Electronic supplementary information (ESI):

Towards atomically precise luminescent Ag$_2$S clusters separable by thin layer chromatography

C. K. Manju, Jyoti Sarita Mohanty, Depanjan Sarkar, Sudhakar Chennu and Thalappil Pradeep[a]*

*DST Unit of Nanoscience (DST UNS) and Thematic Unit of Excellence,
Department of Chemistry, Indian Institute of Technology Madras,
Chennai 600036, India.*

Table of contents

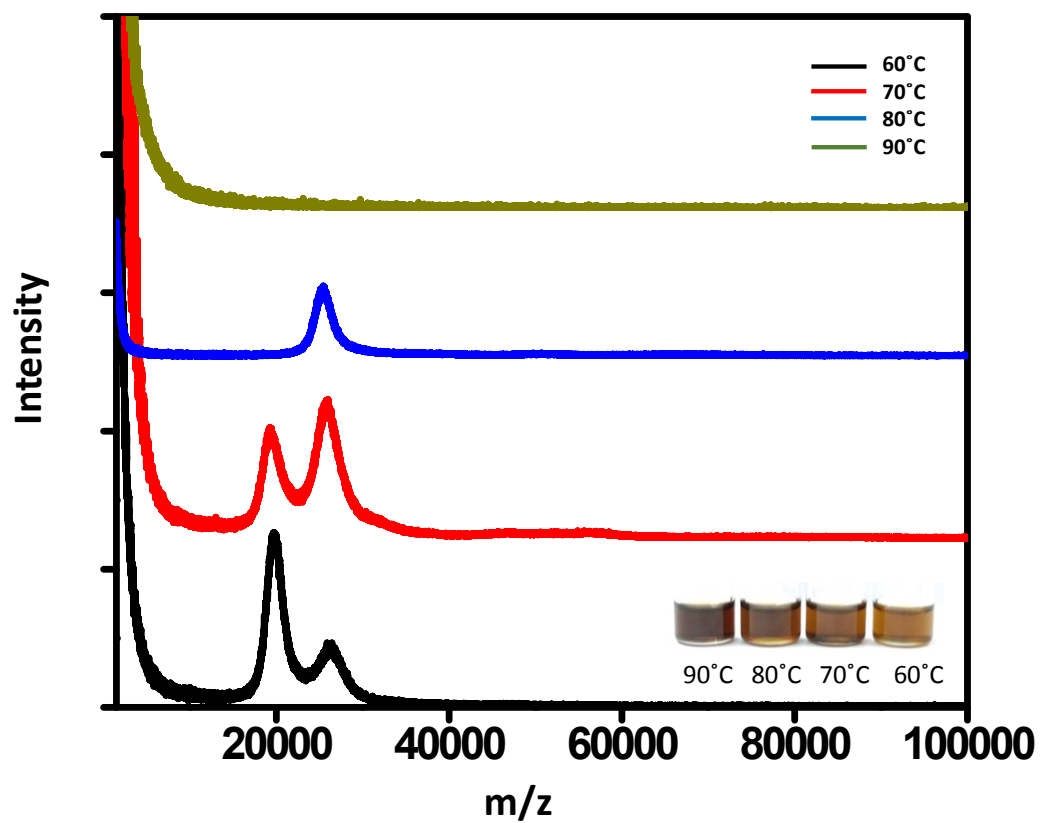# Supporting information 1

Fig. S1. Full range MALDI MS spectra of Ag_2S clusters synthesized at different temperature.
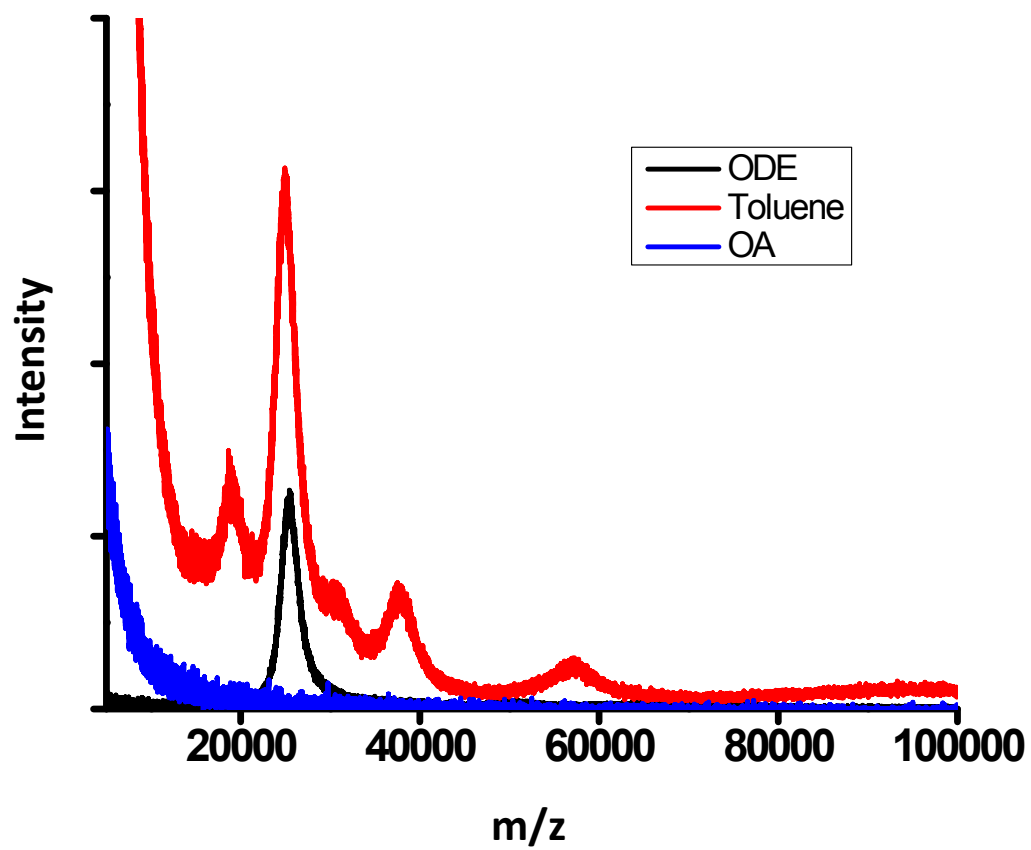
Supporting information 2

