

Supporting Information

Monolayer Protected Noble Metal Clusters as Potential Standards for Negative Ion Mass Spectrometry

Ananya Baksi,[†] Papri Chakraborty,[†] Abhijit Nag, Debasmita Ghosh, Shridevi Bhat and Thalappil Pradeep*

DST Unit of Nanoscience and Thematic Unit of Excellence, Indian Institute of Technology Madras, Chennai, 600036

*Email: pradeep@iitm.ac.in

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Supporting Information 1

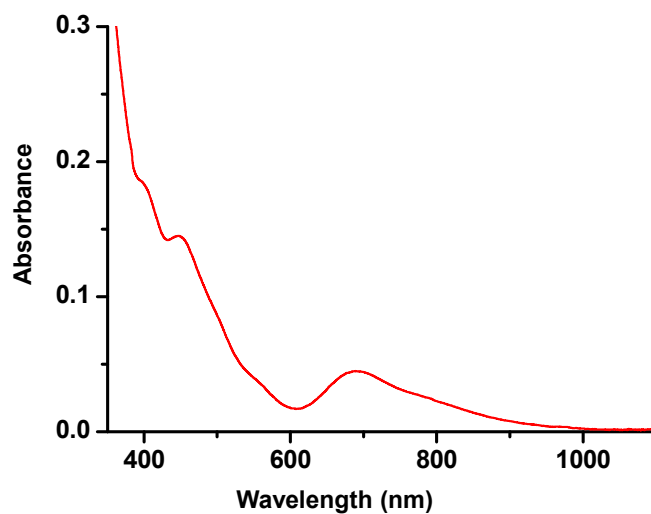


Figure S1. UV-vis spectrum of $[\text{Au}_{25}(\text{PET})_{18}]^-$ showing all the characteristic bands confirming the purity of the cluster.

Supporting Information 2

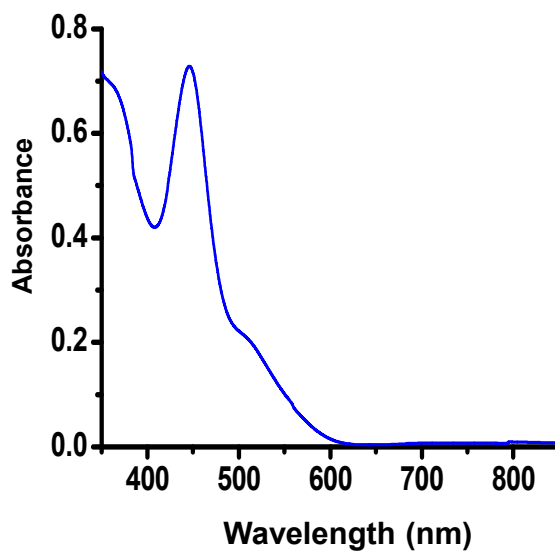


Figure S2. UV-vis spectrum of $[\text{Ag}_{29}(\text{BDT})_{12}(\text{TPP})_4]^{3-}$ showing all the characteristic bands confirming the purity of the cluster.

Supporting Information 3

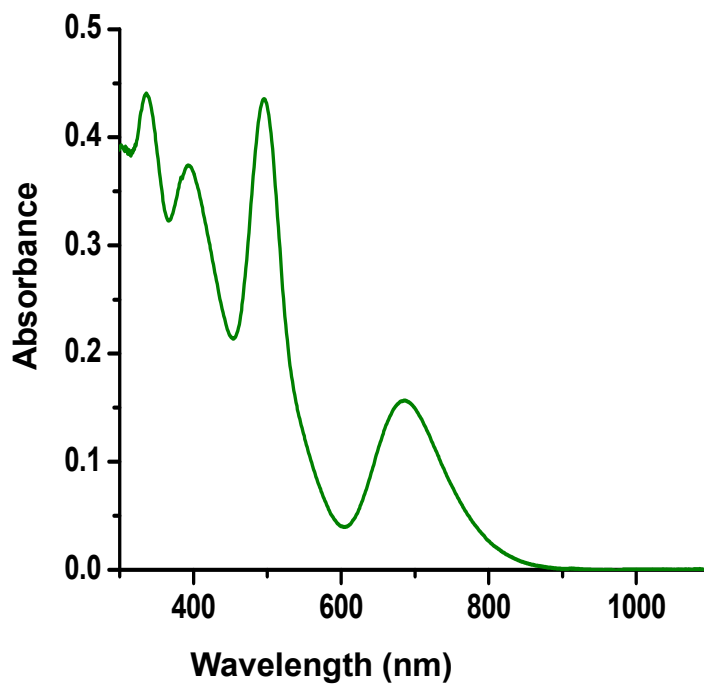


Figure S3. UV-vis spectrum of [Ag₂₅(DMBT)₁₈]⁻ showing all the characteristic bands confirming the purity of the cluster.

Supporting Information 4

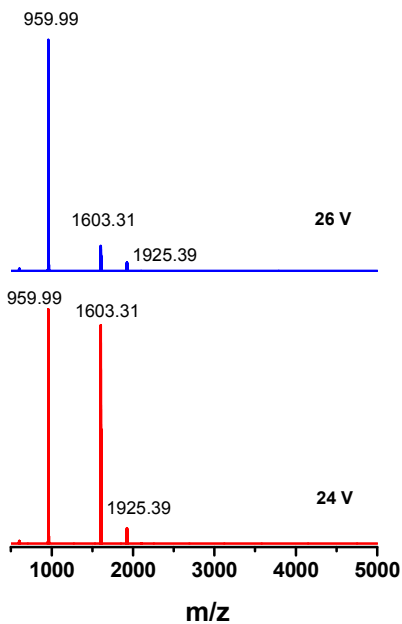


Figure S4. CID mass spectra of [Ag₂₉(BDT)₁₂(TPP)₄]³⁻ at CE 24 V and 26 V laboratory CE showing fragments. Exact masses of the fragments are given.

