Supplementary Information

Ultraviolet photoactivation perturbs the metal-ligand interface of atomically precise nanoclusters

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1. Experimental Section

Materials. All the materials were commercially available. All chemicals, including silver nitrate ($AgNO_3$), 1,3-benzenedithiol (BDT), sodium borohydride ($NaBH_4$), triphenylphosphine (TPP, 97%), and 2,4-dimethylbenzenethiol (DMBT) were purchased from Sigma-Aldrich. HPLC grade dichloromethane (DCM), dimethylformamide (DMF), and methanol (MeOH) were purchased from Rankem. All solvents and chemicals were used as such without further purification.

Synthesis of $Ag_{29}(BDT)_{12}(PPh_3)_4$ (Ag_{29}). The cluster was synthesized by adopting an already-reported method. First, ~20 mg of AgNO3 was dissolved in 5 mL of MeOH, and then 9 mL of DCM was added. After a few mins, ~13.5 µL of BDT (0.5 mL of DCM) was added to the solution. Then, after 5 min of stirring in the dark, ~200 mg of PPh3 (in 0.5 mL of DCM) was added to the mixture, and next, 0.5 mL of an ice-cold aqueous solution containing ~11 mg of $NaBH_4$ was added, which immediately changed the color of the solution to dark brown. The reaction was kept for 3 h under dark conditions. Then, the precipitate (red color) was collected by centrifugation, and the concentrated solution was collected by rotary evaporation. The cluster was washed several times with MeOH and then dissolved in DCM. The reddish-orange colored cluster was collected after the removal of unwanted byproducts.

Synthesis of $PtAg_{24}(DMBT)_{18}$ ($PtAg_{24}$). For the synthesis of $PtAg_{24}$, we followed a reported method after some modifications.46 At first, ~10 mg of AgNO3 was dissolved in MeOH (5 mL) along with ~10

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mg of K_2PtCl_4 (9 mL of DCM). Then, ~10 µL of DMBT in 0.5 mL of DCM was added to the mixture followed by the addition of ~10 mg of PPh_4Br (in 0.5 mL of DCM). After ~20 min, $NaBH_4$ (40 mg in 0.5 mL of ice-cold water) was added, resulting in the reduction of Ag-Pt-phosphine-thiolate to form NCs, and 50 µL of triethylamine was added after 5 min. The solution was kept stirring overnight. The formed cluster solution was evaporated and then washed with MeOH. The clusters were extracted in DCM.

2. Instrumentation

UV-Vis absorption spectra of the cluster in their respective solution were optimized using a PerkinElmer Lambda 25 spectrophotometer in the 200–1100 nm wavelength range. The slit width used for the measurement is 1 nm.

UV Photoactivation -Mass Spectrometry

Static emitters (1.2 mm o.d.) were pulled to a fine tip using a Sutter Instrument P-2000 laser puller (Novato, CA) and coated in an Au/Pd mixture for static electrospray. Emitters were loaded with 5–10 µL of the Ag_{29}(BDT) solution, and a spray voltage of 1.1–1.3 kV was used for direct infusion. Mass spectra were collected in negative mode on a Thermo Scientific Orbitrap Fusion Lumos mass spectrometer (San Jose, CA), modified with a 193 nm Coherent ExciStar excimer laser (Santa Cruz, CA) to perform UVPD in the high-pressure linear ion trap. All data were collected using a maximum injection time of 100 ms, an AGC (automatic gain control) target of 1×10^6, and a resolution of 120,000 at m/z 200. For all spectra, 20 scans were collected and averaged with 1 microscan per scan. Ion activation methods were performed following quadrupole isolation with the isolation width set to 50 m/z. An activation time of 10 ms and q-value of 0.25 were used when performing CID (10–40% NCE) and HCD (5– 25% NCE) at the MS2 and MS3 levels. Activated-electron photodetachment dissociation (a-EPD) experiments were performed using UV photoactivation with various numbers of pulses and laser energies (e.g., 2 pulses at 2 mJ per pulse) to generate charge-reduced radical species (MS2), followed by isolation and collisional activation of the primary charge-reduced precursor ion (MS3).

ESI-MS of $PtAg_{24}$ was performed on a Thermo Scientific Q Exactive HF-X quadrupole-Orbitrap mass spectrometer (Bremen, Germany), which was modified to perform ultraviolet photodissociation (UVPD) with a 500 Hz, 193 nm Coherent ExciStar excimer laser (Santa Cruz, CA) in the higher energy collisional dissociation (HCD) cell as previously described. Ions were generated by nanoelectrospray ionization using Au/Pd-coated borosilicate emitters fabricated in-house and using a spray voltage of 1.2 kV. Mass spectra were collected in negative mode. $PtAg_{24}$ ions were quadrupole-isolated and activated using HCD (1-5% NCE). For the manuscript, experiments involving $PtAg_{24}$ were undertaken using the HF-X mass spectrometer, which does not have the capability to perform a-EPD, which is a

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MS^3 experiment. UV photoactivation of $PtAg_{24}$ using the Lumos mass spectrometer resulted in a product ion of *m/z* 5253, corresponding to $[PtAg_{24}(DMBT)_{18}]$-. The high *m/z* value of this ion exceeds the upper *m/z* limit of ion isolation (which is *m/z* 4000). Therefore, this species ($[PtAg_{24}(DMBT)_{18}]$-) could not be isolated and subjected to collisional activation, and thus no results are reported.

No photodetached species were detected without photoactivation. Both the clusters Ag_{29} and $PtAg_{24}$ ionize in the negative mode. No peaks were observed in the positive mode in the ESI-MS before and after photoactivation.

3. Computational Studies

Geometry optimizations and electronic structure calculations were carried out using the projector-augmented wave (PAW) method, as implemented in the GPAW code.[1,2] Real-space grids with a 0.2 Å grid spacing were used for all computations. Electron-electron interactions were described using the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional[3] in the generalized gradient approximation (GGA). The BFGS (Broyden–Fletcher–Goldfarb–Shanno) method was used in the optimization process to iteratively minimize forces on the atoms. Convergence was reached at a maximum force threshold of 0.05 eV/Å. The initial structure of $[Ag_{29}(BDT)_{12}]^{3-}$ was built using its known crystal structure.[4] Meanwhile, $[PtAg_{24}(DMBT)_{18}]^{2-}$ was designed by modifying the computed structure of $[Ag_{25}(DMBT)_{18}]$,[5] substituting the central Ag atom with a Pt atom, and optimizing the structure for different charge states. The systems studied included $[Ag_{29}(BDT)_{12}]^{3-}$, $[Ag_{29}(BDT)_{12}]^{2-}$, $[Ag_{29}(BDT)_{12}]^{-}$, $[PtAg_{24}(DMBT)_{18}]^{2-}$, and $[PtAg_{24}(DMBT)_{18}]^{-}$ where BDT and DMBT refer to 1,3-benzenedithiol and dimethylbenzenethiol ligands, respectively. To investigate ligand detachment energies, we have computed the energy required to detach one BDT ligand from $[Ag_{29}(BDT)_{12}]^{2-}$ and one DMBT ligand from $[PtAg_{24}(DMBT)_{18}]^{-}$. The ligand detachment energy $E_{detachment}$ was calculated using the following expression:

$$E_{detachment} = E_{fragment1} + E_{fragment2} - E_{cluster}$$

where, $E_{fragment1}$ is the energy of the cluster after detaching single ligand ($[Ag_{29}(BDT)_{11}]^{2-}$ or $[PtAg_{24}(DMBT)_{17}]^{-}$), $E_{fragment2}$ is the energy of the detached ligand (BDT or DMBT), and $E_{cluster}$ is the energy of the intact cluster ($[Ag_{29}(BDT)_{12}]^{2-}$ or $[PtAg_{24}(DMBT)_{18}]^{-}$). All fragments and clusters were optimized as part of this study.