Fig. S2 MALDI MS of solvent dependent Ag_2S cluster formation. Octadecene (ODE) is only one species. Use of toluene gives multiple population and oleylamine (OA) resulted in bigger quantum dots.
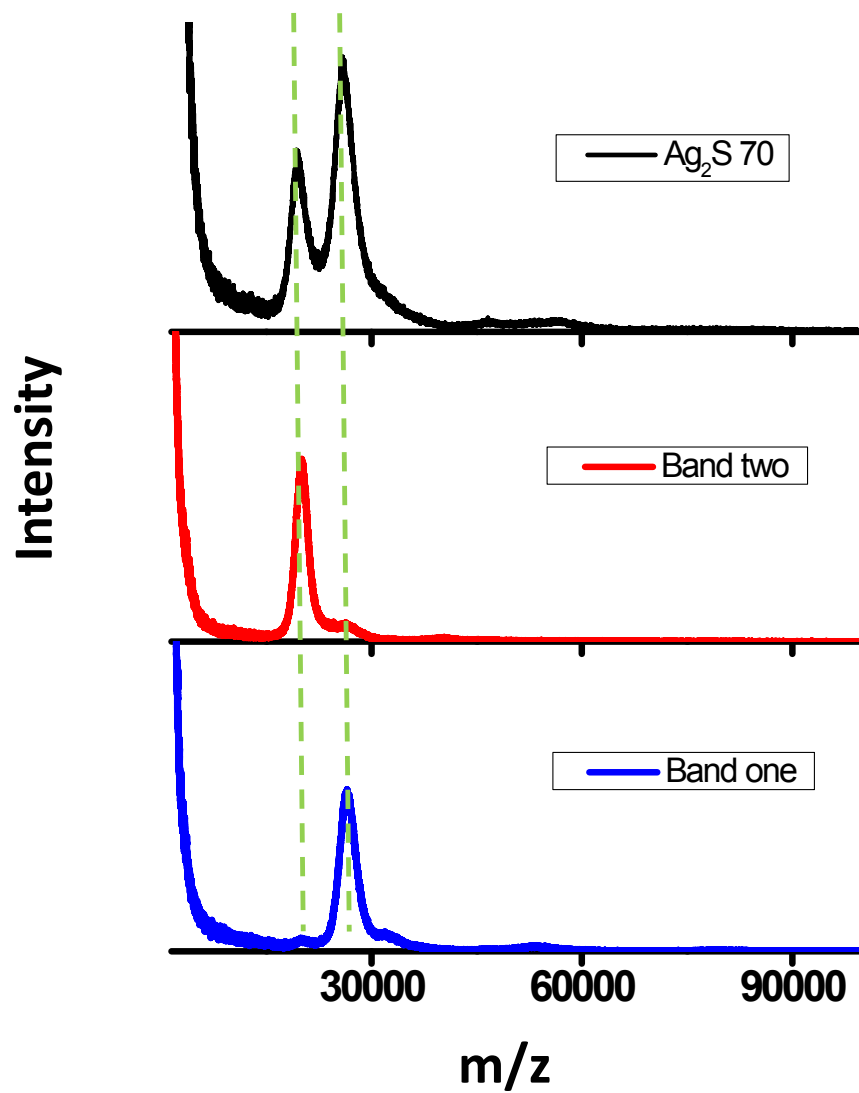
Supporting information 3

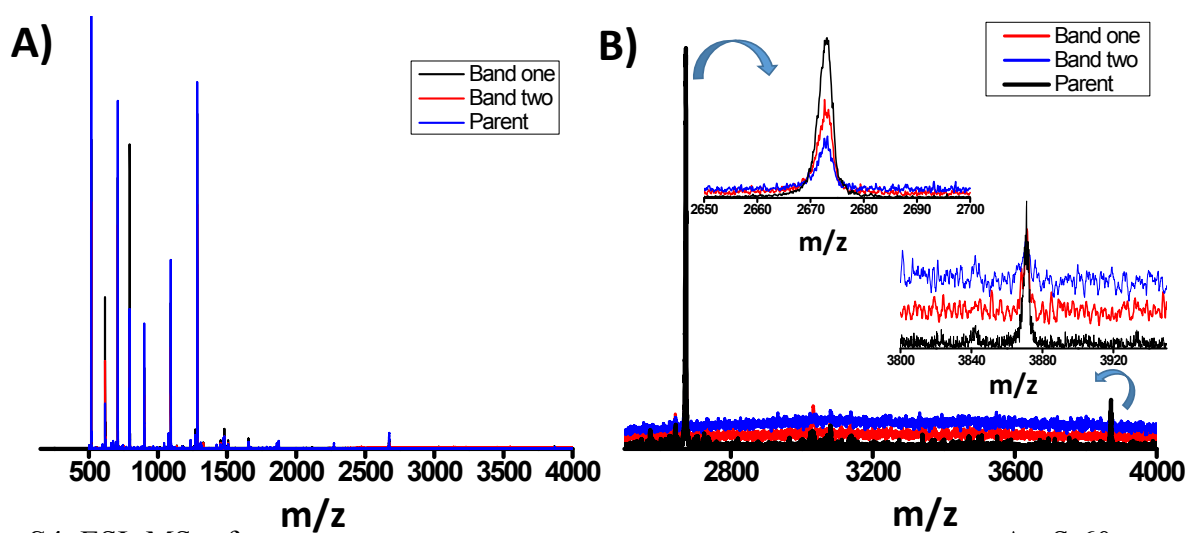**Fig. S3** MALDI MS of parent Ag_2S-70 and TLC separated bands.

