Supporting Information for Publication

Atomically Precise Noble Metal Cluster-Assembled Superstructures in Water: Luminescence Enhancement and Sensing

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Experimental Details

Instrumentation

The UV-vis spectra were measured using a PerkinElmer Lambda 25 UV-vis spectrophotometer. PL spectra were collected using a HORIBA JOBIN YVON Nano Log instrument. The bandpass was set at 3 nm during the measurements. NMR measurements were performed using a Bruker 500 MHz NMR spectrometer. Transmission Electron Microscopy of the samples was performed using a JEOL 3010 instrument with a UHR polepiece.

Computational Details

The interactions of β-CD and CB on the surface of a monolayer of LA protected $Ag_{29}(LA)_{12}^{3-}$ nanocluster was computationally studied by density functional theory (DFT) using GPAW (grid-based projector-augmented wave method) software package[1-2]. For this, $Ag_{29}(LA)_{12}^{3-}$ nanocluster was initially constructed from the crystal structure of $Ag_{29}(BDT)_{12}(TPP)_4^{3-}$ nanocluster by replacing the BDT ligands by LA. The atomic PAW set-ups for each atoms are Ag ($4d^{10}$ $5s^1$), S ($3s^2 3p^4$), O ($2s^2 2p^4$), C ($2s^2 2p^2$) and H ($1s^1$) which tells the valence electronic configuration and the inclusion of scalar-relativistic effects for Ag. First of all, the geometries of $Ag_{29}(LA)_{12}^{3-}$

nanocluster, cyclodextrin, and cucurbituril were separately optimized using the DZP basis set in LCAO mode along with the PBE (Perdew-Burke-Ernzerhof) exchange-correlation functional[3] with a grid spacing of 0.2 Å in LCAO mode. The convergence condition is that the forces acting on atoms were set to be 0.05 eV/Å, without imposing any symmetry constraints. Then the structures of the supramolecular complexes were obtained using molecular docking. The docked structures were re-optimized in DFT with the same level of theory.

Molecular docking studies have been carried out using AutoDock 4.2 and AutoDock Tools programs[4]. The DFT optimized structures of $[Ag_{29}(LA)_{12}]$[5] and β-CD were used for this study. We used $[Ag_{29}(LA)_{12}]$ as the 'ligand'. The 'receptor' molecule was CD and this was the fixed and completely rigid central molecule. We assigned partial charges from DFT for all atoms of $[Ag_{29}(LA)_{12}]^{3-}$. Receptor grids were generated using 126 × 126 × 126 grid points with a grid spacing of 0.375 Å and map types for all the ligand atoms were created using AutoGrid 4.6. The van der Waals radius σ (Å) and well depth ε (kcal/mol) for Ag of 2.63 Å and 4.560 kcal/mol, respectively, were taken from well-tested sources in literature[6-7] and these were added to the AutoDock parameter file which does not contain them by default. The grid parameter file (.gpf) was saved using MGL Tools-1.4.6.50. For docking, the docking parameter files (.dpf) were generated using MGLTools-1.4.6.50 and docking was performed using AutoDock4.2. The results of AutoDock generated an output file (.dlg), and the generated conformers were scored and ranked as per the interaction energy. Ten lowest energy conformers were obtained. The structure showing the lowest binding energy between the interacting molecules was used as an initial structure for DFT optimization. The free energies of binding were calculated subtracting the unbound energies from the sum of the intermolecular and internal energy terms in the adducts, which is a calculation that is performed within the AutoDock program. We obtained the structures of $[Ag_{29}(LA)_{12} \cap CB_n]$ complexes using similar process.

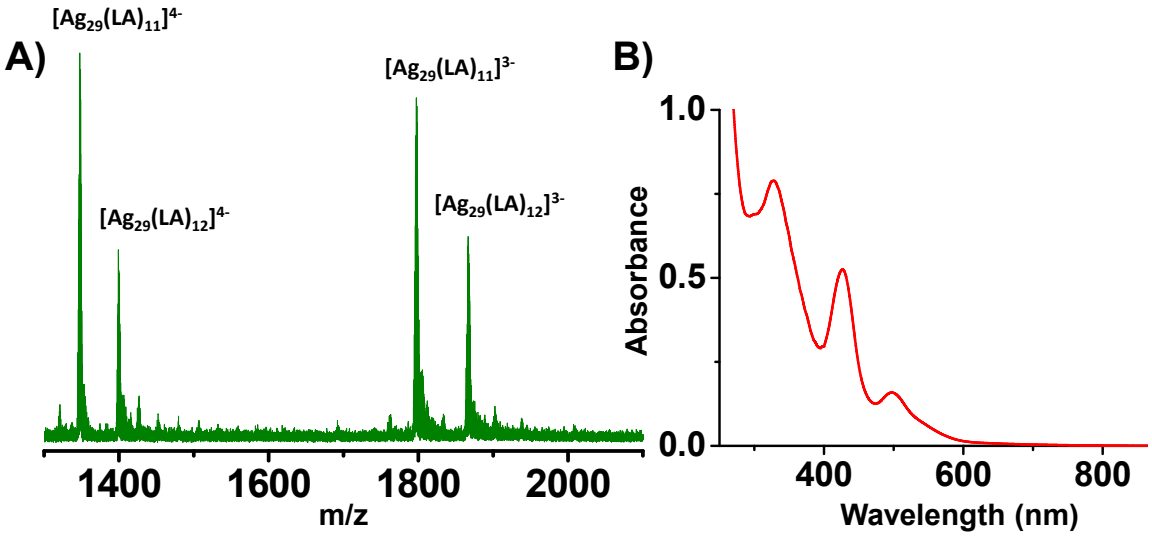


Figure S1. A) HRESI MS and B) UV-vis spectra of $[Ag_{29}(LA)_{12}]$. Different charge states of the cluster (3- and 4-) were observed in ESI MS. One loss of LA was noticed for both 3- and 4- charge states of the cluster.

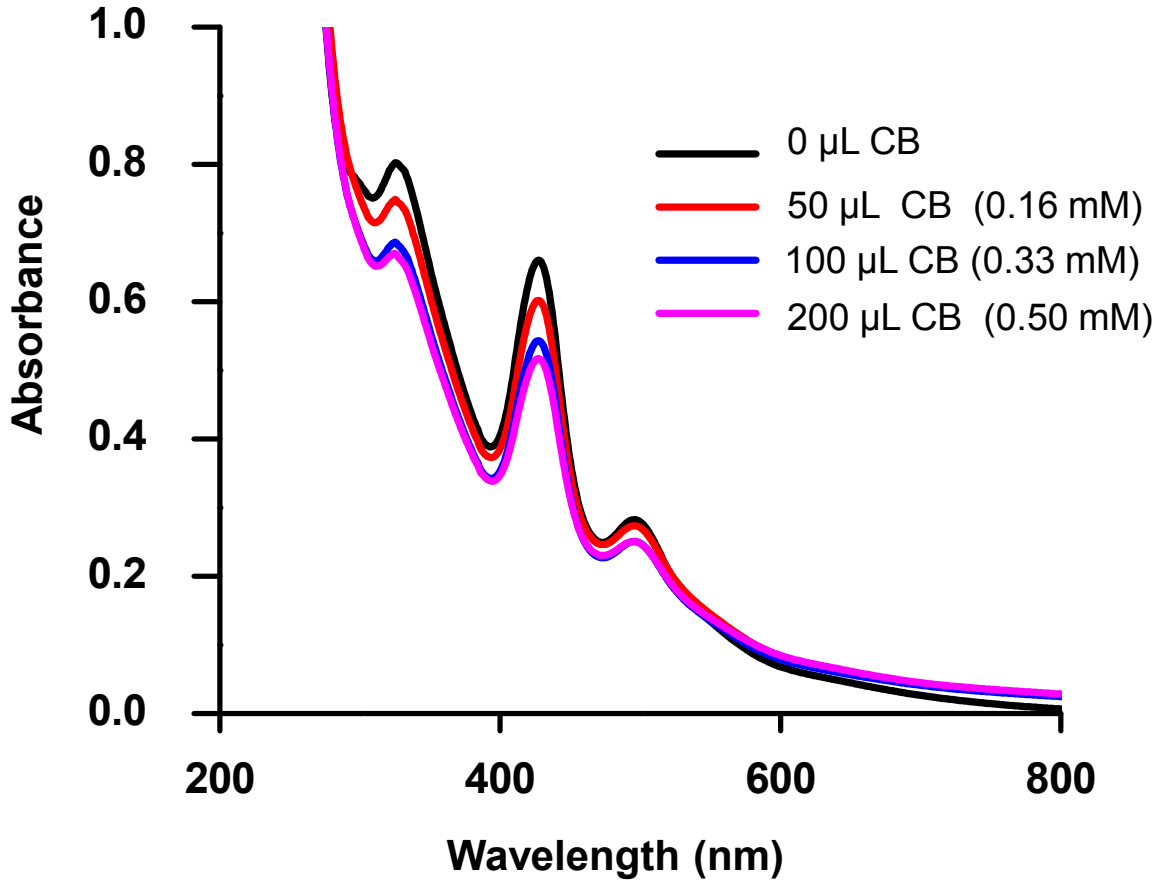


Figure S2. UV-vis spectra of $Ag_{29}(LA)_{12}$ and $[Ag_{29}(LA)_{12} \cap CB_n]$. With increasing the concentration of cucurbituril in the solution, absorbance of the peaks was decreasing and a crossover point was detected at ~550 nm.

