Characterization of two Ag^{I} coordination polymers of the flexible ligand 1,3-bis(4-pyridyl)propane

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Table S1 Crystallographic data and structure refinement parameters for complexes **1** and **2**.

	1	2
Empirical formula	$C_{13}H_{11}AgClN_2O_4$	$C_{41}H_{41}Ag_2ClN_4O_8$
Formula weight	402.56	968.97
Crystal system	Orthorhombic	Orthorhombic
Space group	*Cmca*	*Pbca*
Unit cell dimensions	$a = 7.1013(8)$ Å	$a = 17.7597(12)$ Å
	$b = 15.0391(9)$ Å	$b = 18.1136(10)$ Å
	$c = 27.3815(18)$ Å	$c = 25.4503(11)$ Å
	$\alpha = 90.00^{o}$	$\alpha = 90.00^{o}$
	$\beta = 90.00^{o}$	$\beta = 90.00^{o}$
	$\gamma = 90.00^{o}$	$\gamma = 90.00^{o}$
Volume($Å^3$)	2924.3(4)	8187.2(8)
Z	8	8
Calculated density (mg/m^3)	1.829	1.572
Absorption coefficient (mm^{-1})	1.577	1.078
F(000)	1592	3920
Crystal size (mm^3)	0.25 × 0.16 × 0.12	0.23 × 0.16 × 0.12
θ range for data collection	2.98 to 25.00	3.01 to 25.00
Range of *h, k, l*	−8/5, −13/17, −32/20	−18/21, −15/21, −29/30
Reflections collected	3728	21163
Independent reflections	1399	7196
R_{int}	0.0390	0.0466
Data/restraints/parameters	1399 / 0 / 127	7196 / 0 / 507
Goodness-of-fit on F^2	1.004	1.065
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0311$, $wR_2 = 0.0371$	$R_1 = 0.0371$, $wR_2 = 0.0419$
R indices (all data)	$R_1 = 0.0872$, $wR_2 = 0.0396$	$R_1 = 0.1078$, $wR_2 = 0.0438$
Largest diff. peak and hole (e. Å^{-3})	0.326 and −0.292	0.468 and −0.545

[a]$R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$; [b]$wR_2 = [\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where F_o = observed and F_c = calculated structure factors, respectively.

Table S2 Selected bond lengths (Å) and angles ($^\circ$) for complex **1**[a].

Ag1–N1	2.126(5)	Ag1–N2[#1]	2.128(4)
N1–Ag1–N2[#1]	173.15(19)		

[a] Symmetry transformations used to generate equivalent atoms: #1 = $-x + 1, -y + 1/2, z - 1/2$.

**Table S3** Selected bond lengths (Å) and angles ($^\circ$) for complex **2**[a].

Ag1–N1	2.148(3)	Ag1–Ag2	3.0055(4)
Ag1–N2[#1]	2.148(4)	Ag2–N3	2.170(3)
Ag1–O1	2.560(4)	Ag2–N4[#2]	2.170(3)
N1–Ag1–N2[#1]	167.44(14)	N2[#1]–Ag1–O1	93.14(16)
N1–Ag1–O1	94.70(16)	N3–Ag2–N4[#2]	166.60(14)

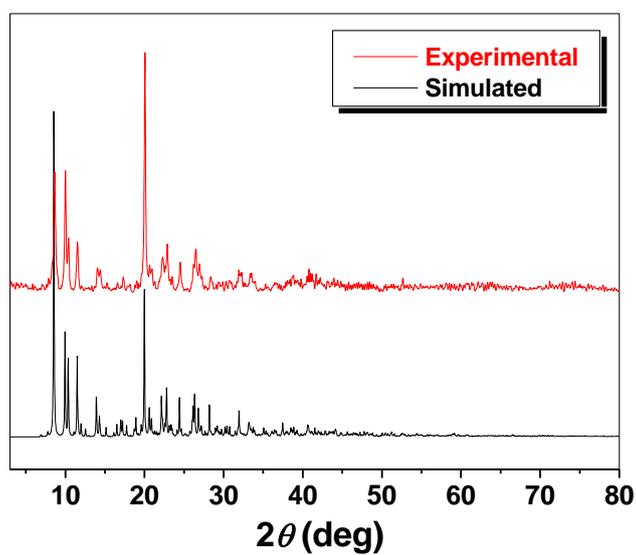[a]Symmetry code: #1 x, $-y + 1/2, z - 1/2$; #2 $-x + 3/2, -y, z + 1/2$.

