

Supplementary Material for New Journal of Chemistry-2014

Influence of ligand environment on the structure and properties of silver (I) dithiocarbamate cluster-based coordination polymers and dimmers

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Supporting information

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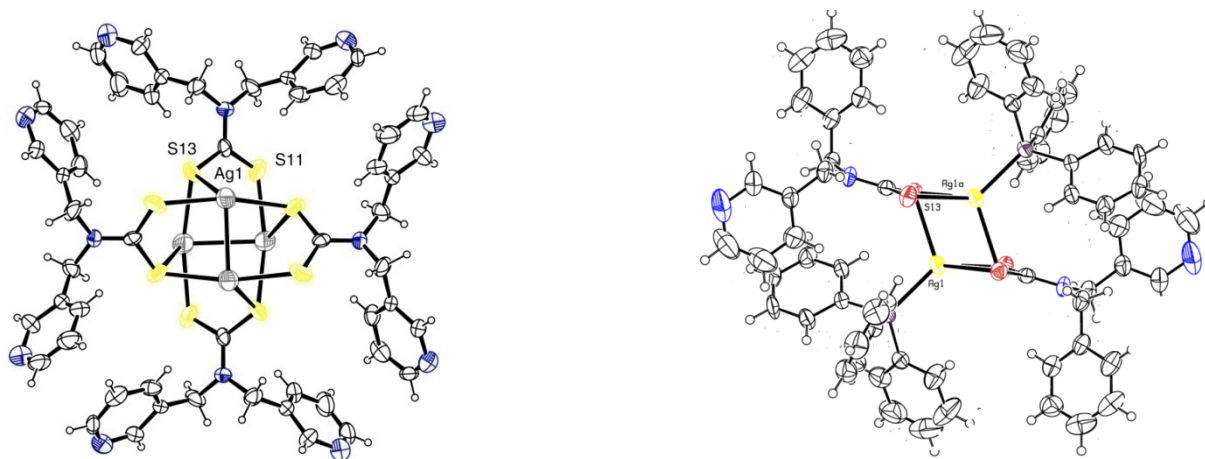


Fig. S1 Structure of **2** and **3** with ellipsoids at 30, 50% probability respectively.

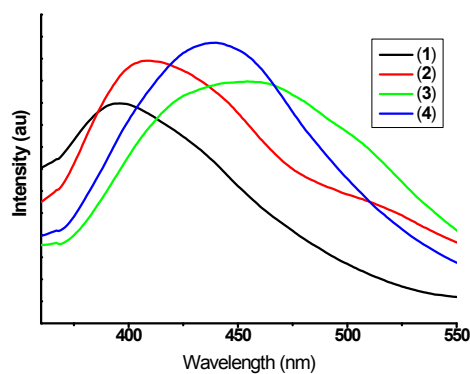


Fig. S2 Emission spectra of **1-4** ($\lambda_{\text{ex}} \sim 320$ and 300 nm) in the solid phase.

Table S1. Selected Bond Lengths (\AA) and Angles ($^\circ$) for complexes **3** and **4**.

	3	4
Ag(1)-P(1)	2.4224(11)	2.4126(10)
Ag(1)-S(11)	2.6187(12)	2.6280(11)
Ag(1)-S(13)\$1	2.6669(9)	2.6830(10)
Ag(1)-S(13)	2.7577(10)	2.7227(11)
Ag(1)-Ag(1)\$1	3.0104(6)	3.0035(6)
P(1)-Ag(1)-S(11)	130.52(4)	130.80(4)
P(1)-Ag(1)-S(13)\$1	117.24(4)	117.38(4)
S(11)-Ag(1)-S(13)\$1	103.65(3)	101.70(3)
P(1)-Ag(1)-S(13)	115.87(3)	117.30(3)
S(11)-Ag(1)-S(13)	67.02(3)	67.35(3)
S(13)-Ag(1)-S(13)\$1	112.61(2)	112.50(3)
P(1)-Ag(1)-Ag(1)\$1	143.62(3)	145.76(3)
S(11)-Ag(1)-Ag(1)\$1	81.46(3)	80.34(3)
S(13)\$1-Ag(1)-Ag(1)\$1	57.74(2)	56.88(2)
S(13)-Ag(1)-Ag(1)\$1	54.87(2)	55.62(2)
C(12)-S(11)-Ag(1)	89.15(16)	87.99(13)
C(12)-S(13)-Ag(1)\$1	98.41(11)	97.06(12)
C(12)-S(13)-Ag(1)	84.15(14)	84.53(13)
Ag(1)-S(13)-Ag(1)\$1	67.39(2)	67.50(3)