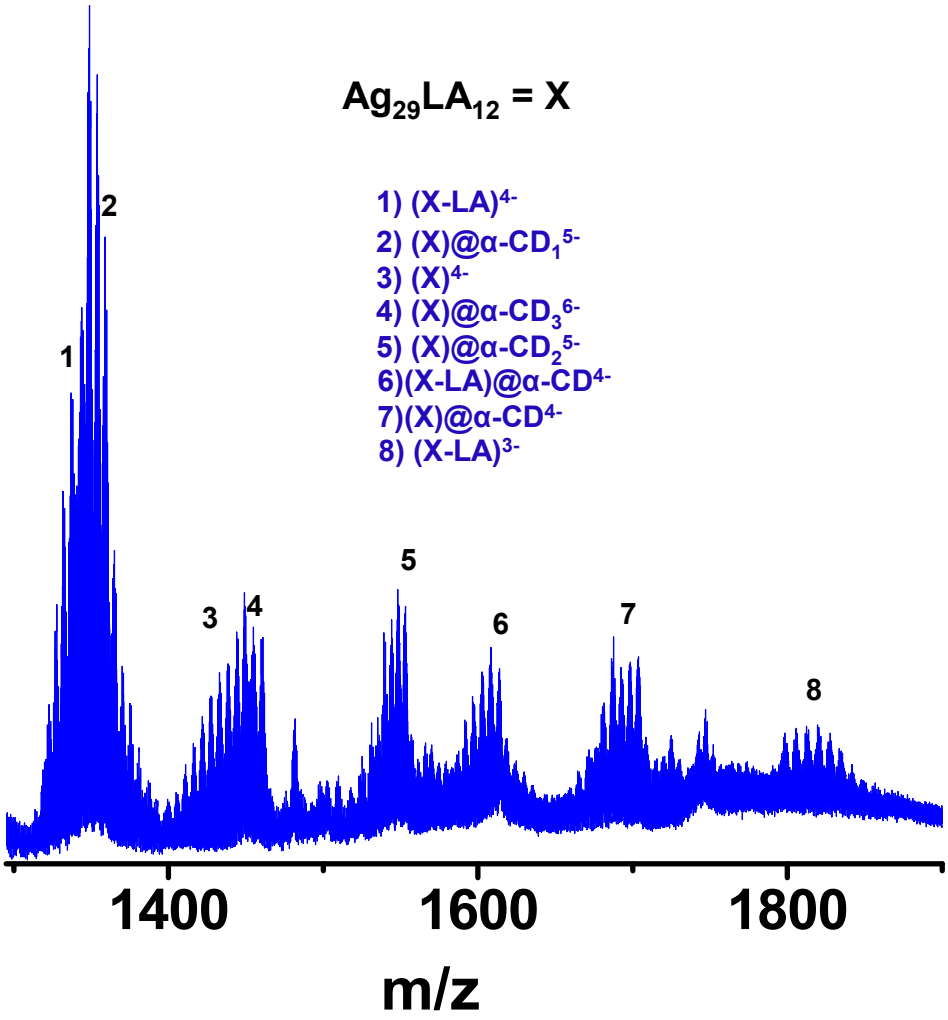


Figure S3. HRESI MS of $[Ag_{29}(LA)_{12}@\alpha\text{-}CD_n]$, where n = 1-3. Assignments of the peaks are provided in the inset of Figure S3 with numbering, where X = $Ag_{29}(LA)_{12}$. Branching of peaks was appearing because of Na adducts.

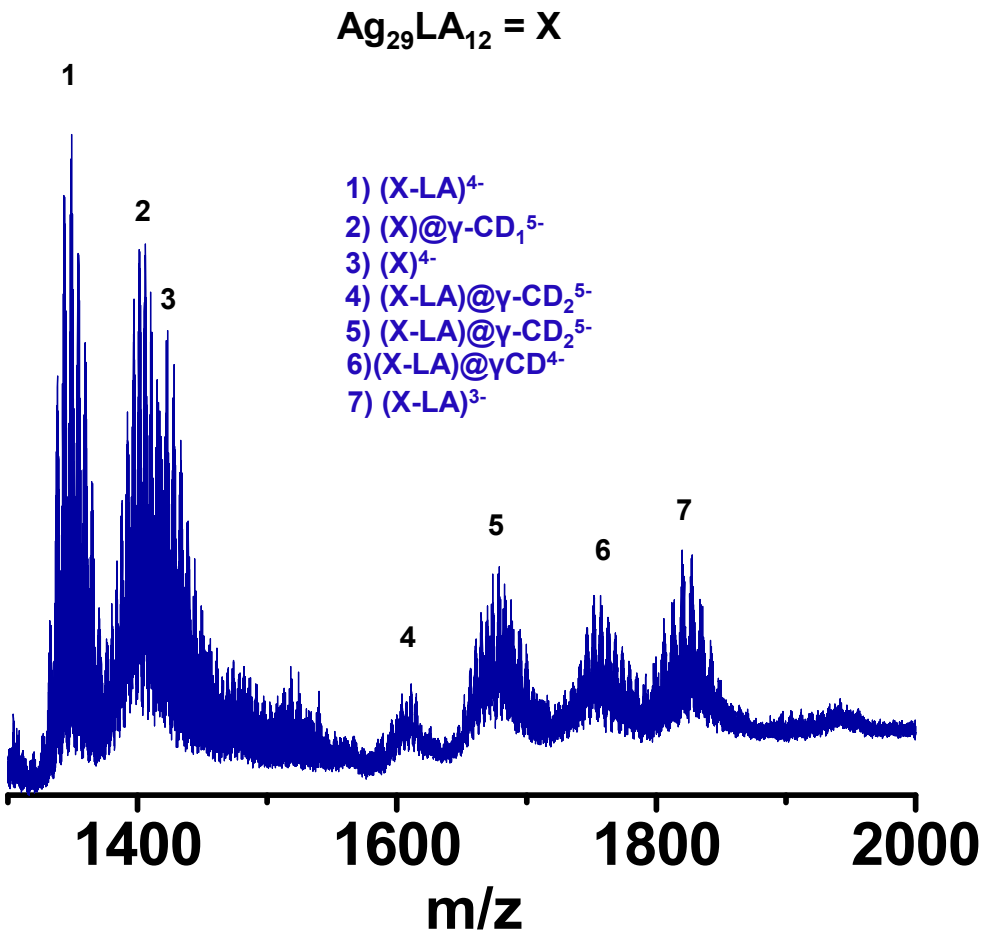


Figure S4. HRESI MS of $[Ag_{29}(LA)_{12}@\gamma\text{-}CD_n]$, where n = 1-3. Assignments of the peaks are provided in the inset of Figure S4 with numbering, where X = $Ag_{29}(LA)_{12}$. Branching of peaks was appearing because of Na adducts.

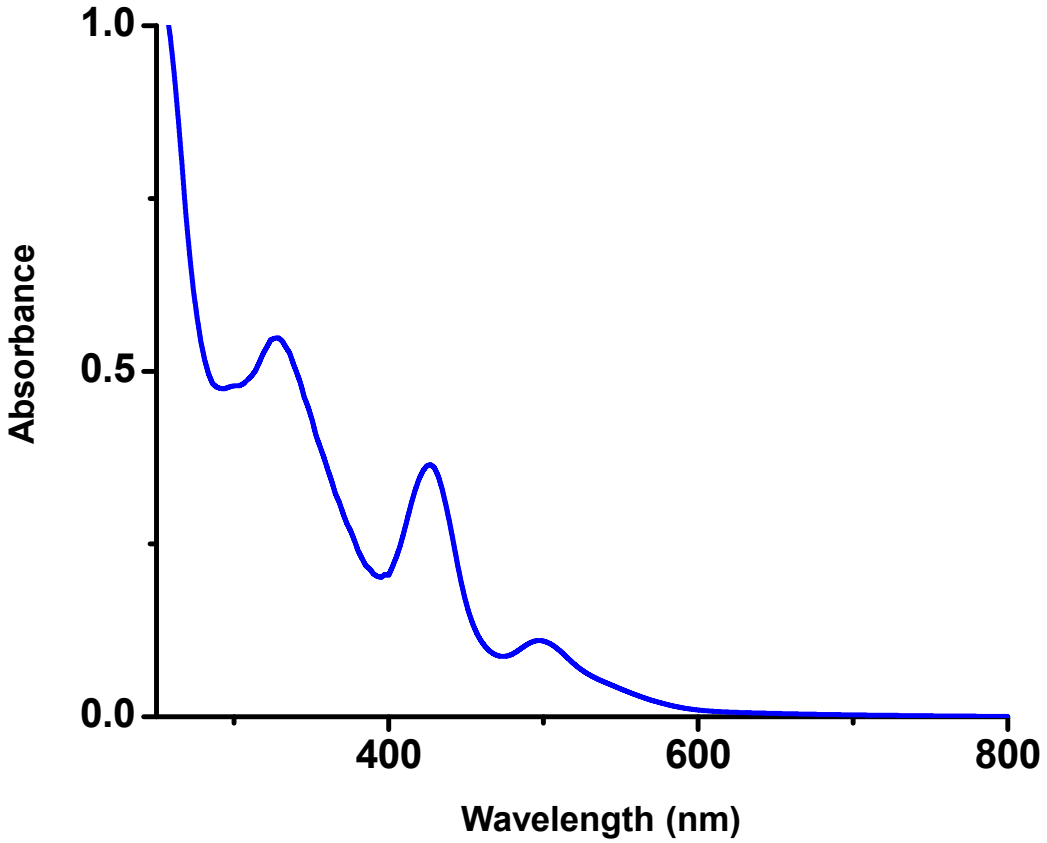


Figure S5. UV-vis spectrum of $[Ag_{29}(LA)_{12}@\beta\text{-}CD_n]$ complexes. UV-vis features are similar to that of the parent cluster.