Table S4 Hydrogen bond lengths (Å) and angles ($^\circ$) for complexes **1** and **2**.

D–H⋯A	d(D–H)	d(H⋯A)	d(D⋯A)	D–H⋯A
1				
C1–H1A⋯O3[a]	0.93	2.54	3.424(5)	160
C9–H9A⋯O2[b]	0.93	2.46	3.297(5)	150
2				
O8–H8⋯O2c	0.82	1.91	2.694(7)	159
C37–H37⋯O4d	0.93	2.51	3.394(8)	159

[a]Symmetry codes for **1**: a = $x - 1/2, y, -z + 1/2$; b = $x, -y, -z + 1$.; for **2**: c $x - 1, y + 1, z$; d $-x + 1, -y, -z$.
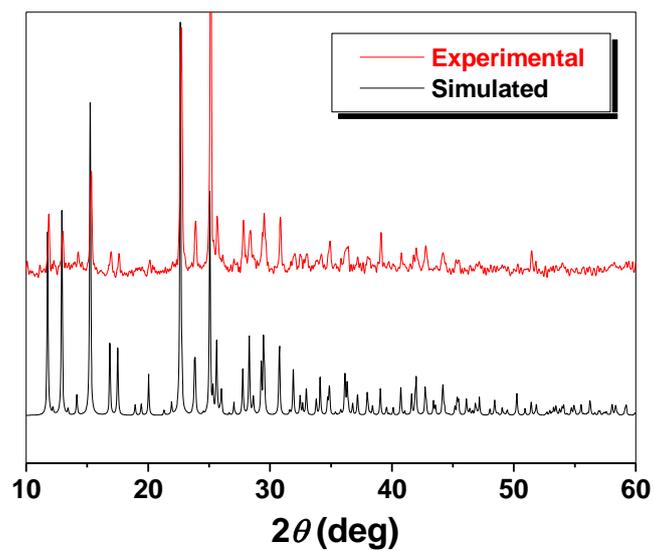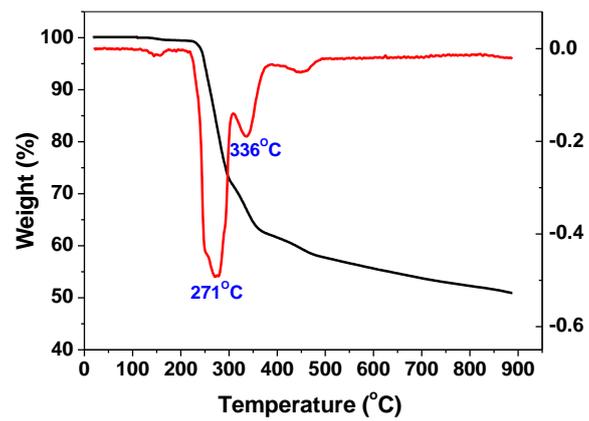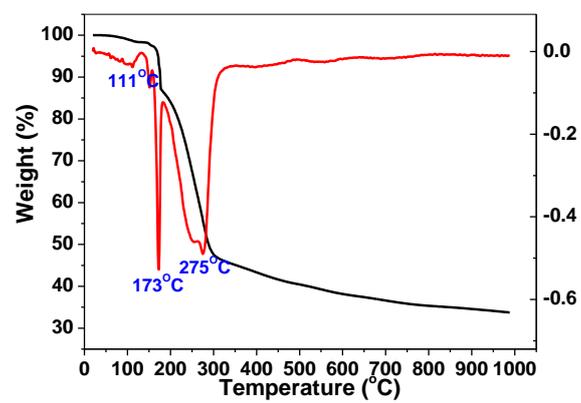
(a)

(b)

Figure S1   X–ray powder diffraction (XRPD) patterns of (a) for **1** and (b) for **2**.

(a)

(b)

Figure S2   Thermogravimetric analysis (TGA) plots of (a) for **1** and (b) for **2**.