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To calculate the ionization potentials (IP1 and IP2) or the energy required to remove one or two electrons, optimizations were done for different charge states of the clusters. The first ionization potential (IP1) was calculated as:

$$IP1 = M_{parent}^{opt+} - M_{parent}^{opt}$$

where, M_{parent}^{opt+} is the energy of the optimized cluster with one electron removed ($[Ag_{29}(BDT)_{12}]^{2-}$ or $[PtAg_{24}(DMBT)_{18}]^{-}$) and M_{parent}^{opt} is the energy of the optimized cluster with the initial charge state ($[Ag_{29}(BDT)_{12}]^{3-}$ or $[PtAg_{24}(DMBT)_{18}]^{2-}$).

The second ionization potential (IP2) was calculated as:

$$IP2 = M_{parent}^{opt++} - M_{parent}^{opt}$$

where, $M_{parent}^{opt++}$is the energy of the optimized cluster with two electron removed ($[Ag_{29}(BDT)_{12}]^{-}$) from M_{parent}^{opt}.

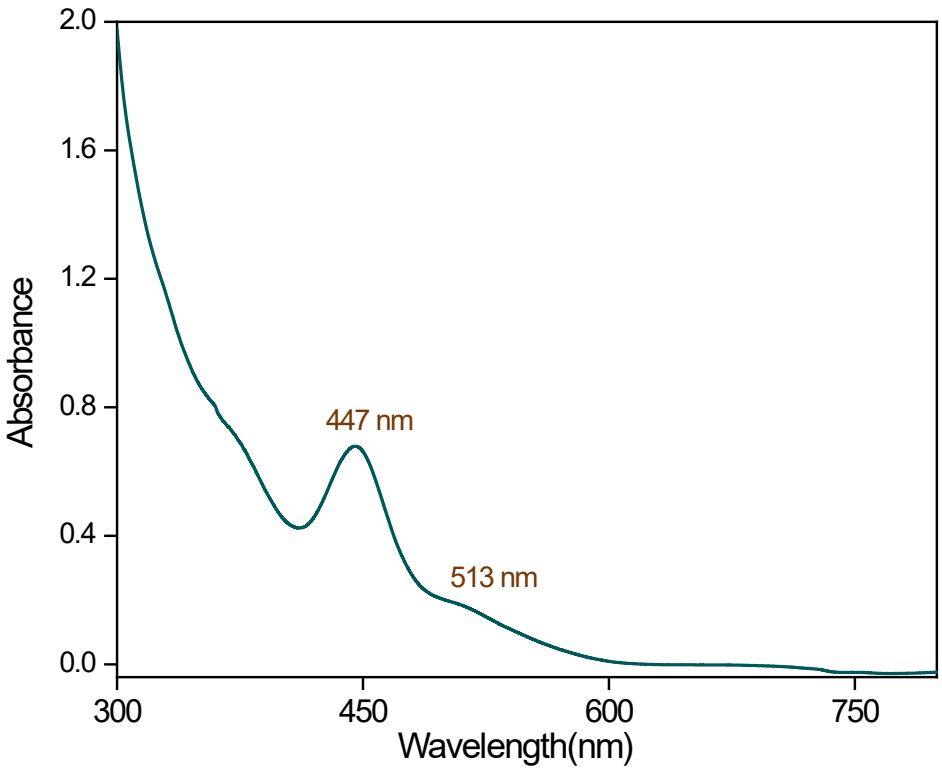

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Fig. S1. UV-Vis absorption spectrum of $[Ag_{29}(BDT)_{12}]^{3-}$ cluster in N,N-Dimethylformamide (DMF).

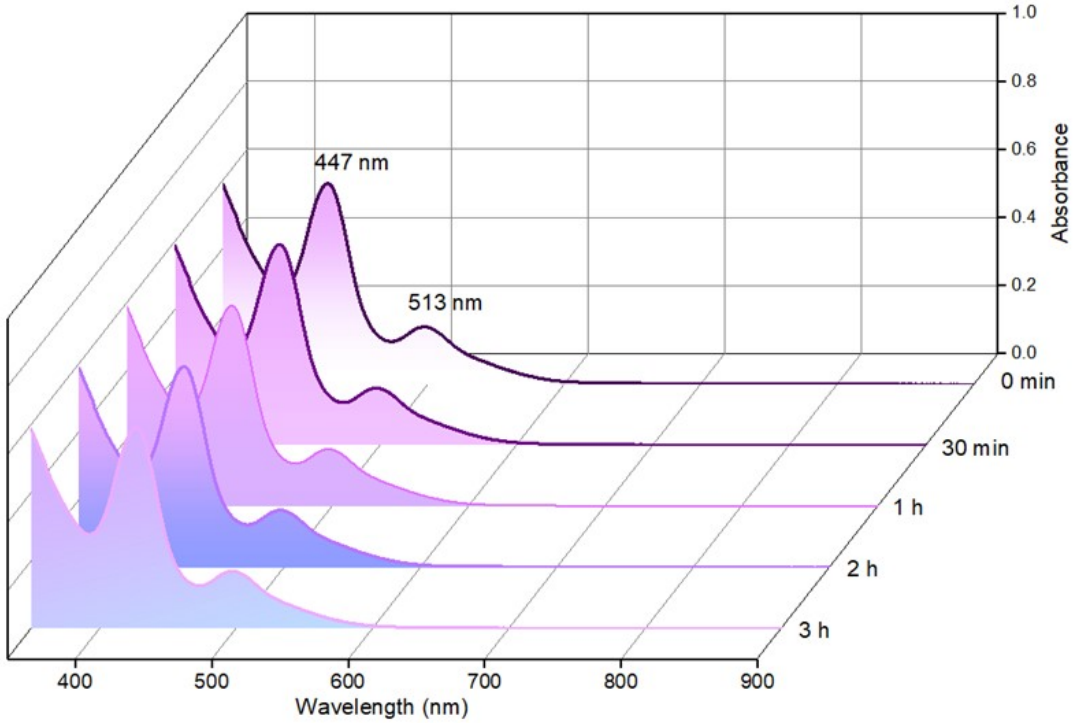

Fig. S2. Stability of $[Ag_{29}(BDT)_{12}]^{3-}$ cluster in DMF based on absorbance profiles acquired over several hours.