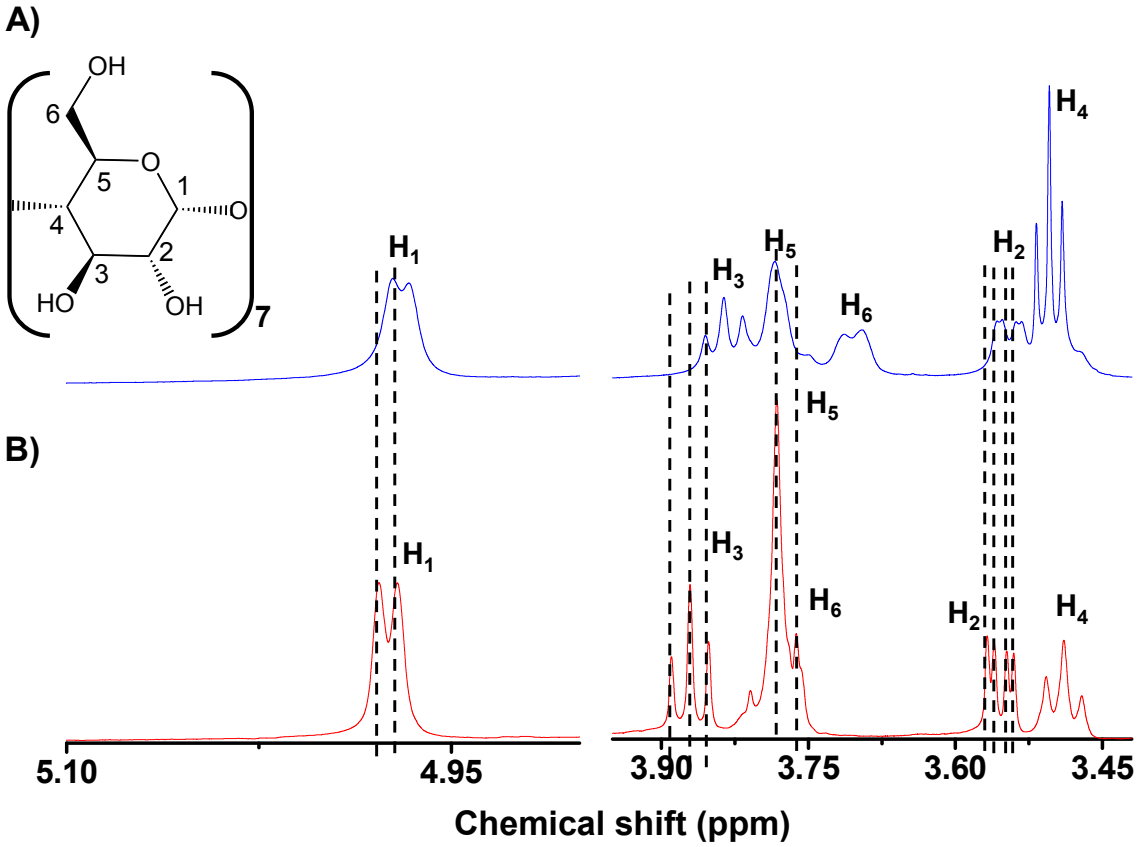


Figure S6. ^{1}H NMR of $[Ag_{29}(LA)_{12}@\beta\text{-}CD_n]$ A) and $Ag_{29}(LA)_{12}$ B). Due to the strong interactions, almost all the peaks H_1 to H_6 got shifted in the upfield region. H_4 of the CD peak is overlapped with the lipoic acid 'e' peak. As a result, the overall peak intensity increased.

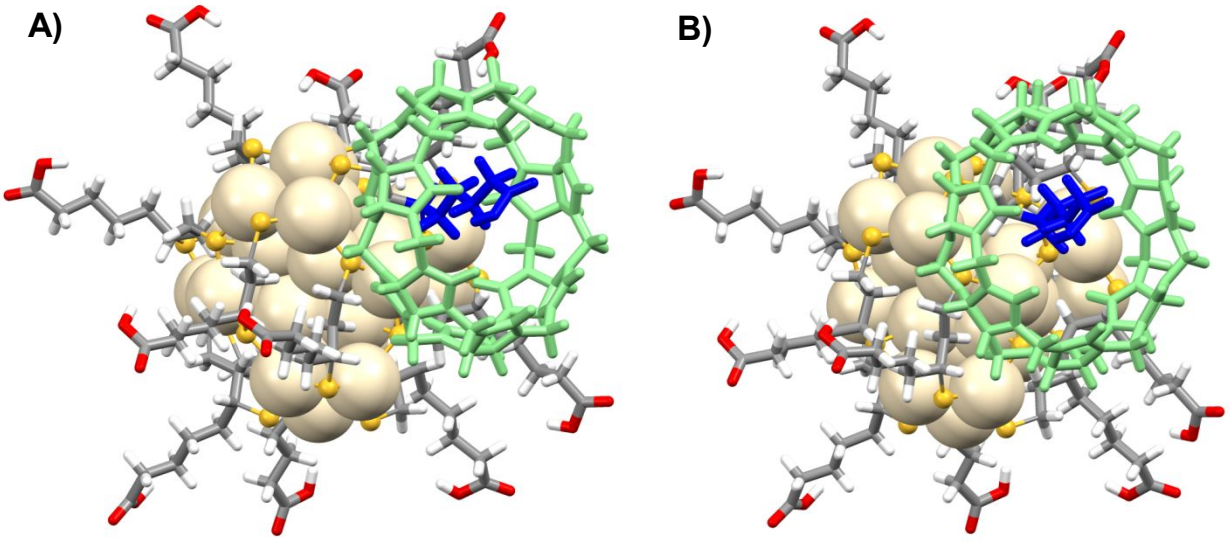


Figure S7. DFT optimised structure of $[Ag_{29}(LA)_{12} \cap CB_1]$ with different orientations, A) and B). Encapsulated LA and CB are shown in blue and light green, respectively.

