Supporting Information for Publication

Selective Extraction of Gold by Niacin

Abhijit Nag† , Md Rabiul Islam† , and Thalappil Pradeep†*

†DST Unit of Nanoscience and Thematic Unit of Excellence, Department of Chemistry,

Indian Institute of Technology Madras, Chennai-600036, India.

*Corresponding Author Email: pradeep@iitm.ac.in; Fax: + 91-44 2257-0545

SUPPORTING INFORMATION CONTENT

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Instrumentation

Inductively coupled plasma-mass spectrometry (ICP MS)

ICP MS was performed using a Perkin Elmer NexION 300X instrument equipped with Ar plasma. Before doing any sample, the instrument was calibrated with gold standard of four different concentrations (0, 10, 100 and 1000 ppb) to get a calibration curve with R^2=0.9999. Blank experiment (0 ppb) was performed with milli-Q water (18.3 MΩ resistance) with 5% (v/v) hydrochloric acid. Standards were also prepared in 5% hydrochloric acid. The same amount (5%) of hydrochloric acid was added to the collected samples also before analyses. For other metals also, the instrument was calibrated with the standard by the same procedure, but 5% nitric acid was used.

Scanning electron microscopy (SEM)

SEM (scanning electron microscopy) and energy dispersive analysis of X-rays (EDS) were performed using an FEI QUANTA-200 SEM.

X-ray photoelectron spectroscopy

XPS measurements were performed with an Omicron ESCA Probe Spectrometer. It consists of EA 125 energy analyzer, XM 1000 MkII X-ray source and monochromator, DAR 400 X-ray source (Al/Mg), VUV source HIS 13, CN 10 and CN 10+ charge neutralizer system, ISE 10 sputter

ion source and MKS residual gas analyzer for temperature programed desorption (TPD). Polychromatic Al Kα X-rays (hν = 1486.6 eV) were used for analysis.

Table S1. Different methods for gold recovery available in the literature.

References	**Method used**	**Uptake percentage of gold**
Precious metal recovery from electronic waste by a porous porphyrin polymer[1]	Adsorption	98.8
High-efficiency gold recovery using Cucurbit[6]uril[2]	Precipitation	99.2
Selective isolation of gold facilitated by second-sphere coordination with α-cyclodextrin[3]	Precipitation	Not available
Environmentally benign, rapid, and selective extraction of gold from ores and waste electronic materials[4]	Chemical leaching	90
Rapid capture of trace precious metals by amyloid-like protein membrane with high adsorption capacity and selectivity[5]	Adsorption	99.6
A simple primary amide for the selective recovery of gold from secondary resources[6]	Solvent extraction	Not available
Selective extraction of trace amounts of gold from complex water mixtures with a metal–organic framework (MOF)/polymer composite[7]	Adsorption	99
This work	Precipitation	99.9

Table S2. ICP MS data for gold extraction at different concentrations of gold.

Initial gold concentration	Gold concentration after niacin treatment
5139 ppm	2.9 ppm
320 ppb	248 ppb

Table S3. Crystal data and structure refinement for I.

Identification code	shelx	
Empirical formula	C12 H11 Au Cl4 N2 O4	
Formula weight	585.99	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 7.2567(18) Å	a= 90°.
	b = 10.516(4) Å	b= 105.095(14)°.
	c = 11.444(4) Å	g = 90°.
Volume	843.2(5) $Å^3$	
Z	2	
Density (calculated)	2.308 Mg/m^3	
Absorption coefficient	9.376 mm^{-1}	
F(000)	552	
Crystal size	0.200 x 0.150 x 0.100 mm^3	
Theta range for data collection	3.580 to 29.980°.	
Index ranges	-9<=h<=10, -14<=k<=14, -15<=l<=16	
Reflections collected	14924	
Independent reflections	2426 [R(int) = 0.0557]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7451 and 0.4461	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2426 / 1 / 112	
Goodness-of-fit on F^2	1.278	
Final R indices [I>2sigma(I)]	R1 = 0.0271, wR2 = 0.0644	
R indices (all data)	R1 = 0.0354, wR2 = 0.0710	
Extinction coefficient	0.0376(16)	
Largest diff. peak and hole	0.681 and -0.928 $e.Å^{-3}$	

