S_4N_4 as an intermediate in Ag_2S nanoparticles synthesis

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Supporting information

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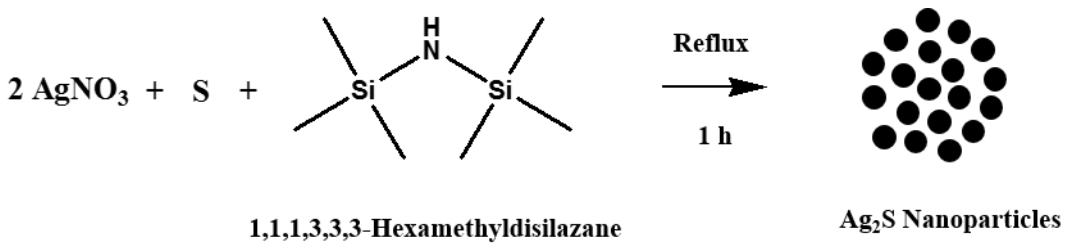
Supplementary information



***Scheme S1**: Synthesis of Ag_2S nanoparticles*

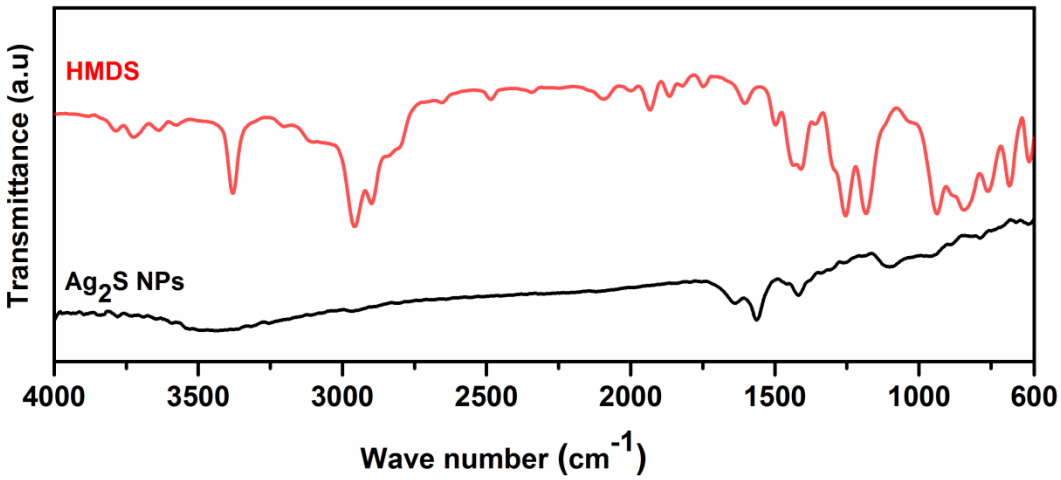


***Figure S1:** Stacked IR plot of Ag_2S nanoparticles along with HMDS (capping agent). Absence of organic peaks explaining complete removal of the capping agent on surface of the NPs. Observed peaks in the spectra were adsorbed water and carbon dioxide molecules.*

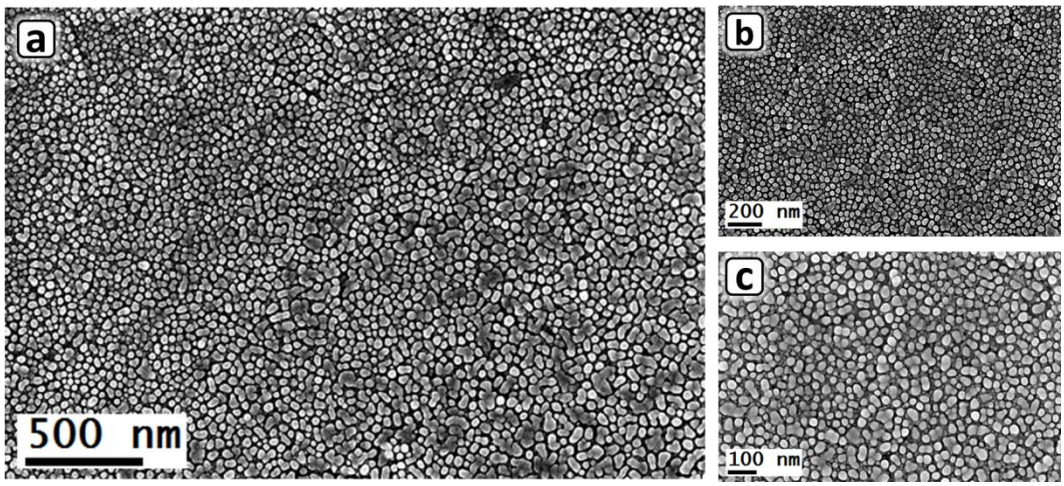


Figure S2: *Large area scanning electron micrographs of Ag_2S NPs. The particles were spherical and distributed uniformly on substrate. Due to resolution limits of FESEM, particles appeared as agglomerated.*

