.112586000000
H	-1.615928000000	-6.269261000000	4.269694000000
H	-1.048593000000	-7.522132000000	3.147602000000
H	1.333916000000	-6.970433000000	3.683645000000
H	0.453244000000	-7.355571000000	5.177782000000
H	1.884139000000	-5.284027000000	5.451887000000
H	0.159872000000	-4.924564000000	5.673263000000
H	-6.556471000000	-5.950137000000	-0.278031000000
H	-3.524873000000	-7.986766000000	-2.271754000000
H	-4.883474000000	-4.174953000000	0.452735000000
H	-1.851221000000	-6.210966000000	-1.541952000000
H	-3.607431000000	-0.826607000000	-3.593166000000
H	-4.958986000000	-2.842629000000	-1.698785000000
H	-5.414463000000	-1.139951000000	-1.923235000000
H	-2.003798000000	-2.668607000000	-4.119918000000
H	-2.875722000000	-3.769593000000	-3.040925000000
H	-6.061222000000	-1.579322000000	-4.288833000000
H	-6.940880000000	-2.673890000000	-3.203846000000
H	-5.324357000000	-4.520589000000	-3.701020000000
H	-6.025332000000	-3.909062000000	-5.214483000000
H	-3.517832000000	-4.206598000000	-5.407578000000
H	-3.995484000000	-2.511356000000	-5.629536000000
H	8.422285000000	-2.704978000000	-0.242012000000
H	8.682698000000	0.927102000000	-2.255421000000
H	6.045845000000	-2.136441000000	0.476374000000
H	6.305030000000	1.495401000000	-1.538851000000
H	2.522894000000	-2.709424000000	-3.591806000000
H	4.938006000000	-2.886559000000	-1.690182000000
H	3.683122000000	-4.124327000000	-1.915870000000
H	3.335566000000	-0.402297000000	-4.112025000000
H	4.721608000000	-0.622669000000	-3.031096000000
H	4.387531000000	-4.471140000000	-4.279892000000
H	5.771998000000	-4.695681000000	-3.192819000000
H	6.582238000000	-2.379452000000	-3.690565000000
H	6.397275000000	-3.291363000000	-5.203973000000
H	5.420283000000	-0.962652000000	-5.398074000000
H	4.181156000000	-2.213930000000	-5.621903000000
H	-1.877687000000	8.648966000000	-0.256788000000
H	-5.159503000000	7.042371000000	-2.247265000000
H	-1.169225000000	6.311210000000	0.462568000000
H	-4.451316000000	4.703699000000	-1.528269000000
H	1.088560000000	3.545771000000	-3.591224000000
H	0.008066000000	5.715085000000	-1.692555000000
H	1.712626000000	5.266842000000	-1.917191000000



H	-1.306846000000	3.071348000000	-4.121579000000
H	-1.829297000000	4.372322000000	-3.039303000000
H	1.653862000000	6.052738000000	-4.280493000000
H	1.139329000000	7.356596000000	-3.192218000000
H	-1.265675000000	6.872142000000	-3.693679000000
H	-0.384950000000	7.180237000000	-5.205338000000
H	-1.888255000000	5.151736000000	-5.404622000000
H	-0.179238000000	4.725444000000	-5.625903000000
N	5.080875000000	7.135610000000	1.076308000000
N	3.236586000000	5.079851000000	0.483600000000
N	-8.721097000000	0.817521000000	1.098148000000
N	-6.020077000000	0.256272000000	0.491308000000
N	3.679104000000	-7.948625000000	1.064018000000
N	2.785391000000	-5.331977000000	0.486919000000
N	-5.144560000000	-7.074295000000	-1.324415000000
N	-3.288950000000	-5.105990000000	-0.512957000000
N	8.696021000000	-0.926372000000	-1.297360000000
N	6.061545000000	-0.295826000000	-0.500072000000
N	-3.558822000000	7.988634000000	-1.300750000000
N	-2.774230000000	5.396161000000	-0.501281000000
S	2.597131000000	1.272974000000	1.618922000000
S	-2.406594000000	1.612620000000	1.622046000000
S	0.149038000000	2.815561000000	-1.504551000000
S	-0.208100000000	-2.884148000000	1.621592000000
S	-2.512118000000	-1.279374000000	-1.503773000000
S	2.365762000000	-1.534638000000	-1.502341000000
O	0.073172000000	4.753837000000	1.549223000000
O	-0.267395000000	3.635522000000	3.519716000000
O	-4.145484000000	-2.318851000000	1.546868000000
O	-3.019802000000	-2.049833000000	3.524189000000
O	4.062891000000	-2.419079000000	1.567170000000
O	3.267560000000	-1.578317000000	3.543880000000
O	-0.098441000000	-4.756575000000	-1.528571000000
O	0.281488000000	-3.535094000000	-3.428888000000
O	4.161098000000	2.282780000000	-1.540174000000
O	2.915817000000	2.009259000000	-3.442873000000
O	-4.064273000000	2.457654000000	-1.524335000000
O	-3.204149000000	1.523001000000	-3.430406000000
F	-0.779954000000	5.989302000000	4.718345000000
F	-2.250425000000	5.966577000000	3.084516000000
F	-0.354354000000	7.059581000000	2.852138000000
F	-4.783444000000	-3.700081000000	4.707833000000
F	-4.015627000000	-4.942583000000	3.065138000000
F	-5.920569000000	-3.862768000000	2.839729000000
F	5.570968000000	-2.301371000000	4.732168000000
F	6.275895000000	-1.013127000000	3.096435000000
F	6.280183000000	-3.201746000000	2.862509000000
F	0.687360000000	-5.851527000000	-4.759291000000
F	2.204276000000	-5.921484000000	-3.168949000000
F	0.301453000000	-6.999460000000	-2.930830000000
F	4.713791000000	3.534404000000	-4.762886000000
F	4.014182000000	4.868952000000	-3.161493000000
F	5.902015000000	3.762187000000	-2.933609000000
F	-5.426625000000	2.309959000000	-4.747428000000
F	-6.233667000000	1.043825000000	-3.141183000000
F	-6.213349000000	3.232687000000	-2.919930000000
H	-0.002434000000	0.004131000000	3.241362000000

**Conf1-Ag<sup>H</sup> (Ag<sub>12</sub>-py):**

C	3.284834000000	-2.368646000000	-3.180716000000
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H	2.937343000000	-3.413856000000	-3.086093000000
C	2.814137000000	-1.801098000000	-4.525430000000
H	3.075625000000	-0.726407000000	-4.576718000000
H	1.715844000000	-1.885786000000	-4.603106000000
C	3.493297000000	-2.559418000000	-5.682228000000
H	3.147032000000	-3.612967000000	-5.679739000000
H	3.171206000000	-2.123720000000	-6.645553000000
C	5.025157000000	-2.522199000000	-5.556901000000
H	5.493137000000	-3.093452000000	-6.379580000000
H	5.371247000000	-1.473990000000	-5.657257000000
C	5.483437000000	-3.072144000000	-4.196365000000
H	6.582058000000	-2.998672000000	-4.095126000000
H	5.227917000000	-4.149265000000	-4.125080000000
C	4.810284000000	-2.316570000000	-3.034638000000
H	5.113183000000	-2.747455000000	-2.062904000000
H	5.139067000000	-1.260078000000	-3.037644000000
C	-3.685907000000	-1.321801000000	-3.008040000000
H	-4.388422000000	-0.469443000000	-2.943329000000
C	-2.925899000000	-1.243262000000	-4.337212000000
H	-2.139415000000	-2.020342000000	-4.355942000000
H	-2.431022000000	-0.260404000000	-4.425179000000
C	-4.457955000000	-2.638617000000	-2.859222000000
H	-5.010914000000	-2.649038000000	-1.902776000000
H	-3.737880000000	-3.478028000000	-2.824489000000
C	-0.632404000000	-4.369009000000	-2.932971000000
C	-1.425624000000	-5.510919000000	-3.634230000000
C	4.340565000000	1.877471000000	-2.790621000000
C	-3.683615000000	2.747575000000	-2.787500000000
C	-4.597139000000	3.824246000000	-3.443080000000
C	6.567535000000	1.270884000000	0.461440000000
H	6.057754000000	1.851488000000	-0.314272000000
C	7.677452000000	1.765823000000	1.156400000000
H	8.063153000000	2.761116000000	0.916632000000
C	8.263613000000	0.976684000000	2.155261000000
H	9.125412000000	1.342390000000	2.722858000000
C	7.723383000000	-0.290931000000	2.411773000000
H	8.142636000000	-0.947700000000	3.179603000000
C	6.616627000000	-0.718855000000	1.669501000000
H	6.152281000000	-1.694691000000	1.837427000000
C	-3.972331000000	-5.303938000000	1.577833000000
H	-4.629409000000	-4.446873000000	1.753698000000
C	-4.081263000000	-6.482498000000	2.325311000000
H	-4.848395000000	-6.560822000000	3.101234000000
C	-3.192204000000	-7.534840000000	2.066059000000
H	-3.245217000000	-8.465124000000	2.640856000000
C	-2.234722000000	-7.371171000000	1.055684000000
H	-1.520377000000	-8.163728000000	0.813807000000
C	-2.187517000000	-6.161840000000	0.351885000000
H	-1.451160000000	-5.970699000000	-0.436719000000
C	2.459443000000	-6.013125000000	-1.709330000000
H	1.392517000000	-6.019674000000	-1.953731000000
C	3.357461000000	-6.910215000000	-2.299783000000
H	2.991597000000	-7.644557000000	-3.023621000000
C	5.115343000000	-5.879305000000	-1.012882000000
H	6.160759000000	-5.787416000000	-0.703426000000
C	4.156289000000	-5.016406000000	-0.467179000000
H	4.416087000000	-4.247301000000	0.269497000000
C	4.713488000000	-6.839348000000	-1.950985000000
H	5.442256000000	-7.521706000000	-2.400612000000
C	-3.895713000000	-1.454783000000	-5.515780000000
H	-4.614988000000	-0.611423000000	-5.554219000000

H	-3.327169000000	-1.428510000000	-6.463246000000
C	-4.663807000000	-2.779697000000	-5.382259000000
H	-5.365208000000	-2.906529000000	-6.227366000000
H	-3.945419000000	-3.622106000000	-5.429223000000
C	-5.419540000000	-2.841049000000	-4.045295000000
H	-5.940456000000	-3.809992000000	-3.932723000000
H	-6.200677000000	-2.053754000000	-4.021008000000
Ag	-0.076166000000	-1.493947000000	-2.172700000000
Ag	1.577160000000	0.887787000000	-2.513127000000
Ag	-1.311747000000	1.129561000000	-2.090415000000
Ag	3.999408000000	-0.493391000000	-0.092132000000
Ag	1.434281000000	-3.311987000000	-0.305931000000
F	-5.789386000000	3.954474000000	-2.786236000000
F	-4.873646000000	3.566825000000	-4.740148000000
F	-3.975304000000	5.044206000000	-3.380982000000
N	6.039834000000	0.049187000000	0.714564000000
N	-3.036624000000	-5.138454000000	0.612828000000
N	2.848452000000	-5.075204000000	-0.813820000000
O	-0.360773000000	-3.355457000000	-3.634561000000
O	3.456882000000	1.601685000000	-3.655007000000
O	-2.850243000000	2.203153000000	-3.566412000000
O	-0.370410000000	-4.602092000000	-1.716530000000
O	4.223128000000	2.020572000000	-1.541681000000
O	-3.836593000000	2.586524000000	-1.542451000000
S	2.481932000000	-1.488341000000	-1.737962000000
S	0.380014000000	2.982004000000	-1.496608000000
S	-2.567528000000	-1.072997000000	-1.522637000000
Ag	-2.474733000000	-3.055199000000	-0.078178000000
C	5.797429000000	1.996157000000	-3.324096000000
C	0.179195000000	3.793179000000	-4.195007000000
H	-0.817469000000	3.313776000000	-4.222863000000
H	0.927516000000	3.016519000000	-4.438928000000
C	0.435577000000	4.334588000000	-2.782534000000
C	0.236202000000	4.937748000000	-5.224921000000
H	1.267919000000	5.342807000000	-5.267684000000
H	0.011882000000	4.536249000000	-6.229898000000
C	-0.471007000000	6.598042000000	-3.446559000000
H	-1.201680000000	7.382960000000	-3.176726000000
H	0.532979000000	7.068721000000	-3.408731000000
C	-0.741491000000	6.068279000000	-4.863956000000
H	-0.670531000000	6.888444000000	-5.601755000000
H	-1.778642000000	5.682306000000	-4.908323000000
C	-0.536831000000	5.460965000000	-2.410270000000
H	-0.310029000000	5.837815000000	-1.396629000000
H	-1.564475000000	5.051017000000	-2.380446000000
H	1.476134000000	4.706630000000	-2.715718000000
C	-3.060252000000	2.194547000000	3.225306000000
H	-2.663831000000	3.226227000000	3.209303000000
C	-2.554925000000	1.474361000000	4.480113000000
H	-2.841936000000	0.407343000000	4.427742000000
H	-1.453030000000	1.532728000000	4.519115000000
C	-3.170690000000	2.112239000000	5.740443000000
H	-2.798492000000	3.151589000000	5.844505000000
H	-2.824824000000	1.560764000000	6.633668000000
C	-4.706593000000	2.118901000000	5.669676000000
H	-5.132593000000	2.591535000000	6.573689000000
H	-5.073983000000	1.073489000000	5.647612000000
C	-5.194005000000	2.846495000000	4.406338000000
H	-6.297352000000	2.819668000000	4.339239000000
H	-4.902402000000	3.915586000000	4.455597000000
C	-4.590964000000	2.214569000000	3.137512000000

H	-4.913030000000	2.766041000000	2.235900000000
H	-4.963191000000	1.178044000000	3.032335000000
C	3.493582000000	1.271726000000	3.117729000000
H	4.222032000000	0.440252000000	3.085041000000
C	2.610166000000	1.118739000000	4.360497000000
H	1.808582000000	1.879963000000	4.334467000000
H	2.137687000000	0.120975000000	4.357120000000
C	4.234069000000	2.613979000000	3.092296000000
H	4.876376000000	2.678831000000	2.195922000000
H	3.496317000000	3.435296000000	3.020705000000
C	0.499406000000	4.328342000000	2.919760000000
C	1.191844000000	5.455523000000	3.742972000000
C	-4.311688000000	-1.914456000000	2.813090000000
C	3.743614000000	-2.730697000000	2.770252000000
C	4.542616000000	-3.816104000000	3.552702000000
C	-6.722560000000	-1.120788000000	-0.306625000000
H	-6.228779000000	-1.772971000000	0.422181000000
C	-7.916354000000	-1.474715000000	-0.946179000000
H	-8.386482000000	-2.435049000000	-0.715062000000
C	-8.478960000000	-0.592474000000	-1.878518000000
H	-9.406854000000	-0.847925000000	-2.400354000000
C	-7.829914000000	0.624560000000	-2.128098000000
H	-8.227835000000	1.349965000000	-2.843731000000
C	-6.641619000000	0.909915000000	-1.446417000000
H	-6.093094000000	1.841614000000	-1.610665000000
C	4.122767000000	5.279902000000	-1.306664000000
H	4.706375000000	4.375439000000	-1.501230000000
C	4.386513000000	6.482927000000	-1.971743000000
H	5.202220000000	6.530340000000	-2.699157000000
C	3.587878000000	7.600678000000	-1.692572000000
H	3.763291000000	8.553491000000	-2.202455000000
C	2.561011000000	7.473390000000	-0.747173000000
H	1.912307000000	8.317081000000	-0.493777000000
C	2.358570000000	6.236157000000	-0.123994000000
H	1.563395000000	6.069811000000	0.611313000000
C	-2.525298000000	5.884238000000	1.703561000000
H	-1.450062000000	5.910688000000	1.904109000000
C	-3.421999000000	6.721280000000	2.378496000000
H	-3.044961000000	7.423795000000	3.127707000000
C	-5.202610000000	5.714642000000	1.105032000000
H	-6.256794000000	5.611061000000	0.830988000000
C	-4.244200000000	4.908362000000	0.478141000000
H	-4.512374000000	4.168430000000	-0.284277000000
C	-4.788512000000	6.632266000000	2.079729000000
H	-5.516024000000	7.268077000000	2.594793000000
C	3.456926000000	1.301111000000	5.635016000000
H	4.191538000000	0.473503000000	5.707796000000
H	2.801788000000	1.221459000000	6.521652000000
C	4.196720000000	2.648992000000	5.629212000000
H	4.813782000000	2.754163000000	6.540503000000
H	3.454226000000	3.471138000000	5.645359000000
C	5.071641000000	2.789877000000	4.373200000000
H	5.570346000000	3.776571000000	4.351483000000
H	5.875537000000	2.025827000000	4.390218000000
Ag	0.116226000000	1.474555000000	1.884739000000
Ag	-1.555367000000	-0.891450000000	2.042808000000
Ag	1.364154000000	-1.129808000000	1.782465000000
Ag	-3.985670000000	0.361452000000	0.146089000000
Ag	-1.476623000000	3.302590000000	0.100791000000
F	5.887087000000	-3.577231000000	3.479835000000
F	4.213968000000	-3.892433000000	4.863786000000

F	4.319493000000	-5.049030000000	3.003200000000
N	-6.090242000000	0.051446000000	-0.555655000000
N	3.122251000000	5.152449000000	-0.403152000000
N	-2.925070000000	4.983456000000	0.775335000000
O	0.175909000000	3.284856000000	3.549097000000
O	-3.285740000000	-1.705717000000	3.517025000000
O	2.860149000000	-2.108833000000	3.422784000000
O	0.357809000000	4.607186000000	1.691598000000
O	-4.410407000000	-2.142586000000	1.570232000000
O	4.075354000000	-2.624875000000	1.553840000000
S	-2.369601000000	1.439087000000	1.657492000000
S	-0.300205000000	-2.933186000000	1.427336000000
S	2.541144000000	1.054615000000	1.517860000000
Ag	2.360437000000	3.102260000000	0.164477000000
F	1.333643000000	5.162540000000	5.055979000000
F	0.483131000000	6.620287000000	3.649861000000
F	2.444310000000	5.704909000000	3.244166000000
C	-5.683674000000	-1.862830000000	3.549217000000
F	-6.375008000000	-3.025113000000	3.357644000000
F	-6.452109000000	-0.847870000000	3.037268000000
F	-5.581484000000	-1.655007000000	4.880998000000
C	-0.154408000000	-3.462441000000	4.206219000000
H	0.808038000000	-2.918203000000	4.221784000000
H	-0.967797000000	-2.728299000000	4.348871000000
C	-0.314797000000	-4.150336000000	2.845785000000
C	-0.171443000000	-4.513096000000	5.334161000000
H	-1.172234000000	-4.989561000000	5.378042000000
H	-0.018833000000	-4.007935000000	6.305262000000
C	0.727828000000	-6.268385000000	3.742401000000
H	1.526779000000	-7.013080000000	3.570341000000
H	-0.235297000000	-6.818535000000	3.717820000000
C	0.900799000000	-5.592684000000	5.112416000000
H	0.858263000000	-6.347756000000	5.918881000000
H	1.903546000000	-5.126043000000	5.160680000000
C	0.745484000000	-5.231066000000	2.604337000000
H	0.575764000000	-5.718206000000	1.626879000000
H	1.742514000000	-4.756013000000	2.556031000000
H	-1.324080000000	-4.599230000000	2.778515000000
F	6.497185000000	0.865493000000	-2.988371000000
F	5.878476000000	2.146627000000	-4.661478000000
F	6.449435000000	3.051866000000	-2.745941000000
F	-2.620246000000	-5.716925000000	-2.994262000000
F	-1.703933000000	-5.261461000000	-4.933457000000
F	-0.728528000000	-6.683540000000	-3.572244000000
H	-0.011140000000	0.169932000000	-3.138462000000

**Conf2-S<sup>H</sup> (Ag<sub>12</sub>-py):**

C	5.981973000000	0.315347000000	-1.961941000000
H	6.765863000000	-0.324184000000	-1.510231000000
C	5.952742000000	0.096550000000	-3.484033000000
H	5.084802000000	0.640120000000	-3.905142000000
H	5.801236000000	-0.973043000000	-3.711620000000
C	7.245447000000	0.625861000000	-4.132682000000
H	8.108087000000	0.021950000000	-3.785020000000
H	7.185922000000	0.490652000000	-5.227835000000
C	7.480772000000	2.103422000000	-3.780018000000
H	8.417964000000	2.465203000000	-4.240955000000
H	6.658370000000	2.713421000000	-4.200885000000
C	7.522785000000	2.303149000000	-2.256041000000
H	7.656882000000	3.371453000000	-2.005285000000

H	8.399656000000	1.766738000000	-1.839302000000
C	6.238367000000	1.779820000000	-1.586526000000
H	6.294868000000	1.884952000000	-0.488717000000
H	5.379838000000	2.393126000000	-1.914267000000
C	-1.450028000000	-3.188852000000	-3.582839000000
H	-2.525631000000	-3.280329000000	-3.828211000000
C	-0.768245000000	-2.248103000000	-4.586889000000
H	0.269184000000	-2.055962000000	-4.252750000000
H	-1.301928000000	-1.281813000000	-4.613406000000
C	-0.798674000000	-4.578596000000	-3.554457000000
H	-1.343618000000	-5.237244000000	-2.851484000000
H	0.233125000000	-4.480263000000	-3.165366000000
C	2.861359000000	-3.408377000000	-2.733220000000
C	3.887332000000	-4.034437000000	-3.720011000000
C	2.799509000000	2.682411000000	-2.956252000000
C	-4.169567000000	0.678849000000	-3.292692000000
C	-4.955578000000	1.661017000000	-4.213891000000
C	4.301528000000	4.287137000000	0.559972000000
H	3.810205000000	4.148781000000	-0.409399000000
C	4.631649000000	5.559957000000	1.043995000000
H	4.399954000000	6.444046000000	0.441962000000
C	5.245314000000	5.670171000000	2.299705000000
H	5.507637000000	6.650873000000	2.710034000000
C	5.512686000000	4.498411000000	3.021064000000
H	5.986056000000	4.531623000000	4.006944000000
C	5.152249000000	3.263513000000	2.465014000000
H	5.318100000000	2.318215000000	2.992941000000
C	-0.615192000000	-6.846718000000	1.421777000000
H	-1.649815000000	-6.623778000000	1.705529000000
C	0.172769000000	-7.756647000000	2.137002000000
H	-0.248781000000	-8.280327000000	3.000203000000
C	1.498208000000	-7.968867000000	1.730126000000
H	2.143454000000	-8.666624000000	2.273875000000
C	1.979392000000	-7.270042000000	0.614579000000
H	3.005509000000	-7.399973000000	0.256978000000
C	1.126513000000	-6.376483000000	-0.046319000000
H	1.476607000000	-5.785949000000	-0.899188000000
C	5.385903000000	-4.211470000000	-0.296975000000
H	4.651522000000	-4.848023000000	-0.798666000000
C	6.757412000000	-4.331898000000	-0.545500000000
H	7.113941000000	-5.100954000000	-1.236452000000
C	7.117451000000	-2.472539000000	0.945407000000
H	7.761208000000	-1.753869000000	1.460902000000
C	5.733238000000	-2.413634000000	1.142854000000
H	5.287544000000	-1.640630000000	1.776969000000
C	7.642104000000	-3.446657000000	0.084728000000
H	8.720020000000	-3.512051000000	-0.095468000000
C	-0.737868000000	-2.883148000000	-5.990475000000
H	-1.773983000000	-2.984423000000	-6.373269000000
H	-0.208435000000	-2.204175000000	-6.683382000000
C	-0.063661000000	-4.264342000000	-5.965777000000
H	-0.070055000000	-4.714245000000	-6.975691000000
H	0.998288000000	-4.146284000000	-5.673708000000
C	-0.765193000000	-5.196952000000	-4.964903000000
H	-0.258904000000	-6.179109000000	-4.922925000000
H	-1.803736000000	-5.387291000000	-5.304751000000
Ag	0.971604000000	-1.634185000000	-1.362905000000
Ag	1.216801000000	1.104912000000	-1.131742000000
Ag	-1.326415000000	0.008734000000	-2.005972000000
Ag	3.497250000000	1.094832000000	0.616001000000
Ag	2.682681000000	-2.935192000000	0.651860000000