Packing in I

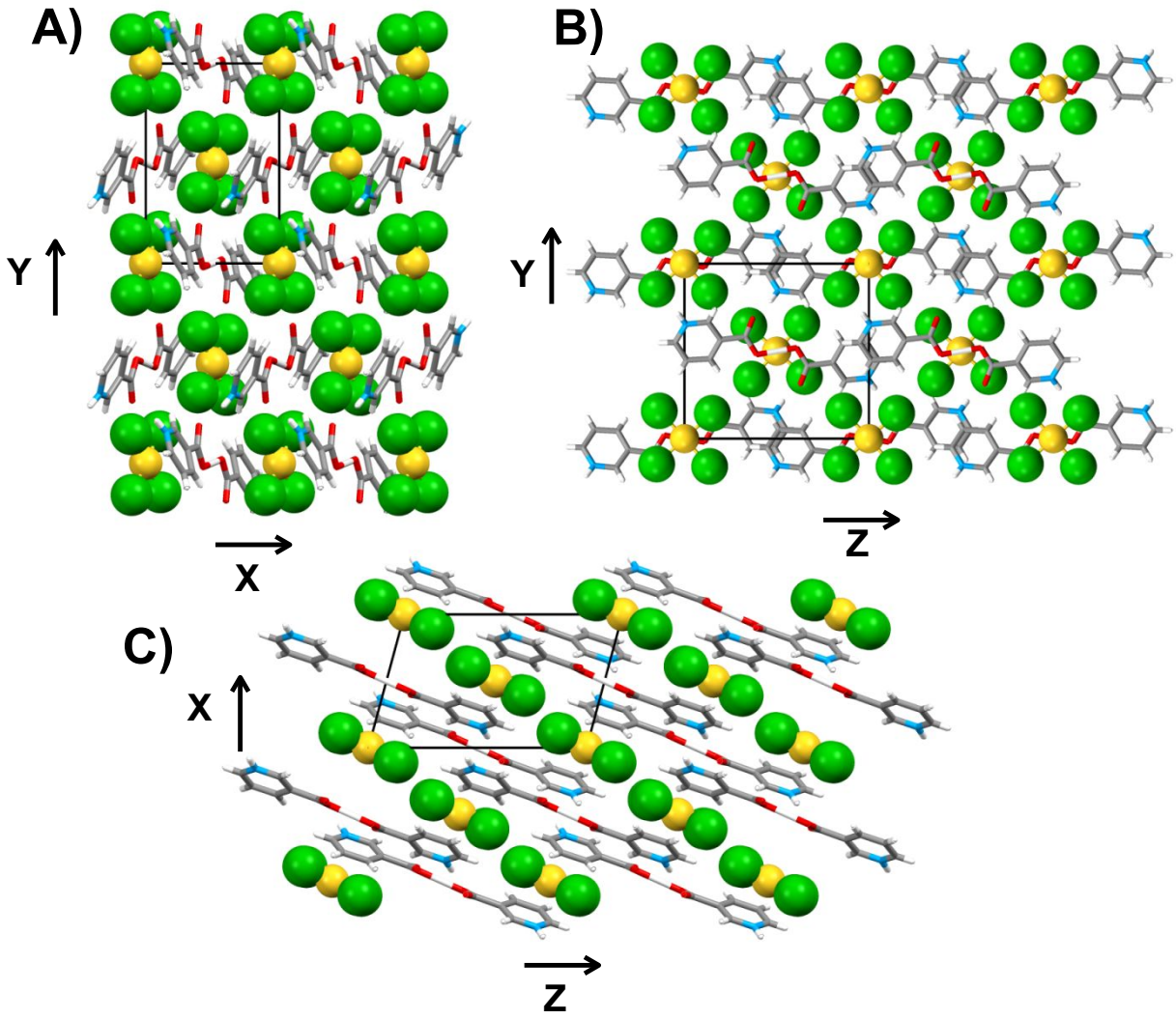

Figure S1. Packing of the crystal. Views from, **A)** Z, **B)** X and **C)** Y axes.