Supporting information 4

Fig. S4 ESI MS of Ag$_2$S-60 and TLC separated clusters. Cesium acetate was used as an ionization enhancer as the cluster was not having any charge. (A) Shows full range mass spectra were cesium clusters are seen in the lower range (below 2000 m/z). (B) MS shows cluster fragments in the positive mode. Specific regions are expanded in the inset.
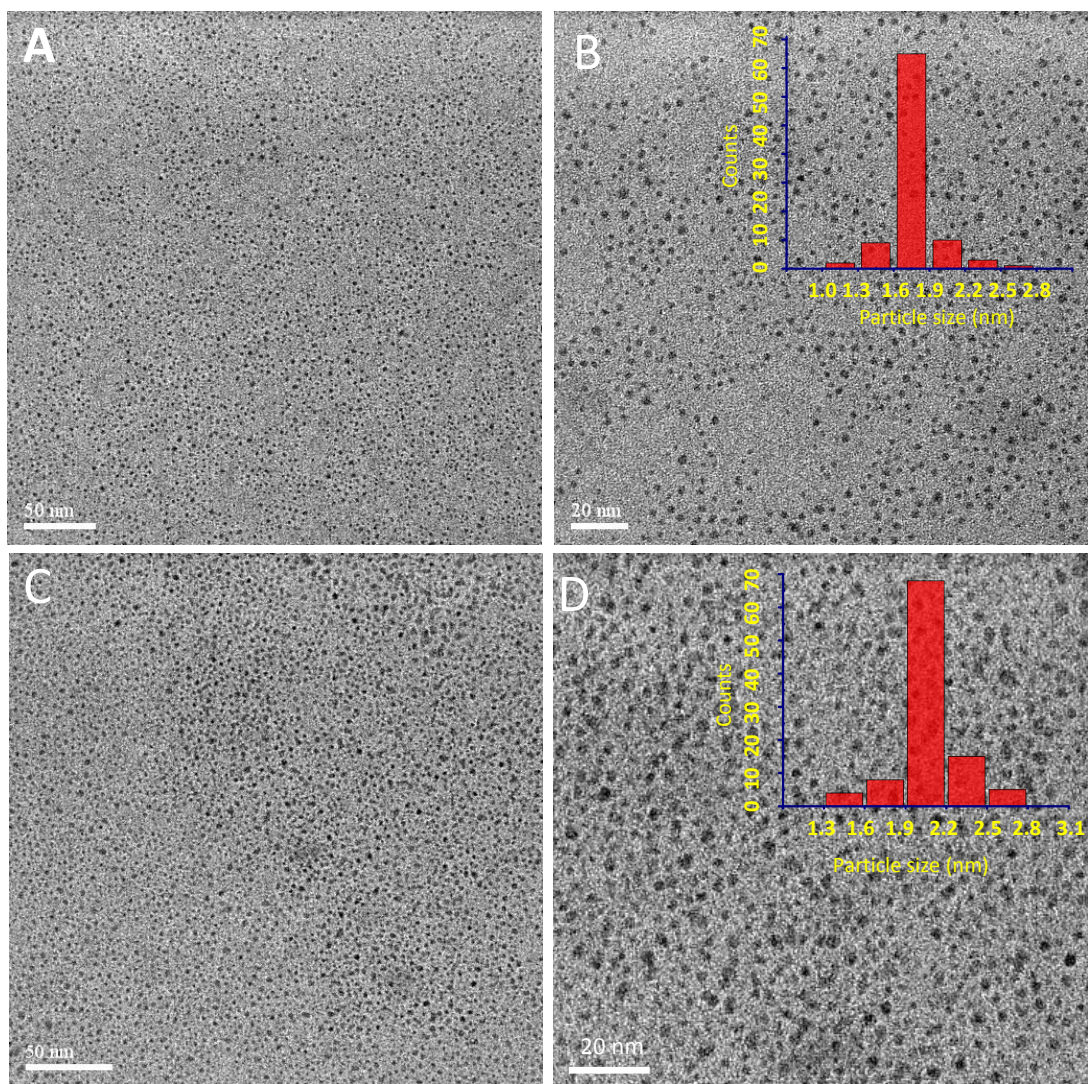
Supporting information 5

