IIT MADRAS
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Technology Transfer Office
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Industrial Consultancy & Sponsored Research (IC&SR)

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

IITM Technology Available for Licensing

Problem Statement

- **Mass Spectrometry (MS)** is vital for identifying and characterizing molecules.
- MS is crucial in materials science for **high-mass molecule characterization.** Challenges exist in **ionizing molecules** in negative ion mode, especially for **high-mass compounds**.
- **Lack of proper standards** in negative ion mode hampers signal quality, peak shape, & intensity. Standards are needed in biology for **sample understanding and instrument calibration**.
- Positive ion standards are available for **bigger proteins and peptides.** Few negative ion standards are available **beyond m/z 3000**. High concentrations of cesium-based salts are required for **traditional calibration methods**.

The present patent introduces **atomically precise clusters** as calibration standards for **negative ion mass spectrometry**.

Technology Category/ Market

Categories: Chemistry & Chemical Analysis, Advance Material & Manufacturing

Applications: Calibrating Mass Spectrometers, Biological and Chemical Research, Proteomics, Ion Mobility Calibration, Molecular Structure Analysis, Metabolomics, Research, Development & Quality Control, Environmental Analysis, Drug Discovery

Industry: Pharmaceutical Industry, Chemical Industry, Forensic & Materials Science, Healthcare

Market: The global nanomaterials market was valued at **$16.3 B** in **2021,** and is projected to reach **$62.8 B** by **2031,** growing at **14.6% CAGR from 2021 to 2031.**

Intellectual Property

IITM IDF Ref. 1732; Patent No: 350803

TRL (Technology Readiness Level)

TRL-4, Proof of Concept & validated in Lab

Technology

The present patent introduces a **Monolayer Protected Noble Metal Clusters as Standards for Negative Ion Mass Spectrometry**.
It discloses a **method** for **calibrating mass spectrometer** in the negative ion mode and in the high mass range, the said method comprises:

- **Dissolving atomically precise monolayer protected metal cluster in a solvent, that is dicholoromethane (DCM) or dimethylformamide (DMF);**
- **Serial dilution of the dissolved metal cluster to achieve 1 µg/mL cluster concentration;**
- **Directly infusing 1 µg/mL of cluster concentration to a MS instrument with a flow rate of 10 µL/min**

wherein, 1 µg/mL conc. of monolayer protected metal cluster calibrates a wide spectral of mass range of 1-100 kDa with maximum signal to noise ratio.

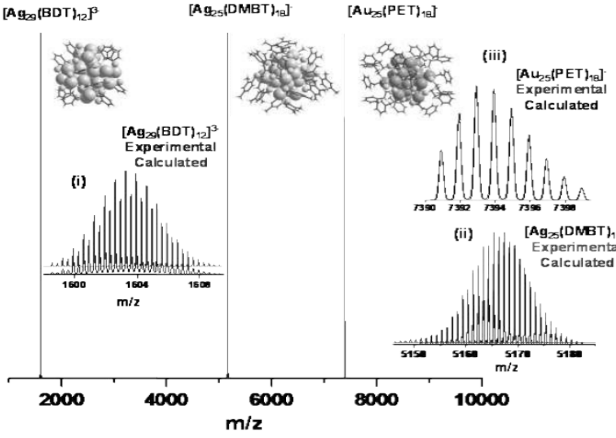

FIG 1 shows **mass spectra** of **[Ag29(BDT)12]3-, [Ag25(DMBT)18]-, and [Au25(PET)18]- in negative ion mode.** They serve as reliable standards for m/z calibration, accurately matching their calculated isotope patterns. Cluster structures are depicted near their molecular ion peaks.

Refer FIG 2 and 3.

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

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Key Features / Value Proposition

- The clusters are selected from **atomically precise noble metals of gold, silver, platinum, palladium, iridium, copper or their alloys with precise composition.**
- The **atomically precise metal clusters** $[Ag_{29}(S2R)_{12}]^{3-}$, $[Ag_{25}(SR)_{18}]^{-}$ and $[Au_{25}(SR)_{18}]^{-}$ are $\mathbf{[Ag_{29}(BDT)_{12}]^{3-}}$, $\mathbf{[Ag_{25}(DMBT)_{18}]^{-}}$ and $\mathbf{[Au_{25}(PET)_{18}]^{-}}$ respectively**.**
- The metal clusters calibrates **ion mobility mass spectrometry (IMS) in negative ion mode** for high mass range up to **m/z 10.**
- The metal cluster monomers and higher aggregates are used to **calibrate collision cross sections (CCSs) for negative ions of higher mass.**
- Similar **monolayer protected metal clusters** are used for calibrating in **positive ion mode** either in **presence or absence of ionization enhancers**.
- The metal clusters are fragmented to well defined **daughter ions** by **tandem mass spectrometry** to calibrate the **mass spectrometer in MS/MS mode.**