\$1 Symmetry element \$1 $-x, 2-y, -z$

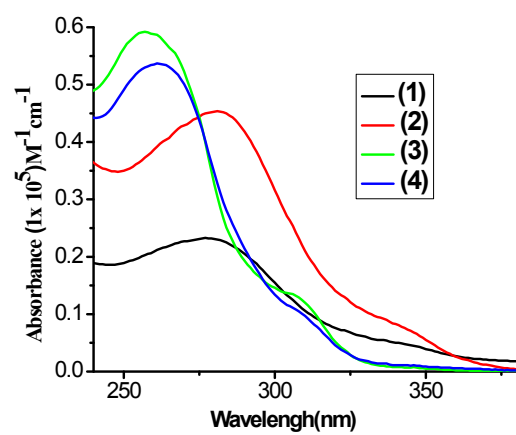


Fig. S3 UV-Vis. spectra of 1-4 in CH_2Cl_2 solution.

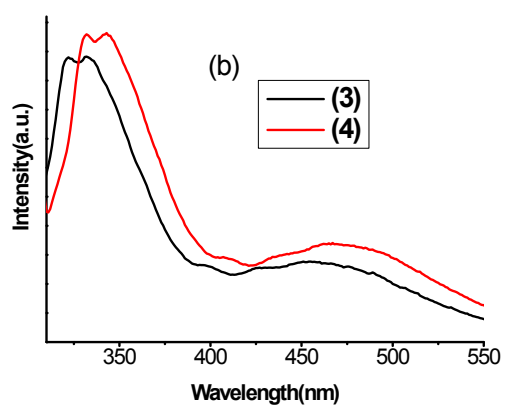
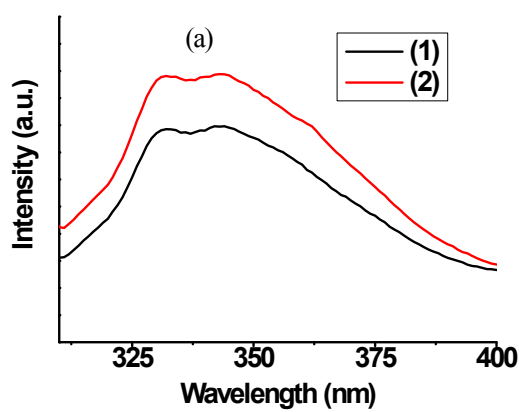


Fig. S4 (a, b) Emission spectra of (1-4) in CH_2Cl_2 solution ($\lambda_{\text{exc}} = 300$ nm).

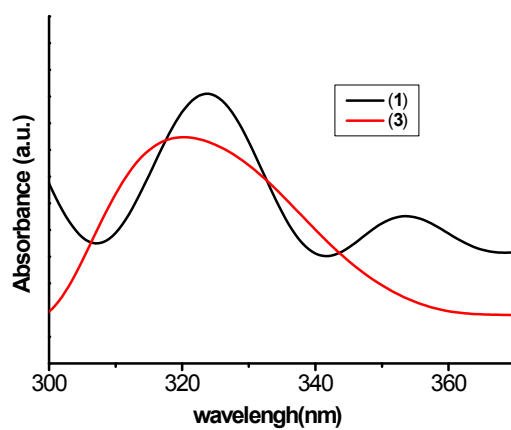


Fig. S5 Solid phase (nujol mull) UV-Vis. spectra of **1** and **3**.