UV-vis spectra

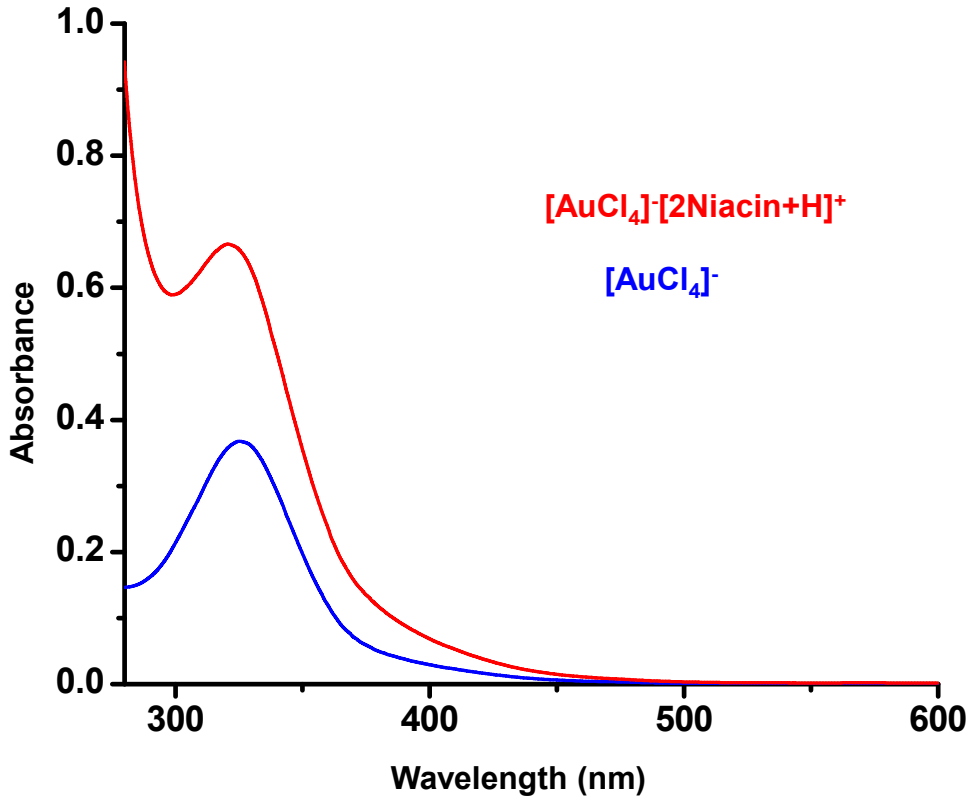

Figure S2. UV-vis spectra of $[AuCl_4]^-$ (blue) and $[AuCl_4]^-[2Niacin+H]^+$ (red) in DMF.

Packing of $AuCl_4^-$ in a crystal of I

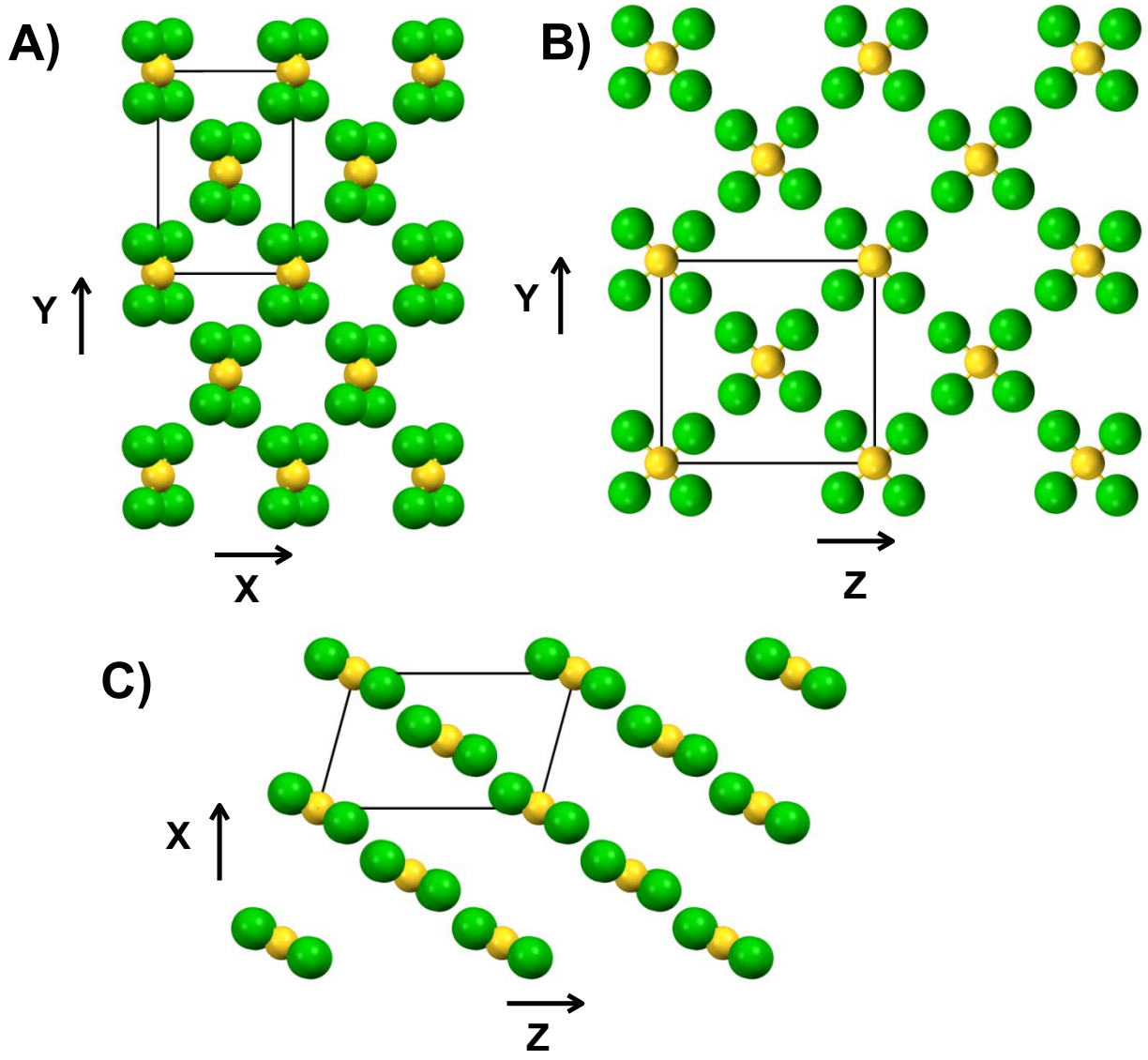

Figure S3. Packing of $AuCl_4^-$ in the crystal. Views from, **A)** Z, **B)** X and **C)** Y axes.