F	-6.193887000000	1.166728000000	-4.494324000000
F	-4.333257000000	1.909289000000	-5.392276000000
F	-5.132590000000	2.869773000000	-3.589296000000
N	4.553528000000	3.155214000000	1.257147000000
N	-0.148980000000	-6.161400000000	0.352350000000
N	4.877440000000	-3.268279000000	0.530527000000
O	2.422361000000	-2.275664000000	-3.079624000000
O	2.541721000000	1.496276000000	-3.299874000000
O	-3.088533000000	0.220375000000	-3.747077000000
O	2.615183000000	-4.075617000000	-1.686231000000
O	2.561069000000	3.250636000000	-1.848696000000
O	-4.739278000000	0.463830000000	-2.179174000000
S	4.405459000000	-0.359838000000	-1.220419000000
S	-0.960993000000	2.424329000000	-1.632773000000
S	-1.424578000000	-2.463289000000	-1.858557000000
Ag	-1.140387000000	-4.124148000000	-0.073001000000
C	3.472931000000	3.604935000000	-4.013524000000
C	-0.613001000000	2.323480000000	-4.458253000000
H	-1.574511000000	1.806512000000	-4.621170000000
H	0.140820000000	1.551324000000	-4.224913000000
C	-0.765122000000	3.291260000000	-3.279724000000
C	-0.182076000000	3.112023000000	-5.725600000000
H	0.918874000000	3.119319000000	-5.806111000000
H	-0.560732000000	2.574705000000	-6.614222000000
C	-2.062513000000	4.656707000000	-5.003016000000
H	-2.775639000000	3.960375000000	-5.480605000000
H	-2.499061000000	5.667558000000	-5.096507000000
C	-0.711028000000	4.567596000000	-5.726845000000
H	0.015668000000	5.230460000000	-5.217204000000
H	-0.795987000000	4.940350000000	-6.763237000000
C	-1.918444000000	4.290378000000	-3.503071000000
H	-1.734702000000	5.192307000000	-2.892413000000
H	-2.866354000000	3.852462000000	-3.141333000000
H	0.184002000000	3.837935000000	-3.142955000000
C	-4.362214000000	0.461190000000	2.403920000000
H	-4.451658000000	1.561643000000	2.476447000000
C	-3.865666000000	-0.092673000000	3.742659000000
H	-3.682980000000	-1.179249000000	3.642267000000
H	-2.911397000000	0.393535000000	4.015023000000
C	-4.923240000000	0.163798000000	4.834845000000
H	-5.019363000000	1.256550000000	4.997775000000
H	-4.574403000000	-0.269549000000	5.790102000000
C	-6.290416000000	-0.423547000000	4.444650000000
H	-7.040590000000	-0.200756000000	5.225653000000
H	-6.205740000000	-1.525085000000	4.381491000000
C	-6.760066000000	0.116371000000	3.083878000000
H	-7.718910000000	-0.349314000000	2.789741000000
H	-6.943993000000	1.207961000000	3.156255000000
C	-5.706707000000	-0.146697000000	1.990595000000
H	-6.035928000000	0.271344000000	1.023053000000
H	-5.583440000000	-1.236410000000	1.849985000000
C	1.806199000000	2.611089000000	3.631577000000
H	2.855264000000	2.282990000000	3.741653000000
C	0.935642000000	1.924052000000	4.689513000000
H	-0.125389000000	2.175042000000	4.502189000000
H	1.044366000000	0.828724000000	4.606920000000
C	1.741066000000	4.139818000000	3.716119000000
H	2.405874000000	4.590987000000	2.958151000000
H	0.713123000000	4.475796000000	3.485177000000
C	-2.118672000000	3.972024000000	2.743508000000
C	-2.249992000000	5.256144000000	3.617193000000

C	-3.501487000000	-4.083457000000	2.119573000000
C	3.787590000000	-0.299501000000	3.496080000000
C	4.276004000000	-0.228829000000	4.975894000000
C	-4.679433000000	-4.281572000000	-1.634037000000
H	-4.228926000000	-4.537644000000	-0.668365000000
C	-4.998829000000	-5.270190000000	-2.573081000000
H	-4.794871000000	-6.318837000000	-2.337063000000
C	-5.568724000000	-4.891215000000	-3.795944000000
H	-5.818159000000	-5.640965000000	-4.553863000000
C	-5.818638000000	-3.531114000000	-4.026457000000
H	-6.269020000000	-3.182713000000	-4.960481000000
C	-5.472787000000	-2.603241000000	-3.037074000000
H	-5.642740000000	-1.530870000000	-3.169766000000
C	0.967722000000	6.016687000000	-1.687720000000
H	1.802096000000	5.337459000000	-1.891343000000
C	0.687641000000	7.111560000000	-2.513324000000
H	1.326538000000	7.307106000000	-3.379384000000
C	-0.418319000000	7.919755000000	-2.215643000000
H	-0.666678000000	8.780286000000	-2.845183000000
C	-1.206555000000	7.597661000000	-1.101750000000
H	-2.083344000000	8.193920000000	-0.832931000000
C	-0.870821000000	6.479007000000	-0.329630000000
H	-1.469644000000	6.156516000000	0.528444000000
C	-5.297317000000	4.172670000000	1.049470000000
H	-4.382218000000	4.663239000000	1.391567000000
C	-6.543522000000	4.463896000000	1.614444000000
H	-6.609053000000	5.200571000000	2.420312000000
C	-7.520953000000	2.861369000000	0.101617000000
H	-8.375029000000	2.312905000000	-0.306075000000
C	-6.240393000000	2.616586000000	-0.408484000000
H	-6.053852000000	1.880379000000	-1.198539000000
C	-7.678083000000	3.794293000000	1.135376000000
H	-8.666532000000	3.995620000000	1.560794000000
C	1.335273000000	2.408938000000	6.097627000000
H	2.366934000000	2.075356000000	6.321898000000
H	0.676299000000	1.931432000000	6.845856000000
C	1.252168000000	3.940711000000	6.201069000000
H	1.556717000000	4.275258000000	7.209783000000
H	0.201247000000	4.260404000000	6.057682000000
C	2.128874000000	4.611641000000	5.131339000000
H	2.041366000000	5.712673000000	5.185563000000
H	3.194118000000	4.365618000000	5.316291000000
Ag	-1.008784000000	1.277334000000	1.839035000000
Ag	-1.524688000000	-1.559613000000	1.507243000000
Ag	1.224727000000	-0.528859000000	1.251487000000
Ag	-3.714495000000	-1.373009000000	-0.749132000000
Ag	-3.107264000000	2.566339000000	-0.503599000000
F	4.653609000000	1.047406000000	5.301794000000
F	3.322589000000	-0.598770000000	5.870994000000
F	5.354135000000	-1.037228000000	5.164973000000
N	-4.899934000000	-2.964631000000	-1.865038000000
N	0.201070000000	5.701350000000	-0.615880000000
N	-5.143453000000	3.259463000000	0.060877000000
O	-2.062931000000	2.873749000000	3.360344000000
O	-2.869382000000	-3.221608000000	2.783989000000
O	2.682002000000	-0.865431000000	3.303455000000
O	-2.077660000000	4.205572000000	1.497757000000
O	-3.136652000000	-4.778633000000	1.120715000000
O	4.594974000000	0.222030000000	2.667843000000
S	-3.119486000000	0.257029000000	1.019376000000
S	0.481198000000	-3.019997000000	1.726159000000



S	1.350445000000	2.046406000000	1.898172000000
Ag	0.448107000000	3.721106000000	0.380965000000
F	-2.186955000000	5.019166000000	4.947041000000
F	-3.438763000000	5.886935000000	3.365125000000
F	-1.252359000000	6.143465000000	3.312008000000
C	-4.991961000000	-4.305820000000	2.523095000000
F	-5.348363000000	-5.612870000000	2.490500000000
F	-5.800462000000	-3.640099000000	1.629885000000
F	-5.283673000000	-3.827005000000	3.758682000000
C	0.036347000000	-2.347848000000	4.458968000000
H	0.843005000000	-1.596195000000	4.465606000000
H	-0.875281000000	-1.858898000000	4.070952000000
C	0.456765000000	-3.496684000000	3.538084000000
C	-0.233449000000	-2.894864000000	5.884451000000
H	-1.292868000000	-3.198463000000	5.969509000000
H	-0.078546000000	-2.073167000000	6.607848000000
C	2.022374000000	-3.996008000000	5.491671000000
H	2.498425000000	-3.026993000000	5.727748000000
H	2.722658000000	-4.782999000000	5.825328000000
C	0.684503000000	-4.092930000000	6.240439000000
H	0.187409000000	-5.043982000000	5.964653000000
H	0.849270000000	-4.136322000000	7.331685000000
C	1.813176000000	-4.100405000000	3.959647000000
H	1.859309000000	-5.152609000000	3.621793000000
H	2.628798000000	-3.556752000000	3.448482000000
H	-0.337015000000	-4.266637000000	3.545155000000
F	4.585941000000	4.210835000000	-3.500308000000
F	3.843306000000	2.954403000000	-5.137241000000
F	2.608288000000	4.606578000000	-4.376034000000
F	4.007823000000	-5.378783000000	-3.553928000000
F	3.561388000000	-3.806561000000	-5.015712000000
F	5.125715000000	-3.489680000000	-3.499666000000
H	3.576959000000	0.095361000000	-2.211425000000

### Ag<sub>12</sub>-BpV

C	3.133368000000	-2.767506000000	3.127525000000
H	4.218116000000	-2.616609000000	2.978024000000
C	2.681668000000	-2.005365000000	4.379298000000
H	1.581568000000	-2.090267000000	4.471956000000
H	2.940206000000	-0.936588000000	4.286879000000
C	3.348572000000	-2.614965000000	5.628601000000
H	4.445834000000	-2.458941000000	5.567073000000
H	3.003807000000	-2.073497000000	6.528218000000
C	3.048845000000	-4.117675000000	5.750097000000
H	3.556764000000	-4.541818000000	6.635594000000
H	1.960375000000	-4.255935000000	5.903869000000
C	3.478004000000	-4.870731000000	4.480506000000
H	3.211808000000	-5.941141000000	4.553902000000
H	4.580585000000	-4.825854000000	4.378599000000
C	2.821578000000	-4.265964000000	3.224780000000
H	3.165498000000	-4.789614000000	2.313245000000
H	1.724000000000	-4.386664000000	3.289138000000
C	0.906813000000	3.568168000000	3.071943000000
H	-0.079748000000	4.066935000000	3.073971000000
C	1.014396000000	2.665510000000	4.305697000000
H	1.957102000000	2.089959000000	4.251781000000
H	0.170850000000	1.953280000000	4.320314000000
C	2.027140000000	4.612804000000	3.021859000000
H	1.915484000000	5.251386000000	2.127502000000

H	3.001582000000	4.098442000000	2.932525000000
C	4.713467000000	1.543924000000	2.546933000000
C	5.613213000000	2.611301000000	3.238276000000
C	-1.421492000000	-4.272289000000	3.450825000000
C	-3.220734000000	2.758094000000	2.823250000000
C	-4.328812000000	3.281832000000	3.792149000000
C	0.432456000000	-6.058293000000	0.676281000000
H	0.477632000000	-5.561267000000	1.649354000000
C	-0.731124000000	-6.720939000000	0.278411000000
H	-1.583758000000	-6.743590000000	0.962308000000
C	-0.793623000000	-7.303679000000	-1.004806000000
C	0.382624000000	-7.258349000000	-1.785984000000
H	0.402666000000	-7.687918000000	-2.792274000000
C	1.499781000000	-6.564348000000	-1.311595000000
H	2.399315000000	-6.443772000000	-1.925780000000
C	4.356639000000	4.908284000000	-2.040051000000
H	3.393419000000	5.424684000000	-2.079054000000
C	5.320736000000	5.093427000000	-3.032740000000
H	5.117156000000	5.779077000000	-3.860462000000
C	6.543398000000	4.394704000000	-2.956992000000
C	6.742479000000	3.571916000000	-1.829924000000
H	7.664415000000	2.993778000000	-1.716236000000
C	5.724079000000	3.427021000000	-0.884559000000
H	5.822588000000	2.750580000000	-0.028224000000
C	6.492274000000	-1.501238000000	1.841192000000
H	6.527741000000	-0.414187000000	1.960883000000
C	7.081746000000	-2.356412000000	2.774827000000
H	7.609851000000	-1.932510000000	3.633966000000
C	6.336391000000	-4.209535000000	1.437022000000
H	6.219186000000	-5.279315000000	1.240062000000
C	5.771474000000	-3.289806000000	0.549261000000
H	5.239447000000	-3.631429000000	-0.345096000000
C	6.987661000000	-3.753221000000	2.600992000000
C	1.003471000000	3.526376000000	5.584204000000
H	0.017836000000	4.025182000000	5.678612000000
H	1.111866000000	2.869911000000	6.466750000000
C	2.119142000000	4.584309000000	5.558401000000
H	2.079192000000	5.208180000000	6.469930000000
H	3.103353000000	4.076876000000	5.554662000000
C	2.011327000000	5.466598000000	4.304304000000
H	2.840539000000	6.197992000000	4.268519000000
H	1.069267000000	6.050502000000	4.341976000000
Ag	1.902646000000	0.365321000000	1.808423000000
Ag	-0.054608000000	-1.827837000000	1.943866000000
Ag	-0.963725000000	0.937849000000	1.765066000000
Ag	2.189106000000	-3.674465000000	-0.312138000000
Ag	4.113434000000	-0.617342000000	0.029442000000
F	-4.484777000000	4.636435000000	3.663872000000
F	-4.072912000000	3.023388000000	5.094158000000
F	-5.538410000000	2.711736000000	3.495015000000
N	1.526331000000	-5.932659000000	-0.112209000000
N	4.532611000000	4.065103000000	-0.993891000000
N	5.816982000000	-1.950476000000	0.755233000000
O	3.779479000000	1.055178000000	3.236659000000
O	-0.521517000000	-3.423823000000	3.691512000000
O	-2.169247000000	2.328143000000	3.372728000000
O	5.046826000000	1.307279000000	1.346222000000
O	-1.887092000000	-4.682329000000	2.344574000000
O	-3.519671000000	2.841389000000	1.596225000000
S	2.366433000000	-2.064662000000	1.573168000000
S	-2.393075000000	-1.089298000000	1.499513000000

S	0.876940000000	2.597269000000	1.467910000000
Ag	2.699007000000	3.080643000000	-0.119866000000
C	-2.095942000000	-4.938161000000	4.686244000000
C	-2.762315000000	-0.891315000000	4.324143000000
H	-2.561938000000	0.194348000000	4.261688000000
H	-1.793637000000	-1.406913000000	4.446964000000
C	-3.440694000000	-1.354725000000	3.030133000000
C	-3.682227000000	-1.186593000000	5.526930000000
H	-3.796091000000	-2.282704000000	5.637935000000
H	-3.198203000000	-0.822876000000	6.451447000000
C	-5.724982000000	-0.982514000000	4.036581000000
H	-6.695403000000	-0.473649000000	3.888670000000
H	-5.939833000000	-2.069514000000	4.078588000000
C	-5.066187000000	-0.538452000000	5.352470000000
H	-5.717867000000	-0.791562000000	6.208625000000
H	-4.956470000000	0.562711000000	5.348645000000
C	-4.810902000000	-0.696609000000	2.830488000000
H	-5.275640000000	-1.056809000000	1.896187000000
H	-4.677243000000	0.395614000000	2.722755000000
H	-3.564213000000	-2.453615000000	3.055397000000
C	-2.745343000000	2.383827000000	-3.126705000000
H	-3.501338000000	1.587494000000	-3.243930000000
C	-1.924956000000	2.504485000000	-4.412524000000
H	-1.102230000000	3.225738000000	-4.267086000000
H	-1.475100000000	1.527663000000	-4.657656000000
C	-2.838364000000	2.977898000000	-5.560576000000
H	-3.599762000000	2.199758000000	-5.766286000000
H	-2.236975000000	3.086642000000	-6.481208000000
C	-3.534649000000	4.302552000000	-5.208348000000
H	-4.196082000000	4.623372000000	-6.033784000000
H	-2.766126000000	5.091237000000	-5.084321000000
C	-4.337688000000	4.172832000000	-3.903483000000
H	-4.804184000000	5.137618000000	-3.631437000000
H	-5.164304000000	3.447173000000	-4.046480000000
C	-3.441030000000	3.695424000000	-2.743835000000
H	-4.031734000000	3.559891000000	-1.819389000000
H	-2.671896000000	4.463194000000	-2.531387000000
C	-0.429571000000	-3.925091000000	-3.041443000000
H	0.180129000000	-4.827565000000	-2.857993000000
C	0.076357000000	-3.211198000000	-4.298953000000
H	-0.457561000000	-2.249951000000	-4.408258000000
H	1.154482000000	-2.995336000000	-4.203869000000
C	-1.906776000000	-4.320299000000	-3.142794000000
H	-2.213995000000	-4.869429000000	-2.233669000000
H	-2.519491000000	-3.402239000000	-3.186211000000
C	-3.255746000000	-0.986553000000	-3.957457000000
C	-4.414721000000	-1.094006000000	-4.987420000000
C	0.956296000000	4.538741000000	-2.693024000000
C	3.956132000000	-3.417129000000	-2.895966000000
C	5.272812000000	-3.670189000000	-3.689031000000
C	-0.203649000000	6.449041000000	0.712169000000
H	0.509070000000	6.224717000000	-0.089039000000
C	-0.030682000000	7.522695000000	1.587972000000
H	0.832025000000	8.183316000000	1.461085000000
C	-0.963550000000	7.747372000000	2.622048000000
C	-2.073502000000	6.879883000000	2.681730000000
H	-2.829552000000	6.978377000000	3.465874000000
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H	-3.024825000000	5.139644000000	1.791497000000
C	-4.762714000000	-4.302900000000	1.299125000000
H	-4.171841000000	-4.884573000000	2.013704000000

C	-6.073044000000	-3.910612000000	1.585926000000
H	-6.524975000000	-4.201929000000	2.538825000000
C	-6.762659000000	-3.069611000000	0.687257000000
C	-6.095859000000	-2.725030000000	-0.505554000000
H	-6.576197000000	-2.095189000000	-1.259415000000
C	-4.790546000000	-3.170422000000	-0.724754000000
H	-4.250575000000	-2.860836000000	-1.624011000000
C	-5.979380000000	0.716254000000	-1.789436000000
H	-5.342381000000	0.036870000000	-2.366340000000
C	-7.265414000000	1.058941000000	-2.213178000000
H	-7.639451000000	0.661698000000	-3.161572000000
C	-7.467366000000	2.430529000000	-0.246408000000
H	-8.030771000000	3.094407000000	0.416235000000
C	-6.171264000000	2.046766000000	0.107943000000
H	-5.682728000000	2.423976000000	1.011295000000
C	-8.052193000000	1.925950000000	-1.426663000000
C	-0.188820000000	-4.082095000000	-5.544115000000
H	0.421250000000	-5.007237000000	-5.487291000000
H	0.148581000000	-3.535828000000	-6.443364000000
C	-1.674457000000	-4.458147000000	-5.665733000000
H	-1.837940000000	-5.098020000000	-6.552062000000
H	-2.270112000000	-3.537177000000	-5.819791000000
C	-2.161043000000	-5.176265000000	-4.396770000000
H	-3.238454000000	-5.414969000000	-4.463497000000
H	-1.631642000000	-6.145122000000	-4.291651000000
Ag	-1.207488000000	-0.685371000000	-1.940975000000
Ag	0.696673000000	1.523632000000	-2.094647000000
Ag	1.677121000000	-1.228801000000	-1.853624000000
Ag	-1.109708000000	3.559319000000	-0.089012000000
Ag	-3.324001000000	0.621994000000	-0.045181000000
F	5.631094000000	-4.974869000000	-3.704851000000
F	5.199528000000	-3.242287000000	-4.973127000000
F	6.285112000000	-2.970303000000	-3.078523000000
N	-1.255087000000	5.598888000000	0.805804000000
N	-4.112387000000	-3.929014000000	0.169843000000
N	-5.437908000000	1.189768000000	-0.641324000000
O	-2.107793000000	-0.743985000000	-4.402900000000
O	1.123128000000	3.529601000000	-3.428171000000
O	3.255896000000	-2.452122000000	-3.296337000000
O	-3.615728000000	-1.126869000000	-2.743279000000
O	1.196468000000	4.688264000000	-1.455338000000
O	3.802569000000	-4.186605000000	-1.895600000000
S	-1.724629000000	1.789741000000	-1.670320000000
S	3.030605000000	0.852095000000	-1.632213000000
S	-0.160761000000	-2.905735000000	-1.487152000000
Ag	-1.805805000000	-3.484922000000	0.274576000000
F	-5.128517000000	0.083507000000	-4.992488000000
F	-5.291412000000	-2.084477000000	-4.660235000000
F	-3.985310000000	-1.321055000000	-6.246069000000
C	0.358894000000	5.812701000000	-3.363698000000
F	1.246826000000	6.846377000000	-3.287338000000
F	-0.781057000000	6.206637000000	-2.712194000000
F	0.034146000000	5.637047000000	-4.665074000000
C	3.243373000000	0.812231000000	-4.460560000000
H	2.968564000000	-0.259041000000	-4.442760000000
H	2.314653000000	1.409867000000	-4.494560000000
C	4.031876000000	1.144104000000	-3.188577000000
C	4.112141000000	1.102043000000	-5.700653000000
H	4.318569000000	2.191144000000	-5.753884000000
H	3.544539000000	0.843405000000	-6.612960000000
C	6.213965000000	0.645618000000	-4.359125000000