Fig. S5 TEM images of TLC separated Ag$_2$S-60 clusters. (A) and (B) Band two and (C) and (D) band one, at different magnifications.
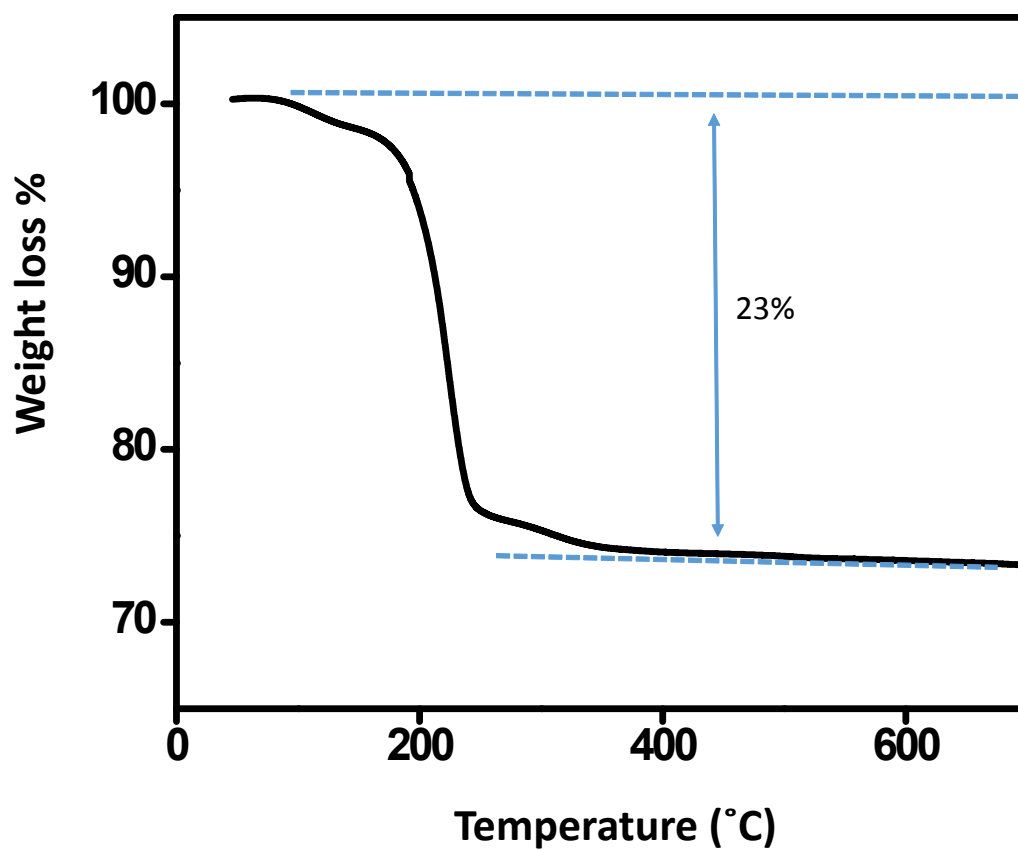
Supporting information 6

Fig. S6 TG data of Ag_2S-80 showing 23% weight loss due to the protecting BBSH group.