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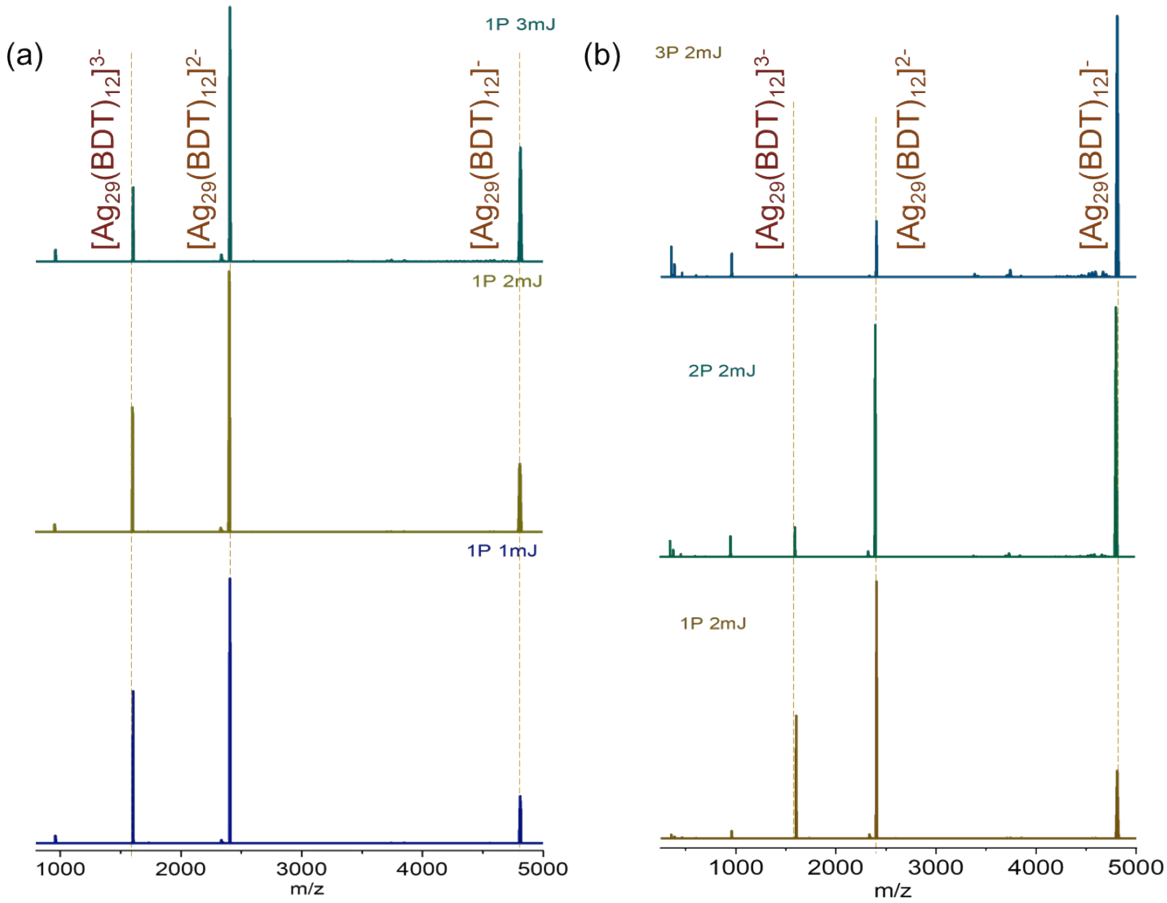

Fig. S3. UV photoactivation of $[Ag_{29}(BDT)_{12}]^{3-}$ obtained us ing (a) Different laser energies, and (b) Different number of laser pulses.

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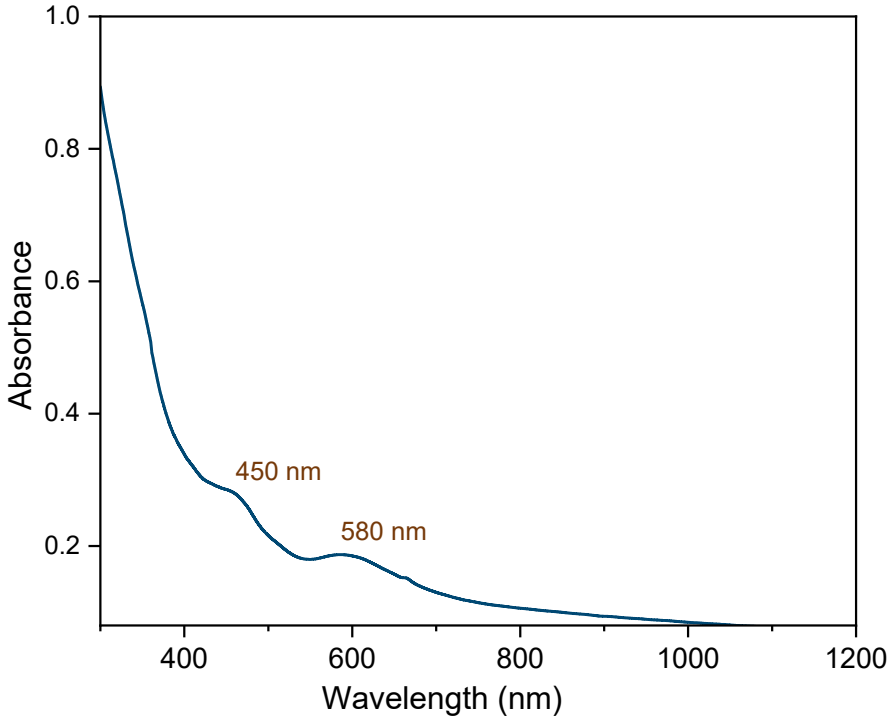

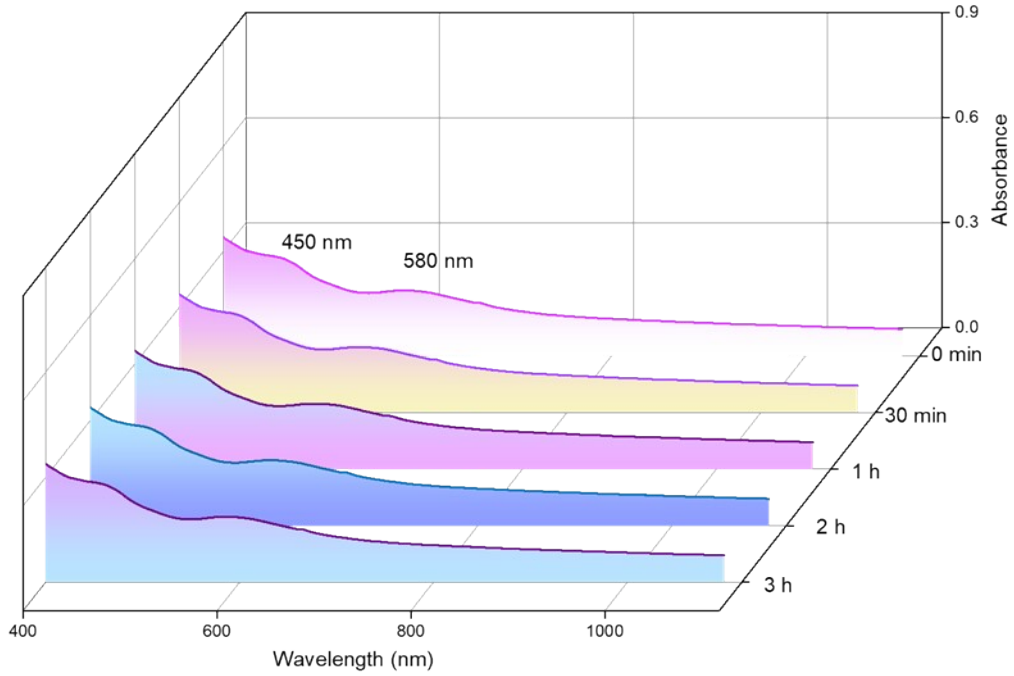

Fig. S4. UV-Vis absorption spectrum of $[PtAg_{24}(DMBT)_{18}]^{2-}$ in dichloromethane (DCM).

Fig. S5. Stability of $[PtAg_{24}(DMBT)_{18}]^{2-}$ in DCM based on absorbance profiles acquired over several

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hours.