H	7.137093000000	0.040272000000	-4.301840000000
H	6.529216000000	1.708087000000	-4.368315000000
C	5.439918000000	0.328958000000	-5.648737000000
H	6.059012000000	0.570010000000	-6.532273000000
H	5.231633000000	-0.757075000000	-5.684440000000
C	5.354837000000	0.375047000000	-3.109101000000
H	5.905036000000	0.655371000000	-2.192161000000
H	5.130898000000	-0.703601000000	-3.041998000000
H	4.222043000000	2.233326000000	-3.152746000000
F	-1.865061000000	-6.277782000000	4.698572000000
F	-1.6711116000000	-4.427813000000	5.862504000000
F	-3.455353000000	-4.754069000000	4.628028000000
F	5.520850000000	3.806251000000	2.573336000000
F	5.280489000000	2.842502000000	4.529774000000
F	6.920429000000	2.227224000000	3.206982000000
C	-0.776293000000	8.834430000000	3.610233000000
C	-1.869904000000	9.550363000000	4.136769000000
C	0.507267000000	9.188065000000	4.073756000000
C	-1.632019000000	10.562760000000	5.075009000000
H	-2.890198000000	9.340099000000	3.800505000000
C	0.630096000000	10.214253000000	5.019115000000
H	1.394957000000	8.648546000000	3.728482000000
H	-2.472292000000	11.135106000000	5.488500000000
H	1.621527000000	10.494856000000	5.397215000000
C	-9.442239000000	2.268340000000	-1.805285000000
C	-10.300564000000	1.303060000000	-2.369501000000
C	-9.968218000000	3.559138000000	-1.599257000000
C	-11.613980000000	1.668313000000	-2.692307000000
H	-9.959146000000	0.274180000000	-2.522782000000
C	-11.295184000000	3.817270000000	-1.966287000000
H	-9.344080000000	4.357545000000	-1.185117000000
H	-12.299335000000	0.926794000000	-3.122068000000
H	-11.718732000000	4.819492000000	-1.822606000000
C	7.516509000000	-4.696645000000	3.612218000000
C	7.431787000000	-4.408251000000	4.989939000000
C	8.098464000000	-5.926542000000	3.246302000000
C	7.917995000000	-5.344155000000	5.911722000000
H	6.961673000000	-3.483269000000	5.339962000000
C	8.558360000000	-6.786335000000	4.252130000000
H	8.214885000000	-6.199033000000	2.192487000000
H	7.849099000000	-5.140050000000	6.987879000000
H	9.021354000000	-7.744637000000	3.984212000000
C	-2.056074000000	-7.861577000000	-1.532345000000
C	-3.297154000000	-7.268935000000	-1.214660000000
C	-2.075905000000	-8.970355000000	-2.407308000000
C	-4.462481000000	-7.788613000000	-1.784729000000
H	-3.340103000000	-6.386403000000	-0.566341000000
H	-1.138343000000	-9.486942000000	-2.653634000000
C	-4.354503000000	-8.884424000000	-2.655275000000
H	-5.438092000000	-7.340469000000	-1.571194000000
H	-5.247811000000	-9.306391000000	-3.133004000000
C	-8.099471000000	-2.518385000000	1.006826000000
C	-8.442049000000	-1.202782000000	0.632065000000
C	-9.068122000000	-3.259516000000	1.711104000000
C	-9.708171000000	-0.706860000000	0.967144000000
H	-7.721857000000	-0.565096000000	0.111829000000
C	-10.305598000000	-2.665278000000	1.992579000000
H	-8.871612000000	-4.292891000000	2.014601000000
H	-9.987697000000	0.316065000000	0.682886000000
H	-11.074330000000	-3.231382000000	2.534081000000
C	7.556087000000	4.486797000000	-4.033233000000

C	7.171521000000	4.546263000000	-5.388315000000
C	8.936970000000	4.488005000000	-3.753913000000
C	8.164886000000	4.600314000000	-6.374462000000
H	6.113957000000	4.515451000000	-5.670638000000
C	9.844868000000	4.551891000000	-4.818716000000
H	9.298375000000	4.464657000000	-2.720826000000
H	7.883245000000	4.635518000000	-7.434619000000
H	10.924036000000	4.562369000000	-4.618956000000
N	-0.409439000000	10.905664000000	5.524420000000
N	-12.122781000000	2.900936000000	-2.504362000000
N	-10.642498000000	-1.410873000000	1.635424000000
N	8.477665000000	-6.520583000000	5.570152000000
N	-3.186255000000	-9.480312000000	-2.963580000000
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### Ag<sub>12</sub>-BPA

C	-3.060985000000	2.574320000000	-3.293295000000
H	-2.707091000000	3.613999000000	-3.169918000000
C	-2.407886000000	1.959990000000	-4.536614000000
H	-2.655611000000	0.882993000000	-4.580955000000
H	-1.310775000000	2.061691000000	-4.464084000000
C	-2.925353000000	2.659184000000	-5.808422000000
H	-2.589592000000	3.715820000000	-5.807927000000
H	-2.471238000000	2.181858000000	-6.695982000000
C	-4.459594000000	2.604401000000	-5.889249000000
H	-4.817155000000	3.120820000000	-6.798974000000
H	-4.783410000000	1.547454000000	-5.967721000000
C	-5.095226000000	3.228542000000	-4.636775000000
H	-6.197912000000	3.160245000000	-4.680210000000
H	-4.842064000000	4.307535000000	-4.590968000000
C	-4.592122000000	2.534094000000	-3.356824000000
H	-5.024272000000	3.012825000000	-2.459476000000
H	-4.930450000000	1.481460000000	-3.353274000000
C	3.490174000000	1.856264000000	-2.825503000000
H	4.122458000000	0.952618000000	-2.892822000000
C	2.671462000000	1.995997000000	-4.111553000000
H	1.951827000000	2.828764000000	-4.005865000000
H	2.095219000000	1.070069000000	-4.282262000000
C	4.362098000000	3.086282000000	-2.555844000000
H	4.947499000000	2.947174000000	-1.628916000000
H	3.703654000000	3.960912000000	-2.400976000000
C	0.311884000000	4.877200000000	-2.487829000000
C	0.760639000000	6.103481000000	-3.341416000000
C	-4.263015000000	-1.538367000000	-3.141915000000
C	3.786236000000	-1.869407000000	-3.148497000000
C	4.768773000000	-2.643258000000	-4.076384000000
C	-6.629400000000	-1.312703000000	0.206537000000
H	-6.119567000000	-1.857117000000	-0.595578000000
C	-7.635131000000	-1.903438000000	0.979656000000
H	-7.923725000000	-2.945159000000	0.782946000000
C	-8.243796000000	-1.159839000000	2.009542000000
C	-7.813078000000	0.168430000000	2.188246000000
H	-8.249821000000	0.801672000000	2.968282000000
C	-6.798467000000	0.686542000000	1.380632000000
H	-6.424791000000	1.704873000000	1.515736000000
C	4.813734000000	4.853283000000	0.707841000000

H	4.871352000000	4.080794000000	1.480585000000
C	5.965913000000	5.453439000000	0.190399000000
H	6.935173000000	5.157342000000	0.597166000000
C	5.862536000000	6.367794000000	-0.872714000000
C	4.559671000000	6.708585000000	-1.289292000000
H	4.400270000000	7.433305000000	-2.094984000000
C	3.453707000000	6.088770000000	-0.705154000000
H	2.431643000000	6.317644000000	-1.019707000000
C	-2.446875000000	6.537047000000	-0.789798000000
H	-1.353352000000	6.591015000000	-0.763188000000
C	-3.235600000000	7.649620000000	-1.097542000000
H	-2.754596000000	8.616629000000	-1.280620000000
C	-5.172799000000	6.240132000000	-0.940134000000
H	-6.251871000000	6.068368000000	-0.991107000000
C	-4.325263000000	5.184228000000	-0.598231000000
H	-4.714237000000	4.197693000000	-0.331704000000
C	-4.635251000000	7.520720000000	-1.170203000000
C	3.613369000000	2.260707000000	-5.302000000000
H	4.255160000000	1.370990000000	-5.462029000000
H	3.014046000000	2.388068000000	-6.221851000000
C	4.493511000000	3.498512000000	-5.059103000000
H	5.178101000000	3.658625000000	-5.912403000000
H	3.844785000000	4.393690000000	-4.991571000000
C	5.292259000000	3.360137000000	-3.752470000000
H	5.877682000000	4.279603000000	-3.555087000000
H	6.021548000000	2.529959000000	-3.848393000000
Ag	0.015281000000	1.865420000000	-1.761554000000
Ag	-1.540474000000	-0.529871000000	-2.215300000000
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Ag	-4.201982000000	0.604251000000	-0.351928000000
Ag	-1.699736000000	3.528509000000	-0.001563000000
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F	4.392416000000	-2.660957000000	-5.376337000000
F	4.899184000000	-3.943978000000	-3.673116000000
N	-6.199716000000	-0.042152000000	0.407987000000
N	3.572480000000	5.135900000000	0.251120000000
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O	-3.245881000000	-1.233847000000	-3.821731000000
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O	0.362211000000	5.031407000000	-1.233273000000
O	-4.349365000000	-1.878917000000	-1.923562000000
O	4.081183000000	-1.919669000000	-1.922770000000
S	-2.489130000000	1.731692000000	-1.717843000000
S	-0.219951000000	-2.596509000000	-1.808722000000
S	2.428294000000	1.517934000000	-1.317863000000
Ag	2.033520000000	3.480513000000	0.289879000000
C	-5.642505000000	-1.467302000000	-3.862636000000
C	-0.084850000000	-2.731571000000	-4.629961000000
H	0.804252000000	-2.077721000000	-4.567079000000
H	-0.983965000000	-2.091047000000	-4.671133000000
C	-0.138084000000	-3.614751000000	-3.377358000000
C	0.013544000000	-3.605131000000	-5.896024000000
H	-0.918883000000	-4.194396000000	-6.013311000000
H	0.087838000000	-2.950610000000	-6.783546000000
C	1.141794000000	-5.442222000000	-4.569272000000
H	2.026304000000	-6.102333000000	-4.500693000000

H	0.254058000000	-6.103722000000	-4.636978000000
C	1.217361000000	-4.558634000000	-5.824918000000
H	1.263476000000	-5.188877000000	-6.732155000000
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C	1.044419000000	-4.588403000000	-3.290503000000
H	0.939801000000	-5.231777000000	-2.396845000000
H	1.977534000000	-4.009056000000	-3.161401000000
H	-1.090444000000	-4.178988000000	-3.356817000000
C	2.840325000000	-2.138617000000	3.184554000000
H	2.738883000000	-3.226521000000	3.011788000000
C	2.004442000000	-1.729102000000	4.404118000000
H	2.005854000000	-0.624919000000	4.481642000000
H	0.962262000000	-2.065951000000	4.265789000000
C	2.599632000000	-2.328590000000	5.692093000000
H	2.515331000000	-3.433823000000	5.658044000000
H	2.003055000000	-1.992359000000	6.559768000000
C	4.074020000000	-1.929288000000	5.861308000000
H	4.493625000000	-2.378150000000	6.780218000000
H	4.144980000000	-0.829883000000	5.974127000000
C	4.899176000000	-2.356291000000	4.637228000000
H	5.952581000000	-2.038646000000	4.749277000000
H	4.905384000000	-3.463506000000	4.565503000000
C	4.320187000000	-1.763337000000	3.338280000000
H	4.893882000000	-2.110704000000	2.459445000000
H	4.410783000000	-0.662558000000	3.369328000000
C	-3.643886000000	-1.447470000000	2.794204000000
H	-4.394184000000	-0.636186000000	2.836310000000
C	-2.744270000000	-1.370372000000	4.033542000000
H	-1.930648000000	-2.113718000000	3.933381000000
H	-2.290680000000	-0.365604000000	4.103342000000
C	-4.339014000000	-2.806668000000	2.673542000000
H	-4.990149000000	-2.820027000000	1.782301000000
H	-3.574399000000	-3.590857000000	2.532172000000
C	-0.515762000000	-4.705704000000	2.210359000000
C	-1.414924000000	-5.825534000000	2.830574000000
C	3.722651000000	2.073751000000	3.325815000000
C	-4.060778000000	2.666977000000	2.567647000000
C	-4.877196000000	3.718233000000	3.382508000000
C	6.606088000000	0.876688000000	0.941104000000
H	5.965236000000	1.590975000000	1.467523000000
C	7.985478000000	0.832260000000	1.143606000000
H	8.447055000000	1.541432000000	1.838265000000
C	8.763353000000	-0.133752000000	0.473927000000
C	8.100232000000	-0.974079000000	-0.436446000000
H	8.650255000000	-1.732079000000	-1.007358000000
C	6.714483000000	-0.865819000000	-0.595383000000
H	6.158662000000	-1.509650000000	-1.285677000000
C	-4.203962000000	-5.044947000000	-1.882634000000
H	-4.681413000000	-4.108399000000	-2.185135000000
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C	-4.181004000000	-7.460302000000	-1.679590000000
C	-2.948983000000	-7.325147000000	-1.015736000000
H	-2.421222000000	-8.202577000000	-0.626204000000
C	-2.418110000000	-6.051904000000	-0.786847000000
H	-1.480970000000	-5.907858000000	-0.236757000000
C	3.084671000000	-5.906144000000	0.541886000000



H	2.057247000000	-6.285762000000	0.547471000000
C	4.181912000000	-6.731610000000	0.807988000000
H	4.021311000000	-7.798731000000	0.996810000000
C	5.599214000000	-4.806203000000	0.600886000000
H	6.575815000000	-4.315064000000	0.621245000000
C	4.459006000000	-4.053995000000	0.311410000000
H	4.526310000000	-2.991103000000	0.069565000000
C	5.481561000000	-6.189774000000	0.837836000000
C	-3.563511000000	-1.672746000000	5.302744000000
H	-4.318649000000	-0.874155000000	5.448825000000
H	-2.896406000000	-1.643960000000	6.183734000000
C	-4.265498000000	-3.036619000000	5.200643000000
H	-4.866414000000	-3.230371000000	6.108223000000
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C	-5.153365000000	-3.103300000000	3.947678000000
H	-5.625577000000	-4.100395000000	3.864356000000
H	-5.978782000000	-2.367223000000	4.032255000000
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Ag	-1.575169000000	1.085150000000	1.712390000000
Ag	3.730084000000	-0.099928000000	0.145712000000
Ag	1.395248000000	-3.247651000000	-0.044278000000
F	-6.222676000000	3.541140000000	3.197271000000
F	-4.646088000000	3.674680000000	4.715875000000
F	-4.578820000000	4.988268000000	2.961372000000
N	5.967944000000	0.023900000000	0.101631000000
N	-3.057124000000	-4.922718000000	-1.174226000000
N	3.216959000000	-4.586609000000	0.278240000000
O	-0.439486000000	-3.643895000000	2.885636000000
O	2.710233000000	1.667095000000	3.963785000000
O	-3.307315000000	1.908075000000	3.238375000000
O	-0.020824000000	-4.997948000000	1.081979000000
O	3.886617000000	2.197829000000	2.077775000000
O	-4.253954000000	2.722625000000	1.319453000000
S	2.170715000000	-1.377579000000	1.610511000000
S	0.027475000000	2.994009000000	1.717231000000
S	-2.715935000000	-1.069419000000	1.210274000000
Ag	-2.442986000000	-2.876055000000	-0.447882000000
F	-1.560432000000	-5.710557000000	4.171845000000
F	-0.947658000000	-7.072976000000	2.566258000000
F	-2.682247000000	-5.754716000000	2.284369000000
C	4.952233000000	2.414157000000	4.222243000000
F	5.943973000000	3.055962000000	3.530263000000
F	5.504232000000	1.264513000000	4.719988000000
F	4.618720000000	3.201301000000	5.271849000000
C	-0.432027000000	3.114901000000	4.507773000000
H	-1.427514000000	2.670581000000	4.321756000000
H	0.297380000000	2.293862000000	4.623958000000
C	-0.037070000000	3.982114000000	3.308280000000
C	-0.481549000000	3.974439000000	5.786193000000
H	0.539237000000	4.335002000000	6.026243000000
H	-0.802428000000	3.344188000000	6.635599000000
C	-1.020089000000	6.031599000000	4.407460000000
H	-1.727516000000	6.869661000000	4.265496000000
H	-0.024253000000	6.483034000000	4.592012000000
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H	-1.431982000000	5.792099000000	6.535922000000

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H	-0.625082000000	5.797786000000	2.262067000000
H	-1.981539000000	4.825928000000	2.874025000000
H	1.008570000000	4.322987000000	3.427754000000
F	-6.440131000000	-0.529350000000	-3.258242000000
F	-5.555359000000	-1.136478000000	-5.171168000000
F	-6.294171000000	-2.663855000000	-3.775678000000
F	2.072266000000	5.947039000000	-3.720682000000
F	0.024449000000	6.256294000000	-4.466154000000
F	0.692710000000	7.274375000000	-2.642993000000
C	-5.524155000000	8.720124000000	-1.390380000000
H	-4.960487000000	9.516639000000	-1.907540000000
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C	-6.074840000000	9.295747000000	-0.047174000000
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C	7.059875000000	6.947837000000	-1.601144000000
H	7.132755000000	6.448673000000	-2.588475000000
H	6.847225000000	8.006545000000	-1.837604000000
C	8.419413000000	6.882689000000	-0.885695000000
H	9.136027000000	7.485318000000	-1.477573000000
H	8.341010000000	7.394605000000	0.091669000000
C	10.231733000000	-0.292028000000	0.781621000000
H	10.688164000000	-1.006661000000	0.074089000000
H	10.728837000000	0.687083000000	0.645660000000
C	10.471838000000	-0.785790000000	2.238883000000
H	11.559650000000	-0.789980000000	2.430413000000
H	10.023895000000	-0.057990000000	2.939957000000
C	6.696056000000	-7.061505000000	1.043749000000
H	6.396790000000	-8.004124000000	1.535711000000
H	7.423454000000	-6.553853000000	1.705624000000
C	7.398456000000	-7.418667000000	-0.305502000000
H	8.162637000000	-8.188050000000	-0.092737000000
H	6.658750000000	-7.869884000000	-0.991055000000
C	-4.934809000000	-8.767071000000	-1.698942000000
H	-5.666294000000	-8.767735000000	-2.526165000000
H	-4.254733000000	-9.623425000000	-1.853472000000
C	-5.694403000000	-8.967355000000	-0.344534000000
H	-6.351356000000	-9.850731000000	-0.439682000000
H	-4.956352000000	-9.187056000000	0.447032000000
C	-9.348519000000	-1.734426000000	2.863271000000
C	-7.030457000000	8.347525000000	0.640108000000
C	-6.607673000000	7.448611000000	1.635520000000
C	-8.378196000000	8.268544000000	0.242071000000
C	-7.522893000000	6.523049000000	2.159652000000
H	-5.570662000000	7.447881000000	1.987440000000
C	-9.214775000000	7.313743000000	0.834929000000
H	-8.771799000000	8.943231000000	-0.527380000000
H	-7.194670000000	5.795086000000	2.909206000000
H	-10.269025000000	7.244454000000	0.535521000000
C	9.040233000000	5.513112000000	-0.664962000000
C	9.968226000000	5.333977000000	0.378899000000
C	8.756628000000	4.385113000000	-1.457061000000
C	10.551850000000	4.077974000000	0.579550000000
H	10.227652000000	6.169698000000	1.038536000000
C	9.385731000000	3.165629000000	-1.166857000000

H	8.033279000000	4.430746000000	-2.277441000000
H	11.275109000000	3.929591000000	1.391858000000
H	9.152374000000	2.272088000000	-1.759653000000
C	9.902734000000	-2.162653000000	2.500011000000
C	8.539446000000	-2.364607000000	2.793892000000
C	10.708135000000	-3.313272000000	2.423905000000
C	8.059566000000	-3.669299000000	2.968503000000
H	7.853590000000	-1.515381000000	2.882272000000
C	10.132701000000	-4.574870000000	2.624749000000
H	11.780060000000	-3.226591000000	2.212173000000
H	6.998172000000	-3.837765000000	3.188677000000
H	10.756449000000	-5.477453000000	2.575084000000
C	8.051294000000	-6.218627000000	-0.950568000000
C	7.419834000000	-5.463463000000	-1.954956000000
C	9.297198000000	-5.752026000000	-0.492985000000
C	8.030750000000	-4.289321000000	-2.418761000000
H	6.445564000000	-5.760798000000	-2.356054000000
C	9.822379000000	-4.565066000000	-1.014863000000
H	9.838620000000	-6.296161000000	0.287700000000
H	7.534898000000	-3.678195000000	-3.179480000000
H	10.779740000000	-4.176870000000	-0.643914000000
C	-6.491285000000	-7.737751000000	0.031481000000
C	-5.996517000000	-6.804152000000	0.959928000000
C	-7.687989000000	-7.405861000000	-0.629860000000
C	-6.687544000000	-5.600771000000	1.153360000000
H	-5.058866000000	-6.986485000000	1.496311000000
C	-8.302067000000	-6.171843000000	-0.374693000000
H	-8.128048000000	-8.090316000000	-1.364492000000
H	-6.300441000000	-4.853256000000	1.856407000000
H	-9.218807000000	-5.883256000000	-0.903742000000
N	-8.812142000000	6.437827000000	1.776705000000
N	10.275260000000	2.992785000000	-0.169211000000
N	8.826102000000	-4.776085000000	2.882832000000
N	9.209667000000	-3.821643000000	-1.958152000000
N	-7.817246000000	-5.265304000000	0.499737000000
H	-9.358749000000	-1.223353000000	3.842521000000
C	-10.758317000000	-1.574200000000	2.214089000000
H	-11.516431000000	-1.789994000000	2.988207000000
H	-10.894028000000	-0.521608000000	1.906940000000
C	-10.958046000000	-2.502214000000	1.039770000000
C	-11.415530000000	-3.817626000000	1.236860000000
C	-10.632671000000	-2.131552000000	-0.277099000000
C	-11.512063000000	-4.682999000000	0.141855000000
H	-11.688592000000	-4.166450000000	2.239367000000
C	-10.748210000000	-3.079768000000	-1.303663000000
H	-10.274149000000	-1.121065000000	-0.500165000000
H	-11.867797000000	-5.712121000000	0.282828000000
H	-10.475942000000	-2.810747000000	-2.332384000000
N	-11.177039000000	-4.343973000000	-1.119437000000
H	-9.163630000000	-2.807438000000	3.049954000000

Ag<sub>12</sub>-Azopy

C	3.835220000000	-0.017295000000	3.025883000000
H	4.326239000000	0.935043000000	2.757695000000
C	3.049366000000	0.161495000000	4.326820000000

H	2.470871000000	-0.753196000000	4.544020000000
H	2.334648000000	0.994559000000	4.215340000000
C	4.026661000000	0.451933000000	5.483071000000
H	4.525213000000	1.424539000000	5.302321000000
H	3.453991000000	0.556404000000	6.422421000000
C	5.083048000000	-0.657475000000	5.613000000000
H	5.785268000000	-0.427677000000	6.435279000000
H	4.577217000000	-1.607205000000	5.874694000000
C	5.852662000000	-0.840363000000	4.295232000000
H	6.580835000000	-1.668649000000	4.375954000000
H	6.438365000000	0.075185000000	4.077482000000
C	4.890899000000	-1.124679000000	3.123097000000
H	5.447830000000	-1.211961000000	2.173042000000
H	4.380550000000	-2.091424000000	3.293719000000
C	-0.260830000000	4.956020000000	1.121194000000
H	-1.141662000000	5.485747000000	0.716682000000
C	-0.417939000000	4.801091000000	2.637100000000
H	0.401908000000	4.169930000000	3.025046000000
H	-1.373943000000	4.299981000000	2.865808000000
C	1.014024000000	5.710993000000	0.724332000000
H	1.049187000000	5.843341000000	-0.373658000000
H	1.892575000000	5.099517000000	0.999236000000
C	3.387351000000	3.463157000000	2.515065000000
C	4.524632000000	4.260192000000	3.210901000000
C	0.740332000000	-3.203097000000	4.124334000000
C	-4.255331000000	2.714876000000	2.067378000000
C	-5.555069000000	3.060011000000	2.853970000000
C	2.299526000000	-5.757938000000	1.551611000000
H	1.729502000000	-5.347532000000	2.392192000000
C	2.071995000000	-7.056875000000	1.087230000000
H	1.335397000000	-7.703828000000	1.571371000000
C	2.734396000000	-7.490855000000	-0.075167000000
C	3.703873000000	-6.647067000000	-0.656413000000
H	4.258556000000	-6.966552000000	-1.541538000000
C	3.900705000000	-5.384203000000	-0.101415000000
H	4.627482000000	-4.687218000000	-0.525501000000
C	3.201015000000	4.407447000000	-3.815508000000
H	2.329705000000	4.664168000000	-4.428349000000
C	4.431766000000	4.077022000000	-4.391499000000
H	4.571019000000	4.070425000000	-5.476130000000
C	5.473490000000	3.648300000000	-3.546975000000
C	5.284787000000	3.708408000000	-2.151423000000
H	6.087778000000	3.417390000000	-1.470648000000
C	4.033744000000	4.086308000000	-1.665876000000
H	3.833690000000	4.094813000000	-0.589283000000
C	6.273400000000	1.578766000000	0.897220000000
H	5.529899000000	2.374432000000	1.022984000000
C	7.418117000000	1.523932000000	1.688708000000
H	7.603818000000	2.281168000000	2.453196000000
C	8.033384000000	-0.497085000000	0.503051000000
H	8.720177000000	-1.331478000000	0.334873000000
C	6.848689000000	-0.382004000000	-0.229160000000
H	6.560358000000	-1.126132000000	-0.974653000000
C	8.311969000000	0.448758000000	1.507161000000
C	-0.360437000000	6.187205000000	3.310509000000
H	-1.231470000000	6.793455000000	2.985961000000
H	-0.451112000000	6.061371000000	4.404593000000