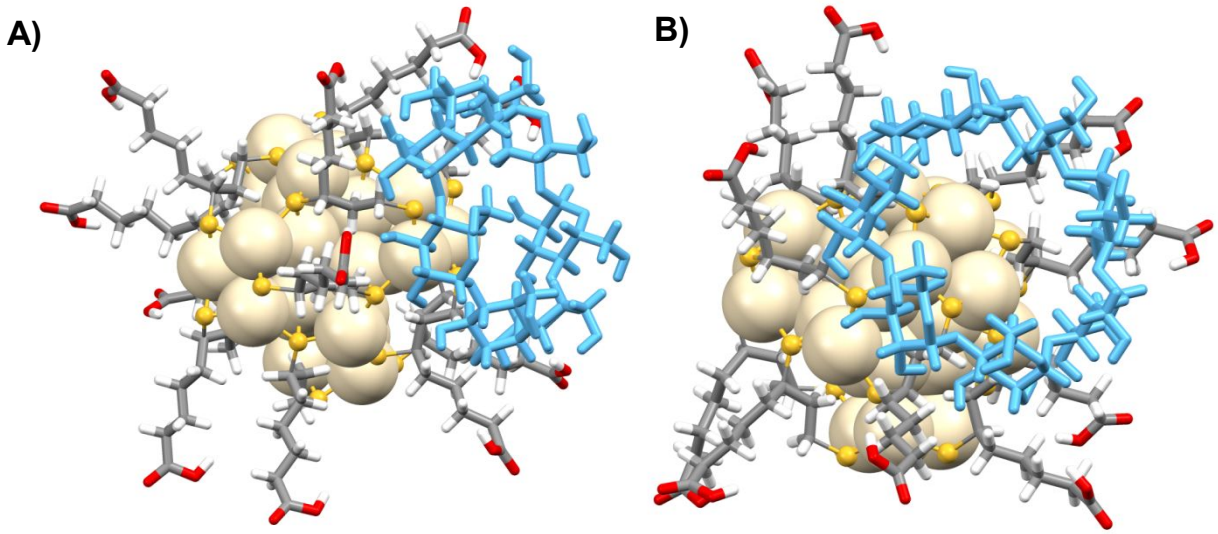
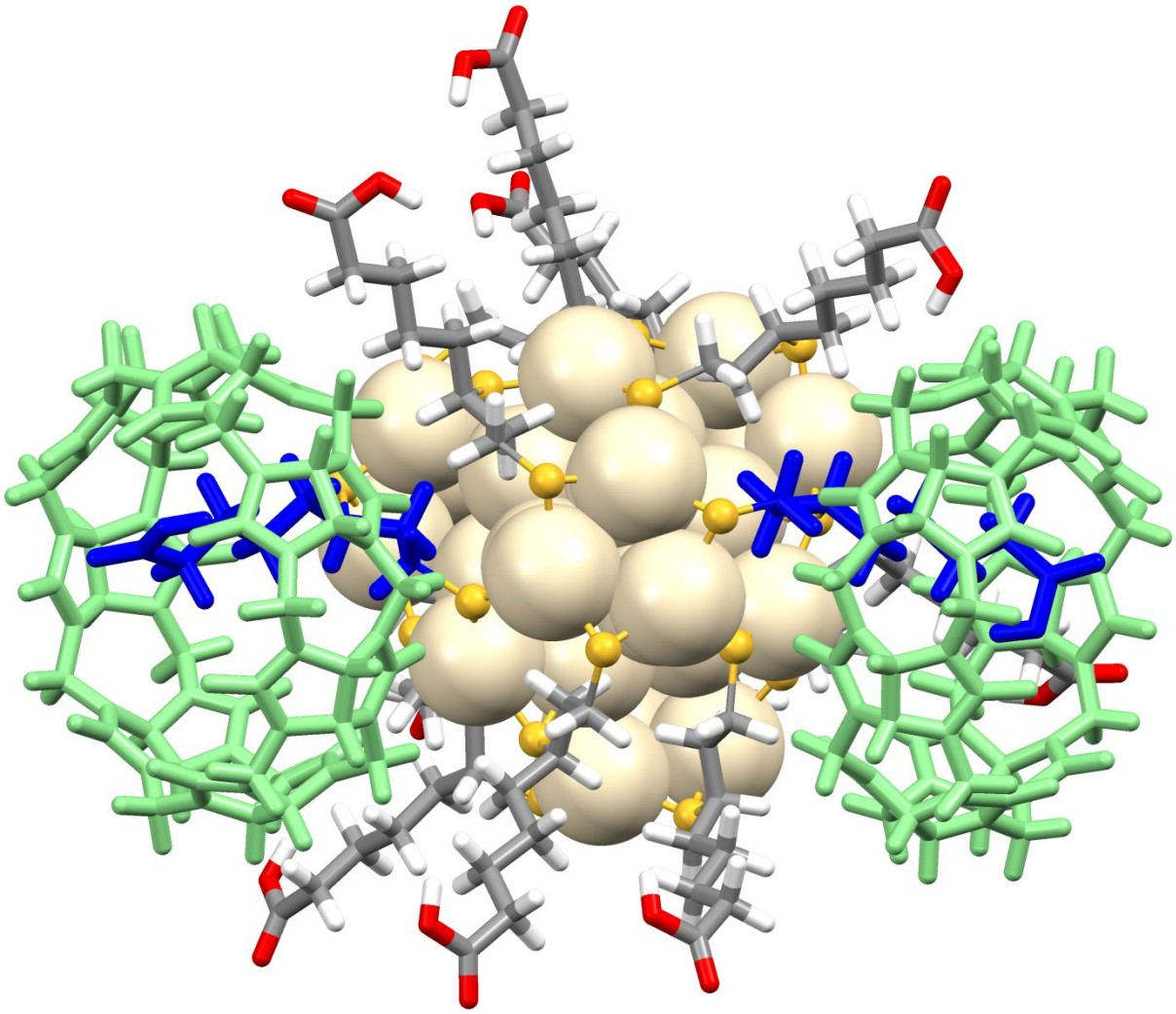
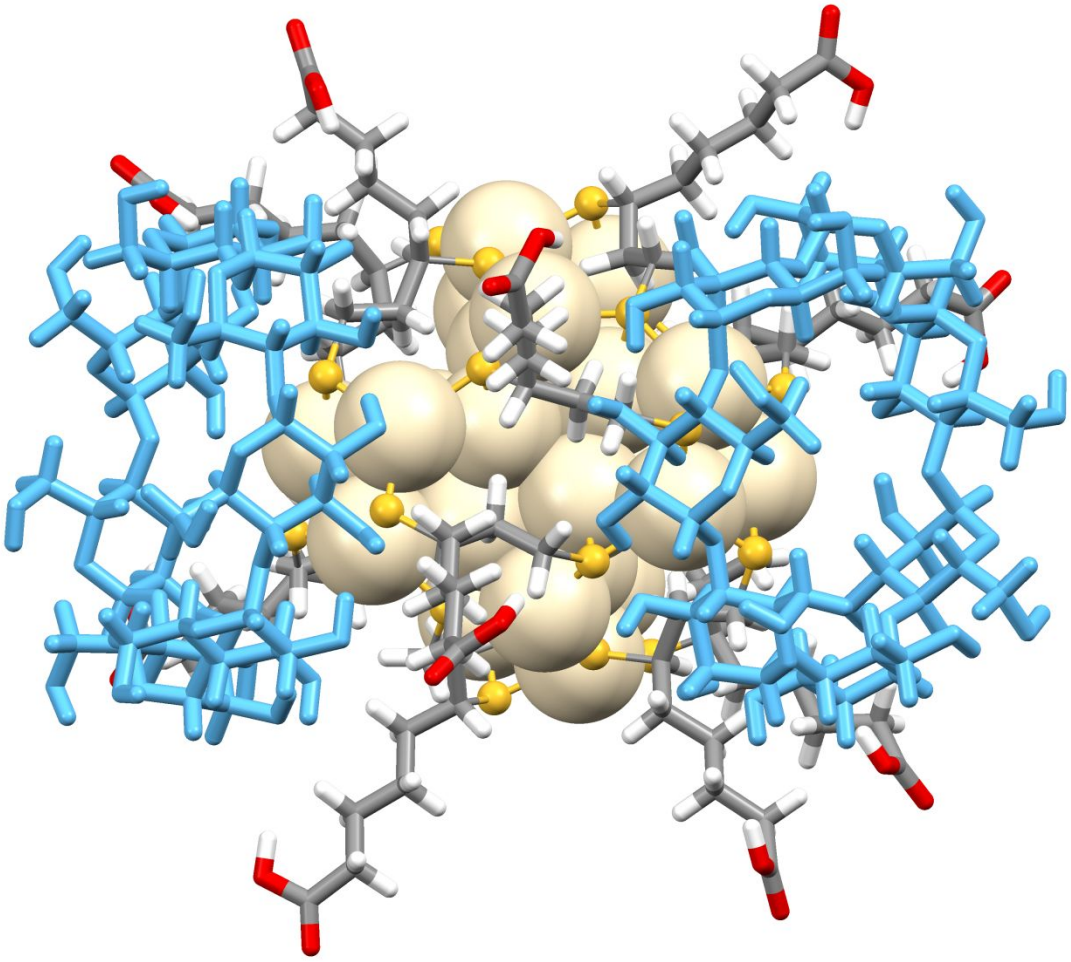


Figure S8. DFT optimised structure of $[Ag_{29}(LA)_{12}@\beta\text{-}CD_1]$ with different orientations, A) and B). β-CD is shown in light blue.



Binding energy = - 10.05 kcal/mol

Figure S9. DFT optimised structure of $[Ag_{29}(LA)_{12} \cap CB_2]$. Encapsulated LA and CB are shown in blue and light green, respectively.



Binding energy = - 64.93 kcal/mol

Figure S10. DFT optimised structure of $[Ag_{29}(LA)_{12}@\beta\text{-}CD_2]$. β-CDs are shown in light blue.