Table S2. Pyrolysis and TGA results for the complexes.

Compound	T °C in TGA	Residue wt. observed (calcd.) (%)	Expected decomposition product of
1	207-401	32.5(32.4)	Ag ₂ S
2	213-405	33.4(32.3)	Ag ₂ S
3	Above 415	24.2(19.17)	Ag ₂ S
4	417-465	21.3 (19.16)	Ag ₂ S

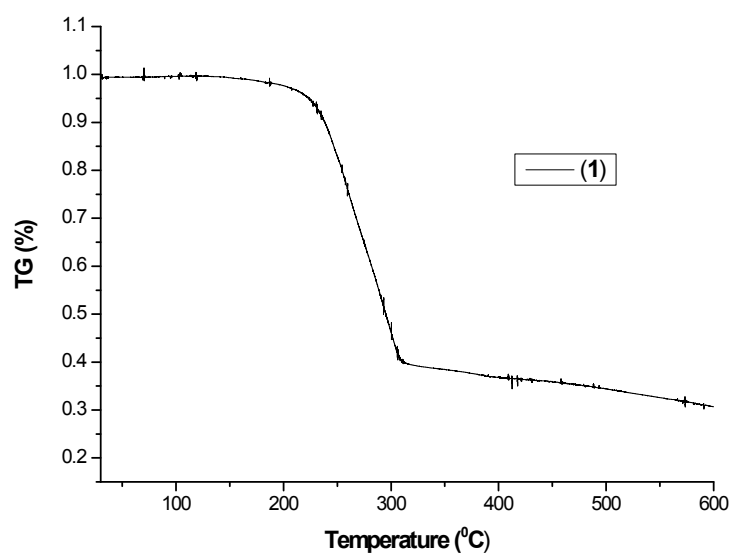


Fig. S6 thermogravimetric (TG) trace of 1.

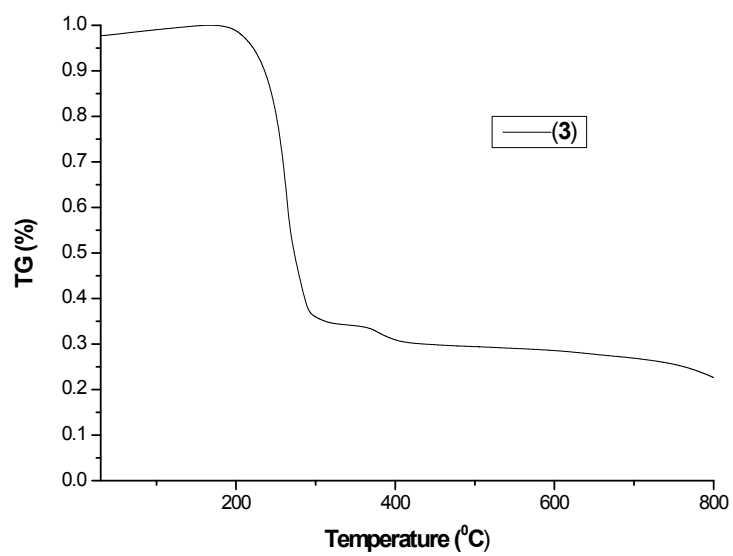
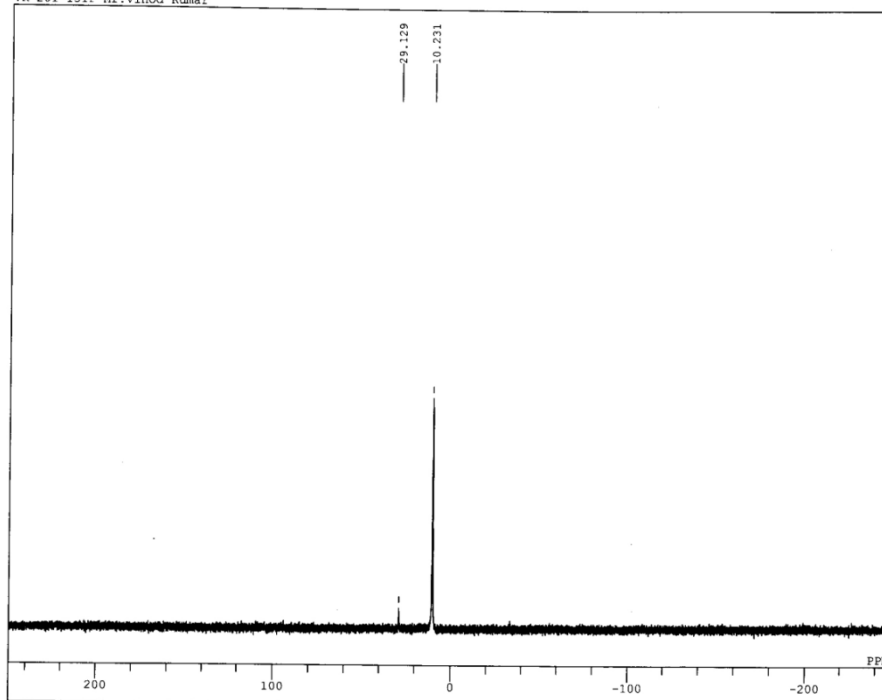