C	0.937674000000	6.930134000000	2.955630000000
H	0.954840000000	7.925621000000	3.436379000000
H	1.801432000000	6.364103000000	3.356871000000
C	1.081858000000	7.077854000000	1.432429000000
H	2.038233000000	7.570763000000	1.175306000000
H	0.274854000000	7.730722000000	1.043416000000
Ag	1.464774000000	1.825749000000	1.159098000000
Ag	0.345383000000	-0.653937000000	2.169174000000
Ag	-1.443600000000	1.542333000000	1.547277000000
Ag	2.694826000000	-2.718380000000	0.902586000000
Ag	3.858794000000	0.460402000000	-0.709535000000
F	-6.226529000000	4.080574000000	2.242322000000
F	-5.331633000000	3.421053000000	4.136083000000
F	-6.394458000000	1.976616000000	2.871991000000
N	3.179448000000	-4.917017000000	0.951838000000
N	2.984523000000	4.380098000000	-2.478546000000
N	5.972609000000	0.632509000000	-0.031457000000
O	2.401129000000	3.140352000000	3.220701000000
O	0.454505000000	-1.983525000000	4.260637000000
O	-3.173852000000	2.790654000000	2.709600000000
O	3.603591000000	3.173940000000	1.292218000000
O	0.261605000000	-4.065134000000	3.326016000000
O	-4.460689000000	2.386510000000	0.858910000000
S	2.720293000000	-0.343129000000	1.549523000000
S	-2.160839000000	-0.760021000000	2.191930000000
S	-0.308315000000	3.303862000000	0.233634000000
Ag	1.024778000000	3.301442000000	-1.855572000000
C	1.896461000000	-3.748994000000	5.020642000000
C	-1.956055000000	0.384973000000	4.775268000000
H	-2.183242000000	1.364937000000	4.315503000000
H	-0.865027000000	0.220709000000	4.724691000000
C	-2.681682000000	-0.717229000000	3.995093000000
C	-2.429805000000	0.391293000000	6.242087000000
H	-2.121097000000	-0.554474000000	6.731628000000
H	-1.920523000000	1.209251000000	6.783179000000
C	-4.670776000000	-0.564916000000	5.550103000000
H	-5.767140000000	-0.425186000000	5.580367000000
H	-4.467828000000	-1.548804000000	6.018329000000
C	-3.956680000000	0.546408000000	6.334990000000
H	-4.280504000000	0.537345000000	7.391928000000
H	-4.249856000000	1.528962000000	5.915452000000
C	-4.206800000000	-0.589683000000	4.080836000000
H	-4.691050000000	-1.418052000000	3.534035000000
H	-4.518690000000	0.347722000000	3.586212000000
H	-2.356589000000	-1.702932000000	4.373797000000
C	-3.854521000000	0.052037000000	-3.135208000000
H	-4.425731000000	-0.843926000000	-2.831138000000
C	-3.074782000000	-0.249320000000	-4.417376000000
H	-2.439806000000	0.617816000000	-4.675124000000
H	-2.418326000000	-1.121405000000	-4.256814000000
C	-4.065748000000	-0.537678000000	-5.563412000000
H	-4.620685000000	-1.468641000000	-5.334567000000
H	-3.499131000000	-0.725188000000	-6.493658000000
C	-5.053919000000	0.624210000000	-5.759999000000
H	-5.774300000000	0.384729000000	-6.563530000000
H	-4.494560000000	1.522911000000	-6.083928000000
C	-5.801388000000	0.943316000000	-4.455020000000

H	-6.473371000000	1.811083000000	-4.588840000000
H	-6.442986000000	0.084062000000	-4.172807000000
C	-4.813753000000	1.234836000000	-3.307527000000
H	-5.357477000000	1.432880000000	-2.367145000000
H	-4.227402000000	2.142425000000	-3.545655000000
C	0.292659000000	-4.868624000000	-1.304715000000
H	1.220610000000	-5.375494000000	-0.987466000000
C	0.322207000000	-4.680496000000	-2.824962000000
H	-0.555091000000	-4.083107000000	-3.133085000000
H	1.234376000000	-4.133184000000	-3.116758000000
C	-0.922264000000	-5.676306000000	-0.830420000000
H	-0.873862000000	-5.825375000000	0.264691000000
H	-1.839440000000	-5.093401000000	-1.032829000000
C	-3.608761000000	-3.410184000000	-2.206794000000
C	-4.789287000000	-4.168486000000	-2.878084000000
C	-0.782697000000	3.269823000000	-4.398795000000
C	4.207906000000	-2.687804000000	-2.250740000000
C	5.461180000000	-3.154225000000	-3.055012000000
C	-2.250504000000	5.752735000000	-1.725920000000
H	-1.635847000000	5.313825000000	-2.520328000000
C	-2.070078000000	7.076477000000	-1.325948000000
H	-1.314649000000	7.707103000000	-1.800351000000
C	-2.857129000000	7.579847000000	-0.269001000000
C	-3.846670000000	6.749218000000	0.288045000000
H	-4.488696000000	7.123665000000	1.089963000000
C	-3.948337000000	5.430166000000	-0.160507000000
H	-4.667987000000	4.734538000000	0.279609000000
C	-2.936804000000	-4.356142000000	3.848863000000
H	-1.924158000000	-4.466926000000	4.251287000000
C	-4.059073000000	-4.344331000000	4.674709000000
H	-3.969605000000	-4.443482000000	5.758924000000
C	-5.327574000000	-4.168381000000	4.081304000000
C	-5.410748000000	-4.086346000000	2.679691000000
H	-6.385847000000	-3.974500000000	2.196655000000
C	-4.230281000000	-4.087872000000	1.929469000000
H	-4.240869000000	-3.969939000000	0.840398000000
C	-6.525386000000	-1.676179000000	-0.798323000000
H	-5.897266000000	-2.567783000000	-0.724995000000
C	-7.684249000000	-1.660491000000	-1.577849000000
H	-7.996223000000	-2.549583000000	-2.131616000000
C	-7.979445000000	0.661202000000	-0.956514000000
H	-8.537302000000	1.598730000000	-1.010673000000
C	-6.808287000000	0.564330000000	-0.209339000000
H	-6.392824000000	1.420988000000	0.329957000000
C	-8.424148000000	-0.468961000000	-1.675581000000
C	0.276142000000	-6.058362000000	-3.516717000000
H	1.193197000000	-6.630446000000	-3.265429000000
H	0.280621000000	-5.913048000000	-4.612517000000
C	-0.960774000000	-6.861906000000	-3.083307000000
H	-0.966783000000	-7.852478000000	-3.574783000000
H	-1.875752000000	-6.330711000000	-3.411190000000
C	-0.993517000000	-7.034295000000	-1.556102000000
H	-1.911132000000	-7.565401000000	-1.242034000000
H	-0.139468000000	-7.664107000000	-1.239091000000
Ag	-1.436349000000	-1.771363000000	-1.257306000000
Ag	-0.399363000000	0.725872000000	-2.323495000000
Ag	1.443268000000	-1.429880000000	-1.671511000000

Ag	-2.654171000000	2.725965000000	-0.991547000000
Ag	-3.970283000000	-0.499846000000	0.555564000000
F	6.082552000000	-4.195599000000	-2.426422000000
F	5.178615000000	-3.543829000000	-4.316578000000
F	6.373648000000	-2.131521000000	-3.138257000000
N	-3.149566000000	4.922591000000	-1.131128000000
N	-3.006948000000	-4.196542000000	2.501962000000
N	-6.079663000000	-0.582874000000	-0.134102000000
O	-2.647422000000	-3.125395000000	-2.970456000000
O	-0.575555000000	2.029268000000	-4.438712000000
O	3.106115000000	-2.743298000000	-2.861354000000
O	-3.749258000000	-3.117248000000	-0.980615000000
O	-0.239582000000	4.162785000000	-3.675611000000
O	4.466782000000	-2.293474000000	-1.073867000000
S	-2.743185000000	0.354901000000	-1.653487000000
S	2.095727000000	0.884967000000	-2.364636000000
S	0.363034000000	-3.242474000000	-0.370116000000
Ag	-1.194830000000	-3.150818000000	1.550460000000
F	-5.566856000000	-3.281680000000	-3.579771000000
F	-5.605693000000	-4.769131000000	-1.965832000000
F	-4.364735000000	-5.119635000000	-3.740874000000
C	-1.922156000000	3.811435000000	-5.315396000000
F	-1.589670000000	4.978248000000	-5.916546000000
F	-3.036405000000	4.051949000000	-4.542652000000
F	-2.288507000000	2.932333000000	-6.279333000000
C	1.854981000000	-0.276006000000	-4.947907000000
H	1.958406000000	-1.270883000000	-4.473823000000
H	0.788098000000	0.006473000000	-4.939745000000
C	2.673073000000	0.742084000000	-4.144790000000
C	2.380252000000	-0.345002000000	-6.396255000000
H	2.192057000000	0.625370000000	-6.898915000000
H	1.804575000000	-1.105525000000	-6.954355000000
C	4.689258000000	0.353549000000	-5.616623000000
H	5.763426000000	0.091668000000	-5.606155000000
H	4.611248000000	1.357872000000	-6.080388000000
C	3.884060000000	-0.664601000000	-6.440149000000
H	4.241966000000	-0.682471000000	-7.485730000000
H	4.055617000000	-1.675530000000	-6.021696000000
C	4.169470000000	0.415513000000	-4.169519000000
H	4.739623000000	1.147614000000	-3.574207000000
H	4.320101000000	-0.567682000000	-3.694211000000
H	2.495019000000	1.757297000000	-4.545672000000
F	3.033056000000	-3.887790000000	4.253317000000
F	2.210939000000	-2.925066000000	6.048562000000
F	1.611208000000	-4.970887000000	5.534035000000
F	5.165582000000	5.098450000000	2.354026000000
F	4.085438000000	4.991561000000	4.257711000000
F	5.467588000000	3.374138000000	3.684227000000
N	-9.568288000000	-0.510778000000	-2.515465000000
N	-6.546060000000	-4.052920000000	4.797564000000
N	9.492220000000	0.242414000000	2.265666000000
N	6.630564000000	3.120520000000	-4.176832000000
N	-2.724906000000	8.875286000000	0.288624000000
N	2.339324000000	-8.744594000000	-0.603292000000
N	-6.374606000000	-3.763521000000	6.026609000000
N	-10.145868000000	0.618278000000	-2.639102000000
N	-1.568240000000	9.377527000000	0.103815000000

N	7.254856000000	2.303643000000	-3.424001000000
N	9.498545000000	0.894273000000	3.360518000000
N	2.536569000000	-8.830771000000	-1.859843000000
C	-11.286787000000	0.591298000000	-3.481865000000
C	-11.771000000000	-0.541766000000	-4.169391000000
C	-11.969663000000	1.811987000000	-3.629971000000
C	-12.910368000000	-0.386884000000	-4.962733000000
H	-11.256870000000	-1.501165000000	-4.073791000000
C	-13.103980000000	1.846290000000	-4.452948000000
H	-11.606025000000	2.700367000000	-3.105509000000
H	-13.316787000000	-1.244440000000	-5.513713000000
H	-13.659370000000	2.782760000000	-4.588747000000
C	8.379674000000	1.686769000000	-4.028013000000
C	8.784242000000	1.855360000000	-5.368752000000
C	9.109700000000	0.809014000000	-3.205998000000
C	9.899574000000	1.137257000000	-5.808158000000
H	8.226424000000	2.522535000000	-6.030394000000
C	10.213644000000	0.144864000000	-3.758352000000
H	8.802771000000	0.658944000000	-2.166206000000
H	10.244462000000	1.238501000000	-6.844959000000
H	10.804555000000	-0.547117000000	-3.145015000000
C	10.676585000000	0.721063000000	4.131785000000
C	10.702081000000	1.391636000000	5.367766000000
C	11.794967000000	-0.053651000000	3.758375000000
C	11.841042000000	1.258809000000	6.174390000000
H	9.841810000000	1.995148000000	5.671523000000
C	12.874004000000	-0.111129000000	4.643849000000
H	11.799396000000	-0.585621000000	2.803906000000
H	11.892736000000	1.768172000000	7.144745000000
H	13.762800000000	-0.702310000000	4.389456000000
C	2.130807000000	-10.066323000000	-2.427146000000
C	1.708653000000	-11.199948000000	-1.701977000000
C	2.157691000000	-10.132720000000	-3.831666000000
C	1.337045000000	-12.335702000000	-2.426050000000
H	1.678973000000	-11.173001000000	-0.609924000000
C	1.754811000000	-11.325362000000	-4.448760000000
H	2.481644000000	-9.260858000000	-4.407637000000
H	1.006004000000	-13.239425000000	-1.898916000000
H	1.758561000000	-11.409316000000	-5.542678000000
C	-7.578457000000	-3.643200000000	6.767570000000
C	-8.870123000000	-3.942850000000	6.286267000000
C	-7.440111000000	-3.188274000000	8.091088000000
C	-9.948116000000	-3.768370000000	7.157844000000
H	-9.004588000000	-4.300261000000	5.262413000000
C	-8.596074000000	-3.047015000000	8.871438000000
H	-6.444927000000	-2.951715000000	8.478812000000
H	-10.968221000000	-3.993446000000	6.821758000000
H	-8.523192000000	-2.690773000000	9.906622000000
C	-1.408409000000	10.681999000000	0.638465000000
C	-0.100974000000	11.199496000000	0.611676000000
C	-2.442046000000	11.477679000000	1.174806000000
C	0.116451000000	12.484317000000	1.128529000000
H	0.711692000000	10.594283000000	0.199011000000
C	-2.106257000000	12.746214000000	1.654870000000
H	-3.466501000000	11.098513000000	1.205119000000
H	1.125041000000	12.916210000000	1.127443000000
H	-2.882383000000	13.397255000000	2.076697000000



N	-9.836553000000	-3.328949000000	8.431280000000
N	1.351157000000	-12.418692000000	-3.775111000000
N	-13.581390000000	0.776690000000	-5.116154000000
N	-0.856173000000	13.260135000000	1.642586000000
N	10.616389000000	0.291879000000	-5.034393000000
N	12.917726000000	0.525440000000	5.835641000000

### Ag<sub>12</sub>-BPA-Ag<sub>1</sub>

C	2.576377000000	2.393034000000	3.345535000000
H	2.289923000000	3.452834000000	3.217685000000
C	1.705271000000	1.765977000000	4.442080000000
H	1.930458000000	0.683384000000	4.500333000000
H	0.635858000000	1.883958000000	4.190351000000
C	2.002917000000	2.432420000000	5.798679000000
H	1.690844000000	3.494910000000	5.754354000000
H	1.388931000000	1.953069000000	6.583062000000
C	3.497078000000	2.341467000000	6.149121000000
H	3.699636000000	2.851726000000	7.108637000000
H	3.775728000000	1.277349000000	6.282908000000
C	4.363641000000	2.943115000000	5.030739000000
H	5.438082000000	2.831501000000	5.266599000000
H	4.163127000000	4.030932000000	4.949053000000
C	4.066149000000	2.269636000000	3.677261000000
H	4.684797000000	2.715871000000	2.878579000000
H	4.334059000000	1.201019000000	3.734536000000
C	-3.847501000000	1.981719000000	2.600778000000
H	-4.446589000000	1.070394000000	2.775721000000
C	-3.087452000000	2.344509000000	3.878688000000
H	-2.413946000000	3.197724000000	3.679935000000
H	-2.466655000000	1.488162000000	4.192233000000
C	-4.765083000000	3.114371000000	2.128965000000
H	-5.304708000000	2.816024000000	1.212089000000
H	-4.145710000000	3.994478000000	1.875036000000
C	-0.545840000000	4.943547000000	2.144860000000
C	-1.099385000000	6.170900000000	2.932583000000
C	4.165617000000	-1.534052000000	2.915943000000
C	-4.065770000000	-1.554496000000	3.536986000000
C	-5.117619000000	-2.008753000000	4.590909000000
C	6.770345000000	-0.677504000000	-0.125628000000
H	6.190725000000	-1.391651000000	0.468055000000
C	7.997564000000	-1.019091000000	-0.700919000000
H	8.377984000000	-2.041642000000	-0.574525000000
C	8.723094000000	-0.041261000000	-1.411639000000
C	8.148768000000	1.238370000000	-1.525455000000
H	8.666508000000	2.046989000000	-2.051251000000
C	6.902364000000	1.494129000000	-0.951128000000
H	6.405703000000	2.461365000000	-1.064278000000
C	-4.912248000000	4.668538000000	-1.248910000000
H	-4.952552000000	3.816744000000	-1.934510000000
C	-6.072200000000	5.350219000000	-0.868207000000
H	-7.026754000000	5.034114000000	-1.294252000000
C	-5.997808000000	6.375969000000	0.090362000000
C	-4.709744000000	6.726214000000	0.544038000000
H	-4.573223000000	7.532211000000	1.273163000000
C	-3.592673000000	6.017620000000	0.097458000000

H	-2.582661000000	6.254720000000	0.445514000000
C	2.499527000000	6.436216000000	0.826636000000
H	1.456843000000	6.692594000000	0.608729000000
C	3.427203000000	7.396173000000	1.247964000000
H	3.120461000000	8.444832000000	1.325604000000
C	5.047566000000	5.638012000000	1.461698000000
H	6.044174000000	5.262920000000	1.711760000000
C	4.082270000000	4.751621000000	0.987343000000
H	4.315117000000	3.697062000000	0.822989000000
C	4.742268000000	7.008077000000	1.566606000000
C	-4.089884000000	2.708893000000	4.990210000000
H	-4.685561000000	1.810478000000	5.249065000000
H	-3.537343000000	2.995491000000	5.903571000000
C	-5.026696000000	3.847380000000	4.551439000000
H	-5.758104000000	4.074026000000	5.349050000000
H	-4.426246000000	4.764254000000	4.393184000000
C	-5.757007000000	3.494357000000	3.244952000000
H	-6.377007000000	4.346687000000	2.904807000000
H	-6.449234000000	2.646478000000	3.422942000000
Ag	-0.305037000000	1.839989000000	1.593276000000
Ag	1.252023000000	-0.618741000000	2.018225000000
Ag	-1.699579000000	-0.698902000000	1.966644000000
Ag	4.118591000000	0.904940000000	0.334263000000
Ag	1.404485000000	3.548017000000	-0.105531000000
F	-6.325633000000	-1.408294000000	4.353068000000
F	-4.765118000000	-1.715598000000	5.864042000000
F	-5.317111000000	-3.361398000000	4.526665000000
N	6.222162000000	0.556739000000	-0.250907000000
N	-3.689410000000	4.969738000000	-0.756660000000
N	2.826428000000	5.134273000000	0.670697000000
O	-0.226344000000	3.959592000000	2.867983000000
O	3.128514000000	-1.327408000000	3.585825000000
O	-3.072196000000	-0.922105000000	3.994362000000
O	-0.528008000000	5.068806000000	0.885158000000
O	4.298832000000	-1.877251000000	1.692833000000
O	-4.331079000000	-1.880988000000	2.345485000000
S	2.207463000000	1.643652000000	1.663526000000
S	-0.177105000000	-2.615328000000	2.066368000000
S	-2.714576000000	1.474011000000	1.202831000000
Ag	-2.229419000000	3.248670000000	-0.522033000000
C	5.539159000000	-1.348686000000	3.633104000000
C	-0.149079000000	-2.321496000000	4.866561000000
H	-0.935990000000	-1.559701000000	4.721813000000
H	0.832413000000	-1.820703000000	4.783145000000
C	-0.276122000000	-3.382726000000	3.765675000000
C	-0.316675000000	-2.961626000000	6.258576000000
H	0.528463000000	-3.652850000000	6.454167000000
H	-0.265070000000	-2.171244000000	7.029783000000
C	-1.734728000000	-4.811355000000	5.270623000000
H	-2.703255000000	-5.341865000000	5.327476000000
H	-0.943918000000	-5.570638000000	5.438090000000
C	-1.643309000000	-3.731898000000	6.361735000000
H	-1.743375000000	-4.192374000000	7.361956000000
H	-2.486371000000	-3.023886000000	6.246333000000
C	-1.571990000000	-4.200911000000	3.865353000000
H	-1.580466000000	-4.989985000000	3.090132000000
H	-2.428109000000	-3.537906000000	3.651390000000