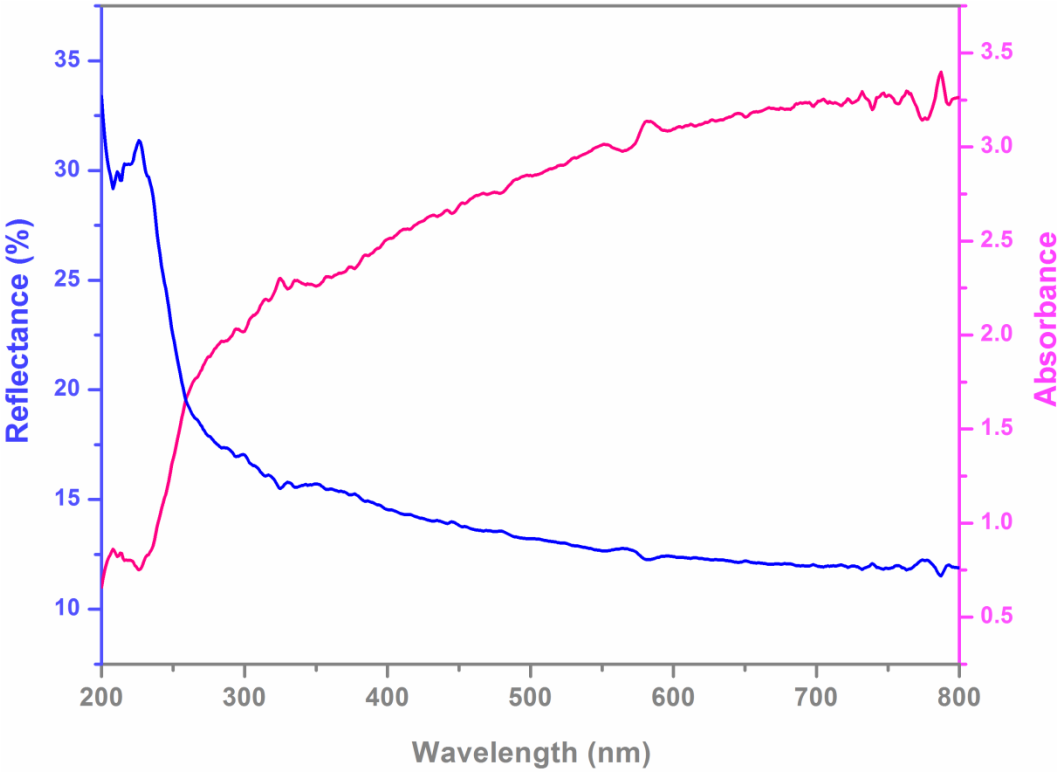


Figure S3: *(a) Solid state UV spectrum of Ag_2S nanoparticles. Ag_2S nanoparticles exhibited broad absorption .*