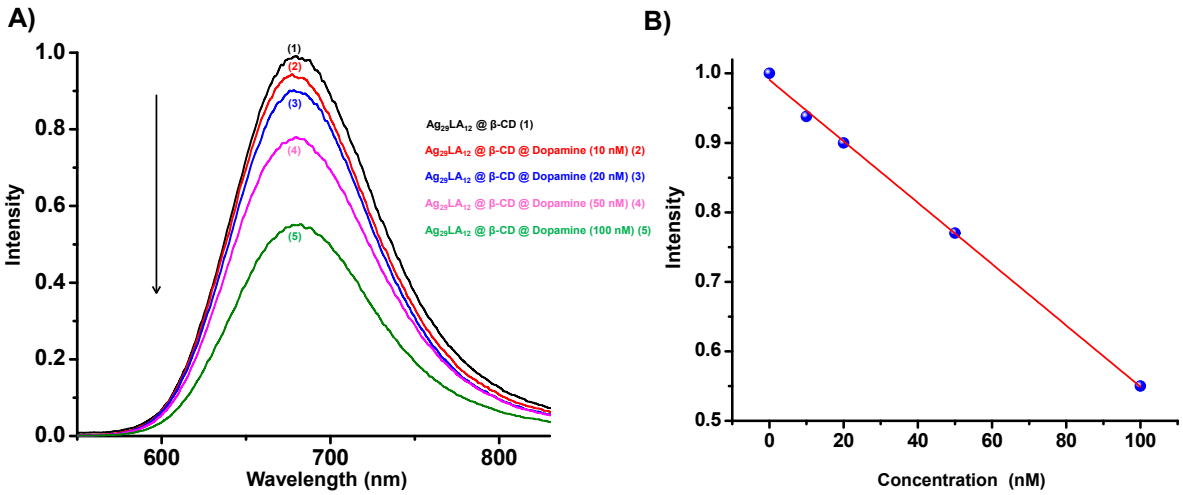


Figure S11. A) Dopamine concentration dependent quenching of a solution of [$Ag_{29}(LA)_{12}$@β-CD_n] complexes. With increase in the concentration of dopamine, PL intensity was decreased. B) Plot between PL quenching efficiency and dopamine concentration shows a linear relationship.

Table S1. Different methods for dopamine detection available in the literature.

Method used and references	**Property used for detection**	**Detection limit**
Periodic cylindrical gold nanoelectrode arrays[8]	Electrochemical	5.83 μM
Colorimetric detection of dopamine using functionalized gold nanoparticles[9]	Plasmon absorption	0.5 nM
Colorimetric sensing of dopamine using hexagonal silver nanoparticles[10]	Plasmon absorption	0.031 μM
Rotating droplet system[11]	Electrochemical	100 nM
Turn-on fluorescent sensing based on in situ formation of visible light emitting polydopamine nanoparticles[12]	Florescence of PDA nanoparticles	40 nM
Colorimetric Detection using cyclodextrin-modified Au nanoparticles[13]	Plasmon absorption	3 nM
Protein conjugated fluorescent gold nanoclusters[14]	Fluorescence of gold nanoclusters	10 nM
This work	Fluorescence of supramolecular complexes of atomically precise cluster	10 nM

Coordinates of the lowest energy geometry of $Ag_{29}LA_{12}\cap CB_1$

O	21.222000	8.150000	5.720000
O	18.093000	12.492000	8.653000
O	24.161000	8.820000	7.958000
O	20.776000	13.095000	10.821000
O	24.856000	7.226000	11.180000
O	21.512000	11.435000	14.072000
O	22.973000	4.478000	12.958000
O	19.654000	8.750000	15.863000
O	19.886000	2.760000	11.993000
O	16.523000	6.986000	14.978000
O	17.846000	3.359000	8.901000
O	14.536000	7.549000	11.938000
O	18.471000	5.734000	6.239000
O	15.274000	9.991000	9.217000
N	19.297000	9.401000	5.574000
N	21.164000	10.414000	6.184000
N	18.050000	11.112000	6.807000
N	19.923000	12.192000	7.286000
N	23.036000	10.820000	7.680000
N	24.253000	10.517000	9.525000
N	21.757000	12.608000	8.799000
N	22.909000	12.212000	10.663000
N	24.770000	9.479000	11.639000
N	24.313000	8.039000	13.249000
N	23.386000	11.155000	12.760000
N	23.010000	9.739000	14.429000
N	23.113000	6.271000	14.423000
N	21.504000	4.793000	14.741000
N	21.796000	7.966000	15.558000

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N	19.450000	3.670000	14.050000
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N	18.133000	5.351000	15.221000
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N	15.912000	4.627000	8.764000
N	15.075000	5.286000	11.895000
N	14.633000	6.323000	9.975000
N	16.355000	6.225000	6.982000
N	17.471000	7.794000	5.911000
N	15.098000	7.920000	8.203000
N	16.275000	9.490000	7.183000
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C	18.908000	10.798000	5.694000
C	20.231000	11.500000	6.061000
C	18.639000	11.973000	7.685000
C	22.592000	10.584000	6.342000
C	20.791000	13.176000	7.915000
C	23.853000	9.938000	8.367000
C	23.058000	12.157000	8.306000
C	23.844000	11.911000	9.603000
C	21.719000	12.670000	10.153000
C	25.272000	9.964000	10.364000
C	23.277000	12.400000	12.030000
C	24.657000	8.175000	11.927000
C	24.586000	10.333000	12.792000
C	24.302000	9.314000	13.917000
C	22.538000	10.828000	13.785000
C	24.399000	6.778000	13.957000
C	22.449000	9.247000	15.670000

C	22.558000	5.110000	13.928000
C	22.476000	6.711000	15.657000
C	21.359000	5.671000	15.843000
C	20.416000	7.836000	15.773000
C	20.779000	3.528000	14.586000
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C	16.818000	3.830000	9.403000
C	15.125000	4.204000	10.927000
C	14.787000	4.934000	9.608000
C	14.724000	6.501000	11.358000
C	15.991000	4.869000	7.335000
C	14.125000	7.357000	9.133000
C	17.555000	6.526000	6.363000
C	15.419000	7.337000	6.920000
C	16.213000	8.430000	6.200000
C	15.532000	9.218000	8.300000
C	18.462000	8.358000	5.017000
C	16.621000	10.854000	6.816000
H	18.396000	11.075000	4.796000
H	20.644000	12.214000	5.379000
H	22.894000	11.417000	5.742000
H	23.035000	9.657000	6.043000
H	20.182000	13.856000	8.473000
H	21.333000	13.662000	7.130000
H	23.426000	12.867000	7.596000

H	24.722000	12.501000	9.767000
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H	24.984000	9.249000	14.739000
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H	24.783000	6.059000	13.264000
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H	23.268000	9.116000	16.346000
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H	20.705000	3.064000	15.547000
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H	16.192000	11.495000	7.557000
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Ag	15.730000	17.600000	13.699000
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Ag	18.207000	16.008000	17.594000
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H	9.214000	13.934000	19.822000
C	7.514000	13.933000	18.512000
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C	5.157000	13.279000	19.255000
C	4.228000	12.523000	20.194000
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C	14.144000	17.787000	10.307000
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C	11.596000	19.645000	4.626000
O	10.258000	19.587000	4.925000
O	11.956000	20.265000	3.651000
H	13.140000	17.241000	7.728000
H	14.327000	18.540000	7.594000

H	11.290000	18.866000	7.371000
H	12.443000	20.196000	7.274000
H	12.374000	17.803000	5.333000
H	13.543000	19.121000	5.256000
H	10.135000	19.073000	5.745000
C	17.015000	14.476000	10.299000
H	16.111000	14.556000	9.682000
H	17.762000	13.901000	9.732000
C	17.568000	15.841000	10.701000
H	16.750000	16.478000	11.073000
H	18.241000	15.687000	11.557000
C	18.377000	16.620000	9.653000
H	19.271000	16.029000	9.391000
C	17.648000	17.006000	8.355000
H	16.661000	17.421000	8.618000
H	18.201000	17.838000	7.892000
C	17.489000	15.896000	7.308000
C	16.672000	16.359000	6.101000
C	16.529000	15.264000	5.028000
C	15.619000	15.656000	3.882000
O	14.289000	15.788000	4.205000
O	15.973000	15.865000	2.744000
H	16.998000	15.012000	7.741000
H	18.484000	15.561000	6.971000
H	15.674000	16.675000	6.449000
H	17.131000	17.253000	5.649000
H	16.137000	14.344000	5.495000
H	17.509000	15.024000	4.596000
H	14.164000	15.572000	5.147000
C	15.297000	22.575000	18.768000
H	15.842000	23.089000	19.575000

H	14.975000	23.339000	18.043000
C	16.179000	21.520000	18.115000
H	16.409000	20.760000	18.876000
H	15.600000	21.004000	17.333000
C	17.512000	22.001000	17.531000
H	17.342000	22.638000	16.648000
C	18.410000	22.754000	18.538000
H	18.176000	22.396000	19.554000
H	19.456000	22.469000	18.348000
C	18.334000	24.285000	18.483000
C	19.344000	24.924000	19.445000
C	19.464000	26.446000	19.308000
C	20.513000	27.141000	20.171000
O	21.009000	26.434000	21.232000
O	20.900000	28.272000	19.978000
H	17.319000	24.645000	18.718000
H	18.555000	24.622000	17.457000
H	19.048000	24.655000	20.477000
H	20.330000	24.462000	19.266000
H	18.503000	26.931000	19.548000
H	19.683000	26.729000	18.267000
H	20.614000	25.541000	21.233000
C	14.048000	21.851000	14.747000
H	14.088000	22.601000	15.550000
H	13.509000	22.298000	13.899000
C	15.441000	21.404000	14.307000
H	16.096000	21.265000	15.178000
H	15.358000	20.418000	13.830000
C	16.105000	22.343000	13.298000
H	15.465000	22.352000	12.400000
C	16.260000	23.803000	13.794000