H	0.599703000000	-4.058728000000	3.807129000000
C	-2.622839000000	-2.524441000000	-3.003189000000
H	-2.353354000000	-3.581557000000	-2.819045000000
C	-1.922618000000	-2.036889000000	-4.275739000000
H	-2.104192000000	-0.952528000000	-4.395792000000
H	-0.835584000000	-2.199673000000	-4.183576000000
C	-2.473421000000	-2.784050000000	-5.505198000000
H	-2.211952000000	-3.859236000000	-5.430874000000
H	-1.978283000000	-2.400193000000	-6.415883000000
C	-3.998736000000	-2.629695000000	-5.613374000000
H	-4.383559000000	-3.184800000000	-6.488545000000
H	-4.246848000000	-1.562185000000	-5.771778000000
C	-4.692925000000	-3.114724000000	-4.330808000000
H	-5.785814000000	-2.960950000000	-4.399835000000
H	-4.532348000000	-4.205904000000	-4.212069000000
C	-4.148769000000	-2.382220000000	-3.088009000000
H	-4.617421000000	-2.773325000000	-2.165372000000
H	-4.407319000000	-1.308213000000	-3.154607000000
C	3.865716000000	-1.097721000000	-2.980570000000
H	4.455786000000	-0.168691000000	-3.089514000000
C	2.900117000000	-1.224220000000	-4.164048000000
H	2.226166000000	-2.085907000000	-3.997251000000
H	2.276646000000	-0.313972000000	-4.233086000000
C	4.797904000000	-2.306996000000	-2.862826000000
H	5.486947000000	-2.163961000000	-2.012454000000
H	4.194114000000	-3.208850000000	-2.654929000000
C	0.860707000000	-4.847795000000	-2.688548000000
C	2.030527000000	-5.661315000000	-3.331956000000
C	-3.729784000000	1.621050000000	-3.472552000000
C	3.967409000000	2.872745000000	-2.712311000000
C	4.850032000000	3.832622000000	-3.569717000000
C	-6.590536000000	0.680910000000	-1.007846000000
H	-5.921131000000	1.325826000000	-1.585571000000
C	-7.971926000000	0.688499000000	-1.198267000000
H	-8.406142000000	1.360036000000	-1.945872000000
C	-8.784041000000	-0.201492000000	-0.467485000000
C	-8.155472000000	-0.984915000000	0.515135000000
H	-8.737145000000	-1.667211000000	1.145592000000
C	-6.764126000000	-0.937509000000	0.654818000000
H	-6.233615000000	-1.548301000000	1.394501000000
C	4.425322000000	-5.024158000000	1.676820000000
H	4.798323000000	-4.119401000000	2.163498000000
C	5.139108000000	-6.221227000000	1.738432000000
H	6.079998000000	-6.256359000000	2.295665000000
C	4.696967000000	-7.336854000000	1.003984000000
C	3.473948000000	-7.210639000000	0.322715000000
H	3.064799000000	-8.041379000000	-0.262342000000
C	2.796898000000	-5.986844000000	0.333526000000
H	1.861356000000	-5.855325000000	-0.220500000000
C	-2.757718000000	-6.175624000000	-0.620603000000
H	-1.839667000000	-6.613206000000	-1.027690000000
C	-3.981925000000	-6.847373000000	-0.668088000000
H	-4.024313000000	-7.855082000000	-1.095161000000
C	-5.005089000000	-4.931079000000	0.343950000000
H	-5.861241000000	-4.371639000000	0.726937000000
C	-3.740919000000	-4.336765000000	0.402647000000
H	-3.619524000000	-3.346312000000	0.856079000000

C	-5.150512000000	-6.234023000000	-0.174343000000
C	3.691840000000	-1.422800000000	-5.470874000000
H	4.280116000000	-0.506864000000	-5.681356000000
H	2.984774000000	-1.548055000000	-6.311310000000
C	4.635201000000	-2.633567000000	-5.375866000000
H	5.214903000000	-2.743561000000	-6.310832000000
H	4.031900000000	-3.554464000000	-5.258628000000
C	5.584455000000	-2.499804000000	-4.174015000000
H	6.233721000000	-3.392063000000	-4.091913000000
H	6.257164000000	-1.630825000000	-4.324211000000
Ag	0.557346000000	-1.590987000000	-1.483587000000
Ag	-1.269097000000	0.601906000000	-2.135838000000
Ag	1.598598000000	1.116331000000	-1.874500000000
Ag	-3.752874000000	-0.400173000000	-0.221989000000
Ag	-0.637141000000	-3.893390000000	-0.154077000000
F	6.158170000000	3.406049000000	-3.550240000000
F	4.475524000000	3.896621000000	-4.869236000000
F	4.834027000000	5.106260000000	-3.079898000000
N	-5.983083000000	-0.151077000000	-0.124994000000
N	3.282483000000	-4.893892000000	0.965337000000
N	-2.628050000000	-4.944093000000	-0.075019000000
O	0.706880000000	-3.684692000000	-3.130864000000
O	-2.670154000000	1.252596000000	-4.050759000000
O	3.250670000000	2.069705000000	-3.377069000000
O	0.266331000000	-5.453039000000	-1.737330000000
O	-3.935857000000	1.841214000000	-2.243319000000
O	4.089417000000	3.010218000000	-1.464379000000
S	-1.998241000000	-1.656791000000	-1.459926000000
S	-0.163401000000	2.828983000000	-1.895441000000
S	2.981555000000	-0.835402000000	-1.351569000000
Ag	2.550220000000	-2.768431000000	0.428431000000
F	2.229373000000	-5.350918000000	-4.636021000000
F	1.867239000000	-7.003742000000	-3.242404000000
F	3.202309000000	-5.360381000000	-2.663352000000
C	-4.976551000000	1.747201000000	-4.400739000000
F	-5.957004000000	2.530359000000	-3.853983000000
F	-5.531282000000	0.507514000000	-4.595963000000
F	-4.677931000000	2.260040000000	-5.614652000000
C	0.275249000000	2.922296000000	-4.693134000000
H	1.296602000000	2.538919000000	-4.510721000000
H	-0.409198000000	2.061832000000	-4.789073000000
C	-0.155783000000	3.788319000000	-3.505283000000
C	0.267230000000	3.764561000000	-5.984435000000
H	-0.773561000000	4.066563000000	-6.219830000000
H	0.613200000000	3.139412000000	-6.827737000000
C	0.710571000000	5.868227000000	-4.641087000000
H	1.374011000000	6.744490000000	-4.519403000000
H	-0.309870000000	6.263845000000	-4.819663000000
C	1.148614000000	5.016410000000	-5.843705000000
H	1.112849000000	5.618415000000	-6.770305000000
H	2.200863000000	4.705415000000	-5.700060000000
C	0.712584000000	5.041373000000	-3.340452000000
H	0.350406000000	5.645116000000	-2.487820000000
H	1.747345000000	4.729360000000	-3.100104000000
H	-1.217571000000	4.075992000000	-3.622846000000
F	6.280749000000	-0.374305000000	3.019520000000
F	5.412169000000	-0.995655000000	4.932167000000

F	6.268779000000	-2.501748000000	3.581267000000
F	-2.435664000000	5.983164000000	3.196780000000
F	-0.472137000000	6.361973000000	4.116145000000
F	-1.000427000000	7.331027000000	2.221894000000
C	5.812295000000	8.012041000000	1.921191000000
H	5.353035000000	8.949845000000	2.280257000000
H	6.439731000000	7.618342000000	2.741593000000
C	6.734070000000	8.346761000000	0.705859000000
H	7.438742000000	9.136249000000	1.024993000000
H	6.114610000000	8.768027000000	-0.105817000000
C	-7.213670000000	7.069928000000	0.674715000000
H	-7.350031000000	6.702592000000	1.711681000000
H	-6.983537000000	8.145435000000	0.786570000000
C	-8.536860000000	6.943252000000	-0.099571000000
H	-9.269723000000	7.620448000000	0.381382000000
H	-8.398477000000	7.336621000000	-1.123873000000
C	-10.235837000000	-0.389698000000	-0.828077000000
H	-10.739321000000	-1.006983000000	-0.063306000000
H	-10.736953000000	0.595858000000	-0.864551000000
C	-10.374544000000	-1.076895000000	-2.222358000000
H	-11.447448000000	-1.135965000000	-2.478003000000
H	-9.896555000000	-0.429791000000	-2.980514000000
C	-6.471305000000	-6.971399000000	-0.190426000000
H	-6.300363000000	-7.975511000000	-0.617581000000
H	-7.189233000000	-6.464705000000	-0.866943000000
C	-7.128694000000	-7.145286000000	1.214492000000
H	-7.820634000000	-8.004798000000	1.147881000000
H	-6.354480000000	-7.414179000000	1.954982000000
C	5.596146000000	-8.533947000000	0.817450000000
H	6.274100000000	-8.633614000000	1.683537000000
H	5.010640000000	-9.467311000000	0.743241000000
C	6.451041000000	-8.375398000000	-0.483674000000
H	7.182869000000	-9.202731000000	-0.520226000000
H	5.787538000000	-8.482297000000	-1.359936000000
C	10.099051000000	-0.318115000000	-1.967673000000
C	7.498322000000	7.143619000000	0.200288000000
C	7.082591000000	6.423455000000	-0.932635000000
C	8.613758000000	6.641186000000	0.897649000000
C	7.771794000000	5.258506000000	-1.300479000000
H	6.215266000000	6.744669000000	-1.517994000000
C	9.229983000000	5.463567000000	0.453112000000
H	8.994174000000	7.156298000000	1.787547000000
H	7.444451000000	4.688211000000	-2.175468000000
H	10.095794000000	5.058691000000	0.993150000000
C	-9.169054000000	5.564506000000	-0.191765000000
C	-9.992981000000	5.246694000000	-1.288508000000
C	-8.991224000000	4.558298000000	0.775530000000
C	-10.580901000000	3.978912000000	-1.369194000000
H	-10.166578000000	5.982023000000	-2.082214000000
C	-9.613903000000	3.314899000000	0.597358000000
H	-8.354154000000	4.715583000000	1.651416000000
H	-11.222764000000	3.722003000000	-2.221748000000
H	-9.459559000000	2.512943000000	1.330276000000
C	-9.759689000000	-2.458943000000	-2.272839000000
C	-8.369528000000	-2.655970000000	-2.401894000000
C	-10.550647000000	-3.615756000000	-2.151176000000
C	-7.853005000000	-3.957368000000	-2.362807000000

H	-7.689464000000	-1.806091000000	-2.520280000000
C	-9.938489000000	-4.876058000000	-2.150752000000
H	-11.639979000000	-3.535306000000	-2.060840000000
H	-6.769937000000	-4.119815000000	-2.430360000000
H	-10.550329000000	-5.784535000000	-2.068987000000
C	-7.909582000000	-5.935433000000	1.681078000000
C	-7.441077000000	-5.057903000000	2.674831000000
C	-9.144081000000	-5.617460000000	1.085207000000
C	-8.185052000000	-3.909224000000	2.984767000000
H	-6.489421000000	-5.238857000000	3.184674000000
C	-9.813298000000	-4.449945000000	1.465837000000
H	-9.565420000000	-6.263318000000	0.308671000000
H	-7.804326000000	-3.199143000000	3.725513000000
H	-10.763459000000	-4.180233000000	0.986994000000
C	7.151333000000	-7.035490000000	-0.538018000000
C	6.658891000000	-5.985682000000	-1.333588000000
C	8.247139000000	-6.742711000000	0.295157000000
C	7.258711000000	-4.722098000000	-1.245396000000
H	5.793041000000	-6.134705000000	-1.988295000000
C	8.765601000000	-5.440686000000	0.328474000000
H	8.679816000000	-7.516177000000	0.940598000000
H	6.879529000000	-3.892428000000	-1.852821000000
H	9.591304000000	-5.183378000000	1.003633000000
N	8.828281000000	4.760974000000	-0.626272000000
N	-10.403063000000	3.008812000000	-0.451558000000
N	-8.608049000000	-5.067652000000	-2.237953000000
N	-9.352693000000	-3.584852000000	2.392256000000
N	8.287637000000	-4.428890000000	-0.426273000000
H	10.304146000000	0.370762000000	-2.806044000000
C	11.217549000000	-0.130662000000	-0.894807000000
H	12.191944000000	-0.112374000000	-1.415311000000
H	11.084991000000	0.853600000000	-0.410861000000
C	11.213625000000	-1.236556000000	0.133766000000
C	11.903283000000	-2.439075000000	-0.105947000000
C	10.467834000000	-1.156850000000	1.323483000000
C	11.807259000000	-3.482921000000	0.820605000000
H	12.505636000000	-2.562525000000	-1.013330000000
C	10.418639000000	-2.268224000000	2.177335000000
H	9.908753000000	-0.248322000000	1.571435000000
H	12.342243000000	-4.425674000000	0.645606000000
H	9.813637000000	-2.230334000000	3.092472000000
N	11.070492000000	-3.425326000000	1.948470000000
H	10.153113000000	-1.348812000000	-2.361744000000
H	1.015791000000	-3.187365000000	-0.421157000000

### Ag<sub>12</sub>-BPA-SH

C	2.278595000000	2.727590000000	3.197867000000
H	2.006914000000	3.782789000000	3.008382000000
C	1.379959000000	2.174121000000	4.311344000000
H	1.576063000000	1.091295000000	4.424683000000
H	0.317362000000	2.306049000000	4.038485000000
C	1.676297000000	2.898006000000	5.638499000000
H	1.387974000000	3.963787000000	5.540664000000
H	1.042090000000	2.469948000000	6.436299000000
C	3.163331000000	2.792317000000	6.013222000000
H	3.364059000000	3.341472000000	6.951403000000

H	3.418498000000	1.730664000000	6.196960000000
C	4.057517000000	3.325784000000	4.881947000000
H	5.125761000000	3.198991000000	5.137202000000
H	3.883713000000	4.413672000000	4.752552000000
C	3.762510000000	2.600170000000	3.555401000000
H	4.401102000000	2.998576000000	2.745144000000
H	4.007900000000	1.530974000000	3.660482000000
C	-4.085058000000	1.837659000000	2.413353000000
H	-4.627485000000	0.901378000000	2.641265000000
C	-3.380408000000	2.336140000000	3.678253000000
H	-2.770356000000	3.224943000000	3.435303000000
H	-2.703569000000	1.552163000000	4.057117000000
C	-5.065066000000	2.874629000000	1.852380000000
H	-5.561584000000	2.486520000000	0.945318000000
H	-4.503311000000	3.780744000000	1.558303000000
C	-1.033587000000	5.094483000000	1.742499000000
C	-1.896490000000	6.218506000000	2.397706000000
C	4.136772000000	-1.205130000000	3.249026000000
C	-3.888648000000	-1.727396000000	3.778270000000
C	-4.806825000000	-2.201281000000	4.942204000000
C	6.537401000000	-0.375883000000	0.176623000000
H	5.766242000000	-1.147776000000	0.103117000000
C	7.894534000000	-0.696869000000	0.123482000000
H	8.197793000000	-1.738686000000	-0.006361000000
C	8.860382000000	0.321423000000	0.246276000000
C	8.388013000000	1.637112000000	0.410543000000
H	9.065043000000	2.495154000000	0.490146000000
C	7.011082000000	1.874840000000	0.445356000000
H	6.620247000000	2.891177000000	0.546864000000
C	-5.197316000000	4.261294000000	-1.924202000000
H	-5.259600000000	3.315507000000	-2.472610000000
C	-6.307318000000	5.099361000000	-1.780606000000
H	-7.249973000000	4.803018000000	-2.247101000000
C	-6.210173000000	6.262294000000	-0.996198000000
C	-4.942392000000	6.561200000000	-0.459267000000
H	-4.785415000000	7.457666000000	0.150424000000
C	-3.870315000000	5.692610000000	-0.671483000000
H	-2.873751000000	5.893240000000	-0.265788000000
C	2.089667000000	6.696942000000	-0.192512000000
H	1.133971000000	6.830839000000	-0.708749000000
C	2.925765000000	7.780661000000	0.094739000000
H	2.635931000000	8.786385000000	-0.227834000000
C	4.421786000000	6.249870000000	1.180139000000
H	5.336702000000	6.015741000000	1.732368000000
C	3.556187000000	5.218273000000	0.817941000000
H	3.790532000000	4.176256000000	1.047412000000
C	4.128391000000	7.571314000000	0.794766000000
C	-4.431715000000	2.684544000000	4.749146000000
H	-4.958028000000	1.756700000000	5.050979000000
H	-3.923305000000	3.067659000000	5.652725000000
C	-5.448353000000	3.714383000000	4.228273000000
H	-6.218599000000	3.916963000000	4.995248000000
H	-4.924392000000	4.669922000000	4.035647000000
C	-6.111191000000	3.233979000000	2.926166000000
H	-6.792366000000	4.010928000000	2.529686000000
H	-6.734658000000	2.340578000000	3.134768000000
Ag	-0.561921000000	1.934345000000	1.480494000000

Ag	1.231732000000	-0.459294000000	1.938111000000
Ag	-1.734121000000	-0.687549000000	2.071205000000
Ag	3.891810000000	1.362426000000	0.125826000000
Ag	1.007485000000	3.710146000000	-0.276832000000
F	-6.063901000000	-1.680488000000	4.786915000000
F	-4.361404000000	-1.829626000000	6.165786000000
F	-4.928534000000	-3.563231000000	4.954935000000
N	6.091988000000	0.890260000000	0.334837000000
N	-3.998707000000	4.533792000000	-1.361802000000
N	2.403707000000	5.427738000000	0.147834000000
O	-0.646066000000	4.198923000000	2.542627000000
O	3.026195000000	-0.845892000000	3.699738000000
O	-3.030772000000	-0.849608000000	4.089796000000
O	-0.871499000000	5.193921000000	0.490640000000
O	4.435219000000	-1.788473000000	2.156079000000
O	-4.111144000000	-2.266576000000	2.660602000000
S	1.927499000000	1.896156000000	1.550731000000
S	-0.106363000000	-2.512654000000	2.211594000000
S	-2.888784000000	1.301031000000	1.080323000000
Ag	-2.601765000000	2.797713000000	-0.909295000000
C	5.393922000000	-0.905358000000	4.122344000000
C	0.009590000000	-2.001550000000	4.981044000000
H	-0.921732000000	-1.421128000000	4.845228000000
H	0.865927000000	-1.328972000000	4.800476000000
C	0.036065000000	-3.149127000000	3.962010000000
C	0.054372000000	-2.555956000000	6.418562000000
H	1.030517000000	-3.052367000000	6.594082000000
H	-0.006043000000	-1.714111000000	7.132497000000
C	-1.031614000000	-4.708624000000	5.649156000000
H	-1.870383000000	-5.411010000000	5.808677000000
H	-0.097832000000	-5.288306000000	5.796539000000
C	-1.083865000000	-3.558741000000	6.667948000000
H	-1.025656000000	-3.958690000000	7.696986000000
H	-2.056288000000	-3.036530000000	6.580623000000
C	-1.079775000000	-4.177477000000	4.203608000000
H	-0.993959000000	-5.008292000000	3.478463000000
H	-2.057646000000	-3.695772000000	4.020547000000
H	1.023065000000	-3.648719000000	3.996380000000
C	-2.173019000000	-3.065199000000	-2.726854000000
H	-1.594452000000	-3.982584000000	-2.514019000000
C	-1.716122000000	-2.480106000000	-4.067378000000
H	-2.227825000000	-1.516847000000	-4.244327000000
H	-0.630418000000	-2.285371000000	-4.035394000000
C	-2.044955000000	-3.458055000000	-5.211274000000
H	-1.441774000000	-4.380911000000	-5.092753000000
H	-1.741320000000	-3.006430000000	-6.173497000000
C	-3.541493000000	-3.809883000000	-5.228222000000
H	-3.760965000000	-4.530191000000	-6.037585000000
H	-4.125179000000	-2.892934000000	-5.444599000000
C	-3.987754000000	-4.379659000000	-3.872310000000
H	-5.070820000000	-4.604121000000	-3.880894000000
H	-3.469340000000	-5.341725000000	-3.683689000000
C	-3.668277000000	-3.403576000000	-2.722298000000
H	-3.961154000000	-3.839656000000	-1.750815000000
H	-4.251410000000	-2.472629000000	-2.851694000000
C	3.921558000000	-1.146861000000	-2.937397000000
H	4.788400000000	-0.460266000000	-2.995779000000



C	2.967836000000	-0.866798000000	-4.106980000000
H	2.046576000000	-1.463031000000	-3.964748000000
H	2.691380000000	0.202316000000	-4.112222000000
C	4.392517000000	-2.607886000000	-2.920518000000
H	5.106526000000	-2.767258000000	-2.091007000000
H	3.517279000000	-3.252020000000	-2.727603000000
C	1.017216000000	-4.809799000000	-2.721981000000
C	1.592628000000	-5.729518000000	-3.844746000000
C	-3.862372000000	0.857606000000	-3.480699000000
C	4.003729000000	3.243313000000	-2.507781000000
C	4.443964000000	4.481005000000	-3.351929000000
C	-6.516260000000	0.349779000000	-0.602654000000
H	-5.880389000000	0.963748000000	-1.248945000000
C	-7.905728000000	0.468198000000	-0.606525000000
H	-8.380047000000	1.211780000000	-1.254963000000
C	-8.685494000000	-0.418835000000	0.161046000000
C	-8.000041000000	-1.301599000000	1.012649000000
H	-8.546869000000	-1.985379000000	1.670902000000
C	-6.602980000000	-1.352642000000	0.980137000000
H	-6.034060000000	-2.032296000000	1.622969000000
C	5.542972000000	-4.436396000000	0.947271000000
H	5.729047000000	-3.659349000000	1.696269000000
C	6.534952000000	-5.348993000000	0.572731000000
H	7.514905000000	-5.306758000000	1.062987000000
C	6.256859000000	-6.303642000000	-0.421934000000
C	4.960887000000	-6.305883000000	-0.973055000000
H	4.675435000000	-7.020724000000	-1.752340000000
C	4.019043000000	-5.374654000000	-0.527433000000
H	2.999105000000	-5.366120000000	-0.923669000000
C	-2.258419000000	-6.257727000000	-0.502213000000
H	-1.396702000000	-6.669687000000	-1.037604000000
C	-3.532397000000	-6.822502000000	-0.606509000000
H	-3.672132000000	-7.719882000000	-1.218565000000
C	-4.357922000000	-5.082167000000	0.821708000000
H	-5.144007000000	-4.547267000000	1.359414000000
C	-3.052609000000	-4.587678000000	0.899168000000
H	-2.839553000000	-3.691757000000	1.489660000000
C	-4.625286000000	-6.244152000000	0.069918000000
C	3.621539000000	-1.252476000000	-5.446736000000
H	4.496188000000	-0.596243000000	-5.631500000000
H	2.905920000000	-1.064653000000	-6.268201000000
C	4.067126000000	-2.722455000000	-5.443668000000
H	4.557771000000	-2.978997000000	-6.400595000000
H	3.178241000000	-3.373751000000	-5.350441000000
C	5.020025000000	-3.004646000000	-4.271321000000
H	5.280354000000	-4.079575000000	-4.248793000000
H	5.967376000000	-2.447384000000	-4.422078000000
Ag	0.803922000000	-1.695451000000	-1.281993000000
Ag	-1.188260000000	0.275844000000	-2.078933000000
Ag	1.606030000000	1.111344000000	-1.805117000000
Ag	-3.688551000000	-0.897858000000	-0.201936000000
Ag	-0.006203000000	-4.114823000000	0.166166000000
F	5.800496000000	4.633572000000	-3.353874000000
F	4.047872000000	4.422419000000	-4.646108000000
F	3.910697000000	5.629760000000	-2.819496000000
N	-5.868995000000	-0.577965000000	0.146198000000
N	4.303313000000	-4.440288000000	0.407301000000