Supporting information 7

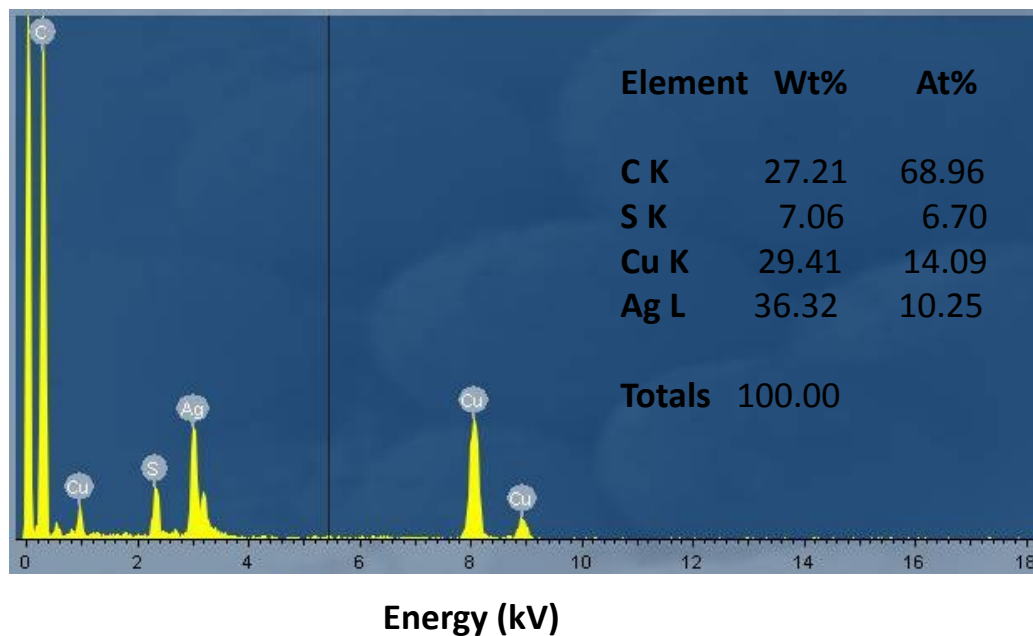| Element	Wt%	At%
C K	27.21	68.96
S K	7.06	6.70
Cu K	29.41	14.09
Ag L	36.32	10.25
Totals	100.00	

Energy (kV)

Fig S7. EDS spectrum of purified Ag_2S-80 cluster. Ag:S ratio of 1:0.65.

Supporting information 8

Jacobian correction:

This uses the equations

$E = hc/\lambda$

$f(E) \, dE = f(\lambda) \, d(\lambda)$

$f(E) = f(\lambda) \, (dE/d\lambda) = f(\lambda) \, (d/dE)(hc/E)$

$\qquad = f(\lambda) \, (hc/E^2)$

The factor (hc/E^2), known as the Jacobian factor, is used to scale the signal values along with wavelength conversion [wavelength (in nm) = 1239.8/(energy (eV))]. Normally, it is plotted by multiplying the absorbance value with the factor $1/W^2$, where W is the value in electronvolts corresponding to the wavelength in nanometers

Supporting information 9

Cluster assignment:

MALDI MS peak for Ag_2S-80 = 25450 Da

TG showed 23% weight loss.

This weight loss is due to organic ligand.

$$23\% \text{ of } 25450 = (23*25450)/100$$

$$= 5854 = \text{Total ligand mass}$$

$$\text{Mass of one SBB ligand} = 179.41$$

$$\text{No of ligands} = 5854/179.41$$

$$\sim 32$$

Cluster core mass is calculated by subtracting the total ligand mass from cluster mass

$$\text{This is} = 25450\text{-}5854 = 19596 \text{ Da}$$

This cluster core mass can contain 79 Ag_2S units

$$\text{Mass of } Ag_2S = 248$$

$$19596/248 \approx 79$$

From this, the cluster core can be assigned as $Ag_{158}S_{79}$. Hence the total molecular formula may be given as $(Ag_{158}S_{79})SBB_{32}$. This is in agreement with the Ag:S ratio of 1:0.65 obtained from EDS measurement.