Supporting information:

Contrasting crystallographic signatures of Ag(I)- and Cu(II)-N6,N6'-bisadenine complexes: Extended vs. foldback geometries

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Experimental section:

N, N-Dimethylformamide was distilled prior to use. ^{1}H and ^{13}C NMR were recorded on JEOL-JNM LAMBDA 400 model operating at 400, 100 MHz, respectively. HRMS mass spectra for the ligand and metalated complexes were recorded at IIT Kanpur, India, on Waters, Q-Tof Premier Micromass HAB 213 mass spectrometer using capillary voltage 2.6-3.2 kV. Solvents were evaporated using rotary evaporator under reduce pressure. NaH was purchased from sd fine chemicals pvt. Ltd. Mumbai, India, n-propyl bromide was purchased from Spectrochem Pvt.Ltd. Mumbai; 6-chloro purine was purchased from SRL, India and used without further purification. All solvents were distilled prior to use using standards procedures.

Synthesis of 9-propyl 6-choloro purine: Experimental details for the synthesis of 9-propyl 6-choloro purine have been reported earlier.[1] A similar protocol was followed and the purity of product so obtained was confirmed by spectroscopic analysis.

Synthesis of trimethylene-N^6,N$^{6'}$-Bis-(9-propyladenine): 9-propyl 6-choloro purine (0.900g, 4.57mmol) was dissolved in butanol (5ml), followed by addition of 1,3-diaminopropane (0.191ml, 2.28mmol) and stir for 15min. After this, triethylamine (0.764ml, 5.49mmol) is added and the reaction mixture was refluxed for 3 hours. After this time, butanol is removed via distillation and compound is separated by coloumn chromatography (0.360g, 40% yield). HRMS: (M+H)$^+$ =395.2421, found 395.2420; M.P.=117^{O}C. ^{1}H NMR: (400MHz, $CDCl_3$, 22.6^{0}C, TMS) δ(ppm) 0.91-0.94(t, *J* = 7.32 Hz, 6H), 1.84-1.93(m, 2H), 2.00(bs, 4H), 3.74 (bs, 4H), 4.10-4.14(t, *J* = 7.32Hz, 4H), 6.98 (bs, 2H, D_2O exchange), 7.73 (s, 2H), 8.42(s, 2H). ^{13}C NMR (100MHz, $CDCl_3$, 20.9^{O}C, TMS); δ (ppm) 11.5, 23.38, 29.95, 37.31, 45.37, 119.65, 139.67, 148.83, 152.96, 155.00

Synthesis of silver complex 1: In a 25 ml round bottom flask, wrapped with aluminum foil, trimethylene-N^6, N$^{6'}$ -Bis-(9-propyladenine) (100mg, 0.253mmol) was dissolved in methanol (3ml) and to this added silver nitrate solution (43mg, 0.253mmol in 3ml water) drop wise with stirring. The complex started precipitating out with the addition of silver salt solution. Stirring was continued for another one hour. After this time, the precipitate was filtered carefully to avoid direct light and washed with water (4x 5 mL) and methanol (4 x 5 ml) to remove any traces of unreacted metal salt and ligand. The product so obtained was dried under high vacuum. HRMS [M+Ag]$^+$ = 501.1393, found 501.1342; M.P. = 132^{O}C. ^{1}H NMR: (400MHz, d_6-DMSO, 21.4^{0}C, TMS) δ(ppm) 0.79-0.83 (t, *J* = 7.56, 6H), 1.75-1.84 (m, 2H), 1.88-1.91 (m, 4H), 3.57 (bs, 2H), 4.08-4.12 (t, *J* = 7.08, 4H), 7.88 (bs, 2H, D_2O exchange), 8.17 (s, 2H), 8.21 (s, 2H). ^{13}C NMR (100MHz, d_6-DMSO, 23.1 ^{O}C, TMS); δ (ppm) 10.82, 22.69, 44.88, 48.57, 118.29, 142.23, 152.72, 153.07.

Synthesis of copper complex 2: Trimethylene-N^6, N$^{6'}$-Bis-(9-propyladenine) (100mg, 0.253mmol) was dissolved in methanol (3ml), followed by addition of copper chloride (43mg, 0.252 mmol) and stir for 30min. After this, solvent is evaporated and the brownish solid thus obtained is washed with water (4x 5 ml) and methanol (4x 5 ml) to remove any traces of unreacted metal salt and ligand. The product so obtained is dried under high vacuum. HRMS [M+Cu^{63}]$^+$ = 457.1606 (found 457.1638) and [M+Cu^{65}]$^+$ = 459.1613 (found 459.1620); M.P. = 127^{O}C.