N	-2.012166000000	-5.164231000000	0.254950000000
O	1.098984000000	-3.579797000000	-2.956741000000
O	-2.733235000000	0.672190000000	-4.004741000000
O	3.228853000000	2.437700000000	-3.093533000000
O	0.591403000000	-5.435769000000	-1.698885000000
O	-4.162448000000	1.377979000000	-2.364423000000
O	4.469028000000	3.241199000000	-1.333430000000
S	-1.752363000000	-1.968095000000	-1.261972000000
S	-0.344159000000	2.607137000000	-2.041165000000
S	3.152115000000	-0.739115000000	-1.276893000000
Ag	2.888290000000	-2.595059000000	0.736587000000
F	1.363948000000	-5.217270000000	-5.081489000000
F	1.087702000000	-6.983384000000	-3.815828000000
F	2.954993000000	-5.829769000000	-3.689705000000
C	-5.105829000000	0.338867000000	-4.269116000000
F	-6.051814000000	1.313970000000	-4.393954000000
F	-5.696629000000	-0.699340000000	-3.581769000000
F	-4.814711000000	-0.121937000000	-5.505028000000
C	0.287597000000	2.476803000000	-4.799554000000
H	1.348677000000	2.343736000000	-4.517528000000
H	-0.197058000000	1.484147000000	-4.819043000000
C	-0.395116000000	3.361260000000	-3.752552000000
C	0.204706000000	3.147866000000	-6.185013000000
H	-0.855623000000	3.196941000000	-6.505613000000
H	0.730813000000	2.519548000000	-6.926987000000
C	0.121830000000	5.434380000000	-5.087982000000
H	0.588870000000	6.435757000000	-5.045136000000
H	-0.942497000000	5.590150000000	-5.357591000000
C	0.802592000000	4.564541000000	-6.157582000000
H	0.710293000000	5.039377000000	-7.151643000000
H	1.882714000000	4.498449000000	-5.927894000000
C	0.201703000000	4.772309000000	-3.698298000000
H	-0.328101000000	5.379585000000	-2.940907000000
H	1.260028000000	4.699791000000	-3.382686000000
H	-1.480086000000	3.410729000000	-3.960991000000
F	6.288569000000	-0.125702000000	3.441287000000
F	5.093403000000	-0.259951000000	5.272546000000
F	6.036203000000	-2.063431000000	4.456549000000
F	-3.190219000000	5.774704000000	2.551167000000
F	-1.442831000000	6.576476000000	3.620478000000
F	-1.963110000000	7.345463000000	1.634238000000
C	5.105121000000	8.693552000000	1.051265000000
H	4.580342000000	9.665070000000	1.035707000000
H	5.554690000000	8.578648000000	2.054356000000
C	6.252803000000	8.734459000000	-0.006217000000
H	6.878303000000	9.620249000000	0.207143000000
H	5.810348000000	8.875957000000	-1.008219000000
C	-7.388072000000	7.171675000000	-0.697913000000
H	-7.470021000000	7.280298000000	0.401109000000
H	-7.149063000000	8.188312000000	-1.063731000000
C	-8.748310000000	6.764065000000	-1.285175000000
H	-9.479122000000	7.552933000000	-1.020792000000
H	-8.692850000000	6.777495000000	-2.390073000000
C	-10.174451000000	-0.518300000000	-0.054341000000
H	-10.622692000000	-1.180010000000	0.707426000000
H	-10.638233000000	0.482786000000	0.028182000000
C	-10.478376000000	-1.085049000000	-1.479169000000

H	-11.573584000000	-1.177522000000	-1.590081000000
H	-10.136815000000	-0.347838000000	-2.228318000000
C	-5.994950000000	-6.882060000000	-0.004370000000
H	-5.905578000000	-7.821281000000	-0.577895000000
H	-6.692449000000	-6.240587000000	-0.579520000000
C	-6.622592000000	-7.207829000000	1.388253000000
H	-7.276333000000	-8.089479000000	1.259250000000
H	-5.825079000000	-7.503649000000	2.092612000000
C	7.324257000000	-7.249613000000	-0.920070000000
H	8.132691000000	-7.327440000000	-0.171809000000
H	6.898314000000	-8.260753000000	-1.053064000000
C	7.932747000000	-6.803238000000	-2.282625000000
H	8.633011000000	-7.588610000000	-2.619409000000
H	7.122112000000	-6.746643000000	-3.031783000000
C	10.335869000000	0.004731000000	0.254382000000
C	7.098020000000	7.481809000000	0.014582000000
C	6.874563000000	6.427844000000	-0.887155000000
C	8.079218000000	7.280015000000	1.004154000000
C	7.605937000000	5.239054000000	-0.749928000000
H	6.116794000000	6.508293000000	-1.671132000000
C	8.757209000000	6.055659000000	1.058094000000
H	8.305208000000	8.065017000000	1.735264000000
H	7.413174000000	4.403520000000	-1.431431000000
H	9.520660000000	5.881271000000	1.827344000000
C	-9.315783000000	5.424131000000	-0.847958000000
C	-10.277246000000	4.776885000000	-1.647645000000
C	-8.931868000000	4.765700000000	0.333899000000
C	-10.791316000000	3.538679000000	-1.245720000000
H	-10.615353000000	5.231448000000	-2.585801000000
C	-9.497691000000	3.521038000000	0.644439000000
H	-8.177880000000	5.192654000000	1.002100000000
H	-11.538165000000	3.023888000000	-1.863891000000
H	-9.183635000000	2.985943000000	1.549399000000
C	-9.812936000000	-2.419424000000	-1.738982000000
C	-8.479768000000	-2.509068000000	-2.187015000000
C	-10.474259000000	-3.634361000000	-1.485728000000
C	-7.873308000000	-3.766764000000	-2.297826000000
H	-7.905201000000	-1.610532000000	-2.430871000000
C	-9.786462000000	-4.843392000000	-1.657218000000
H	-11.519066000000	-3.639868000000	-1.154057000000
H	-6.823848000000	-3.839666000000	-2.610768000000
H	-10.301002000000	-5.796462000000	-1.474286000000
C	-7.453327000000	-6.084979000000	1.971588000000
C	-7.016648000000	-5.270348000000	3.030744000000
C	-8.722772000000	-5.801770000000	1.435002000000
C	-7.833319000000	-4.216710000000	3.469325000000
H	-6.043003000000	-5.431274000000	3.504303000000
C	-9.463577000000	-4.730698000000	1.943532000000
H	-9.120844000000	-6.404785000000	0.612967000000
H	-7.489147000000	-3.556838000000	4.271762000000
H	-10.446168000000	-4.490168000000	1.517592000000
C	8.650412000000	-5.475325000000	-2.206929000000
C	7.978404000000	-4.263509000000	-2.447126000000
C	10.011328000000	-5.387997000000	-1.863553000000
C	8.676114000000	-3.053908000000	-2.336121000000
H	6.920123000000	-4.262367000000	-2.722420000000
C	10.617079000000	-4.127630000000	-1.772141000000

H	10.597443000000	-6.294212000000	-1.672038000000
H	8.161068000000	-2.103189000000	-2.525323000000
H	11.679264000000	-4.047297000000	-1.506420000000
N	8.533357000000	5.032559000000	0.207791000000
N	-10.416251000000	2.898667000000	-0.120381000000
N	-8.495838000000	-4.934041000000	-2.033564000000
N	-9.040619000000	-3.928221000000	2.941352000000
N	9.978045000000	-2.962810000000	-1.995634000000
H	10.908235000000	0.907323000000	-0.023236000000
C	10.830861000000	-0.474316000000	1.656048000000
H	11.935602000000	-0.491680000000	1.637333000000
H	10.525478000000	0.264031000000	2.418876000000
C	10.309441000000	-1.846950000000	2.010127000000
C	10.935633000000	-3.000953000000	1.504476000000
C	9.143856000000	-2.038744000000	2.774128000000
C	10.367080000000	-4.256350000000	1.745503000000
H	11.848358000000	-2.916588000000	0.904301000000
C	8.655251000000	-3.339552000000	2.961564000000
H	8.595685000000	-1.189479000000	3.192956000000
H	10.835356000000	-5.161640000000	1.338054000000
H	7.737613000000	-3.497453000000	3.538880000000
N	9.235394000000	-4.446461000000	2.452852000000
H	10.554072000000	-0.780505000000	-0.493715000000
H	1.533668000000	-3.275918000000	-0.161399000000

### Ag<sub>12</sub>-Bpv-AgH

C	2.854593000000	-3.171631000000	2.949415000000
H	3.948300000000	-3.123960000000	2.797042000000
C	2.484326000000	-2.410625000000	4.228220000000
H	1.381695000000	-2.393985000000	4.327317000000
H	2.843630000000	-1.369543000000	4.167957000000
C	3.095778000000	-3.122197000000	5.451785000000
H	4.202765000000	-3.072780000000	5.385638000000
H	2.811060000000	-2.578187000000	6.370713000000
C	2.649655000000	-4.591053000000	5.528948000000
H	3.117601000000	-5.091787000000	6.396327000000
H	1.553582000000	-4.625841000000	5.686817000000
C	2.995377000000	-5.340905000000	4.232309000000
H	2.624173000000	-6.381444000000	4.273226000000
H	4.096408000000	-5.402812000000	4.122414000000
C	2.395343000000	-4.633275000000	3.002269000000
H	2.676554000000	-5.160262000000	2.071721000000
H	1.292238000000	-4.642548000000	3.076932000000
C	1.396402000000	3.408173000000	3.109216000000
H	0.495108000000	4.047926000000	3.143072000000
C	1.393473000000	2.470877000000	4.321944000000
H	2.232429000000	1.756629000000	4.228703000000
H	0.449749000000	1.898411000000	4.345824000000
C	2.658178000000	4.277308000000	3.051849000000
H	2.618192000000	4.951290000000	2.177470000000
H	3.542703000000	3.626930000000	2.918151000000
C	4.896431000000	0.882734000000	2.550419000000
C	5.952615000000	1.734530000000	3.315603000000
C	-1.882070000000	-4.163429000000	3.363502000000
C	-2.840598000000	3.084644000000	2.935099000000
C	-3.805116000000	3.770786000000	3.952497000000

C	-0.265830000000	-6.130757000000	0.662383000000
H	-0.111215000000	-5.658017000000	1.636421000000
C	-1.517328000000	-6.647074000000	0.320377000000
H	-2.331008000000	-6.580722000000	1.047216000000
C	-1.717232000000	-7.185964000000	-0.967380000000
C	-0.587038000000	-7.261631000000	-1.811812000000
H	-0.671296000000	-7.667804000000	-2.824514000000
C	0.627156000000	-6.713398000000	-1.388484000000
H	1.499942000000	-6.687559000000	-2.050941000000
C	4.887252000000	4.496280000000	-1.797062000000
H	3.954751000000	5.067339000000	-1.804733000000
C	5.853714000000	4.676054000000	-2.788807000000
H	5.684566000000	5.414336000000	-3.578295000000
C	7.032743000000	3.902769000000	-2.761602000000
C	7.190856000000	3.013424000000	-1.679106000000
H	8.077411000000	2.376510000000	-1.605071000000
C	6.170642000000	2.878059000000	-0.734183000000
H	6.230069000000	2.148355000000	0.081011000000
C	6.309401000000	-2.295841000000	1.625257000000
H	6.480906000000	-1.225533000000	1.775682000000
C	6.821694000000	-3.247245000000	2.510168000000
H	7.428295000000	-2.920231000000	3.359791000000
C	5.804074000000	-4.950650000000	1.151769000000
H	5.547751000000	-5.991237000000	0.931681000000
C	5.324528000000	-3.939837000000	0.314492000000
H	4.717244000000	-4.180038000000	-0.564856000000
C	6.550508000000	-4.615482000000	2.299807000000
C	1.551518000000	3.288347000000	5.618943000000
H	0.659328000000	3.932290000000	5.755869000000
H	1.579832000000	2.599065000000	6.482473000000
C	2.817508000000	4.160209000000	5.582315000000
H	2.901968000000	4.755809000000	6.509597000000
H	3.710123000000	3.506513000000	5.533746000000
C	2.809872000000	5.085183000000	4.354901000000
H	3.739814000000	5.682669000000	4.309695000000
H	1.970277000000	5.804614000000	4.439490000000
Ag	1.971782000000	0.127818000000	1.727325000000
Ag	-0.225508000000	-1.858695000000	1.839434000000
Ag	-0.790133000000	1.008219000000	1.804964000000
Ag	1.572440000000	-3.889606000000	-0.443456000000
Ag	4.010985000000	-1.073739000000	-0.113982000000
F	-3.794231000000	5.130850000000	3.789442000000
F	-3.501224000000	3.513125000000	5.244635000000
F	-5.092615000000	3.351758000000	3.746898000000
N	0.792147000000	-6.113771000000	-0.183420000000
N	5.017588000000	3.588401000000	-0.799589000000
N	5.545908000000	-2.624181000000	0.554890000000
O	3.891458000000	0.503263000000	3.209344000000
O	-0.815382000000	-3.511955000000	3.521615000000
O	-1.831903000000	2.512304000000	3.431708000000
O	5.188186000000	0.690817000000	1.331399000000
O	-2.518590000000	-4.450156000000	2.304879000000
O	-3.202631000000	3.199446000000	1.727743000000
S	2.154315000000	-2.341922000000	1.422506000000
S	-2.472225000000	-0.838073000000	1.550790000000
S	1.193302000000	2.486544000000	1.489209000000
Ag	3.133699000000	2.596486000000	-0.021669000000

C	-2.549574000000	-4.723708000000	4.654311000000
C	-2.666166000000	-0.654125000000	4.386020000000
H	-2.330203000000	0.397268000000	4.315558000000
H	-1.766792000000	-1.292374000000	4.449691000000
C	-3.467366000000	-1.009637000000	3.127807000000
C	-3.545983000000	-0.836734000000	5.639284000000
H	-3.796096000000	-1.908952000000	5.757825000000
H	-2.967196000000	-0.544977000000	6.534456000000
C	-5.626313000000	-0.367216000000	4.268612000000
H	-6.533237000000	0.258889000000	4.178667000000
H	-5.970316000000	-1.419835000000	4.328036000000
C	-4.840508000000	-0.012724000000	5.541560000000
H	-5.469005000000	-0.179347000000	6.435422000000
H	-4.588863000000	1.065285000000	5.523798000000
C	-4.758191000000	-0.190270000000	3.008492000000
H	-5.317918000000	-0.488611000000	2.104014000000
H	-4.501238000000	0.878780000000	2.889196000000
H	-3.720480000000	-2.085820000000	3.146834000000
C	-2.757774000000	2.887366000000	-2.932492000000
H	-3.553453000000	2.139404000000	-3.099304000000
C	-1.987501000000	3.108472000000	-4.236727000000
H	-1.137737000000	3.788799000000	-4.049695000000
H	-1.575446000000	2.149359000000	-4.593272000000
C	-2.928214000000	3.718786000000	-5.293651000000
H	-3.717088000000	2.982147000000	-5.542936000000
H	-2.361294000000	3.904042000000	-6.223969000000
C	-3.574600000000	5.019013000000	-4.787182000000
H	-4.266997000000	5.427156000000	-5.546083000000
H	-2.783276000000	5.779963000000	-4.633084000000
C	-4.315799000000	4.792237000000	-3.458988000000
H	-4.737190000000	5.740996000000	-3.077992000000
H	-5.172068000000	4.106927000000	-3.623928000000
C	-3.382416000000	4.180952000000	-2.394926000000
H	-3.929879000000	3.982601000000	-1.456167000000
H	-2.570361000000	4.895261000000	-2.150780000000
C	-1.133518000000	-3.933084000000	-3.129912000000
H	-0.631208000000	-4.913340000000	-3.039622000000
C	-0.601677000000	-3.199096000000	-4.367640000000
H	-1.021383000000	-2.175753000000	-4.395450000000
H	0.497083000000	-3.104919000000	-4.310395000000
C	-2.650810000000	-4.142185000000	-3.185975000000
H	-2.989663000000	-4.696112000000	-2.292221000000
H	-3.145035000000	-3.154042000000	-3.161373000000
C	-3.373277000000	-0.495258000000	-3.930693000000
C	-4.726559000000	-0.467958000000	-4.701454000000
C	1.506495000000	4.260388000000	-2.758356000000
C	3.353232000000	-3.651247000000	-3.080692000000
C	4.583343000000	-4.021744000000	-3.959727000000
C	0.660778000000	6.427218000000	0.695262000000
H	1.305831000000	6.160181000000	-0.149233000000
C	1.001353000000	7.431536000000	1.603603000000
H	1.927399000000	7.995459000000	1.457968000000
C	0.152452000000	7.711398000000	2.695712000000
C	-1.046532000000	6.973981000000	2.781029000000
H	-1.746508000000	7.119908000000	3.608657000000
C	-1.324400000000	5.995306000000	1.825109000000
H	-2.239329000000	5.399394000000	1.870611000000

C	-5.327167000000	-3.617248000000	1.361489000000
H	-4.777296000000	-4.225206000000	2.087597000000
C	-6.603226000000	-3.119828000000	1.639845000000
H	-7.068650000000	-3.343246000000	2.604574000000
C	-7.242580000000	-2.274741000000	0.708654000000
C	-6.556856000000	-2.016691000000	-0.495569000000
H	-7.001316000000	-1.392571000000	-1.275588000000
C	-5.283193000000	-2.552581000000	-0.698820000000
H	-4.721417000000	-2.313716000000	-1.606595000000
C	-5.831254000000	1.268782000000	-1.552957000000
H	-5.233313000000	0.518656000000	-2.079497000000
C	-7.039189000000	1.739675000000	-2.072380000000
H	-7.379851000000	1.374083000000	-3.045435000000
C	-7.234506000000	3.142225000000	-0.124798000000
H	-7.773202000000	3.865118000000	0.495155000000
C	-6.012112000000	2.630552000000	0.319809000000
H	-5.550801000000	2.964987000000	1.254339000000
C	-7.780329000000	2.695994000000	-1.347083000000
C	-1.012538000000	-3.952335000000	-5.648851000000
H	-0.504042000000	-4.938074000000	-5.677121000000
H	-0.657792000000	-3.387462000000	-6.529669000000
C	-2.534083000000	-4.163232000000	-5.720518000000
H	-2.799649000000	-4.731403000000	-6.630714000000
H	-3.034594000000	-3.178507000000	-5.801888000000
C	-3.048715000000	-4.893717000000	-4.469227000000
H	-4.148056000000	-5.007439000000	-4.502062000000
H	-2.628758000000	-5.919851000000	-4.436651000000
Ag	-1.353826000000	-0.544747000000	-1.820610000000
Ag	0.801367000000	1.449768000000	-2.118208000000
Ag	1.475262000000	-1.376986000000	-1.946171000000
Ag	-0.594735000000	3.674527000000	-0.123875000000
Ag	-3.176878000000	1.120977000000	0.161732000000
F	4.713496000000	-5.358689000000	-4.120064000000
F	4.543107000000	-3.454071000000	-5.189085000000
F	5.715468000000	-3.565797000000	-3.331518000000
N	-0.477765000000	5.701382000000	0.809913000000
N	-4.660132000000	-3.331867000000	0.216720000000
N	-5.319842000000	1.699949000000	-0.376933000000
O	-2.339666000000	-0.243959000000	-4.577739000000
O	1.333316000000	3.232955000000	-3.477841000000
O	2.745429000000	-2.596815000000	-3.423175000000
O	-3.497307000000	-0.747128000000	-2.676761000000
O	1.651510000000	4.347419000000	-1.505171000000
O	3.165807000000	-4.425011000000	-2.097010000000
S	-1.690300000000	2.105096000000	-1.615432000000
S	3.238603000000	0.605630000000	-1.718632000000
S	-0.658139000000	-3.044815000000	-1.554615000000
Ag	-2.314313000000	-3.260710000000	0.240731000000
F	-5.181767000000	0.825779000000	-4.793070000000
F	-5.709301000000	-1.175979000000	-4.066270000000
F	-4.612700000000	-0.957785000000	-5.953307000000
C	1.453658000000	5.618650000000	-3.512955000000
F	2.244557000000	6.556606000000	-2.913165000000
F	0.169173000000	6.092454000000	-3.483126000000
F	1.834066000000	5.527571000000	-4.805861000000
C	3.607188000000	0.633384000000	-4.511720000000
H	3.226720000000	-0.405103000000	-4.536741000000

H	2.741746000000	1.317224000000	-4.568293000000
C	4.359981000000	0.852271000000	-3.192424000000
C	4.559194000000	0.868391000000	-5.701232000000
H	4.871089000000	1.933603000000	-5.713968000000
H	4.016232000000	0.687684000000	-6.646690000000
C	6.540214000000	0.179869000000	-4.277389000000
H	7.403525000000	-0.506195000000	-4.197375000000
H	6.947808000000	1.209901000000	-4.237730000000
C	5.805125000000	-0.028007000000	-5.611192000000
H	6.486909000000	0.175175000000	-6.457238000000
H	5.496380000000	-1.087852000000	-5.691265000000
C	5.598295000000	-0.045059000000	-3.078762000000
H	6.124034000000	0.150588000000	-2.126395000000
H	5.273315000000	-1.101193000000	-3.059149000000
H	4.659319000000	1.915055000000	-3.115499000000
F	-2.490183000000	-6.082536000000	4.672456000000
F	-1.976771000000	-4.263932000000	5.789114000000
F	-3.873948000000	-4.367959000000	4.693047000000
F	6.027026000000	2.988872000000	2.767079000000
F	5.675486000000	1.885926000000	4.631589000000
F	7.189827000000	1.171179000000	3.212666000000
C	0.512488000000	8.722957000000	3.715788000000
C	-0.465109000000	9.527197000000	4.334989000000
C	1.850292000000	8.912535000000	4.118196000000
C	-0.066549000000	10.461056000000	5.299814000000
H	-1.518996000000	9.445662000000	4.050546000000
C	2.136631000000	9.872269000000	5.097360000000
H	2.653135000000	8.297191000000	3.699889000000
H	-0.814850000000	11.100348000000	5.785517000000
H	3.171834000000	10.024758000000	5.428566000000
C	-9.091134000000	3.187114000000	-1.830121000000
C	-10.002844000000	2.321225000000	-2.467533000000
C	-9.487597000000	4.528023000000	-1.656836000000
C	-11.239370000000	2.827448000000	-2.888846000000
H	-9.764492000000	1.261321000000	-2.603771000000
C	-10.745758000000	4.929309000000	-2.123989000000
H	-8.814196000000	5.254039000000	-1.190017000000
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H	-11.067217000000	5.972049000000	-2.006392000000
C	6.998630000000	-5.649232000000	3.260470000000
C	6.995543000000	-5.401375000000	4.648576000000
C	7.419890000000	-6.924455000000	2.834607000000
C	7.401074000000	-6.418830000000	5.521684000000
H	6.648662000000	-4.441069000000	5.044351000000
C	7.811248000000	-7.866203000000	3.795033000000
H	7.466836000000	-7.171274000000	1.769132000000
H	7.393750000000	-6.246077000000	6.605478000000
H	8.149933000000	-8.861522000000	3.480157000000
C	-3.065148000000	-7.570649000000	-1.434963000000
C	-4.204764000000	-6.843035000000	-1.028996000000
C	-3.269543000000	-8.636078000000	-2.339463000000
C	-5.454605000000	-7.195381000000	-1.545309000000
H	-4.102468000000	-5.985468000000	-0.354551000000
H	-2.418070000000	-9.254143000000	-2.654972000000
C	-5.530092000000	-8.263527000000	-2.452952000000
H	-6.353983000000	-6.639215000000	-1.262298000000
H	-6.493121000000	-8.555581000000	-2.890651000000



C	-8.553527000000	-1.648412000000	0.996206000000
C	-8.843485000000	-0.344515000000	0.545279000000
C	-9.553178000000	-2.308790000000	1.736966000000
C	-10.089110000000	0.220430000000	0.845718000000
H	-8.098521000000	0.232081000000	-0.009808000000
C	-10.766224000000	-1.650306000000	1.979094000000
H	-9.400499000000	-3.330764000000	2.098600000000
H	-10.326488000000	1.235522000000	0.500975000000
H	-11.558103000000	-2.153663000000	2.548508000000
C	8.036756000000	3.983490000000	-3.846591000000
C	7.639306000000	4.130830000000	-5.191288000000
C	9.418381000000	3.884325000000	-3.589348000000
C	8.621251000000	4.168547000000	-6.189526000000
H	6.578388000000	4.179959000000	-5.457985000000
C	10.314643000000	3.941157000000	-4.664368000000
H	9.790880000000	3.789101000000	-2.564340000000
H	8.328704000000	4.271193000000	-7.242308000000
H	11.394783000000	3.874235000000	-4.481532000000
N	1.208768000000	10.647049000000	5.691262000000
N	-11.624042000000	4.108393000000	-2.731350000000
N	-11.052134000000	-0.405888000000	1.549686000000
N	7.807997000000	-7.639145000000	5.122710000000
N	-4.462888000000	-8.985808000000	-2.845786000000
N	9.943988000000	4.078850000000	-5.952000000000
H	0.336180000000	-0.115653000000	-1.144261000000