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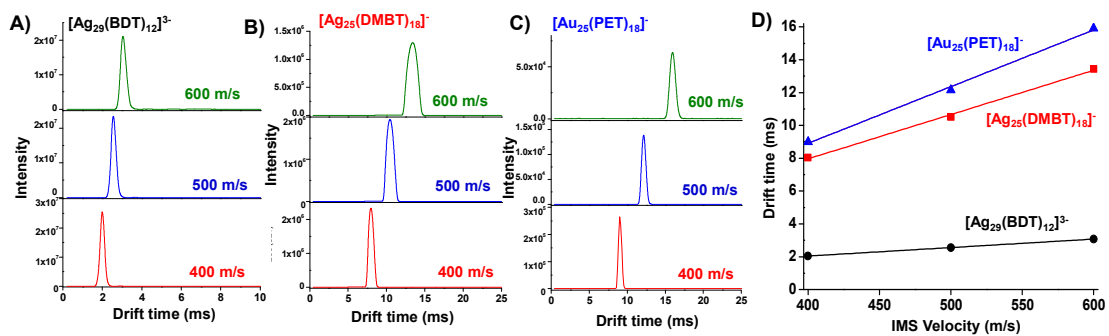


Figure S5. Drift time plots at different IMS velocity for A) $[\text{Au}_{25}(\text{PET})_{18}]^{-}$, B) $[\text{Ag}_{25}(\text{DMBT})_{18}]^{-}$ and C) $[\text{Ag}_{29}(\text{BDT})_{12}]^{3-}$ clusters. IMS velocity and drift time shows linear relation for the clusters as shown in D).

Supporting Tables

Table S1. Detail of the peak envelope of the isotope pattern with relative abundances and m/z positions for $[\text{Ag}_{29}(\text{BDT})_{12}]^{3-}$, $[\text{Ag}_{25}(\text{DMBT})_{18}]^{-}$ and $[\text{Au}_{25}(\text{PET})_{18}]^{-}$ clusters, respectively.

$\text{Ag}_{29}(\text{BDT})_{12}^{3-}$		$\text{Ag}_{25}(\text{DMBT})_{18}^{-}$		$\text{Au}_{25}(\text{PET})_{18}^{-}$	
m/z	Relative abundance	m/z	Relative abundance	m/z	Relative abundance
1597.98	1.36	5151.39	1.74	7390.93	42.79
1598.32	1.23	5152.39	2.37	7391.93	75.31
1598.65	3.81	5153.39	5.02	7392.93	100
1598.98	3.38	5154.39	6.53	7393.93	97.96
1599.32	9.10	5155.39	12.11	7394.93	81.56
1599.65	7.94	5156.39	15.02	7395.93	58.39
1599.98	18.79	5157.39	24.75	7396.93	37.35
1600.32	16.09	5158.39	29.28	7397.93	21.58
1600.65	33.78	5159.39	43.37	7398.93	11.44
1600.98	28.36	5160.39	48.88	7399.93	5.615
1601.32	53.29	5161.39	65.66	7400.93	2.56
1601.65	43.80	5162.39	70.42	7401.93	1.10
1601.98	74.13	5163.39	86.42		
1602.32	59.60	5164.39	88.10		
1602.65	91.34	5165.39	99.31		
1602.98	71.73	5166.39	96.12		
1603.32	100	5167.39	100		
1603.65	76.59	5168.39	91.77		
1603.98	97.51	5169.39	88.42		
1604.32	72.73	5170.39	76.83		
1604.65	84.85	5171.39	68.76		
1604.98	61.53	5172.39	56.50		
1605.32	65.96	5173.39	47.07		
1605.65	46.42	5174.39	36.51		
1605.98	45.84	5175.39	28.36		
1606.32	31.26	5176.39	20.73		
1606.65	28.50	5177.39	15.03		
1606.98	18.78	5178.39	10.34		
1607.32	15.84	5179.39	7.00		
1607.65	10.07	5180.39	4.53		
1607.98	7.87	5181.39	2.86		
1608.32	4.81	5182.39	1.73		
1608.65	3.49	5183.39	1.02		
1608.98	2.05				
1609.31	1.38				

Table S2. Assignment of the fragments obtained in the MS/MS spectra of A) $[\text{Ag}_{25}(\text{DMBT})_{18}]^-$ and B) $[\text{Ag}_{29}(\text{BDT})_{12}]^{3-}$ clusters.

A) Assignment of the fragments of $[\text{Ag}_{25}(\text{DMBT})_{18}]^-$

m/z	Assignment of the peaks
5167.39	$[\text{Ag}_{25}(\text{DMBT})_{18}]^-$
4431.59	$[\text{Ag}_{22}(\text{DMBT})_{15}]^-$
4185.65	$[\text{Ag}_{21}(\text{DMBT})_{14}]^-$
1362.94	$[\text{Ag}_5(\text{DMBT})_6]^-$
627.09	$[\text{Ag}_2(\text{DMBT})_3]^-$
381.12	$[\text{Ag}(\text{DMBT})_2]^-$

B) Assignment of the fragments of $[\text{Ag}_{29}(\text{BDT})_{12}]^{3-}$

m/z	Assignment of the peaks
1603.31	$[\text{Ag}_{29}(\text{BDT})_{12}]^{3-}$
1925.39	$[\text{Ag}_{24}(\text{BDT})_9]^{2-}$
959.99	$[\text{Ag}_5(\text{BDT})_3]^-$