Table S1: Crystallographic data for complexes 1 and 2

Identification code	1	2
Empirical formula	C19 H32 N11 O6 Ag1	C21 H29 Cl2 Cu N10 O2
Formula weight	612.38	587.98
Crystal colour	Colorless	greenish
Crystal size (mm)	0.2, 0.2, 0.2	0.2, 0.18, 0.18
Crystal system	Orthorhombic	Triclinic
Space group	Ibca	P -1
a (Å)	8.7535 (14)	9.6584(6)
b (Å)	13.673 (2)	11.3064(7)
c (Å)	43.743 (7)	13.3168(8)
α (^{0})	90	69.1570(1)
β (^{0})	90	84.6630(1)
λ (^{0})	90	78.6340(1)
V (A^3)	5235.4 (15)	1331.98 (6)
Dcal (mg m^{-3})	1.55	1.47
Z	8	2
μ (M$_o$Kα)(mm^{-1})	0.826	1.060
F (000)	2496	607.8
2θ range	2.8 to 23.4	2.1 to 28.3
Reflection measured	10898	8830
Independent reflection	1903 [R(int) = 0.0583]	6315[R(int) = 0.024]
Reflection observed (I>2σ(I))	1422	4837
Parameters	173	347
Final R1, wR2 (observed data)	R1 = 0.0728, wR2 = 0.2114	R1=0.068 wR2=0.177
Goodness-of-fit (observed data)	1.046	1.148
CCDC number*	684613	682049

Table S2: Selected hydrogen bonding distances (Å) and bond angles (^{o}) in complexes **1** and **2**

Complex	D-H…A	Symmetry of A	d$_{H...A}$	$^{\#}$D - H...A
1	N(6)-H(6)...O(6)	x, y, z	2.13	141
2	O(2)-H(2A)...N(1)	x, y, z	1.99	165
	N(6)-H(6)...Cl(2)	1-x, 1-y, 1-z	2.51	145
	N(6')-H(6')...O(1)	1-x, 1-y, 1-z	2.17	160

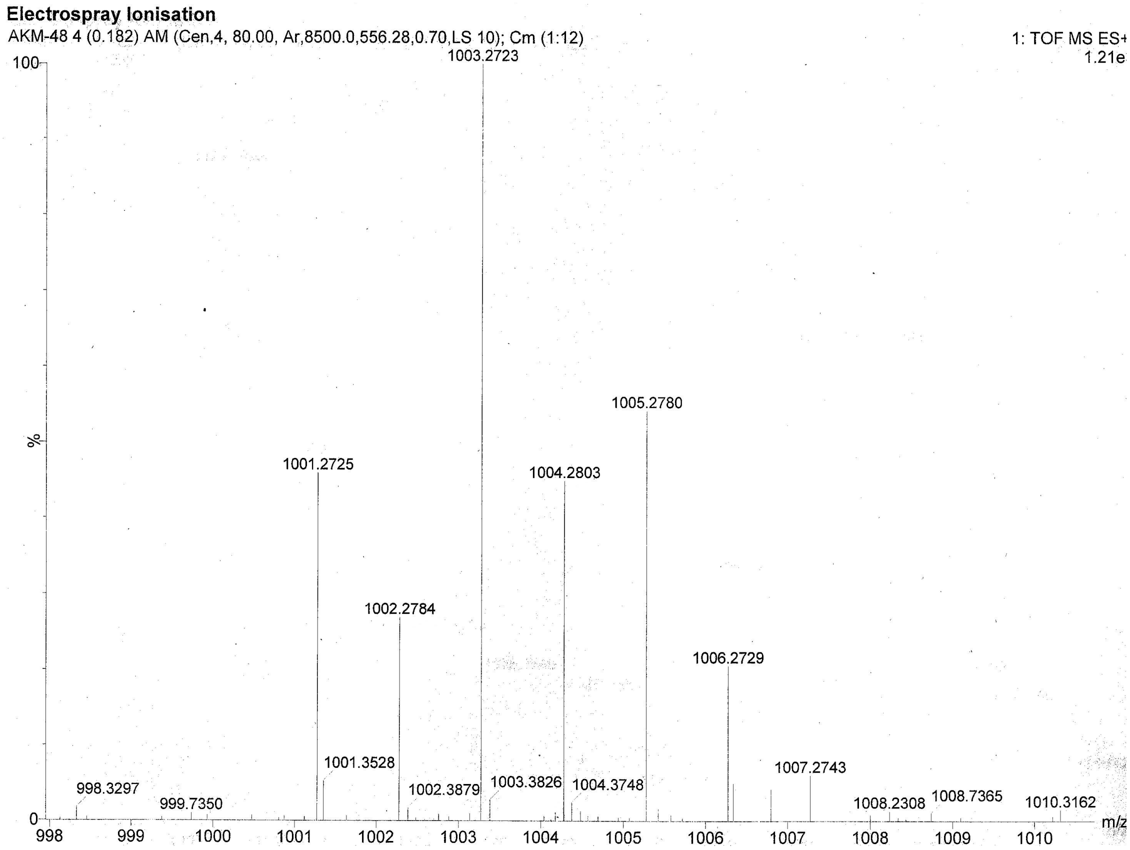

Figure S1: Mass spectroscopic data for complex **1**, showing peaks corresponding to $[L_2Ag_2^{107} +1]$ and $[L_2Ag_2^{109} +1]$.