### Ag<sub>12</sub>-BPvSH

C	3.153163000000	-2.488350000000	3.274936000000
H	4.203030000000	-2.162607000000	3.162204000000
C	2.551881000000	-1.830050000000	4.523136000000
H	1.475212000000	-2.087139000000	4.579775000000
H	2.637647000000	-0.731347000000	4.450133000000
C	3.271715000000	-2.344680000000	5.784847000000
H	4.330550000000	-2.013481000000	5.756334000000
H	2.820713000000	-1.880826000000	6.680853000000
C	3.214261000000	-3.878091000000	5.878276000000
H	3.761772000000	-4.229820000000	6.771886000000
H	2.158963000000	-4.192231000000	6.001515000000
C	3.789848000000	-4.532967000000	4.611982000000
H	3.693663000000	-5.632857000000	4.666078000000
H	4.873884000000	-4.313873000000	4.543956000000
C	3.082169000000	-4.019134000000	3.343769000000
H	3.536465000000	-4.463031000000	2.437765000000
H	2.017160000000	-4.318833000000	3.365008000000
C	0.301356000000	3.534469000000	3.129255000000
H	-0.777638000000	3.776526000000	3.139662000000
C	0.634083000000	2.668322000000	4.348604000000
H	1.696249000000	2.364838000000	4.301880000000
H	0.013019000000	1.756332000000	4.337207000000
C	1.112692000000	4.836514000000	3.112658000000
H	0.849767000000	5.441756000000	2.227556000000
H	2.188548000000	4.593689000000	3.031689000000
C	4.338115000000	2.091921000000	2.661852000000
C	4.969149000000	3.334210000000	3.358603000000
C	-1.217354000000	-4.920863000000	3.099932000000
C	-3.064184000000	1.921391000000	3.005520000000

C	-3.954840000000	2.323803000000	4.218378000000
C	1.189622000000	-6.137474000000	0.510484000000
H	1.071845000000	-5.720959000000	1.515343000000
C	0.184467000000	-6.932911000000	-0.046041000000
H	-0.710764000000	-7.141125000000	0.545443000000
C	0.323576000000	-7.404028000000	-1.368081000000
C	1.539060000000	-7.111773000000	-2.026612000000
H	1.712877000000	-7.445113000000	-3.054421000000
C	2.488000000000	-6.302684000000	-1.395994000000
H	3.405321000000	-5.993454000000	-1.909029000000
C	3.696363000000	5.409313000000	-1.981196000000
H	2.679358000000	5.801740000000	-2.059050000000
C	4.661379000000	5.696748000000	-2.948005000000
H	4.398677000000	6.334526000000	-3.796998000000
C	5.959565000000	5.161241000000	-2.819415000000
C	6.224828000000	4.393677000000	-1.667285000000
H	7.208642000000	3.940972000000	-1.511828000000
C	5.202544000000	4.136190000000	-0.750802000000
H	5.355759000000	3.492115000000	0.122166000000
C	6.355090000000	-0.701737000000	2.175134000000
H	6.238702000000	0.380200000000	2.275630000000
C	7.015761000000	-1.455495000000	3.147107000000
H	7.435341000000	-0.952454000000	4.023121000000
C	6.613379000000	-3.404949000000	1.800915000000
H	6.663853000000	-4.481201000000	1.611104000000
C	5.963889000000	-2.583553000000	0.875504000000
H	5.538093000000	-3.002305000000	-0.042408000000
C	7.133265000000	-2.852114000000	2.988657000000
C	0.379426000000	3.469853000000	5.640539000000
H	-0.704225000000	3.690192000000	5.727796000000
H	0.645941000000	2.847662000000	6.514296000000
C	1.175925000000	4.785635000000	5.651067000000
H	0.961136000000	5.359582000000	6.570965000000
H	2.258592000000	4.553228000000	5.658950000000
C	0.857751000000	5.632074000000	4.408338000000
H	1.465269000000	6.556432000000	4.398112000000
H	-0.203621000000	5.950560000000	4.436522000000
Ag	1.775824000000	0.520974000000	1.917583000000
Ag	-0.114579000000	-2.197669000000	1.978512000000
Ag	-1.025213000000	0.458008000000	1.390121000000
Ag	2.589875000000	-3.427895000000	-0.196127000000
Ag	4.044549000000	-0.124953000000	0.163449000000
F	-3.851581000000	3.667422000000	4.454815000000
F	-3.631828000000	1.682374000000	5.363751000000
F	-5.269039000000	2.055870000000	3.953602000000
N	2.312732000000	-5.780824000000	-0.156394000000
N	3.943548000000	4.613920000000	-0.912158000000
N	5.803047000000	-1.250680000000	1.065894000000
O	3.569939000000	1.376181000000	3.358827000000
O	-0.404432000000	-4.031918000000	3.476608000000
O	-2.071537000000	1.183885000000	3.287254000000
O	4.695106000000	1.952468000000	1.452345000000
O	-1.537409000000	-5.291632000000	1.931530000000
O	-3.433683000000	2.376392000000	1.891499000000
S	2.311584000000	-1.878296000000	1.725544000000
S	-2.514297000000	-1.788739000000	1.303977000000
S	0.517882000000	2.622790000000	1.503074000000

Ag	2.243011000000	3.480702000000	0.004524000000
C	-1.967350000000	-5.695277000000	4.224383000000
C	-3.066004000000	-1.880197000000	4.103488000000
H	-2.813399000000	-0.808086000000	4.181280000000
H	-2.127756000000	-2.447668000000	4.229260000000
C	-3.676050000000	-2.160142000000	2.723755000000
C	-4.074493000000	-2.271080000000	5.203122000000
H	-4.236900000000	-3.366546000000	5.174189000000
H	-3.639334000000	-2.042191000000	6.192911000000
C	-6.004663000000	-1.791503000000	3.626124000000
H	-6.941743000000	-1.222406000000	3.482039000000
H	-6.268768000000	-2.863035000000	3.517974000000
C	-5.418236000000	-1.543513000000	5.025318000000
H	-6.135402000000	-1.866248000000	5.802096000000
H	-5.264177000000	-0.456411000000	5.163933000000
C	-4.997682000000	-1.408719000000	2.525492000000
H	-5.415496000000	-1.621427000000	1.526024000000
H	-4.802166000000	-0.320038000000	2.567869000000
H	-3.855211000000	-3.247599000000	2.623979000000
C	-3.021292000000	2.213713000000	-3.209357000000
H	-3.779698000000	1.413790000000	-3.289578000000
C	-2.200211000000	2.263939000000	-4.502473000000
H	-1.375636000000	2.990681000000	-4.389263000000
H	-1.744225000000	1.276287000000	-4.691553000000
C	-3.104510000000	2.679863000000	-5.679673000000
H	-3.865421000000	1.893210000000	-5.853696000000
H	-2.497143000000	2.743672000000	-6.600799000000
C	-3.802202000000	4.020767000000	-5.398004000000
H	-4.457863000000	4.299884000000	-6.242967000000
H	-3.034693000000	4.814449000000	-5.308335000000
C	-4.613719000000	3.957445000000	-4.093575000000
H	-5.084355000000	4.934102000000	-3.876395000000
H	-5.438360000000	3.223870000000	-4.204781000000
C	-3.725009000000	3.542468000000	-2.904286000000
H	-4.323824000000	3.450202000000	-1.979467000000
H	-2.963181000000	4.323806000000	-2.720746000000
C	0.208614000000	-3.922254000000	-3.241180000000
H	0.925674000000	-4.756014000000	-3.126864000000
C	0.650510000000	-3.024441000000	-4.403328000000
H	-0.009019000000	-2.139293000000	-4.443218000000
H	1.686068000000	-2.678920000000	-4.241429000000
C	-1.199580000000	-4.489192000000	-3.453147000000
H	-1.478482000000	-5.145316000000	-2.608726000000
H	-1.912886000000	-3.645945000000	-3.469084000000
C	-3.174990000000	-1.229214000000	-3.618022000000
C	-3.935304000000	-1.398526000000	-4.964424000000
C	0.410943000000	4.690405000000	-2.743165000000
C	4.505110000000	-2.931695000000	-2.700167000000
C	5.897770000000	-3.011358000000	-3.393096000000
C	-1.127745000000	6.425295000000	0.609605000000
H	-0.482170000000	6.287077000000	-0.264126000000
C	-1.072169000000	7.574997000000	1.400573000000
H	-0.388207000000	8.383070000000	1.124641000000
C	-1.892016000000	7.684642000000	2.542633000000
C	-2.774120000000	6.616276000000	2.803084000000
H	-3.421660000000	6.623221000000	3.684844000000
C	-2.776938000000	5.501072000000	1.963095000000

H	-3.419619000000	4.638453000000	2.158890000000
C	-4.326050000000	-5.163015000000	0.712088000000
H	-3.740579000000	-5.753716000000	1.422362000000
C	-5.635455000000	-4.772000000000	1.001816000000
H	-6.089741000000	-5.084253000000	1.946963000000
C	-6.315776000000	-3.899533000000	0.125440000000
C	-5.645662000000	-3.534640000000	-1.059529000000
H	-6.105930000000	-2.873813000000	-1.798663000000
C	-4.346440000000	-3.995148000000	-1.284075000000
H	-3.806261000000	-3.691202000000	-2.182587000000
C	-6.171146000000	0.624152000000	-1.759467000000
H	-5.676050000000	-0.017734000000	-2.495802000000
C	-7.442635000000	1.156282000000	-1.987332000000
H	-7.951055000000	0.949247000000	-2.933885000000
C	-7.302248000000	2.218964000000	0.164450000000
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C	-6.031971000000	1.655802000000	0.315525000000
H	-5.422714000000	1.853767000000	1.202967000000
C	-8.048584000000	1.966320000000	-1.004541000000
C	0.553408000000	-3.798884000000	-5.734001000000
H	1.287685000000	-4.630465000000	-5.730017000000
H	0.841151000000	-3.128670000000	-6.564344000000
C	-0.857306000000	-4.366210000000	-5.961130000000
H	-0.893643000000	-4.937966000000	-6.906348000000
H	-1.573855000000	-3.527922000000	-6.063976000000
C	-1.285745000000	-5.257370000000	-4.784032000000
H	-2.316331000000	-5.631647000000	-4.925166000000
H	-0.631763000000	-6.151502000000	-4.733256000000
Ag	-0.892382000000	-0.764845000000	-1.670818000000
Ag	0.471226000000	1.725869000000	-2.118339000000
Ag	1.953604000000	-1.103215000000	-1.829125000000
Ag	-1.589912000000	3.373496000000	-0.015504000000
Ag	-3.375929000000	-0.079535000000	-0.325261000000
F	6.445516000000	-4.246798000000	-3.322425000000
F	5.853197000000	-2.648105000000	-4.698043000000
F	6.747865000000	-2.143775000000	-2.752370000000
N	-1.956339000000	5.389895000000	0.890936000000
N	-3.665529000000	-4.765465000000	-0.403557000000
N	-5.472971000000	0.854696000000	-0.621502000000
O	-1.918758000000	-1.093758000000	-3.713638000000
O	0.695636000000	3.702822000000	-3.475859000000
O	3.700641000000	-2.099644000000	-3.195601000000
O	-3.908250000000	-1.269539000000	-2.594718000000
O	0.562239000000	4.843577000000	-1.494730000000
O	4.394015000000	-3.671532000000	-1.674007000000
S	-1.995863000000	1.691038000000	-1.733037000000
S	2.821495000000	1.202061000000	-1.548915000000
S	0.302848000000	-3.052200000000	-1.582316000000
Ag	-1.452374000000	-3.889134000000	-0.017352000000
F	-4.949165000000	-0.483109000000	-5.056161000000
F	-4.496262000000	-2.640034000000	-5.028316000000
F	-3.147399000000	-1.245746000000	-6.053316000000
C	-0.214591000000	5.926945000000	-3.454653000000
F	0.648293000000	6.985116000000	-3.398272000000
F	-1.369800000000	6.311478000000	-2.827698000000
F	-0.517897000000	5.708286000000	-4.754900000000
C	3.264247000000	1.176757000000	-4.344401000000

H	3.118977000000	0.079831000000	-4.327395000000
H	2.274166000000	1.654635000000	-4.458339000000
C	3.903851000000	1.612057000000	-3.020431000000
C	4.184615000000	1.554796000000	-5.521659000000
H	4.265746000000	2.660066000000	-5.580610000000
H	3.723592000000	1.221174000000	-6.469135000000
C	6.216570000000	1.369457000000	-4.018987000000
H	7.197232000000	0.878663000000	-3.880020000000
H	6.403946000000	2.461494000000	-4.029777000000
C	5.586152000000	0.945371000000	-5.354803000000
H	6.238060000000	1.247258000000	-6.194983000000
H	5.510537000000	-0.158198000000	-5.382245000000
C	5.303109000000	1.014937000000	-2.830337000000
H	5.744056000000	1.373285000000	-1.881936000000
H	5.210055000000	-0.082859000000	-2.757174000000
H	3.956411000000	2.716496000000	-2.989214000000
F	-1.611565000000	-7.006836000000	4.228833000000
F	-1.739526000000	-5.192083000000	5.456718000000
F	-3.322368000000	-5.637449000000	4.005584000000
F	4.681538000000	4.475894000000	2.656123000000
F	4.528494000000	3.521354000000	4.624670000000
F	6.325712000000	3.214324000000	3.401023000000
C	-1.807965000000	8.854349000000	3.446569000000
C	-2.951857000000	9.391664000000	4.069398000000
C	-0.571004000000	9.466438000000	3.732699000000
C	-2.806959000000	10.492506000000	4.923341000000
H	-3.944239000000	8.974250000000	3.870846000000
C	-0.540037000000	10.560138000000	4.607153000000
H	0.357592000000	9.074443000000	3.305283000000
H	-3.688803000000	10.928809000000	5.409830000000
H	0.415972000000	11.042461000000	4.848085000000
C	-9.413157000000	2.512695000000	-1.185951000000
C	-10.423521000000	1.759950000000	-1.817926000000
C	-9.760536000000	3.798054000000	-0.724820000000
C	-11.702505000000	2.315759000000	-1.952033000000
H	-10.225043000000	0.743309000000	-2.172911000000
C	-11.069222000000	4.258360000000	-0.917963000000
H	-9.014479000000	4.441328000000	-0.247245000000
H	-12.503226000000	1.738689000000	-2.431772000000
H	-11.354159000000	5.260655000000	-0.573334000000
C	7.744503000000	-3.701896000000	4.035854000000
C	7.551640000000	-3.420739000000	5.404086000000
C	8.516386000000	-4.835651000000	3.713581000000
C	8.123255000000	-4.270323000000	6.359798000000
H	6.935209000000	-2.572423000000	5.719363000000
C	9.047114000000	-5.613098000000	4.751065000000
H	8.722081000000	-5.094521000000	2.670036000000
H	7.972828000000	-4.072364000000	7.428766000000
H	9.657236000000	-6.495029000000	4.517782000000
C	-0.783573000000	-8.100734000000	-2.055734000000
C	-2.127189000000	-7.742023000000	-1.813223000000
C	-0.548727000000	-9.111954000000	-3.013863000000
C	-3.139623000000	-8.381754000000	-2.533785000000
H	-2.371196000000	-6.940462000000	-1.106559000000
H	0.477962000000	-9.450815000000	-3.208098000000
C	-2.781782000000	-9.359861000000	-3.474636000000
H	-4.189690000000	-8.113311000000	-2.380349000000

H	-3.550984000000	-9.869070000000	-4.069124000000
C	-7.642561000000	-3.339677000000	0.474616000000
C	-7.985167000000	-2.018343000000	0.120325000000
C	-8.594126000000	-4.071582000000	1.212070000000
C	-9.225670000000	-1.504675000000	0.518250000000
H	-7.281395000000	-1.385908000000	-0.427990000000
C	-9.808576000000	-3.461430000000	1.552616000000
H	-8.402005000000	-5.109812000000	1.500949000000
H	-9.498039000000	-0.472297000000	0.261490000000
H	-10.561227000000	-4.021141000000	2.122558000000
C	6.985912000000	5.357309000000	-3.868484000000
C	6.638271000000	5.340894000000	-5.234685000000
C	8.347101000000	5.534377000000	-3.551160000000
C	7.647006000000	5.496541000000	-6.194049000000
H	5.601608000000	5.173982000000	-5.545372000000
C	9.272255000000	5.687429000000	-4.591748000000
H	8.677260000000	5.576744000000	-2.508261000000
H	7.395495000000	5.474919000000	-7.262112000000
H	10.335461000000	5.834688000000	-4.362625000000
N	-1.629081000000	11.082899000000	5.202929000000
N	-12.041234000000	3.544776000000	-1.518200000000
N	-10.139869000000	-2.197386000000	1.225117000000
N	8.864312000000	-5.354296000000	6.060221000000
N	-1.510026000000	-9.734276000000	-3.714794000000
N	8.949722000000	5.670246000000	-5.899397000000
H	-0.254290000000	-0.240355000000	-0.066737000000

### Ag<sub>12</sub>-Azopy-AgH

C	3.996413000000	-0.274244000000	3.094918000000
H	4.451723000000	0.694969000000	2.823411000000
C	3.264235000000	-0.130767000000	4.432977000000
H	2.711011000000	-1.058295000000	4.657257000000
H	2.526887000000	0.687376000000	4.366923000000
C	4.283297000000	0.156050000000	5.552781000000
H	4.760570000000	1.139189000000	5.370238000000
H	3.748974000000	0.236034000000	6.516799000000
C	5.360219000000	-0.939003000000	5.618120000000
H	6.089243000000	-0.718809000000	6.419366000000
H	4.877500000000	-1.902855000000	5.876109000000
C	6.081753000000	-1.079902000000	4.268365000000
H	6.828281000000	-1.894941000000	4.303700000000
H	6.640976000000	-0.148345000000	4.048495000000
C	5.081029000000	-1.358689000000	3.127926000000
H	5.600829000000	-1.412610000000	2.154480000000
H	4.597065000000	-2.340164000000	3.294706000000
C	-0.268579000000	5.015075000000	1.259248000000
H	-1.128870000000	5.583680000000	0.861587000000
C	-0.449261000000	4.816054000000	2.769224000000
H	0.351482000000	4.154407000000	3.147630000000
H	-1.413608000000	4.319783000000	2.973139000000
C	1.031401000000	5.751262000000	0.909548000000
H	1.095728000000	5.909123000000	-0.183207000000
H	1.890527000000	5.114335000000	1.190094000000
C	3.181245000000	3.230162000000	2.741876000000
C	4.364042000000	4.063234000000	3.308178000000
C	0.779782000000	-3.336908000000	4.003930000000

C	-4.136611000000	2.669248000000	2.197154000000
C	-5.368828000000	3.155192000000	3.014320000000
C	2.182296000000	-5.972771000000	1.358311000000
H	1.625799000000	-5.603714000000	2.226329000000
C	1.924867000000	-7.231290000000	0.807671000000
H	1.175477000000	-7.894426000000	1.248216000000
C	2.577354000000	-7.600266000000	-0.382832000000
C	3.562628000000	-6.739854000000	-0.910572000000
H	4.107872000000	-7.010269000000	-1.817610000000
C	3.788873000000	-5.521963000000	-0.272726000000
H	4.528211000000	-4.812219000000	-0.651731000000
C	3.284949000000	4.528239000000	-3.519353000000
H	2.422914000000	4.811858000000	-4.133523000000
C	4.531416000000	4.246893000000	-4.087978000000
H	4.692899000000	4.306037000000	-5.167952000000
C	5.563495000000	3.788028000000	-3.248133000000
C	5.345091000000	3.761800000000	-1.855614000000
H	6.140696000000	3.443518000000	-1.178929000000
C	4.077108000000	4.084675000000	-1.375894000000
H	3.848808000000	4.020174000000	-0.306387000000
C	6.176309000000	1.510283000000	0.923863000000
H	5.387517000000	2.246118000000	1.114974000000
C	7.356036000000	1.506455000000	1.663225000000
H	7.525291000000	2.243163000000	2.451160000000
C	8.053362000000	-0.416934000000	0.364306000000
H	8.787523000000	-1.193254000000	0.130251000000
C	6.831982000000	-0.353228000000	-0.312614000000
H	6.564636000000	-1.082670000000	-1.080881000000
C	8.313757000000	0.505587000000	1.395201000000
C	-0.377104000000	6.178412000000	3.486647000000
H	-1.233118000000	6.809176000000	3.169187000000
H	-0.484215000000	6.021241000000	4.575194000000
C	0.937786000000	6.910269000000	3.171560000000
H	0.963230000000	7.891313000000	3.680592000000
H	1.786747000000	6.320137000000	3.570268000000
C	1.110568000000	7.097440000000	1.655519000000
H	2.079446000000	7.580767000000	1.429107000000
H	0.321208000000	7.773735000000	1.270437000000
Ag	1.422884000000	1.637869000000	1.136042000000
Ag	0.279373000000	-0.806708000000	2.284870000000
Ag	-1.484385000000	1.414690000000	1.611114000000
Ag	2.701388000000	-2.924962000000	0.968636000000
Ag	3.731338000000	0.254679000000	-0.560157000000
F	-5.844111000000	4.330192000000	2.504279000000
F	-5.106382000000	3.350915000000	4.324787000000
F	-6.376615000000	2.235050000000	2.926490000000
N	3.081612000000	-5.114657000000	0.814334000000
N	3.041880000000	4.416214000000	-2.191986000000
N	5.899525000000	0.587967000000	-0.034963000000
O	2.260476000000	2.910828000000	3.519130000000
O	0.602234000000	-2.095480000000	4.180831000000
O	-3.054148000000	2.556431000000	2.845331000000
O	3.315232000000	2.922550000000	1.501496000000
O	0.253244000000	-4.122713000000	3.166679000000
O	-4.371784000000	2.436706000000	0.978315000000
S	2.811322000000	-0.605757000000	1.682409000000
S	-2.371104000000	-0.972384000000	2.236078000000