Fig. S7 thermogravimetric (TG) trace of 3.

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VK-201 131P Mr. Vinod Kumar



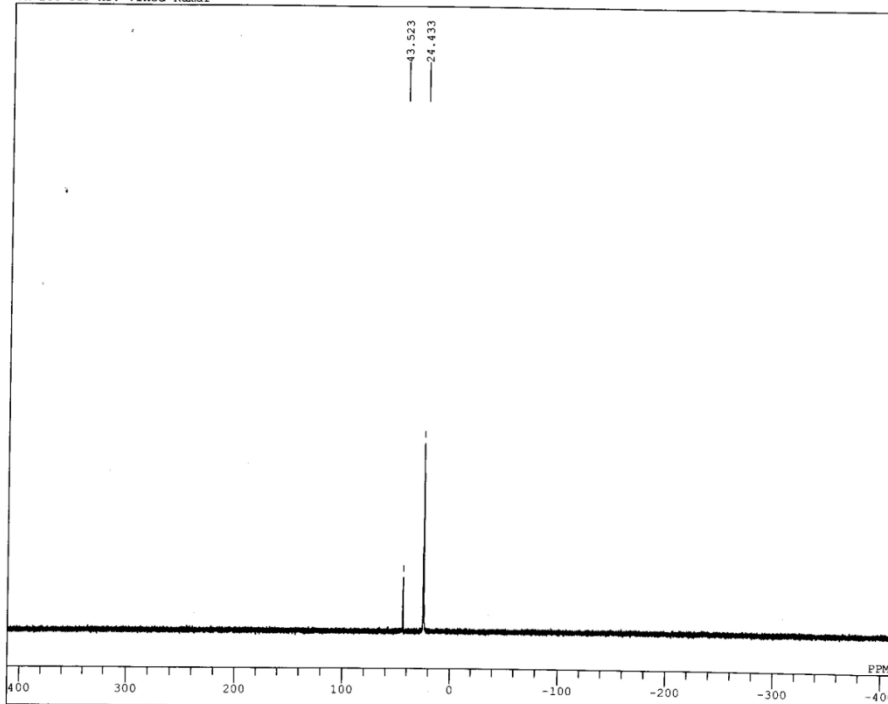
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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RGAIN 23

(a)

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VK-200 31P Mr. Vinod Kumar



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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RGAIN 23

(b)

Fig. S8 (a, b) ³¹P NMR spectra of complexes 3 and 4.