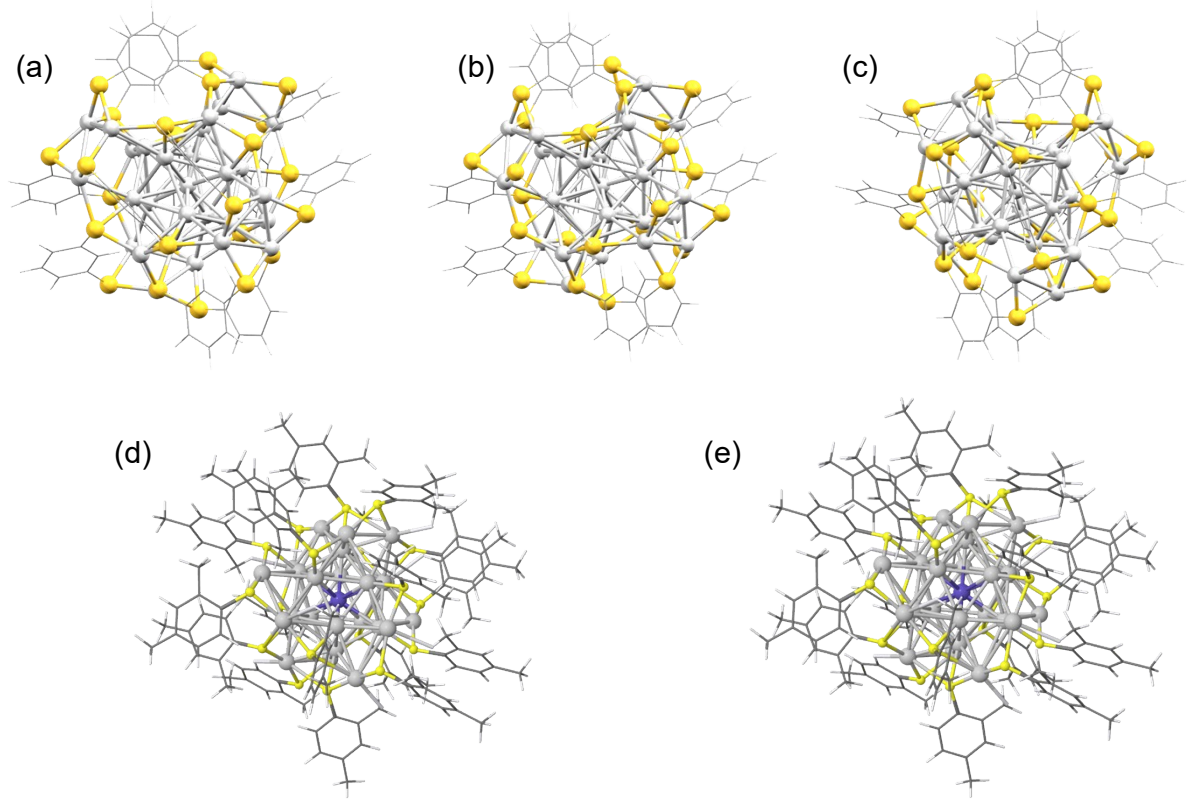

Fig. S6. DFT-optimized structures of (a) $[Ag_{29}(BDT)_{12}]^{-}$, (b) $[Ag_{29}(BDT)_{12}]^{2-}$, (c) $[Ag_{29}(BDT)_{12}]^{3-}$, (d) $[PtAg_{24}(DMBT)_{18}]^{-}$ and ,(c) $[PtAg_{24}(DMBT)_{18}]^{2-}$. Grey: Ag, Blue: Pt, yellow: S, grey: C, white: H.

Coordinates

$Ag_{29}BDT_{12}^{3-}$

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Ag	15.028012	15.028011	15.028012
Ag	12.582394	14.895607	13.574644
Ag	15.073122	16.55673	12.633689
Ag	13.500071	17.404522	15.18863
Ag	17.47649	14.928692	16.483813
Ag	10.745465	13.224404	11.642769
Ag	12.295271	17.665137	12.466397
Ag	16.685302	18.511054	10.850022
Ag	11.62222	19.226633	16.916808
Ag	18.435767	19.364443	13.243939
Ag	17.669079	17.66908	17.669078

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S	15.828985	12.374723	10.568225
S	14.087933	17.829536	10.683036
S	12.194337	19.394556	14.314548
S	19.427366	15.866048	17.778226
S	11.689744	13.000161	9.338203
S	18.206702	17.231623	9.353563
S	16.965626	20.784359	11.836986
S	20.711545	18.373122	12.980928
C	16.319954	13.603427	9.35947
C	16.221632	13.307485	7.991011
H	15.75969	12.375362	7.663128
C	16.731759	14.220059	7.06356
H	16.663376	13.992581	5.99682
C	17.333787	15.411833	7.471539
H	17.738574	16.111648	6.739443
C	17.417307	15.723016	8.840304
C	16.897378	14.810433	9.761322
H	16.957949	15.047953	10.823696
C	13.595037	16.626126	9.454577
C	13.728742	16.938555	8.093847
H	14.2088	17.869305	7.79335
C	13.23836	16.044208	7.138965
H	13.342084	16.284894	6.078178
C	12.622331	14.848739	7.513495
H	12.23851	14.15742	6.761287
C	12.500941	14.519708	8.875561
C	12.996996	15.41838	9.825484
H	12.907138	15.166916	10.883331
C	13.414884	20.62589	13.86992
C	14.58134	20.270559	13.186046
H	14.773687	19.218927	12.972846
C	15.507884	21.227226	12.759835
C	15.24871	22.580492	13.041973
H	15.962193	23.341624	12.724375
C	14.089828	22.938385	13.733043
H	13.906452	23.991222	13.961475
C	13.166151	21.976565	14.151096
H	12.269792	22.259861	14.702466
C	20.638668	16.458972	16.603956
C	20.260431	17.00052	15.37156
H	19.210605	16.976244	15.076873
C	21.190281	17.596459	14.513537
C	22.541615	17.620635	14.905126
H	23.283833	18.080189	14.251358
C	22.924903	17.053899	16.121532
H	23.976735	17.06749	16.414806

v

C	21.988974	16.47513	16.980739
H	22.290224	16.047256	17.937179
Ag	13.574645	12.582393	14.895606
Ag	12.633689	15.073121	16.556732
Ag	15.18863	13.50007	17.404522
Ag	16.483816	17.476488	14.92869
Ag	11.642773	10.745462	13.224404
Ag	12.466395	12.295273	17.665138
Ag	10.850023	16.685304	18.511053
Ag	16.916809	11.622219	19.226633
Ag	13.243947	18.435765	19.364444
S	10.568225	15.828983	12.374724
S	10.68303	14.087941	17.829541
S	14.314546	12.194339	19.394558
S	17.778228	19.427365	15.866047
S	9.338207	11.689741	13.000162
S	9.353563	18.2067	17.231625
S	11.836985	16.965626	20.784356
S	12.980931	20.711542	18.373119
C	9.35947	16.319952	13.603429
C	7.99101	16.22163	13.307487
H	7.663127	15.759689	12.375364
C	7.063561	16.731757	14.22006
H	5.996821	16.663375	13.992583
C	7.471539	17.333785	15.411835
H	6.739444	17.738572	16.11165
C	8.840305	17.417304	15.723017
C	9.761321	16.897376	14.810434
H	10.823696	16.957949	15.047954
C	9.454578	13.595037	16.626125
C	8.093845	13.72874	16.938553
H	7.793348	14.2088	17.869301
C	7.138967	13.238355	16.044205
H	6.078178	13.342078	16.284891
C	7.513497	12.622325	14.848738
H	6.76129	12.238502	14.15742
C	8.875565	12.500938	14.519708
C	9.825485	12.996995	15.418381
H	10.883332	12.907138	15.166916
C	13.86992	13.414884	20.625891
C	13.186049	14.581341	20.27056
H	12.972846	14.773694	19.218929
C	12.759837	15.507884	21.227229
C	13.041976	15.248709	22.580495
H	12.72438	15.962194	23.341628
C	13.733043	14.089827	22.938388