H	15.868000	23.898000	14.821000
H	17.328000	24.064000	13.845000
C	15.532000	24.794000	12.884000
C	15.671000	26.257000	13.308000
C	14.865000	27.196000	12.402000
C	15.015000	28.687000	12.645000
O	15.220000	29.074000	13.943000
O	14.941000	29.529000	11.779000
H	14.461000	24.530000	12.846000
H	15.913000	24.681000	11.855000
H	15.326000	26.342000	14.357000
H	16.734000	26.545000	13.299000
H	13.789000	26.968000	12.498000
H	15.116000	27.031000	11.345000
H	15.293000	28.276000	14.502000
C	13.285000	16.741000	22.521000
H	12.477000	16.259000	23.091000
H	14.045000	17.082000	23.242000
C	13.875000	15.771000	21.504000
H	14.657000	16.291000	20.929000
H	13.081000	15.526000	20.782000
C	14.437000	14.448000	22.035000
H	15.355000	14.627000	22.617000
C	13.447000	13.632000	22.896000
H	12.422000	13.843000	22.546000
H	13.620000	12.561000	22.714000
C	13.555000	13.875000	24.407000
C	12.459000	13.147000	25.193000
C	12.588000	13.336000	26.711000
C	11.531000	12.674000	27.580000
O	10.236000	12.782000	27.147000

O	11.764000	12.106000	28.623000
H	13.507000	14.951000	24.637000
H	14.542000	13.528000	24.755000
H	11.482000	13.525000	24.834000
H	12.478000	12.073000	24.948000
H	12.554000	14.415000	26.946000
H	13.558000	12.966000	27.069000
H	10.230000	13.228000	26.279000
C	17.331000	17.853000	21.891000
H	16.526000	17.804000	22.639000
H	18.154000	18.444000	22.318000
C	17.815000	16.468000	21.473000
H	18.362000	16.569000	20.526000
H	16.952000	15.819000	21.253000
C	18.743000	15.741000	22.454000
H	19.667000	16.334000	22.560000
C	18.136000	15.531000	23.858000
H	17.045000	15.404000	23.757000
H	18.514000	14.590000	24.285000
C	18.440000	16.687000	24.823000
C	17.559000	16.711000	26.074000
C	17.849000	17.943000	26.949000
C	16.979000	18.086000	28.183000
O	15.627000	18.082000	27.966000
O	17.395000	18.211000	29.313000
H	18.320000	17.650000	24.304000
H	19.500000	16.638000	25.123000
H	16.502000	16.707000	25.751000
H	17.698000	15.792000	26.668000
H	17.718000	18.856000	26.342000
H	18.890000	17.933000	27.295000

H	15.453000	17.945000	27.016000
C	15.267000	9.724000	13.443000
H	15.765000	9.336000	12.543000
H	15.040000	8.864000	14.093000
C	16.152000	10.740000	14.156000
H	15.636000	11.092000	15.061000
H	16.244000	11.619000	13.500000
C	17.573000	10.292000	14.524000
H	17.546000	9.530000	15.320000
C	18.412000	9.769000	13.336000
H	18.096000	10.308000	12.427000
H	19.461000	10.056000	13.505000
C	18.389000	8.256000	13.084000
C	19.295000	7.891000	11.898000
C	19.442000	6.385000	11.658000
C	20.305000	5.950000	10.480000
O	20.371000	6.810000	9.419000
O	20.888000	4.890000	10.425000
H	17.366000	7.895000	12.892000
H	18.743000	7.728000	13.986000
H	18.873000	8.386000	11.002000
H	20.290000	8.337000	12.059000
H	18.450000	5.931000	11.491000
H	19.859000	5.884000	12.543000
H	19.882000	7.627000	9.640000
C	14.250000	10.269000	17.604000
H	14.341000	9.591000	16.743000
H	13.708000	9.735000	18.398000
C	15.607000	10.754000	18.106000
H	15.444000	11.678000	18.678000
H	16.251000	11.039000	17.258000

C	16.375000	9.797000	19.020000
H	15.767000	9.623000	19.924000
C	16.738000	8.434000	18.403000
H	17.023000	8.575000	17.346000
H	17.641000	8.060000	18.910000
C	15.648000	7.364000	18.522000
C	16.131000	5.985000	18.071000
C	15.061000	4.899000	18.259000
C	15.496000	3.493000	17.900000
O	16.070000	3.338000	16.664000
O	15.363000	2.523000	18.613000
H	14.750000	7.643000	17.948000
H	15.328000	7.297000	19.576000
H	16.446000	6.052000	17.012000
H	17.036000	5.711000	18.639000
H	14.172000	5.143000	17.650000
H	14.731000	4.866000	19.304000
H	16.148000	4.213000	16.239000
C	22.118000	18.733000	15.416000
H	22.665000	19.557000	15.898000
H	22.862000	17.992000	15.081000
C	21.111000	18.118000	16.381000
H	20.554000	17.327000	15.854000
H	20.371000	18.893000	16.630000
C	21.650000	17.560000	17.705000
H	22.261000	16.660000	17.527000
C	22.456000	18.568000	18.552000
H	22.041000	19.575000	18.378000
H	22.279000	18.344000	19.616000
C	23.972000	18.576000	18.328000
C	24.654000	19.654000	19.180000

C	26.181000	19.651000	19.048000
C	26.947000	20.676000	19.868000
O	26.360000	21.903000	20.020000
O	28.041000	20.480000	20.348000
H	24.221000	18.739000	17.269000
H	24.382000	17.587000	18.597000
H	24.239000	20.634000	18.876000
H	24.372000	19.515000	20.237000
H	26.462000	19.823000	17.994000
H	26.593000	18.671000	19.323000
H	25.472000	21.881000	19.613000
C	21.527000	14.703000	14.411000
H	22.268000	15.515000	14.446000
H	21.967000	13.869000	13.845000
C	21.112000	14.240000	15.805000
H	20.138000	13.738000	15.726000
H	20.951000	15.104000	16.468000
C	22.073000	13.254000	16.477000
H	22.081000	12.335000	15.868000
C	23.531000	13.753000	16.615000
H	23.555000	14.853000	16.540000
H	23.903000	13.504000	17.621000
C	24.473000	13.134000	15.576000
C	25.923000	13.609000	15.693000
C	26.846000	12.864000	14.722000
C	28.324000	13.201000	14.777000
O	28.641000	14.512000	15.015000
O	29.212000	12.398000	14.599000
H	24.109000	13.338000	14.556000
H	24.452000	12.037000	15.694000
H	25.947000	14.699000	15.502000

H	26.277000	13.465000	16.727000
H	26.523000	13.053000	13.684000
H	26.765000	11.778000	14.874000
H	27.817000	15.017000	15.159000

Coordinates of the lowest energy geometry of $Ag_{29}LA_{12}\cap CD_1$

H	10.830000	17.282000	7.240000
O	13.263000	15.494000	6.489000
C	11.912000	15.131000	6.247000
O	11.021000	16.661000	7.989000
C	11.798000	13.667000	5.769000
O	10.452000	13.331000	5.426000
C	10.979000	15.322000	7.460000
C	9.546000	14.885000	7.097000
H	13.664000	14.777000	7.065000
O	12.677000	10.604000	3.938000
O	8.725000	17.559000	9.481000
H	15.647000	13.522000	7.028000
C	9.524000	13.448000	6.550000
C	8.177000	13.004000	5.980000
H	13.505000	10.067000	3.966000
C	7.564000	15.783000	8.249000
H	8.978000	11.669000	4.826000
C	7.601000	16.692000	9.494000
H	9.505000	17.039000	9.127000
O	12.291000	12.841000	6.835000
O	14.928000	13.467000	7.707000
O	8.232000	11.662000	5.477000
O	8.750000	14.976000	8.297000

O	6.383000	15.001000	8.177000
C	13.385000	11.958000	6.526000
C	12.001000	10.282000	5.163000
C	14.427000	12.112000	7.648000
C	12.880000	10.507000	6.396000
C	15.556000	11.075000	7.455000
O	14.007000	9.596000	6.238000
O	3.743000	14.262000	9.057000
C	7.493000	15.802000	10.751000
C	6.210000	14.114000	9.314000
H	6.810000	17.302000	11.827000
O	7.459000	16.568000	11.973000
C	4.877000	13.388000	9.085000
O	16.562000	11.117000	8.452000
H	3.553000	14.514000	9.998000
C	6.252000	14.903000	10.637000
C	14.930000	9.671000	7.327000
H	16.255000	10.561000	9.230000
O	14.294000	9.385000	8.577000
O	6.260000	14.002000	11.764000
H	6.659000	15.699000	13.425000
C	5.071000	13.935000	12.571000
O	13.812000	6.043000	7.210000
O	6.001000	15.554000	14.168000
C	14.583000	8.121000	9.213000
C	12.823000	6.810000	7.906000
O	16.327000	9.231000	10.551000
H	17.040000	8.676000	10.132000
O	4.417000	12.687000	12.446000
C	5.483000	14.242000	14.024000
C	13.309000	7.267000	9.280000