Packing of $[2Niacin+H]^+$ in a crystal of I

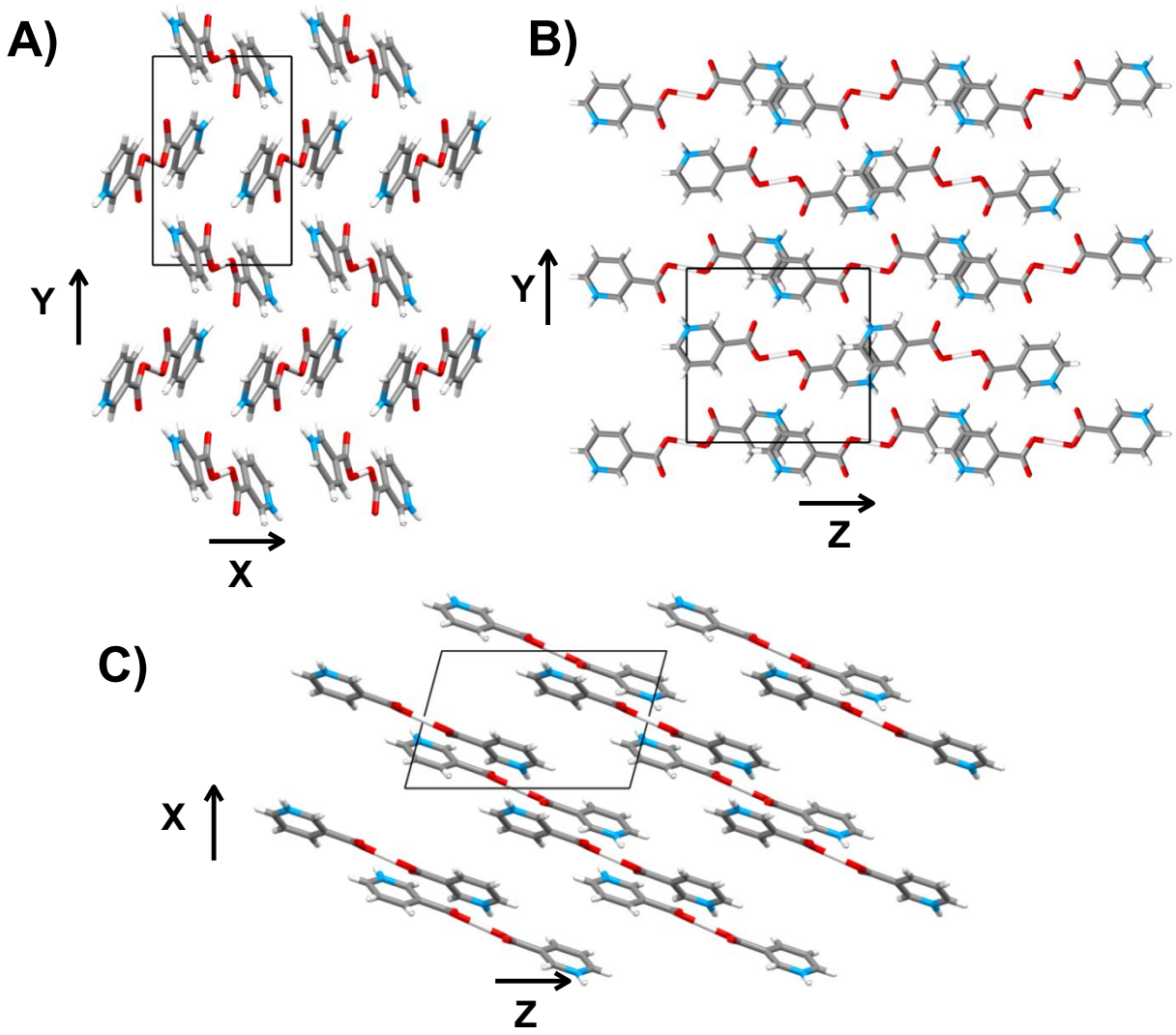

Figure S4. Packing of $[2Niacin+H]^+$ in the crystal. Views from, **A)** Z, **B)** X and **C)** Y axes.