v

H	13.961476	13.906449	23.991221
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H	15.076877	19.210603	16.976241
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C	14.905129	22.541612	17.620633
H	14.251359	23.283829	18.080188
C	16.121535	22.9249	17.053899
H	16.414808	23.976733	17.067491
C	16.980742	21.988973	16.475129
H	17.937184	22.290224	16.047257
Ag	14.895608	13.574643	12.582393
Ag	16.556733	12.633688	15.073123
Ag	17.404524	15.188628	13.50007
Ag	14.928693	16.483813	17.476489
Ag	13.224407	11.642767	10.745463
Ag	17.66514	12.466396	12.295272
Ag	18.511055	10.850022	16.685305
Ag	19.226636	16.916808	11.622221
Ag	19.364447	13.243945	18.435765
S	12.374726	10.568225	15.828984
S	17.829542	10.683032	14.087939
S	19.394563	14.314545	12.19434
S	15.86605	17.778224	19.427366
S	13.000165	9.3382	11.689742
S	17.231626	9.353563	18.206701
S	20.784359	11.836981	16.965626
S	18.373118	12.980927	20.711544
C	13.60343	9.359471	16.319953
C	13.307489	7.991011	16.221631
H	12.375366	7.663127	15.759689
C	14.220062	7.063561	16.731757
H	13.992586	5.996821	16.663375
C	15.411836	7.471538	17.333786
H	16.111652	6.739444	17.738573
C	15.723019	8.840304	17.417306
C	14.810436	9.761321	16.897378
H	15.047955	10.823696	16.957953
C	16.626129	9.454576	13.595039
C	16.93856	8.093845	13.728743
H	17.869311	7.793351	14.2088
C	16.044214	7.138965	13.23836
H	16.284902	6.078178	13.342084
C	14.848745	7.513492	12.622331

v

H	14.157426	6.761285	12.23851
C	14.519712	8.875558	12.500941
C	15.418383	9.825481	12.996998
H	15.166917	10.883329	12.90714
C	20.625895	13.86992	13.414886
C	20.270564	13.186048	14.581343
H	19.218932	12.972844	14.773696
C	21.227233	12.759835	15.507885
C	22.580499	13.041974	15.248711
H	23.341632	12.724376	15.962195
C	22.938391	13.733042	14.089829
H	23.991226	13.961474	13.90645
C	21.976569	14.151094	13.166152
H	22.259862	14.702462	12.269794
C	16.458971	16.603956	20.638668
C	17.00052	15.371562	20.26043
H	16.976244	15.076874	19.210604
C	17.596457	14.513537	21.19028
C	17.620635	14.905125	22.541614
H	18.08019	14.251356	23.283831
C	17.0539	16.121531	22.924902
H	17.067493	16.414804	23.976734
C	16.47513	16.980738	21.988975
H	16.047258	17.937179	22.290226

$Ag_{29}BDT_{12}^{2-}$

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Ag	15.028289	15.028288	15.028289
Ag	12.582858	14.898226	13.575545
Ag	15.068508	16.55596	12.632862
Ag	13.499918	17.404718	15.188258
Ag	17.474978	14.928041	16.481726
Ag	10.745468	13.219828	11.643011
Ag	12.293164	17.66361	12.464453
Ag	16.689187	18.509962	10.851678
Ag	11.622733	19.225419	16.919835
Ag	18.438992	19.366703	13.237902
Ag	17.668742	17.668742	17.668742
S	15.824819	12.373866	10.5652
S	14.094125	17.832057	10.681078
S	12.192185	19.395768	14.31991
S	19.429572	15.859463	17.776957
S	11.695501	13.005915	9.347632
S	18.201653	17.225402	9.362158
S	16.963347	20.781522	11.842287

v

S	20.705663	18.363985	12.988617
C	16.317707	13.602535	9.360668
C	16.2212	13.30825	7.991773
H	15.761726	12.376485	7.66169
C	16.730643	14.220569	7.064593
H	16.664316	13.992792	5.99826
C	17.331569	15.4123	7.473254
H	17.7397	16.11007	6.740852
C	17.4153	15.718772	8.843362
C	16.894795	14.80825	9.765063
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C	12.504838	14.521998	8.877837
C	12.999143	15.420467	9.828435
H	12.907677	15.16678	10.886152
C	13.412916	20.625122	13.872166
C	14.578616	20.26667	13.188545
H	14.7737	19.215169	12.973485
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H	15.960426	23.340533	12.724752
C	14.091175	22.938069	13.735565
H	13.90554	23.99084	13.961112
C	13.167089	21.976822	14.152893
H	12.269888	22.262177	14.700966
C	20.637113	16.456425	16.604986
C	20.25647	16.995886	15.373633
H	19.20661	16.974522	15.077533
C	21.187229	17.592122	14.518395
C	22.539887	17.616399	14.905439
H	23.281433	18.078415	14.252743
C	22.924225	17.051062	16.121151
H	23.975452	17.068032	16.414886
C	21.988063	16.47365	16.980562
H	22.291384	16.048632	17.936854
Ag	13.575547	12.582857	14.898227
Ag	12.632862	15.068507	16.555962
Ag	15.188259	13.499917	17.404718
Ag	16.481729	17.474977	14.92804
Ag	11.643015	10.745466	13.219828

v

Ag	12.464452	12.293165	17.663611
Ag	10.85168	16.689193	18.509965
Ag	16.919836	11.622732	19.225419
Ag	13.237912	18.438989	19.366703
S	10.565199	15.824817	12.373866
S	10.681072	14.094132	17.832062
S	14.319908	12.192188	19.39577
S	17.776961	19.42957	15.859461
S	9.347636	11.695498	13.005916
S	9.362158	18.201652	17.225404
S	11.842286	16.963346	20.781518
S	12.988619	20.70566	18.363982
C	9.360669	16.317705	13.602537
C	7.991772	16.221198	13.308252
H	7.66169	15.761724	12.376487
C	7.064594	16.730642	14.220571
H	5.99826	16.664315	13.992793
C	7.473253	17.331567	15.412302
H	6.740852	17.739698	16.110072
C	8.843363	17.415298	15.718773
C	9.765062	16.894793	14.808251
H	10.827781	16.956956	15.047089
C	9.455375	13.596969	16.627252
C	8.094043	13.730044	16.938419
H	7.792806	14.206385	17.870426
C	7.139039	13.240038	16.044058
H	6.078511	13.341044	16.286409
C	7.514907	12.624678	14.848857
H	6.761241	12.238519	14.160674
C	8.877841	12.504836	14.521998
C	9.828435	12.999142	15.420467
H	10.886153	12.907678	15.16678
C	13.872165	13.412918	20.625123
C	13.188547	14.578617	20.266671
H	12.973485	14.773706	19.215171
C	12.764109	15.505557	21.223912
C	13.044872	15.249338	22.578378
H	12.724757	15.960426	23.340537
C	13.735564	14.091173	22.938071
H	13.961112	13.905536	23.990839
C	14.152891	13.167086	21.976822
H	14.700961	12.269886	22.262175
C	16.604989	20.637111	16.456422
C	15.373637	20.256467	16.995883
H	15.077537	19.206608	16.974519
C	14.518399	21.187225	17.59212

v

C	14.905441	22.539883	17.616397
H	14.252745	23.281427	18.078414
C	16.121154	22.924223	17.051061
H	16.414889	23.975451	17.068034
C	16.980565	21.988061	16.473649
H	17.936858	22.291384	16.048632
Ag	14.898228	13.575545	12.582857
Ag	16.555963	12.632861	15.068509
Ag	17.40472	15.188257	13.499916
Ag	14.928043	16.481726	17.474977
Ag	13.219831	11.643009	10.745467
Ag	17.663613	12.464452	12.293164
Ag	18.509967	10.851679	16.689194
Ag	19.225421	16.919835	11.622734
Ag	19.366706	13.23791	18.43899
S	12.373869	10.5652	15.824818
S	17.832062	10.681075	14.09413
S	19.395776	14.319907	12.192188
S	15.859464	17.776956	19.42957
S	13.005918	9.347628	11.695499
S	17.225405	9.362158	18.201652
S	20.781522	11.842283	16.963345
S	18.363982	12.988614	20.705662
C	13.602538	9.360669	16.317707
C	13.308254	7.991773	16.221199
H	12.376489	7.661691	15.761724
C	14.220573	7.064594	16.730642
H	13.992796	5.998261	16.664315
C	15.412303	7.473254	17.331568
H	16.110073	6.740853	17.739699
C	15.718775	8.843363	17.415299
C	14.808252	9.765062	16.894795
H	15.047091	10.827781	16.95696
C	16.627256	9.455372	13.596972
C	16.938426	8.094042	13.730047
H	17.870436	7.792809	14.206385
C	16.044067	7.139037	13.240044
H	16.28642	6.07851	13.341049
C	14.848864	7.514902	12.624684
H	14.160681	6.761235	12.238528
C	14.522002	8.877835	12.504839
C	15.420469	9.828432	12.999145
H	15.166781	10.886149	12.907679
C	20.625127	13.872165	13.412919
C	20.266675	13.188546	14.57862
H	19.215174	12.973483	14.773709