H	14.072000	5.341000	7.856000
C	15.141000	8.412000	10.615000
C	5.243000	11.564000	12.870000
C	6.433000	13.119000	14.501000
O	13.587000	6.032000	10.018000
C	4.387000	10.303000	12.686000
C	15.375000	7.085000	11.366000
C	5.747000	11.763000	14.310000
O	6.870000	13.303000	15.864000
O	3.208000	10.264000	13.492000
C	14.068000	6.260000	11.347000
O	15.869000	7.240000	12.689000
O	13.098000	6.977000	12.124000
O	6.721000	10.730000	14.650000
H	6.066000	13.525000	16.394000
H	15.105000	7.532000	13.269000
H	3.517000	10.145000	14.440000
C	10.953000	4.805000	11.850000
H	7.450000	11.758000	16.700000
C	12.501000	6.287000	13.238000
C	11.043000	5.925000	12.888000
C	6.350000	9.768000	15.639000
C	7.414000	7.949000	14.467000
C	12.605000	7.200000	14.474000
O	13.979000	7.495000	14.805000
O	6.202000	8.452000	15.087000
O	7.508000	11.043000	17.402000
O	9.796000	7.559000	14.838000
C	8.755000	9.275000	16.191000
C	7.047000	6.557000	13.947000
O	11.553000	3.594000	12.328000

C	7.410000	9.786000	16.756000
C	8.561000	7.918000	15.494000
H	14.361000	6.674000	15.207000
O	10.342000	5.400000	14.054000
O	9.772000	9.175000	17.215000
C	10.373000	6.294000	15.171000
H	11.191000	8.080000	16.750000
C	11.819000	6.567000	15.646000
H	11.132000	3.458000	13.213000
O	6.698000	5.654000	15.004000
O	11.843000	7.321000	16.845000
H	9.371000	8.654000	17.954000
H	5.988000	6.128000	15.505000
H	11.589000	15.804000	5.480000
H	12.373000	13.516000	4.879000
H	11.335000	14.693000	8.249000
H	9.154000	15.519000	6.330000
H	9.774000	12.841000	7.395000
H	7.904000	13.663000	5.182000
H	7.454000	13.036000	6.768000
H	7.544000	16.374000	7.358000
H	6.764000	17.358000	9.497000
H	13.834000	12.207000	5.587000
H	11.709000	9.253000	5.133000
H	11.154000	10.930000	5.246000
H	13.962000	11.919000	8.592000
H	12.315000	10.325000	7.286000
H	16.072000	11.328000	6.553000
H	8.374000	15.197000	10.799000
H	7.003000	13.400000	9.395000
H	4.930000	12.873000	8.149000

H	4.738000	12.722000	9.911000
H	5.376000	15.518000	10.641000
H	15.686000	8.944000	7.112000
H	4.355000	14.657000	12.238000
H	15.308000	7.568000	8.653000
H	11.947000	6.209000	8.033000
H	12.615000	7.683000	7.324000
H	4.626000	14.242000	14.665000
H	12.569000	7.885000	9.744000
H	14.422000	8.979000	11.168000
H	6.133000	11.476000	12.283000
H	7.320000	13.156000	13.904000
H	4.988000	9.452000	12.932000
H	4.059000	10.304000	11.667000
H	16.153000	6.563000	10.849000
H	4.886000	11.710000	14.943000
H	14.252000	5.291000	11.762000
H	9.923000	4.618000	11.629000
H	11.481000	5.117000	10.974000
H	13.008000	5.370000	13.455000
H	10.613000	6.833000	12.520000
H	5.393000	10.031000	16.038000
H	7.764000	8.567000	13.667000
H	12.159000	8.147000	14.255000
H	9.094000	9.993000	15.474000
H	7.885000	6.157000	13.416000
H	6.193000	6.661000	13.311000
H	7.103000	9.118000	17.534000
H	8.298000	7.192000	16.235000
H	9.813000	5.815000	15.947000
H	12.309000	5.652000	15.907000

Ag	15.738000	16.112000	16.160000
Ag	13.280000	15.986000	14.712000
Ag	15.730000	17.600000	13.699000
Ag	14.208000	18.524000	16.286000
Ag	18.207000	16.008000	17.594000
Ag	11.460000	14.296000	12.816000
Ag	12.989000	18.739000	13.521000
Ag	17.396000	19.398000	11.783000
Ag	12.483000	20.500000	17.993000
Ag	19.090000	20.407000	14.297000
Ag	18.491000	18.797000	18.716000
Ag	14.295000	13.621000	16.081000
Ag	13.320000	16.183000	17.690000
Ag	15.882000	14.662000	18.604000
Ag	17.191000	18.587000	16.000000
Ag	12.402000	11.709000	14.515000
Ag	13.122000	13.398000	18.890000
Ag	11.505000	17.805000	19.524000
Ag	17.588000	12.888000	20.516000
Ag	14.120000	19.606000	20.490000
Ag	15.609000	14.660000	13.707000
Ag	17.248000	13.683000	16.228000
Ag	18.133000	16.271000	14.600000
Ag	15.679000	17.630000	18.568000
Ag	14.003000	12.682000	11.887000
Ag	18.395000	13.500000	13.467000
Ag	19.123000	11.799000	17.884000
Ag	20.031000	17.817000	12.630000
Ag	20.198000	14.401000	19.411000
S	16.562000	13.376000	11.718000
S	14.746000	18.878000	11.703000

S	12.924000	20.510000	15.347000
S	20.246000	16.981000	18.788000
S	12.349000	13.929000	10.521000
S	19.055000	18.186000	10.388000
S	17.726000	21.705000	12.660000
S	21.373000	19.468000	13.894000
S	11.244000	16.912000	13.485000
S	11.346000	15.203000	18.992000
S	14.981000	13.358000	20.620000
S	18.516000	20.558000	16.902000
S	10.128000	12.681000	14.146000
S	10.201000	19.548000	18.319000
S	12.517000	18.249000	21.785000
S	13.770000	21.905000	19.553000
S	13.093000	11.615000	17.094000
S	18.548000	11.713000	15.259000
S	20.148000	15.286000	13.324000
S	16.707000	18.909000	20.509000
S	13.657000	10.390000	12.832000
S	17.933000	10.572000	19.656000
S	21.442000	12.686000	18.124000
S	19.328000	14.124000	21.754000
C	9.416000	13.473000	15.650000
H	8.813000	12.689000	16.131000
H	8.727000	14.260000	15.303000
C	10.449000	14.029000	16.620000
H	11.074000	14.764000	16.088000
H	11.123000	13.206000	16.903000
C	9.923000	14.663000	17.911000
H	9.371000	15.590000	17.690000
C	9.016000	13.742000	18.756000

H	9.301000	12.693000	18.573000
H	9.214000	13.934000	19.822000
C	7.514000	13.933000	18.512000
C	6.664000	13.077000	19.457000
C	5.157000	13.279000	19.255000
C	4.228000	12.523000	20.194000
O	4.620000	11.259000	20.550000
O	3.173000	12.955000	20.603000
H	7.254000	13.699000	17.467000
H	7.259000	14.995000	18.667000
H	6.941000	12.018000	19.298000
H	6.935000	13.315000	20.498000
H	4.879000	12.978000	18.230000
H	4.891000	14.341000	19.344000
H	5.499000	11.082000	20.164000
C	9.920000	17.494000	14.633000
H	9.167000	16.695000	14.683000
H	9.466000	18.344000	14.103000
C	10.394000	17.923000	16.024000
H	11.431000	18.281000	15.949000
H	10.426000	17.059000	16.702000
C	9.569000	19.048000	16.651000
H	9.727000	19.945000	16.031000
C	8.043000	18.770000	16.701000
H	7.835000	17.743000	16.358000
H	7.689000	18.835000	17.740000
C	7.267000	19.767000	15.836000
C	5.755000	19.536000	15.773000
C	5.070000	20.587000	14.884000
C	3.569000	20.457000	14.699000
O	3.105000	19.197000	14.422000

O	2.787000	21.380000	14.745000
H	7.667000	19.746000	14.808000
H	7.460000	20.784000	16.217000
H	5.574000	18.514000	15.388000
H	5.321000	19.563000	16.785000
H	5.521000	20.552000	13.876000
H	5.256000	21.596000	15.274000
H	3.848000	18.565000	14.479000
C	13.021000	15.491000	9.810000
H	12.186000	15.929000	9.243000
H	13.805000	15.211000	9.089000
C	13.549000	16.481000	10.842000
H	12.718000	16.739000	11.516000
H	14.303000	15.967000	11.462000
C	14.144000	17.787000	10.307000
H	15.054000	17.569000	9.728000
C	13.181000	18.614000	9.422000
H	12.146000	18.449000	9.764000
H	13.387000	19.684000	9.572000
C	13.298000	18.314000	7.921000
C	12.320000	19.123000	7.061000
C	12.517000	18.875000	5.556000
C	11.596000	19.645000	4.626000
O	10.258000	19.587000	4.925000
O	11.956000	20.265000	3.651000
H	13.140000	17.241000	7.728000
H	14.327000	18.540000	7.594000
H	11.290000	18.866000	7.371000
H	12.443000	20.196000	7.274000
H	12.374000	17.803000	5.333000
H	13.543000	19.121000	5.256000