Crystal structure of $Cu(H_2O)_4(Niacin\text{-}H)_2$

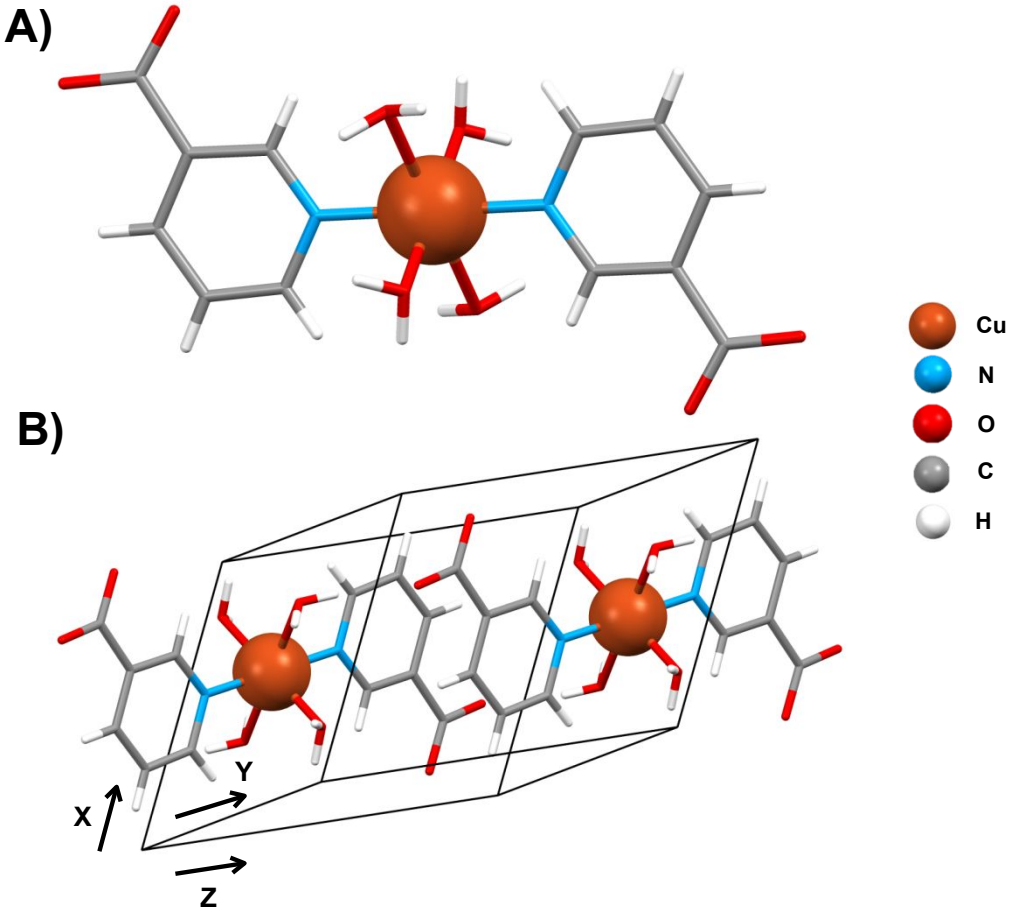

Figure S5. A) Crystal structure of $Cu(H_2O)_4(Niacin\text{-}H)_2$. Color codes for the atoms are also shown. B) Unit cell of $Cu(H_2O)_4(Niacin\text{-}H)_2$. Crystal structure of this system was reported earlier.[8]

Selectivity towards gold

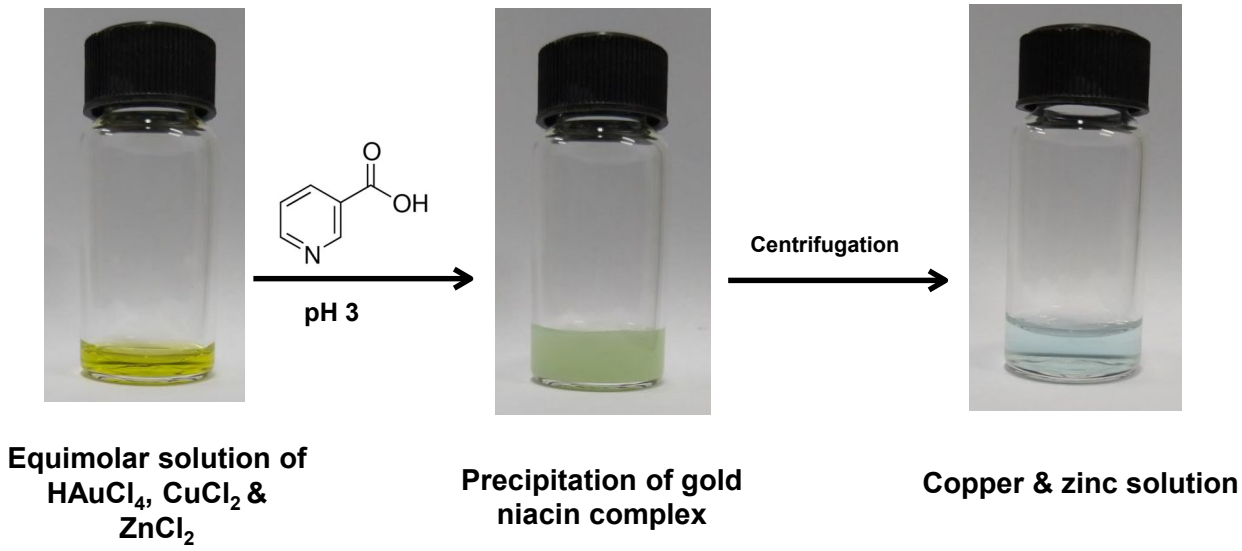

Figure S6. Separation of gold from an equimolar mixture of $HAuCl_4$, $CuCl_2$ and $ZnCl_2$, using saturated (125 mM) solution of niacin.