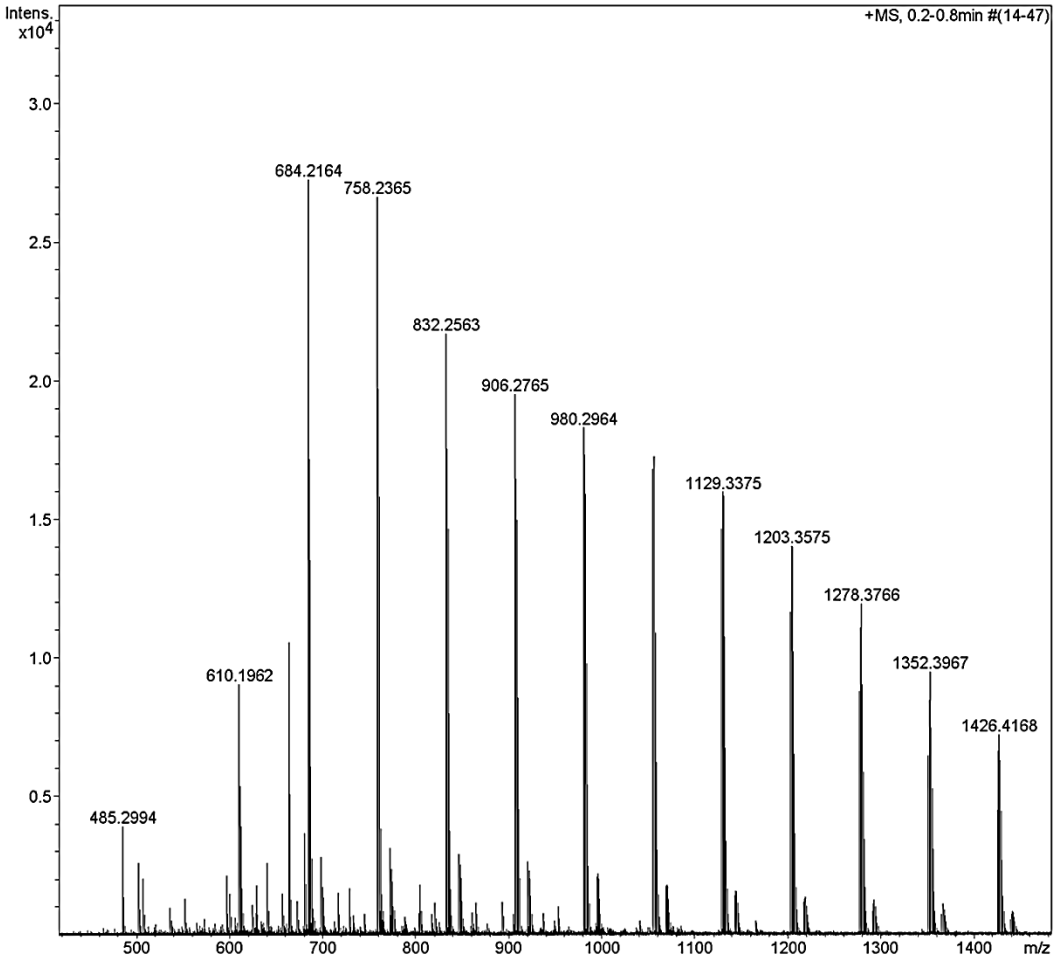


Figure S4: *Full range spectrum of S-N polymer. Polymeric pattern with repeating unit of S-N-Si found*

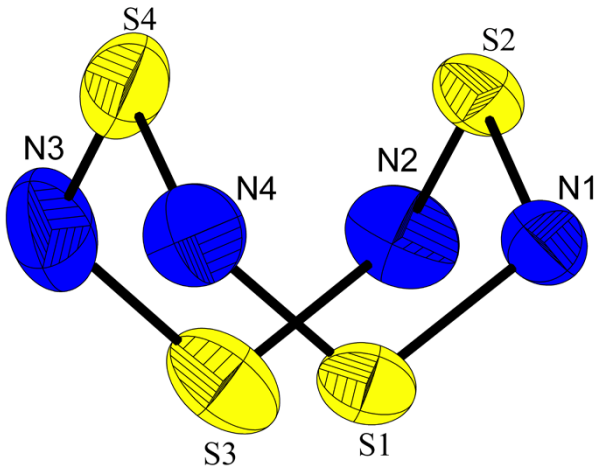


Figure S5: *ORTEP diagram and refinement details of S_4N_4 crystal* ***(CCDC 961232)***

Parameters	Value
Empirical formula	S_4N_4
Color	Orange
Formula weight	184.28
Crystal System	Monoclinic
Space group	P 1 21/n 1
a (Å)	8.7232(6)
b (Å)	7.1849(6)
c (Å)	c = 8.8033(5)
α (°)	90
β (°)	92.428(6)
γ (°)	90
V (Å^3)	551.25(7)
T (K)	298

Z	4
μ (mm^{-1})	1.601
ρ_c ($Mg\ m^{-3}$)	2.220
F(000)	368
Size (mm^3)	0.20 × 0.20 × 0.15
θ range (°)	3.22 to 26.01
hkl Index ranges	–9 < = h < = 10 –4 < = k < = 8 –10 < = l < = 10
Reflections collected / unique	1982 / 1080 R_{int} = 0.0208
Data completeness (%)	99.9
Transmission (max/min)	0.7952 / 0.7401
Data / restraints / parameters	1080 / 0 / 74
Goodness-of-fit on F^2	1.092
Final R indices [I > 2σ (I)]	R_1 = 0.0310 wR_2 = 0.0786
R indices (all data)	R_1 = 0.0332 wR_2 = 0.0811
Largest diff. peak / hole ($e.Å^{-3}$)	0.305 / –0.378