v

C	21.223916	12.764108	15.505558
C	22.578382	13.04487	15.24934
H	23.340541	12.724754	15.960427
C	22.938074	13.735563	14.091175
H	23.990843	13.96111	13.905538
C	21.976826	14.152891	13.16709
H	22.262177	14.700962	12.26989
C	16.456425	16.604986	20.637112
C	16.995886	15.373634	20.25647
H	16.974522	15.077534	19.20661
C	17.592121	14.518395	21.187228
C	17.616398	14.905438	22.539885
H	18.078416	14.252741	23.28143
C	17.051063	16.121149	22.924224
H	17.068036	16.414885	23.975453
C	16.47365	16.980561	21.988064
H	16.048634	17.936854	22.291386

$Ag_{29}BDT_{12}^{1-}$

173

Ag	15.026122	15.02612	15.026121
Ag	12.584916	14.901964	13.574422
Ag	15.082743	16.561511	12.630195
Ag	13.50937	17.408223	15.179691
Ag	17.470971	14.930864	16.493393
Ag	10.750389	13.231101	11.644455
Ag	12.310113	17.668071	12.46886
Ag	16.690625	18.534352	10.816364
Ag	11.608329	19.239538	16.933398
Ag	18.445137	19.354144	13.224324
Ag	17.674331	17.67433	17.674332
S	15.82627	12.365529	10.568829
S	14.108569	17.847552	10.680997
S	12.190924	19.39707	14.327009
S	19.432029	15.862173	17.787448
S	11.716411	13.021797	9.371212
S	18.199772	17.22321	9.362196
S	16.963093	20.776811	11.851196
S	20.711453	18.360658	12.994976
C	16.313297	13.599083	9.368895
C	16.221319	13.306614	7.998363
H	15.772529	12.370746	7.664356
C	16.727923	14.221658	7.07229
H	16.667069	13.993334	6.007191

v

C	17.321417	15.415615	7.4837
H	17.727977	16.115163	6.753604
C	17.400188	15.719995	8.854058
C	16.882284	14.808245	9.776066
H	16.943285	15.04415	10.839034
C	13.611317	16.637995	9.457008
C	13.734778	16.942166	8.092273
H	14.206521	17.874569	7.783184
C	13.240486	16.042004	7.14486
H	13.333424	16.277753	6.082673
C	12.632607	14.846799	7.530998
H	12.244801	14.153267	6.783561
C	12.522464	14.530397	8.897347
C	13.017918	15.433698	9.84018
H	12.926899	15.187621	10.898521
C	13.412937	20.62507	13.876864
C	14.577545	20.26268	13.195277
H	14.76871	19.212018	12.979437
C	15.506229	21.216824	12.771891
C	15.254713	22.573125	13.048733
H	15.966338	23.332115	12.722491
C	14.095564	22.937217	13.735749
H	13.909478	23.989698	13.955539
C	13.169294	21.979327	14.154565
H	12.26972	22.271127	14.696323
C	20.640411	16.451766	16.612533
C	20.257034	16.98641	15.379621
H	19.207107	16.959851	15.086303
C	21.183363	17.584121	14.521773
C	22.537529	17.613547	14.906549
H	23.273836	18.081319	14.252468
C	22.926691	17.053487	16.123613
H	23.978361	17.077053	16.41464
C	21.993051	16.475478	16.986648
H	22.30212	16.061253	17.94645
Ag	13.574423	12.584914	14.901965
Ag	12.630197	15.082743	16.561511
Ag	15.179691	13.509368	17.408223
Ag	16.493394	17.470968	14.930866
Ag	11.644458	10.750388	13.231102
Ag	12.46886	12.310113	17.668074
Ag	10.816366	16.690624	18.534357
Ag	16.933398	11.608327	19.239538
Ag	13.224322	18.445134	19.354148
S	10.568828	15.826267	12.365531
S	10.680999	14.108567	17.84755

v

S 14.327009 12.190926 19.397071
S 17.78745 19.432026 15.862174
S 9.371215 11.716408 13.021798
S 9.362195 18.199769 17.223213
S 11.85119 16.96309 20.776817
S 12.994979 20.711449 18.360659
C 9.368894 16.313295 13.599085
C 7.998362 16.221318 13.306616
H 7.664354 15.772529 12.370747
C 7.072288 16.727922 14.22166
H 6.00719 16.667068 13.993336
C 7.483698 17.321416 15.415618
H 6.753602 17.727975 16.115166
C 8.854056 17.400187 15.719997
C 9.776064 16.882282 14.808247
H 10.839031 16.943283 15.044152
C 9.457006 13.611317 16.637996
C 8.092271 13.734777 16.942167
H 7.78318 14.206519 17.874571
C 7.14486 13.240482 16.042005
H 6.082673 13.333414 16.277753
C 7.531 12.632605 14.8468
H 6.783566 12.244795 14.153267
C 8.897349 12.522464 14.530397
C 9.84018 13.017919 15.433699
H 10.898522 12.926902 15.187627
C 13.876863 13.41294 20.62507
C 13.195279 14.57755 20.262682
H 12.97944 14.768715 19.21202
C 12.771889 15.506231 21.216827
C 13.048732 15.254713 22.573127
H 12.72249 15.966336 23.332119
C 13.735747 14.095564 22.937219
H 13.955539 13.909476 23.9897
C 14.154562 13.169294 21.979328
H 14.696321 12.269719 22.271127
C 16.612535 20.640409 16.451765
C 15.379623 20.257032 16.986409
H 15.086305 19.207105 16.959848
C 14.521775 21.183361 17.584121
C 14.906551 22.537527 17.613547
H 14.25247 23.273834 18.081318
C 16.123615 22.926688 17.053487
H 16.414643 23.978359 17.077054
C 16.98665 21.993049 16.475478
H 17.946452 22.302118 16.061254

v

Ag	14.901966	13.574421	12.584915
Ag	16.561514	12.630195	15.082743
Ag	17.408225	15.17969	13.50937
Ag	14.930867	16.493391	17.47097
Ag	13.231103	11.644454	10.750387
Ag	17.668076	12.46886	12.310114
Ag	18.53436	10.816366	16.690623
Ag	19.239541	16.933396	11.608329
Ag	19.354148	13.224319	18.445135
S	12.365533	10.568829	15.826269
S	17.847554	10.680997	14.108568
S	19.397077	14.32701	12.19093
S	15.862173	17.787445	19.432028
S	13.021803	9.371213	11.716409
S	17.223215	9.362195	18.199769
S	20.776822	11.851186	16.963092
S	18.360659	12.994974	20.711451
C	13.599087	9.368894	16.313297
C	13.306618	7.998362	16.221319
H	12.37075	7.664355	15.772529
C	14.221662	7.072288	16.727922
H	13.993338	6.00719	16.667067
C	15.41562	7.483698	17.321417
H	16.115168	6.753602	17.727975
C	15.719999	8.854056	17.400188
C	14.808248	9.776064	16.882286
H	15.044152	10.839032	16.94329
C	16.638	9.457005	13.611319
C	16.942171	8.09227	13.73478
H	17.874576	7.783179	14.206522
C	16.042008	7.144858	13.240488
H	16.277756	6.082671	13.333425
C	14.846803	7.530998	12.632609
H	14.153271	6.783561	12.244802
C	14.530401	8.897346	12.522466
C	15.433703	9.840178	13.017921
H	15.187628	10.898519	12.926904
C	20.625075	13.876863	13.412946
C	20.262686	13.195278	14.577555
H	19.212024	12.979438	14.76872
C	21.216831	12.771887	15.506235
C	22.573132	13.048729	15.254717
H	23.332123	12.722486	15.96634
C	22.937224	13.735746	14.095569
H	23.989705	13.955537	13.90948
C	21.979333	14.154563	13.169301

v

H	22.271132	14.696321	12.269725
C	16.451765	16.61253	20.640413
C	16.98641	15.379619	20.257035
H	16.95985	15.086302	19.207107
C	17.584122	14.52177	21.183363
C	17.613549	14.906547	22.537529
H	18.081321	14.252465	23.273836
C	17.053488	16.123609	22.926691
H	17.077056	16.414636	23.978362
C	16.475477	16.986645	21.993053
H	16.061253	17.946446	22.302123