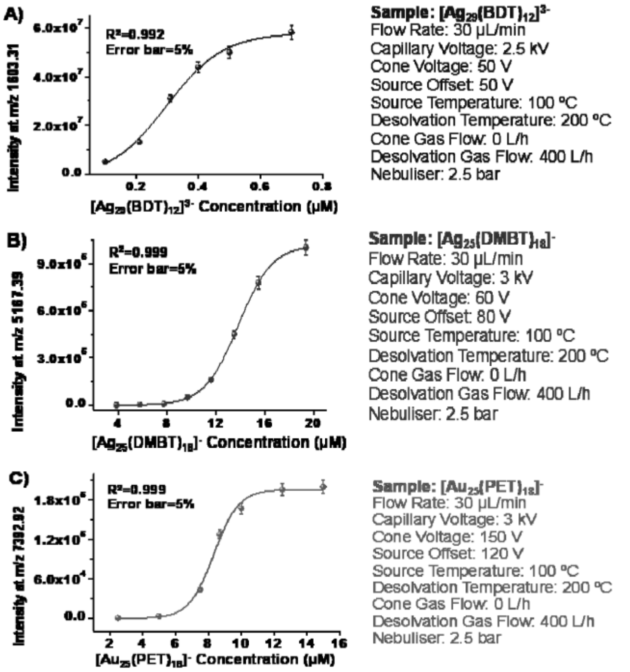
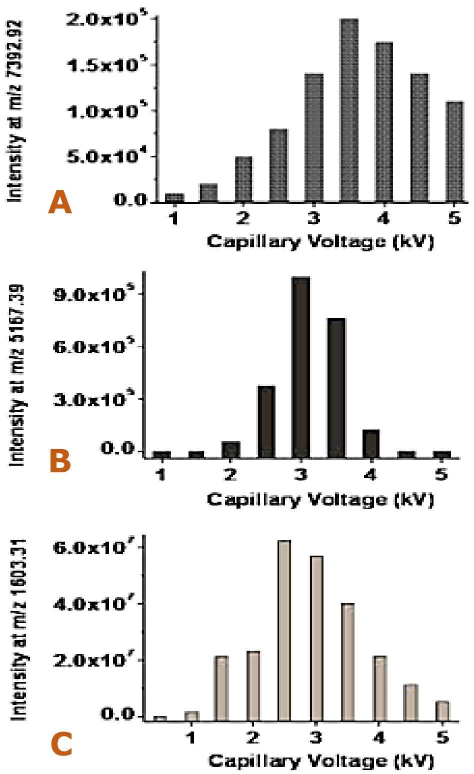
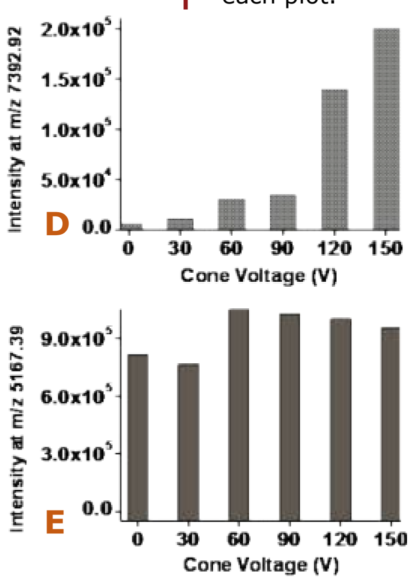


FIG 2 Concentration vs. intensity of
A) [Ag29(BDT)12]3-,
B) [Ag25(DMBT)18]-
C) [Au25(PET)18]-
Optimized experimental conditions are listed along with each plot.





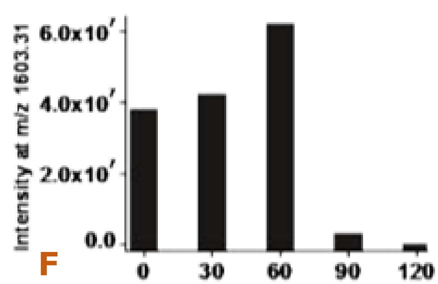


FIG 3 Capillary voltage vs. intensity of cluster ion is plotted for :
A) [Au25(PET)18]-,
B) [Ag25(DMBT)18]- and
C) [Ag29(BDT)12]3-.
Dependence of cone voltage is shown in **D-F** for respective ions.

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