SEM/EDAX of the precipitate

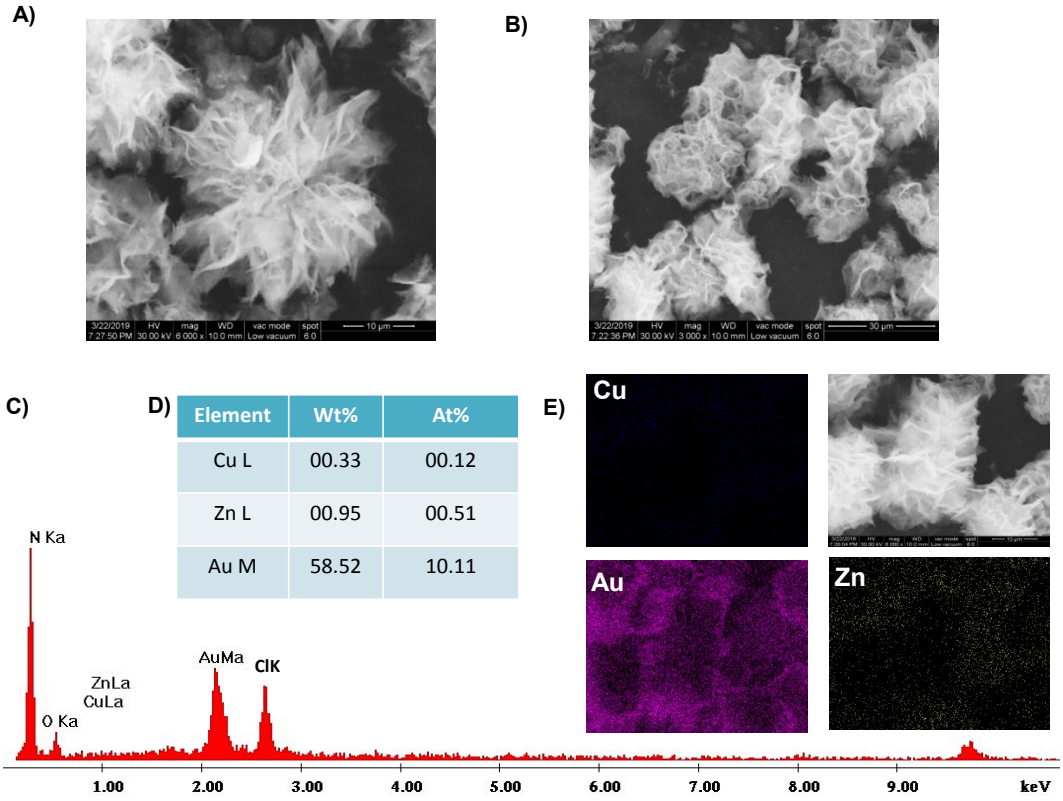

Figure S7. A)-B) SEM images of the precipitate. C) EDS spectrum of the precipitate. D) Elemental analyses data copper, gold and zinc. E) Elemental maps corresponding to zinc, copper, and gold are shown, along with a SEM image. Scale bar is the same for all the images.

Table S4. ICP MS data for gold extraction from the mixtures of $HAuCl_4$, $CuCl_2$ and $ZnCl_2$.

Ions	Initial concentration (ppm)	Final concentration in solution after niacin treatment (ppm)
Cu^{2+}	1710	1616
Au^{3+}	5139	3.9
Zn^{2+}	1745	1639