$PtAg_{24}DMBT_{18}^{2-}$

349

Ag	15.338793	19.811962	17.273493
Ag	18.097825	20.962818	17.842104
Ag	19.857245	18.425739	18.801524
Ag	17.747447	16.098949	18.953449
Ag	13.831386	18.772406	19.56637
Ag	12.264645	20.865519	17.812253
Ag	13.743635	20.77739	14.998654
Ag	15.334239	17.689424	15.120843
Ag	16.805771	18.808226	19.583549
Ag	15.238087	19.008323	22.246282
Ag	12.160677	17.437615	21.735239
Ag	12.983921	15.995719	18.996981
Ag	15.376126	14.355408	18.537688
Ag	12.639618	13.032944	17.728815
Ag	10.79198	15.913332	17.02201
Ag	12.944924	18.076864	16.802248
Ag	16.807581	15.379898	16.226804
Ag	18.213428	13.248301	17.85327
Ag	17.1352	13.525433	20.772314
Ag	15.391187	16.441684	20.634551
Ag	13.888948	15.350871	16.190212
Ag	15.669501	15.136539	13.284329
Ag	18.335822	16.69739	14.094161
Ag	17.703872	18.155669	16.75156
Pt	15.33466	17.089175	17.894467
S	16.038462	22.249416	17.580419
S	20.489874	20.681779	18.115363
S	20.229485	16.047643	19.212069
S	12.332935	22.474183	15.994943
S	15.301599	19.656259	13.544595
S	11.62767	19.97354	19.976069

v

S 17.571508 19.601088 21.850027
S 13.096507 18.959057 23.384167
S 10.736779 16.158369 20.229603
S 14.833703 11.97748 17.866126
S 10.312065 13.550747 17.363308
S 10.450421 18.261321 16.452537
S 18.463539 11.756662 19.762324
S 15.631315 14.579001 22.357107
S 18.806918 13.985784 15.597826
S 13.38149 14.582513 13.827958
S 17.798786 15.287563 12.155046
S 19.836428 18.163999 15.369946
C 20.173348 11.845041 20.268093
C 21.1725 12.203866 19.351998
C 20.549835 11.440157 21.572541
C 22.518936 12.174482 19.703903
C 21.912536 11.422202 21.895049
C 19.534441 11.036987 22.603935
C 22.914773 11.786732 20.988425
C 24.364955 11.802461 21.396146
C 14.878572 10.522292 18.902588
C 15.638265 9.445709 18.413914
C 14.213554 10.387976 20.143372
C 15.746088 8.253624 19.128455
C 14.338381 9.174899 20.832894
C 13.393504 11.492786 20.733789
C 15.090832 8.095623 20.354481
C 15.18976 6.818018 21.149507
C 18.486738 12.620332 14.488233
C 17.220191 12.036565 14.360676
C 19.552505 12.141405 13.686509
C 16.992873 10.999354 13.456874
C 19.291716 11.099721 12.788623
C 20.932322 12.734635 13.760341
C 18.027042 10.513989 12.650496
C 17.793028 9.396947 11.663902
C 13.227729 12.861815 13.364903
C 12.928625 12.523701 12.023506
C 13.347737 11.836044 14.310953
C 12.778103 11.169378 11.693135
C 12.77924 13.573115 10.95944
C 13.195183 10.500256 13.953469
C 12.90974 10.139364 12.630937
C 12.779048 8.691986 12.230334
C 9.819892 12.809304 15.8166
C 9.520834 11.426713 15.767546

v

C 9.63901 13.589315 14.665583
C 9.058421 10.889834 14.559444
C 9.695514 10.539584 16.968153
C 9.176534 13.02655 13.479332
C 8.879148 11.660827 13.404677
C 8.426553 11.034009 12.111558
C 9.866644 18.278834 14.768941
C 8.555036 17.834187 14.472466
C 10.655357 18.810454 13.737992
C 8.106959 17.927636 13.147241
C 7.646754 17.272121 15.530074
C 10.177747 18.90256 12.435362
C 8.890933 18.45173 12.113618
C 8.364051 18.543708 10.705124
C 10.738266 22.498255 15.190429
C 10.61491 23.02613 13.883148
C 9.583797 22.091304 15.876
C 9.334844 23.104286 13.317887
C 11.808071 23.493536 13.098293
C 8.326818 22.185093 15.286483
C 8.179344 22.690837 13.989536
C 6.826167 22.747826 13.329254
C 11.380985 21.330188 21.109287
C 10.134588 21.365231 21.754534
C 12.336721 22.331176 21.395531
C 9.821945 22.372171 22.664346
C 11.989007 23.332752 22.311283
C 13.686277 22.34411 20.752082
C 10.747076 23.381878 22.955779
C 10.416749 24.500473 23.912549
C 17.585001 21.344131 22.244079
C 17.388503 22.325643 21.266574
C 17.853343 21.745889 23.577377
C 17.43911 23.681214 21.582944
C 17.897643 23.115286 23.864528
C 18.093955 20.740236 24.66839
C 17.690473 24.103465 22.891897
C 17.727181 25.567927 23.251053
C 20.986813 21.84153 19.381162
C 20.698795 23.201267 19.172109
C 21.754182 21.4686 20.509302
C 21.145558 24.181461 20.052161
C 22.177832 22.481102 21.382703
C 22.136979 20.045279 20.797429
C 21.890723 23.835121 21.185452
C 22.334769 24.875583 22.181549

v

C 20.883488 15.922498 20.866054
C 20.057404 15.677992 21.973391
C 22.281913 16.021155 21.059665
C 20.586237 15.538644 23.253324
C 22.782661 15.888461 22.361125
C 23.226766 16.250348 19.913952
C 21.965607 15.6494 23.470644
C 22.55398 15.501603 24.850144
C 16.387426 14.277676 23.952845
C 16.366422 12.951362 24.417171
C 16.946351 15.283478 24.774087
C 16.893533 12.608411 25.659829
C 17.463238 14.905324 26.022443
C 17.000071 16.72026 24.35065
C 17.455051 13.586016 26.490453
C 18.013839 13.245204 27.849211
C 13.398072 18.280202 25.008037
C 13.634738 19.171585 26.082848
C 13.366896 16.900642 25.260116
C 13.835589 18.630914 27.360655
C 13.66584 20.662731 25.888527
C 13.574518 16.395811 26.539922
C 13.813532 17.256186 27.618855
C 14.05805 16.711584 29.003129
C 16.309058 23.341886 16.18952
C 15.72462 24.630918 16.214235
C 17.09862 22.977313 15.087459
C 15.964631 25.492017 15.132383
C 14.865061 25.099994 17.354838
C 17.325622 23.859139 14.034576
C 16.759417 25.141396 14.036639
C 17.004551 26.107413 12.904621
C 20.167462 19.521735 14.256743
C 21.49035 20.024246 14.174255
C 19.180533 20.058796 13.417582
C 21.759132 21.036748 13.244786
C 22.599419 19.495499 15.04146
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C 20.783639 21.570447 12.393543
C 21.134221 22.647938 11.398688
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C 18.733776 16.954505 10.126187
C 16.501199 16.045187 9.829569
C 18.588518 17.575509 8.877308
C 20.020393 17.113082 10.88422
C 16.394068 16.662638 8.587354