H	10.135000	19.073000	5.745000
C	17.015000	14.476000	10.299000
H	16.111000	14.556000	9.682000
H	17.762000	13.901000	9.732000
C	17.568000	15.841000	10.701000
H	16.750000	16.478000	11.073000
H	18.241000	15.687000	11.557000
C	18.377000	16.620000	9.653000
H	19.271000	16.029000	9.391000
C	17.648000	17.006000	8.355000
H	16.661000	17.421000	8.618000
H	18.201000	17.838000	7.892000
C	17.489000	15.896000	7.308000
C	16.672000	16.359000	6.101000
C	16.529000	15.264000	5.028000
C	15.619000	15.656000	3.882000
O	14.289000	15.788000	4.205000
O	15.973000	15.865000	2.744000
H	16.998000	15.012000	7.741000
H	18.484000	15.561000	6.971000
H	15.674000	16.675000	6.449000
H	17.131000	17.253000	5.649000
H	16.137000	14.344000	5.495000
H	17.509000	15.024000	4.596000
H	14.164000	15.572000	5.147000
C	15.297000	22.575000	18.768000
H	15.842000	23.089000	19.575000
H	14.975000	23.339000	18.043000
C	16.179000	21.520000	18.115000
H	16.409000	20.760000	18.876000
H	15.600000	21.004000	17.333000

C	17.512000	22.001000	17.531000
H	17.342000	22.638000	16.648000
C	18.410000	22.754000	18.538000
H	18.176000	22.396000	19.554000
H	19.456000	22.469000	18.348000
C	18.334000	24.285000	18.483000
C	19.344000	24.924000	19.445000
C	19.464000	26.446000	19.308000
C	20.513000	27.141000	20.171000
O	21.009000	26.434000	21.232000
O	20.900000	28.272000	19.978000
H	17.319000	24.645000	18.718000
H	18.555000	24.622000	17.457000
H	19.048000	24.655000	20.477000
H	20.330000	24.462000	19.266000
H	18.503000	26.931000	19.548000
H	19.683000	26.729000	18.267000
H	20.614000	25.541000	21.233000
C	14.048000	21.851000	14.747000
H	14.088000	22.601000	15.550000
H	13.509000	22.298000	13.899000
C	15.441000	21.404000	14.307000
H	16.096000	21.265000	15.178000
H	15.358000	20.418000	13.830000
C	16.105000	22.343000	13.298000
H	15.465000	22.352000	12.400000
C	16.260000	23.803000	13.794000
H	15.868000	23.898000	14.821000
H	17.328000	24.064000	13.845000
C	15.532000	24.794000	12.884000
C	15.671000	26.257000	13.308000

C	14.865000	27.196000	12.402000
C	15.015000	28.687000	12.645000
O	15.220000	29.074000	13.943000
O	14.941000	29.529000	11.779000
H	14.461000	24.530000	12.846000
H	15.913000	24.681000	11.855000
H	15.326000	26.342000	14.357000
H	16.734000	26.545000	13.299000
H	13.789000	26.968000	12.498000
H	15.116000	27.031000	11.345000
H	15.293000	28.276000	14.502000
C	13.285000	16.741000	22.521000
H	12.477000	16.259000	23.091000
H	14.045000	17.082000	23.242000
C	13.875000	15.771000	21.504000
H	14.657000	16.291000	20.929000
H	13.081000	15.526000	20.782000
C	14.437000	14.448000	22.035000
H	15.355000	14.627000	22.617000
C	13.447000	13.632000	22.896000
H	12.422000	13.843000	22.546000
H	13.620000	12.561000	22.714000
C	13.555000	13.875000	24.407000
C	12.459000	13.147000	25.193000
C	12.588000	13.336000	26.711000
C	11.531000	12.674000	27.580000
O	10.236000	12.782000	27.147000
O	11.764000	12.106000	28.623000
H	13.507000	14.951000	24.637000
H	14.542000	13.528000	24.755000
H	11.482000	13.525000	24.834000

H	12.478000	12.073000	24.948000
H	12.554000	14.415000	26.946000
H	13.558000	12.966000	27.069000
H	10.230000	13.228000	26.279000
C	17.331000	17.853000	21.891000
H	16.526000	17.804000	22.639000
H	18.154000	18.444000	22.318000
C	17.815000	16.468000	21.473000
H	18.362000	16.569000	20.526000
H	16.952000	15.819000	21.253000
C	18.743000	15.741000	22.454000
H	19.667000	16.334000	22.560000
C	18.136000	15.531000	23.858000
H	17.045000	15.404000	23.757000
H	18.514000	14.590000	24.285000
C	18.440000	16.687000	24.823000
C	17.559000	16.711000	26.074000
C	17.849000	17.943000	26.949000
C	16.979000	18.086000	28.183000
O	15.627000	18.082000	27.966000
O	17.395000	18.211000	29.313000
H	18.320000	17.650000	24.304000
H	19.500000	16.638000	25.123000
H	16.502000	16.707000	25.751000
H	17.698000	15.792000	26.668000
H	17.718000	18.856000	26.342000
H	18.890000	17.933000	27.295000
H	15.453000	17.945000	27.016000
C	15.267000	9.724000	13.443000
H	15.765000	9.336000	12.543000
H	15.040000	8.864000	14.093000

C	16.152000	10.740000	14.156000
H	15.636000	11.092000	15.061000
H	16.244000	11.619000	13.500000
C	17.573000	10.292000	14.524000
H	17.546000	9.530000	15.320000
C	18.412000	9.769000	13.336000
H	18.096000	10.308000	12.427000
H	19.461000	10.056000	13.505000
C	18.389000	8.256000	13.084000
C	19.295000	7.891000	11.898000
C	19.442000	6.385000	11.658000
C	20.305000	5.950000	10.480000
O	20.371000	6.810000	9.419000
O	20.888000	4.890000	10.425000
H	17.366000	7.895000	12.892000
H	18.743000	7.728000	13.986000
H	18.873000	8.386000	11.002000
H	20.290000	8.337000	12.059000
H	18.450000	5.931000	11.491000
H	19.859000	5.884000	12.543000
H	19.882000	7.627000	9.640000
C	14.250000	10.269000	17.604000
H	14.341000	9.591000	16.743000
H	13.708000	9.735000	18.398000
C	15.607000	10.754000	18.106000
H	15.444000	11.678000	18.678000
H	16.251000	11.039000	17.258000
C	16.375000	9.797000	19.020000
H	15.767000	9.623000	19.924000
C	16.738000	8.434000	18.403000
H	17.023000	8.575000	17.346000

H	17.641000	8.060000	18.910000
C	15.648000	7.364000	18.522000
C	16.131000	5.985000	18.071000
C	15.061000	4.899000	18.259000
C	15.496000	3.493000	17.900000
O	16.070000	3.338000	16.664000
O	15.363000	2.523000	18.613000
H	14.750000	7.643000	17.948000
H	15.328000	7.297000	19.576000
H	16.446000	6.052000	17.012000
H	17.036000	5.711000	18.639000
H	14.172000	5.143000	17.650000
H	14.731000	4.866000	19.304000
H	16.148000	4.213000	16.239000
C	22.118000	18.733000	15.416000
H	22.665000	19.557000	15.898000
H	22.862000	17.992000	15.081000
C	21.111000	18.118000	16.381000
H	20.554000	17.327000	15.854000
H	20.371000	18.893000	16.630000
C	21.650000	17.560000	17.705000
H	22.261000	16.660000	17.527000
C	22.456000	18.568000	18.552000
H	22.041000	19.575000	18.378000
H	22.279000	18.344000	19.616000
C	23.972000	18.576000	18.328000
C	24.654000	19.654000	19.180000
C	26.181000	19.651000	19.048000
C	26.947000	20.676000	19.868000
O	26.360000	21.903000	20.020000
O	28.041000	20.480000	20.348000

H	24.221000	18.739000	17.269000
H	24.382000	17.587000	18.597000
H	24.239000	20.634000	18.876000
H	24.372000	19.515000	20.237000
H	26.462000	19.823000	17.994000
H	26.593000	18.671000	19.323000
H	25.472000	21.881000	19.613000
C	21.527000	14.703000	14.411000
H	22.268000	15.515000	14.446000
H	21.967000	13.869000	13.845000
C	21.112000	14.240000	15.805000
H	20.138000	13.738000	15.726000
H	20.951000	15.104000	16.468000
C	22.073000	13.254000	16.477000
H	22.081000	12.335000	15.868000
C	23.531000	13.753000	16.615000
H	23.555000	14.853000	16.540000
H	23.903000	13.504000	17.621000
C	24.473000	13.134000	15.576000
C	25.923000	13.609000	15.693000
C	26.846000	12.864000	14.722000
C	28.324000	13.201000	14.777000
O	28.641000	14.512000	15.015000
O	29.212000	12.398000	14.599000
H	24.109000	13.338000	14.556000
H	24.452000	12.037000	15.694000
H	25.947000	14.699000	15.502000
H	26.277000	13.465000	16.727000
H	26.523000	13.053000	13.684000
H	26.765000	11.778000	14.874000
H	27.817000	15.017000	15.159000

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