Selectivity towards gold

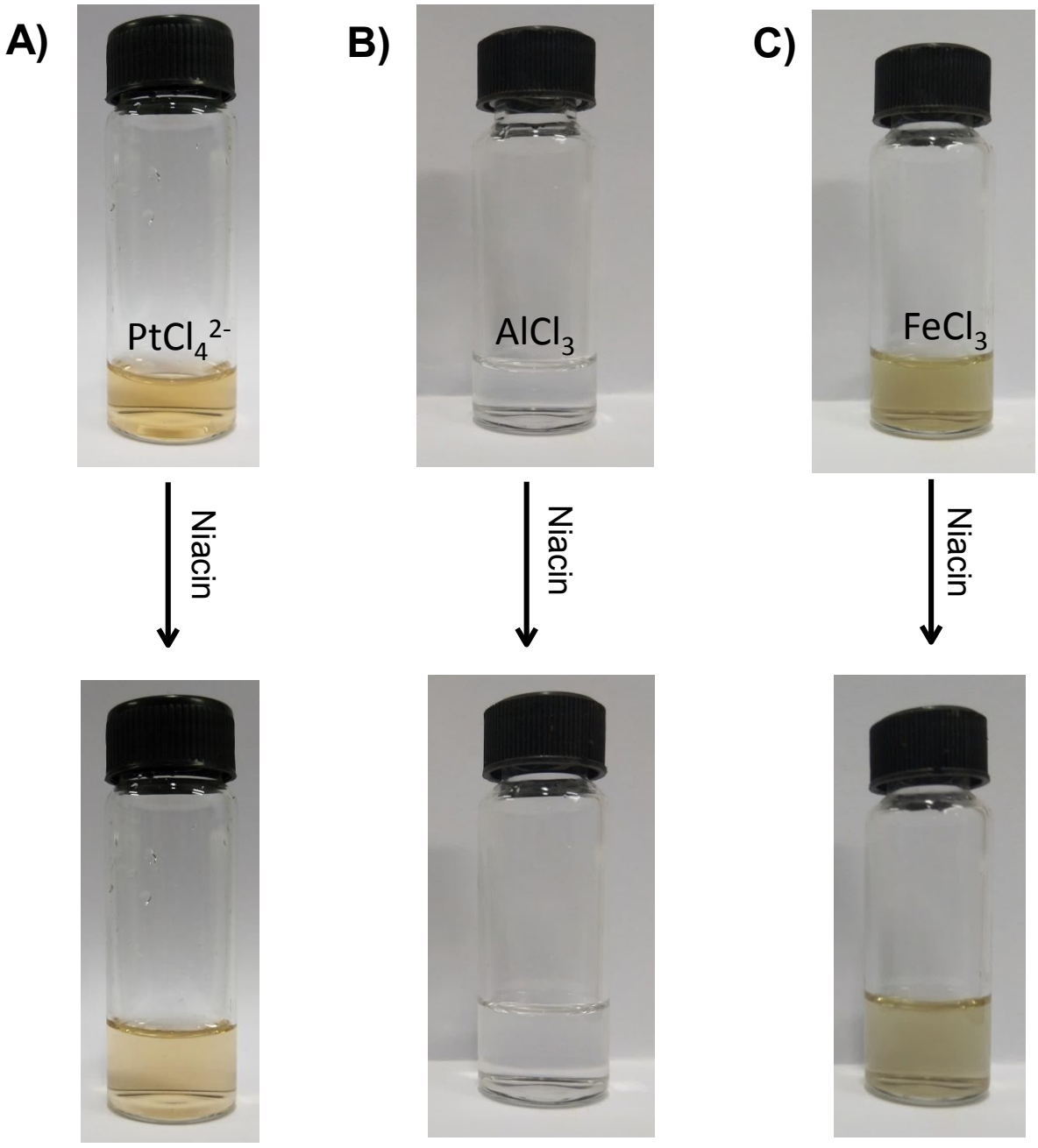

Figure S8. About 125 mM solution of niacin (2 mL) was added to 27 mM 2 mL solutions of A) $PtCl_4^{2-}$, B) $AlCl_3$ and C) $FeCl_3$ at pH 3. No precipitation was observed.