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C	13.489642	19.452882	9.860385
C	13.658483	17.663146	11.616938
C	13.712392	20.731628	9.338117
C	13.230161	21.106814	7.958992
C	9.899416	14.761221	20.962313
C	8.606034	14.509604	20.471009
C	10.412389	13.938928	21.990423
C	7.825405	13.476076	20.977971
C	9.600218	12.903925	22.478524
C	11.773421	14.149142	22.57428
C	8.313104	12.647717	21.997314
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H	23.272173	12.465391	18.967749
H	22.198485	11.112138	22.905147
H	18.881411	10.230865	22.236966
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H	16.352613	7.436775	18.728048
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H	12.961493	11.190776	21.696843
H	12.56539	11.786709	20.06585
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H	15.990476	10.574432	13.37255
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H	21.617489	12.201204	13.086635
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H	16.656291	25.701846	11.941992
H	18.076263	26.330932	12.784036
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H	22.783306	21.41854	13.180077
H	22.727842	18.410555	14.911412
H	22.380491	19.655865	16.108687
H	23.549871	19.992451	14.799521
H	18.692527	21.440943	11.849289
H	21.747181	23.436215	11.862516
H	20.231445	23.121481	10.987884
H	21.712813	22.246142	10.549423
H	15.678671	15.436449	10.206663
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H	20.475516	16.138931	11.117742
H	19.867452	17.619153	11.851406
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H	15.480509	16.534812	8.000989
H	18.295761	18.472343	6.38445
H	16.722073	19.114109	6.896309
H	16.803767	17.578812	6.01839
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H	14.599062	17.116958	11.790997
H	13.062849	17.092947	10.891977
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H	12.873294	22.147016	7.922889
H	12.408549	20.454018	7.630324
H	14.036124	21.018448	7.211752
H	8.22315	15.136306	19.665321
H	6.827929	13.303273	20.566872
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H	11.847061	15.14368	23.048051
H	12.56375	14.127028	21.811282
H	12.002447	13.388363	23.331686
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Ag	17.690062	16.025576	18.964507
Ag	13.813106	18.752482	19.571884
Ag	12.215133	20.856664	17.801467
Ag	13.72279	20.770092	14.955794
Ag	15.32585	17.619247	15.071536
Ag	16.76561	18.796149	19.553022
Ag	15.216327	18.991638	22.259011
Ag	12.14181	17.379797	21.771006
Ag	12.985386	15.897262	19.009251
Ag	15.351624	14.312013	18.523036
Ag	12.615021	12.993862	17.706427
Ag	10.819503	15.891664	16.988331
Ag	12.963451	18.12479	16.71702
Ag	16.744938	15.327931	16.175299
Ag	18.180239	13.19257	17.814535
Ag	17.089713	13.482134	20.787864
Ag	15.354219	16.440296	20.638346
Ag	13.835604	15.319258	16.172949
Ag	15.630149	15.102483	13.257576
Ag	18.297787	16.701008	14.060428
Ag	17.646151	18.166052	16.730516
Pt	15.297584	17.054894	17.873132
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S	20.162009	16.025925	19.179871
S	12.315998	22.435857	15.982226
S	15.262086	19.607951	13.528447
S	11.611618	19.925422	19.936897
S	17.532214	19.564795	21.822005
S	13.070352	18.929827	23.363338
S	10.764578	16.124195	20.218337
S	14.801883	11.956114	17.845134
S	10.301607	13.550657	17.347918
S	10.486531	18.225769	16.434076
S	18.425193	11.758648	19.757562
S	15.59118	14.566597	22.32652
S	18.766699	13.97392	15.58388
S	13.349673	14.56432	13.813635
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S	19.763976	18.142791	15.366331
C	20.13855	11.846969	20.260032
C	21.138959	12.195807	19.341839
C	20.510277	11.437167	21.562939

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C 22.878679 11.769255 20.98124
C 24.325999 11.779092 21.39535
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C 15.60833 9.434748 18.406585
C 14.175627 10.375406 20.132232
C 15.709948 8.243465 19.121022
C 14.300385 9.163316 20.823639
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C 15.055708 8.085655 20.347582
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C 17.171568 12.02566 14.346752
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C 17.983089 10.501821 12.639299
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C 13.200091 12.840528 13.36154
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C 12.745209 8.675541 12.224661
C 9.810507 12.811244 15.794201
C 9.508949 11.429509 15.750002
C 9.628146 13.591336 14.643321
C 9.041288 10.892574 14.544536
C 9.678744 10.542034 16.9501
C 9.161834 13.025359 13.459515
C 8.861326 11.659981 13.388601
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References

[1]. Mortensen, J. J.; Larsen, A. H.; Kuisma, M.; Ivanov, A. V.; Taghizadeh, A.; Peterson, A.; Haldar, A.; Dohn, A. O.; Schäfer, C.; Jónsson, E. Ö.; Hermes, E. D.; Nilsson, F. A.; Kastlunger, G.; Levi, G.; Jónsson, H.; Häkkinen, H.; Fojt, J.; Kangsabanik, J.; Sødequist, J.; Lehtomäki, J.; Heske, J.; Enkovaara, J.; Winther, K. T.; Dulak, M.; Melander, M. M.; Ovesen, M.; Louhivuori, M.; Walter, M.; Gjerding, M.; Lopez-Acevedo, O.; Erhart, P.; Warmbier, R.; Würdemann, R.; Kaappa, S.; Latini, S.; Boland, T. M.; Bligaard, T.; Skovhus, T.; Susi, T.; Maxson, T.; Rossi, T.; Chen, X.; Schmerwitz, Y. L. A.; Schiøtz, J.; Olsen, T.; Jacobsen, K. W.; Thygesen, K. S. GPAW: An Open Python Package for Electronic Structure Calculations. *J. Chem. Phys.* 2024, **160** (9), 092503.

[2]. Enkovaara J; Rostgaard C.; Mortensen J. J.; Chen J.; Dułak M.; Ferrighi L.; Gavnholt J.; Glinsvad C.; Haikola V.; Hansen H. A.; Kristoffersen H. H.; Kuisma M.; Larsen A. H.; Lehtovaara L.; Ljungberg M.; Lopez-Acevedo O.; Moses P. G.; Ojanen J; Olsen T.; Petzold V.; Romero N. A.; Stausholm-Møller J.;

v

Strange M.; Tritsaris G. A.; Vanin M.; Walter M.; Hammer B.; Häkkinen H.; Madsen G. K. H.; Nieminen R. M.; Nørskov J. K.; Puska M.; Rantala T. T.; Schiøtz J.; Thygesen K. S.; Jacobsen K. W., Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method, *J. Phys. Condens. Matter.* 2010, **22**, 253202.

[3]. Perdew J. P.; Burke K.; Ernzerhof M., Generalized Gradient Approximation Made Simple*, Phys. Rev. Lett.*, 1996, **77**, 3865-3868.

[4]. L. G. AbdulHalim, M. S. Bootharaju, Q. Tang, S. Del Gobbo, R. G. AbdulHalim, M. Eddaoudi, D. E. Jiang and O. M. Bakr, *J. Am. Chem. Soc.*, 2015, **137**, 11970–11975.

[5]. Neumaier, M., Baksi, A., Weis, P., Schneider, E. K., Chakraborty, P., Hahn, H., Pradeep, T. and Kappes, M. M., *J. Am. Chem. Soc.*, 2021**, 143**, 6969–6980.

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