S	-0.355596000000	3.386962000000	0.342611000000
Ag	1.052139000000	3.323852000000	-1.682147000000
C	1.871296000000	-3.992729000000	4.905969000000
C	-2.290646000000	-0.053295000000	4.897293000000
H	-2.390718000000	0.973111000000	4.498550000000
H	-1.217162000000	-0.313906000000	4.909426000000
C	-3.049144000000	-1.022130000000	3.979239000000
C	-2.873603000000	-0.106890000000	6.323176000000
H	-2.687672000000	-1.109315000000	6.759747000000
H	-2.339309000000	0.620414000000	6.960972000000
C	-5.127178000000	-0.804856000000	5.403427000000
H	-6.208110000000	-0.573686000000	5.373291000000
H	-5.036419000000	-1.834252000000	5.804487000000
C	-4.384491000000	0.178274000000	6.321593000000
H	-4.787740000000	0.120767000000	7.349287000000
H	-4.560360000000	1.211643000000	5.963301000000
C	-4.560805000000	-0.760806000000	3.970683000000
H	-5.070570000000	-1.499940000000	3.326873000000
H	-4.752333000000	0.235514000000	3.532121000000
H	-2.855570000000	-2.060976000000	4.305021000000
C	-3.830146000000	0.203783000000	-3.175723000000
H	-4.431531000000	-0.682786000000	-2.904999000000
C	-3.029398000000	-0.090572000000	-4.446827000000
H	-2.363655000000	0.763683000000	-4.669038000000
H	-2.402884000000	-0.985401000000	-4.291512000000
C	-3.999547000000	-0.320661000000	-5.623405000000
H	-4.589767000000	-1.238183000000	-5.430984000000
H	-3.415643000000	-0.504279000000	-6.543658000000
C	-4.945152000000	0.876803000000	-5.815248000000
H	-5.650853000000	0.681081000000	-6.643277000000
H	-4.349612000000	1.765357000000	-6.100554000000
C	-5.716938000000	1.184669000000	-4.521973000000
H	-6.359060000000	2.075684000000	-4.649566000000
H	-6.391052000000	0.338310000000	-4.279749000000
C	-4.752175000000	1.416679000000	-3.341842000000
H	-5.315484000000	1.605381000000	-2.411103000000
H	-4.135139000000	2.313431000000	-3.540193000000
C	0.235858000000	-4.807485000000	-1.441317000000
H	1.148795000000	-5.353795000000	-1.146481000000
C	0.275208000000	-4.550329000000	-2.951332000000
H	-0.586941000000	-3.918658000000	-3.232125000000
H	1.200729000000	-4.012435000000	-3.217050000000
C	-1.001099000000	-5.605966000000	-1.009903000000
H	-0.962227000000	-5.808947000000	0.076788000000
H	-1.901549000000	-4.989995000000	-1.187889000000
C	-3.676213000000	-3.273868000000	-2.273416000000
C	-4.834514000000	-3.983425000000	-3.032685000000
C	-0.678014000000	3.406318000000	-4.305839000000
C	4.184032000000	-2.705498000000	-2.306004000000
C	5.411311000000	-3.220109000000	-3.120623000000
C	-2.212419000000	5.850355000000	-1.616353000000
H	-1.589402000000	5.440553000000	-2.419459000000
C	-2.042607000000	7.160395000000	-1.170583000000
H	-1.290528000000	7.812584000000	-1.620450000000
C	-2.835527000000	7.623175000000	-0.098039000000
C	-3.817432000000	6.764102000000	0.429611000000
H	-4.460771000000	7.102104000000	1.246595000000



C	-3.909896000000	5.461573000000	-0.066396000000
H	-4.618825000000	4.744102000000	0.354778000000
C	-2.926022000000	-4.662571000000	3.645361000000
H	-1.904998000000	-4.779307000000	4.024786000000
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H	-6.409937000000	-4.232824000000	2.081411000000
C	-4.259068000000	-4.295375000000	1.770430000000
H	-4.293479000000	-4.099117000000	0.693153000000
C	-6.598837000000	-1.446292000000	-0.984010000000
H	-6.026664000000	-2.377549000000	-0.955091000000
C	-7.738964000000	-1.308054000000	-1.779211000000
H	-8.092237000000	-2.135458000000	-2.399904000000
C	-7.917941000000	0.975876000000	-0.993634000000
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C	-6.769785000000	0.757710000000	-0.236130000000
H	-6.323188000000	1.547408000000	0.375860000000
C	-8.407403000000	-0.071273000000	-1.803524000000
C	0.197377000000	-5.892128000000	-3.707661000000
H	1.098787000000	-6.498554000000	-3.481470000000
H	0.210136000000	-5.695045000000	-4.795313000000
C	-1.061219000000	-6.683701000000	-3.317012000000
H	-1.089053000000	-7.650276000000	-3.853600000000
H	-1.960847000000	-6.115409000000	-3.623691000000
C	-1.106121000000	-6.925635000000	-1.799664000000
H	-2.039619000000	-7.445131000000	-1.514033000000
H	-0.271686000000	-7.593513000000	-1.509691000000
Ag	-1.436427000000	-1.697049000000	-1.274647000000
Ag	-0.379902000000	0.799444000000	-2.321205000000
Ag	1.452531000000	-1.387162000000	-1.678675000000
Ag	-2.579721000000	2.795069000000	-0.965364000000
Ag	-3.992833000000	-0.519829000000	0.472850000000
F	5.986486000000	-4.298958000000	-2.510994000000
F	5.107235000000	-3.578899000000	-4.387249000000
F	6.368290000000	-2.239086000000	-3.193506000000
N	-3.108365000000	4.993742000000	-1.054808000000
N	-3.022700000000	-4.421647000000	2.312226000000
N	-6.105840000000	-0.430163000000	-0.236405000000
O	-2.674466000000	-2.978020000000	-2.980763000000
O	-0.500693000000	2.162689000000	-4.388957000000
O	3.084967000000	-2.678347000000	-2.924937000000
O	-3.874436000000	-3.029538000000	-1.046085000000
O	-0.133296000000	4.258417000000	-3.536827000000
O	4.459018000000	-2.356791000000	-1.119353000000
S	-2.738251000000	0.444046000000	-1.667037000000
S	2.114601000000	0.949989000000	-2.296910000000
S	0.351726000000	-3.225482000000	-0.434220000000
Ag	-1.286849000000	-3.183680000000	1.420028000000
F	-5.598151000000	-3.045903000000	-3.684839000000
F	-5.669453000000	-4.652853000000	-2.189860000000
F	-4.385647000000	-4.863536000000	-3.956299000000
C	-1.783578000000	4.005748000000	-5.228660000000
F	-1.420773000000	5.195102000000	-5.764778000000
F	-2.916950000000	4.225067000000	-4.476881000000
F	-2.133279000000	3.177489000000	-6.242370000000

C	2.024415000000	-0.094110000000	-4.935998000000
H	2.087343000000	-1.108141000000	-4.497563000000
H	0.962024000000	0.202011000000	-4.980632000000
C	2.797815000000	0.881879000000	-4.042286000000
C	2.640741000000	-0.110962000000	-6.349696000000
H	2.494216000000	0.880519000000	-6.824469000000
H	2.096216000000	-0.842583000000	-6.973813000000
C	4.901593000000	0.534352000000	-5.400996000000
H	5.970770000000	0.260625000000	-5.333269000000
H	4.861966000000	1.555160000000	-5.832728000000
C	4.141492000000	-0.445047000000	-6.309944000000
H	4.565256000000	-0.428505000000	-7.330687000000
H	4.277025000000	-1.472820000000	-5.920465000000
C	4.293762000000	0.552730000000	-3.986941000000
H	4.826043000000	1.267126000000	-3.336885000000
H	4.417863000000	-0.444524000000	-3.531855000000
H	2.647738000000	1.914845000000	-4.408132000000
F	3.022548000000	-4.143158000000	4.165168000000
F	2.189807000000	-3.249702000000	5.990460000000
F	1.504229000000	-5.226550000000	5.330467000000
F	4.916392000000	4.879074000000	2.368326000000
F	4.001477000000	4.827030000000	4.359415000000
F	5.358553000000	3.210460000000	3.729262000000
N	-9.533393000000	0.013986000000	-2.664316000000
N	-6.518755000000	-4.469414000000	4.677131000000
N	9.540123000000	0.354415000000	2.088634000000
N	6.743241000000	3.323419000000	-3.885703000000
N	-2.712183000000	8.896431000000	0.505472000000
N	2.157983000000	-8.809302000000	-0.990511000000
N	-6.331014000000	-4.206529000000	5.910965000000
N	-10.026518000000	1.186703000000	-2.736014000000
N	-1.560315000000	9.418332000000	0.330706000000
N	7.402445000000	2.515460000000	-3.153305000000
N	9.560891000000	0.973296000000	3.203642000000
N	2.348949000000	-8.814683000000	-2.251044000000
C	-11.150340000000	1.286541000000	-3.596148000000
C	-11.707196000000	0.226881000000	-4.343138000000
C	-11.735338000000	2.561704000000	-3.696244000000
C	-12.816987000000	0.505347000000	-5.144600000000
H	-11.269714000000	-0.772707000000	-4.285271000000
C	-12.848550000000	2.721151000000	-4.533222000000
H	-11.314570000000	3.394381000000	-3.125169000000
H	-13.277915000000	-0.292182000000	-5.740957000000
H	-13.328218000000	3.702910000000	-4.632842000000
C	8.550362000000	1.962693000000	-3.775129000000
C	8.905314000000	2.130019000000	-5.130123000000
C	9.358802000000	1.150007000000	-2.959543000000
C	10.052518000000	1.477378000000	-5.589151000000
H	8.285214000000	2.744594000000	-5.787229000000
C	10.489809000000	0.551032000000	-3.531184000000
H	9.090929000000	0.999353000000	-1.909269000000
H	10.359479000000	1.578521000000	-6.637815000000
H	11.142910000000	-0.087027000000	-2.922447000000
C	10.784595000000	0.853392000000	3.909799000000
C	10.836135000000	1.496819000000	5.159622000000
C	11.925294000000	0.153751000000	3.462099000000
C	12.021052000000	1.413770000000	5.904005000000

H	9.959621000000	2.042046000000	5.521634000000
C	13.050084000000	0.140085000000	4.290450000000
H	11.910892000000	-0.356489000000	2.495954000000
H	12.093484000000	1.904313000000	6.882740000000
H	13.956731000000	-0.392880000000	3.977065000000
C	1.922565000000	-10.002960000000	-2.897667000000
C	1.503566000000	-11.182385000000	-2.247579000000
C	1.926424000000	-9.969425000000	-4.303680000000
C	1.111412000000	-12.261354000000	-3.044073000000
H	1.492540000000	-11.233206000000	-1.156019000000
C	1.503202000000	-11.112175000000	-4.996856000000
H	2.248144000000	-9.061124000000	-4.821688000000
H	0.782624000000	-13.198308000000	-2.576997000000
H	1.487966000000	-11.118125000000	-6.093850000000
C	-7.520871000000	-4.158490000000	6.681198000000
C	-8.809243000000	-4.501551000000	6.220019000000
C	-7.372841000000	-3.732969000000	8.013637000000
C	-9.873848000000	-4.396981000000	7.118789000000
H	-8.951205000000	-4.837270000000	5.189851000000
C	-8.515861000000	-3.662880000000	8.821925000000
H	-6.380463000000	-3.463682000000	8.387062000000
H	-10.890635000000	-4.657317000000	6.798373000000
H	-8.434919000000	-3.331195000000	9.864674000000
C	-1.411538000000	10.702932000000	0.911485000000
C	-0.113483000000	11.244448000000	0.881147000000
C	-2.446943000000	11.460524000000	1.498373000000
C	0.092803000000	12.511885000000	1.442812000000
H	0.700978000000	10.669946000000	0.429893000000
C	-2.122581000000	12.714840000000	2.021364000000
H	-3.464238000000	11.062995000000	1.533485000000
H	1.094050000000	12.960684000000	1.439033000000
H	-2.901025000000	13.335265000000	2.483334000000
N	-9.752967000000	-3.986656000000	8.401054000000
N	1.102356000000	-12.247955000000	-4.395636000000
N	-13.394234000000	1.723047000000	-5.252783000000
N	-0.881788000000	13.250913000000	2.005631000000
N	10.845779000000	0.697629000000	-4.821175000000
N	13.119329000000	0.752112000000	5.493852000000
H	-0.006319000000	0.464444000000	0.905857000000

### Ag<sub>12</sub>-AzopySH

C	2.914943000000	-0.793954000000	4.048627000000
H	3.581898000000	0.062253000000	3.844478000000
C	1.915026000000	-0.417663000000	5.145654000000
H	1.183954000000	-1.234939000000	5.280882000000
H	1.355845000000	0.485234000000	4.842085000000
C	2.666884000000	-0.165000000000	6.467753000000
H	3.323344000000	0.720923000000	6.354308000000
H	1.936684000000	0.079325000000	7.260568000000
C	3.512090000000	-1.385950000000	6.866164000000
H	4.055808000000	-1.187829000000	7.807827000000
H	2.838171000000	-2.244512000000	7.055186000000
C	4.501102000000	-1.758949000000	5.749886000000
H	5.081932000000	-2.658526000000	6.024456000000
H	5.231742000000	-0.936125000000	5.613098000000
C	3.767584000000	-2.014029000000	4.417428000000

H	4.489807000000	-2.230339000000	3.608479000000
H	3.111203000000	-2.897983000000	4.519719000000
C	-0.089617000000	4.968655000000	1.551529000000
H	-0.827984000000	5.646612000000	1.081808000000
C	-0.480419000000	4.733320000000	3.015770000000
H	0.204017000000	3.983898000000	3.453446000000
H	-1.506777000000	4.330937000000	3.072079000000
C	1.313164000000	5.576044000000	1.413431000000
H	1.549457000000	5.754387000000	0.347935000000
H	2.055075000000	4.847010000000	1.790999000000
C	3.094884000000	2.528354000000	3.066059000000
C	3.688614000000	3.363249000000	4.236075000000
C	-0.594366000000	-3.507873000000	4.264652000000
C	-4.396585000000	3.248757000000	1.528369000000
C	-5.782284000000	3.778964000000	2.001051000000
C	1.027046000000	-6.321520000000	1.852386000000
H	0.371407000000	-5.858989000000	2.598111000000
C	0.704905000000	-7.539681000000	1.247466000000
H	-0.202897000000	-8.081694000000	1.526043000000
C	1.516442000000	-8.017953000000	0.202605000000
C	2.697747000000	-7.315859000000	-0.113704000000
H	3.364403000000	-7.672599000000	-0.901948000000
C	2.968242000000	-6.132503000000	0.570049000000
H	3.853090000000	-5.534791000000	0.340972000000
C	4.160265000000	4.152027000000	-2.632639000000
H	3.320783000000	4.466143000000	-3.262300000000
C	5.439171000000	3.940675000000	-3.159482000000
H	5.649256000000	4.094420000000	-4.221729000000
C	6.452562000000	3.460964000000	-2.309111000000
C	6.159822000000	3.291077000000	-0.939863000000
H	6.930318000000	2.928709000000	-0.255991000000
C	4.860525000000	3.530310000000	-0.500150000000
H	4.576371000000	3.354651000000	0.542504000000
C	6.631094000000	0.698101000000	1.631583000000
H	6.062566000000	1.543558000000	2.033817000000
C	8.024314000000	0.689264000000	1.602576000000
H	8.605539000000	1.535133000000	1.977309000000
C	7.902924000000	-1.521888000000	0.618432000000
H	8.387509000000	-2.412244000000	0.208829000000
C	6.509756000000	-1.429896000000	0.683765000000
H	5.862308000000	-2.242303000000	0.337556000000
C	8.681132000000	-0.440297000000	1.066395000000
C	-0.379695000000	6.057498000000	3.799457000000
H	-1.129325000000	6.774519000000	3.406014000000
H	-0.641132000000	5.875456000000	4.857755000000
C	1.023955000000	6.675093000000	3.687738000000
H	1.065598000000	7.635273000000	4.234076000000
H	1.757572000000	5.999801000000	4.168944000000
C	1.418362000000	6.886421000000	2.217153000000
H	2.450977000000	7.276042000000	2.142971000000
H	0.758331000000	7.648085000000	1.755887000000
Ag	1.020695000000	1.220502000000	1.337269000000
Ag	-0.387975000000	-0.892064000000	2.566419000000
Ag	-1.771044000000	1.734358000000	1.553869000000
Ag	2.025514000000	-3.391770000000	1.608486000000
Ag	3.670939000000	-0.049172000000	0.689240000000
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F	-5.816919000000	4.108111000000	3.310538000000
F	-6.740495000000	2.823431000000	1.790475000000
N	2.128343000000	-5.609680000000	1.502523000000
N	3.858959000000	3.920000000000	-1.333342000000
N	5.878744000000	-0.332496000000	1.162924000000
O	1.850677000000	2.292849000000	3.146356000000
O	-0.831109000000	-2.294106000000	4.515465000000
O	-3.508249000000	3.137176000000	2.417940000000
O	3.918354000000	2.183297000000	2.178610000000
O	-0.902149000000	-4.200934000000	3.248758000000
O	-4.344884000000	2.971992000000	0.293018000000
S	2.078916000000	-1.092475000000	2.393144000000
S	-2.762852000000	-0.524370000000	1.945105000000
S	-0.219651000000	3.415304000000	0.514765000000
Ag	1.779602000000	3.021317000000	-0.926512000000
C	0.233173000000	-4.292652000000	5.330321000000
C	-3.096925000000	0.475695000000	4.561806000000
H	-3.036970000000	1.491272000000	4.126739000000
H	-2.070000000000	0.133414000000	4.784952000000
C	-3.744700000000	-0.467606000000	3.540297000000
C	-3.939798000000	0.525071000000	5.851141000000
H	-3.922714000000	-0.470337000000	6.339334000000
H	-3.476199000000	1.234310000000	6.560695000000
C	-6.029699000000	-0.035071000000	4.537347000000
H	-7.061490000000	0.278482000000	4.293170000000
H	-6.104880000000	-1.049677000000	4.977346000000
C	-5.393452000000	0.927127000000	5.552350000000
H	-5.986157000000	0.945954000000	6.485306000000
H	-5.410963000000	1.954196000000	5.137112000000
C	-5.201447000000	-0.095315000000	3.239386000000
H	-5.640542000000	-0.818837000000	2.529541000000
H	-5.226090000000	0.893912000000	2.748246000000
H	-3.687297000000	-1.505242000000	3.915758000000
C	-3.175402000000	0.558133000000	-3.642288000000
H	-3.914548000000	-0.247893000000	-3.481908000000
C	-2.193632000000	0.139223000000	-4.739677000000
H	-1.403711000000	0.903472000000	-4.838430000000
H	-1.711564000000	-0.813327000000	-4.463221000000
C	-2.951864000000	-0.018500000000	-6.072638000000
H	-3.670285000000	-0.857015000000	-5.984530000000
H	-2.234932000000	-0.295410000000	-6.866918000000
C	-3.700862000000	1.270925000000	-6.448408000000
H	-4.257809000000	1.132988000000	-7.393253000000
H	-2.963157000000	2.078656000000	-6.622085000000
C	-4.658650000000	1.700516000000	-5.325228000000
H	-5.160714000000	2.652588000000	-5.578517000000
H	-5.457802000000	0.941008000000	-5.205688000000
C	-3.908515000000	1.859716000000	-3.987794000000
H	-4.609942000000	2.134811000000	-3.180108000000
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C	-0.124265000000	-4.861835000000	-1.257323000000
H	0.645518000000	-5.506821000000	-0.797888000000
C	0.214234000000	-4.662483000000	-2.738752000000
H	-0.497518000000	-3.940227000000	-3.178006000000
H	1.231510000000	-4.248284000000	-2.840397000000
C	-1.509035000000	-5.489526000000	-1.048022000000
H	-1.686025000000	-5.665387000000	0.029880000000

H	-2.279190000000	-4.772566000000	-1.385817000000
C	-3.586903000000	-2.897469000000	-2.766650000000
C	-4.688654000000	-3.480129000000	-3.698048000000
C	0.464684000000	3.186637000000	-3.908538000000
C	4.075158000000	-3.472418000000	-1.458476000000
C	5.314283000000	-4.222964000000	-2.038733000000
C	-1.280215000000	6.009668000000	-1.686425000000
H	-0.547297000000	5.494290000000	-2.317393000000
C	-1.035411000000	7.289366000000	-1.191680000000
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C	-3.342984000000	5.900090000000	-0.604435000000
H	-4.228342000000	5.299135000000	-0.379547000000
C	-4.160492000000	-4.067724000000	3.202758000000
H	-3.251711000000	-4.302068000000	3.766330000000
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C	-6.523908000000	-3.630419000000	3.033393000000
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H	-7.211147000000	-3.266661000000	1.007416000000
C	-5.064501000000	-3.599579000000	1.107378000000
H	-4.871263000000	-3.446208000000	0.040216000000
C	-6.488621000000	-0.843516000000	-1.899063000000
H	-6.024500000000	-1.818432000000	-1.730192000000
C	-7.469829000000	-0.661398000000	-2.876393000000
H	-7.806441000000	-1.498519000000	-3.493257000000
C	-7.524268000000	1.683323000000	-2.275999000000
H	-7.917409000000	2.693321000000	-2.412203000000
C	-6.538312000000	1.417936000000	-1.328851000000
H	-6.109482000000	2.207126000000	-0.703054000000
C	-7.993086000000	0.626664000000	-3.085737000000
C	0.103790000000	-6.008935000000	-3.481998000000
H	0.863113000000	-6.715710000000	-3.087589000000
H	0.338555000000	-5.852366000000	-4.550762000000
C	-1.296287000000	-6.622800000000	-3.320580000000
H	-1.352906000000	-7.595121000000	-3.844465000000
H	-2.044465000000	-5.955647000000	-3.791194000000
C	-1.643700000000	-6.808273000000	-1.834768000000
H	-2.673626000000	-7.194335000000	-1.719510000000
H	-0.970802000000	-7.568697000000	-1.393670000000
Ag	-1.402141000000	-1.571523000000	-1.394512000000
Ag	0.207960000000	0.771757000000	-1.890538000000
Ag	1.658756000000	-1.665601000000	-1.242279000000
Ag	-2.199976000000	3.055800000000	-1.227814000000
Ag	-4.043670000000	-0.037688000000	-0.104840000000
F	5.436695000000	-5.464693000000	-1.479001000000
F	5.266078000000	-4.384086000000	-3.379933000000
F	6.463107000000	-3.534979000000	-1.752174000000
N	-2.401393000000	5.304311000000	-1.375413000000
N	-3.977204000000	-3.857592000000	1.873950000000
N	-6.013865000000	0.175542000000	-1.143630000000
O	-2.460192000000	-2.731611000000	-3.307806000000
O	0.446306000000	1.922847000000	-3.936189000000
O	3.200035000000	-3.135579000000	-2.305376000000
O	-3.939652000000	-2.611046000000	-1.583538000000

O	0.914616000000	3.979112000000	-3.030825000000
O	4.107405000000	-3.281934000000	-0.208871000000
S	-2.360950000000	0.716244000000	-1.958393000000
S	2.779316000000	0.568933000000	-1.545181000000
S	0.013075000000	-3.271371000000	-0.266833000000
Ag	-1.920672000000	-3.025053000000	1.275308000000
F	-5.196477000000	-2.481915000000	-4.490805000000
F	-5.737948000000	-3.997926000000	-2.997489000000
F	-4.215459000000	-4.452451000000	-4.510314000000
C	-0.231851000000	3.895880000000	-5.110912000000
F	0.483218000000	4.956846000000	-5.557680000000
F	-1.455295000000	4.370486000000	-4.698011000000
F	-0.457186000000	3.070322000000	-6.160778000000
C	3.302425000000	-0.288650000000	-4.177016000000
H	3.077509000000	-1.316569000000	-3.836715000000
H	2.351224000000	0.188147000000	-4.473396000000
C	3.931355000000	0.491573000000	-3.015868000000
C	4.283284000000	-0.352067000000	-5.364747000000
H	4.443428000000	0.668981000000	-5.767927000000
H	3.830952000000	-0.946232000000	-6.179347000000
C	6.253846000000	-0.155830000000	-3.784158000000
H	7.206629000000	-0.611899000000	-3.456195000000
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C	5.635227000000	-0.952637000000	-4.943947000000
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C	-11.751733000000	1.345118000000	-7.122012000000
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C	12.028739000000	1.505118000000	-2.378585000000
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C	0.893111000000	11.113528000000	1.310222000000
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