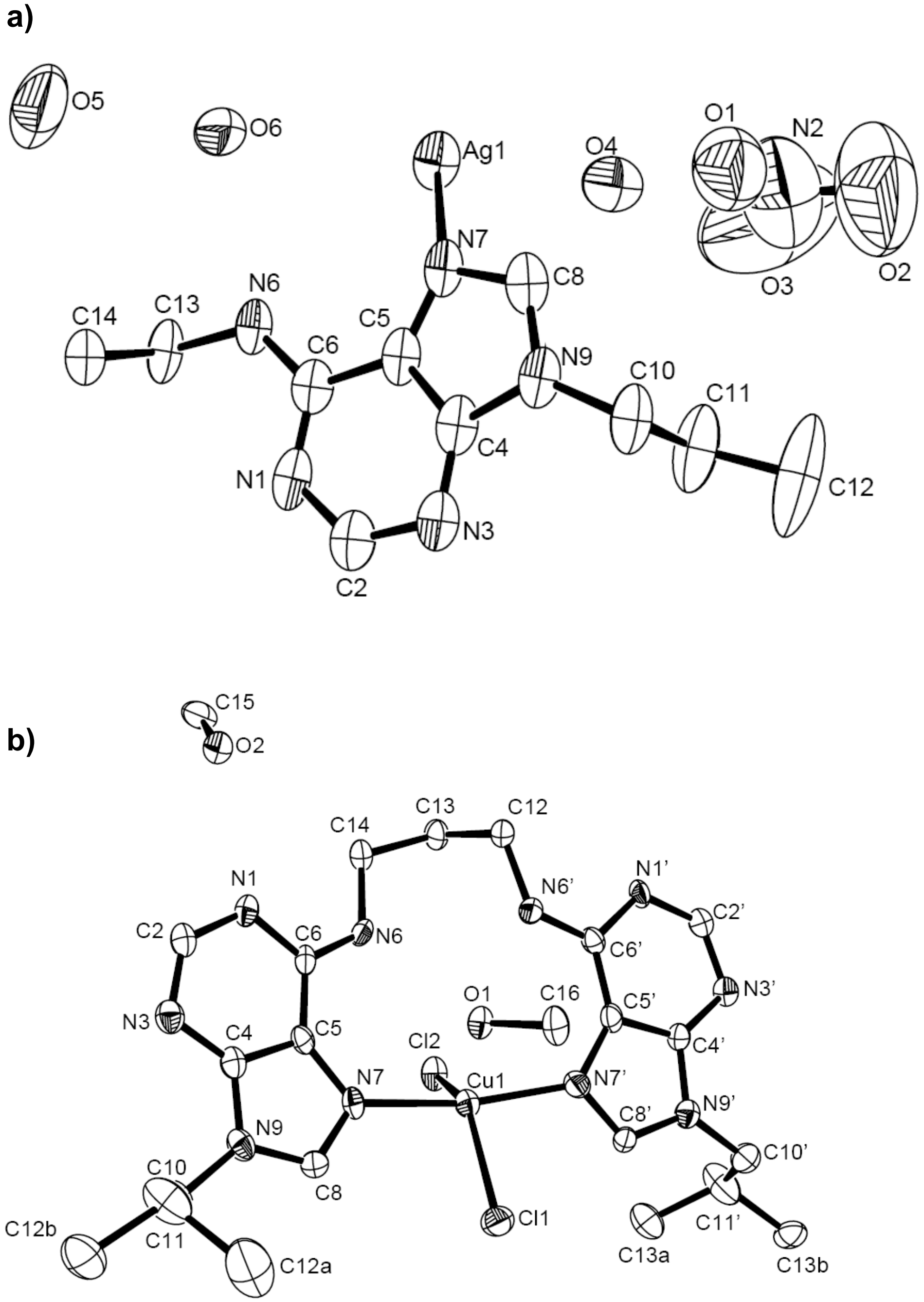

Figure S2: ORTEP diagrams a) for **1** and b) for **2,** with 50 % ellipsoid probability.

References:

(1) C. S. Purohit, A. K. Mishra and S. Verma, *Inorg. Chem.,* 2007, **46**, 8493.