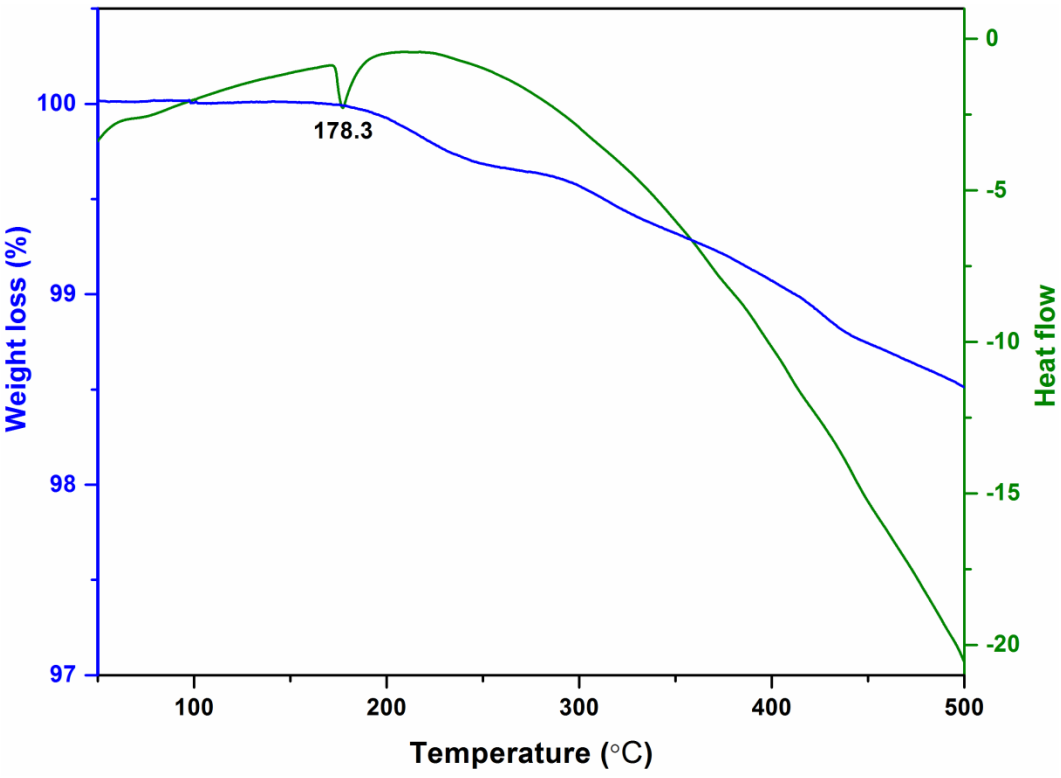


***Figure S6**: TGA/DTA curves of tetrasulfur tetranitride. S_4N_4 was melted at 178 ℃ and then decomposed.*

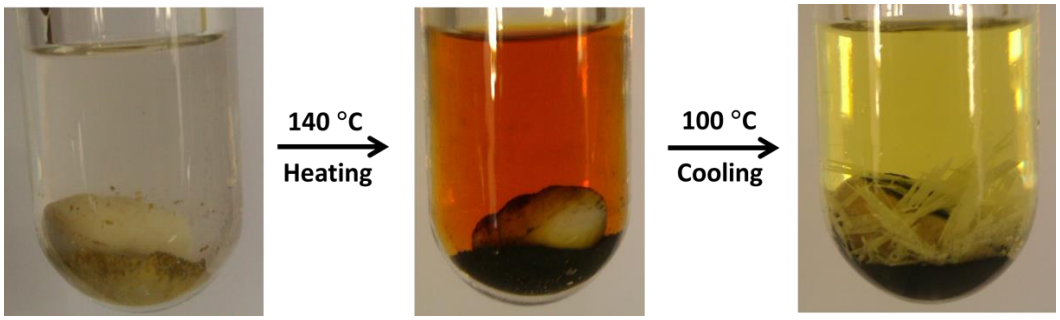


***Figure S7:** Photographs of thermochromic S_4N_4 formation. Reaction mixture (shown with pellet) was colorless at initial and changed to red and yellow after temperature variation. In the higher stoichiometric ratio of sulfur in the reaction, color change was apparent.*