Recovery of gold from nanowaste

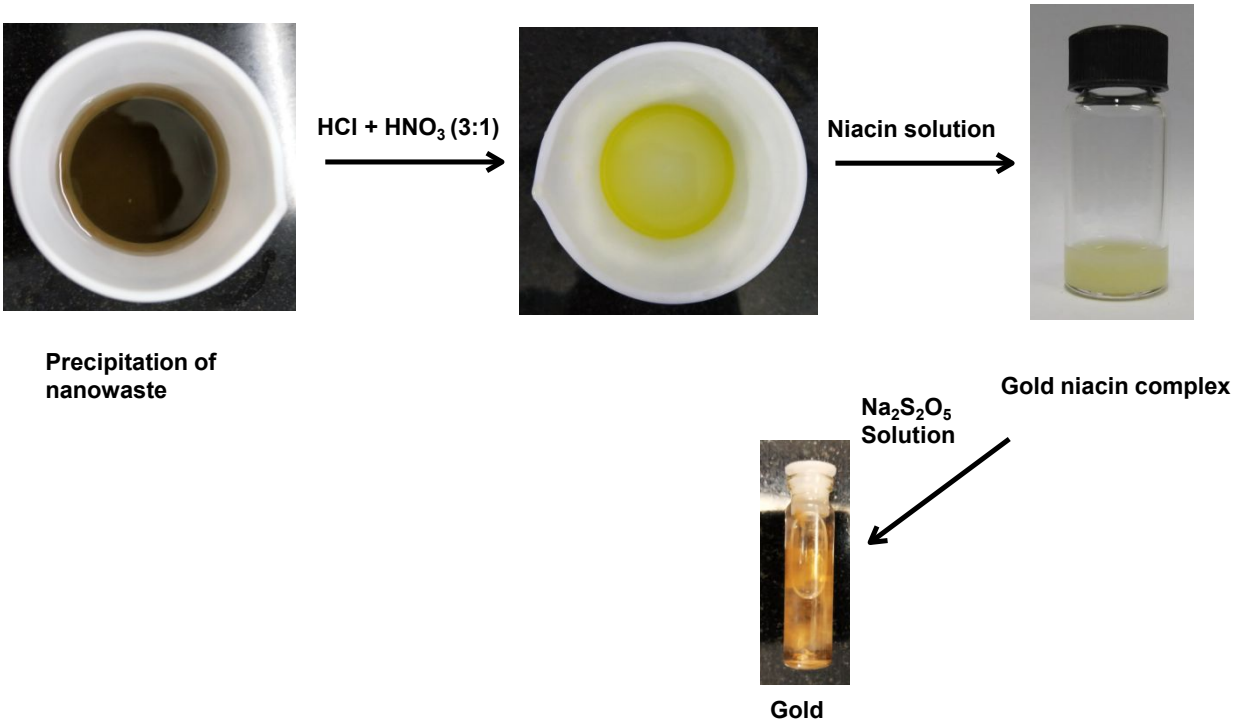

Figure S9. Schematic of the gold recovery process from gold nanowaste. Precipitation of bulk gold by reduction with $Na_2S_2O_5$ is shown.

Table S5. ICP MS data for gold extraction from electronic wastes.

Ions	Initial concentration (ppm)	Final concentration in solution after niacin treatment (ppm)
Ni^{2+}	770	760
Au^{3+}	25	0.85
Cu^{2+}	22320	21120

Table S6. ICP MS data for gold extraction in presence of NaCl and $MgCl_2$.

Initial gold concentration	Gold concentration after niacin treatment
1 ppm	344 ppb

Co-precipitation of copper-niacin in ethanol

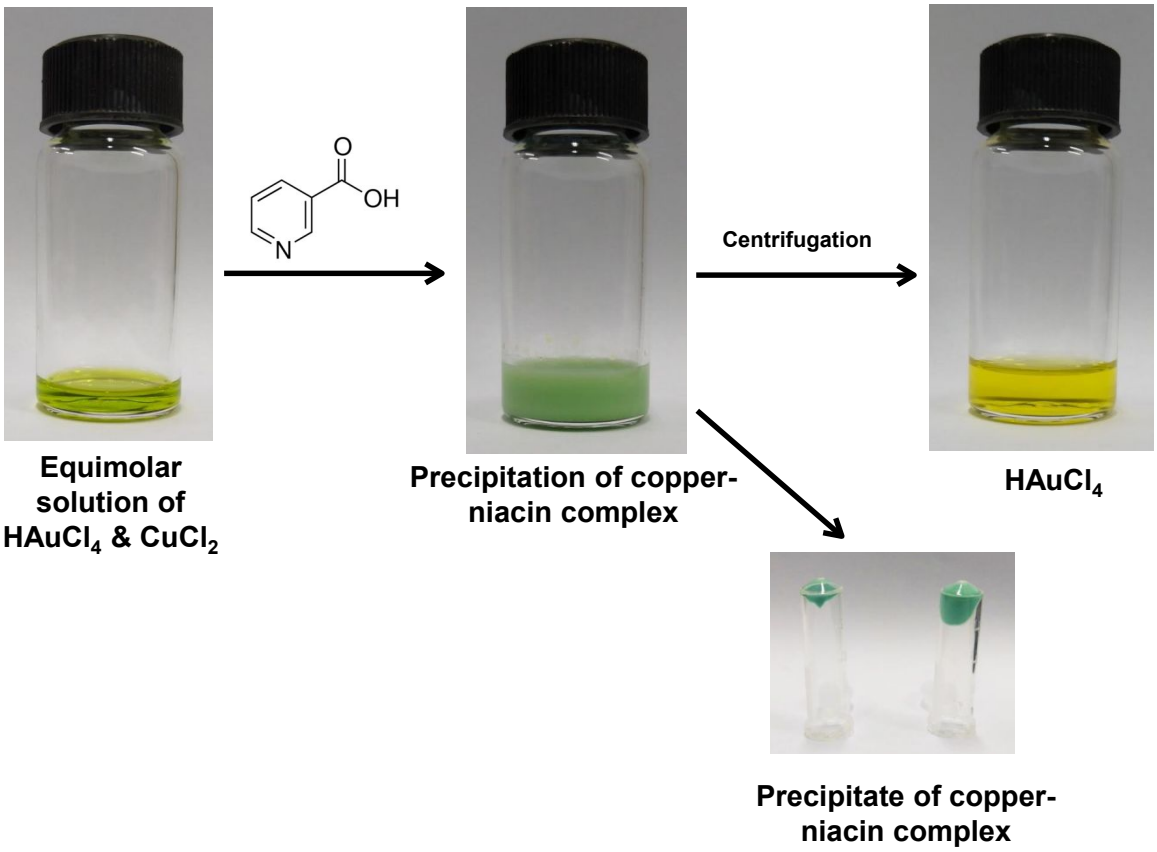

Figure S10. Co-precipitation of copper-niacin complex after addition of saturated niacin solution (1 mL) to an equimolar mixture (27 mM each) of $HAuCl_4$ and $CuCl_2$ (1 mL) in ethanol. By centrifugation, gold and copper can be separated.

References

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