Electronic supplementary information

for

Regioisomer-directed structural diversity in one-dimensional silver(I) coordination polymers

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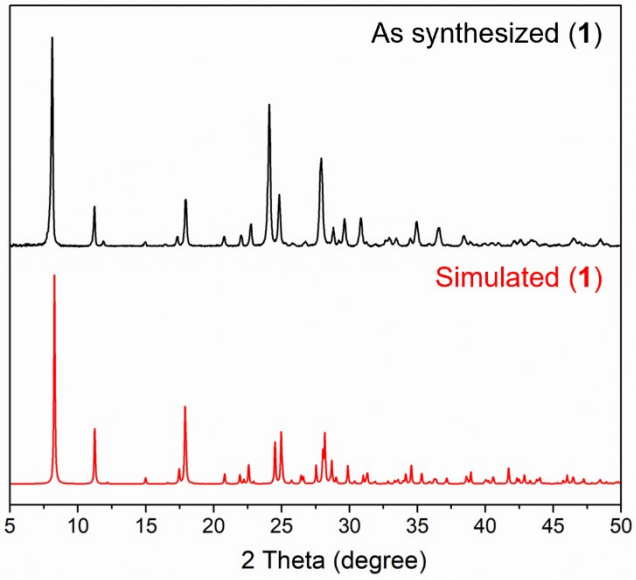
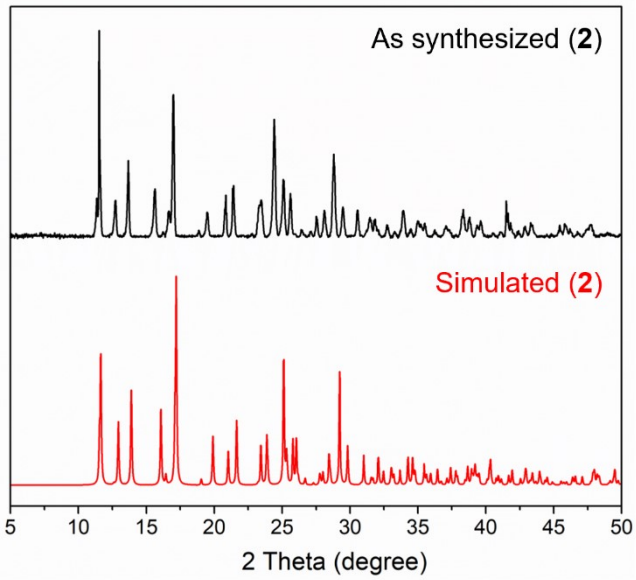
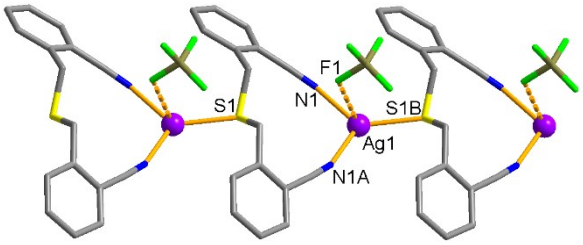


(a)

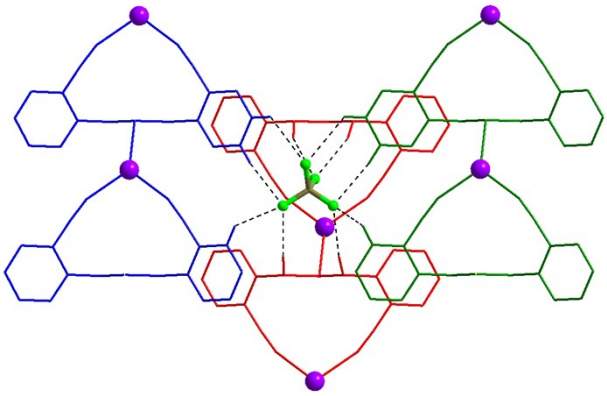


(b)

Fig. S1 Comparison of PXRD patterns for (a) **1** and (b) **2**: (top) as synthesized and (bottom) simulated from the single crystal X-ray data.

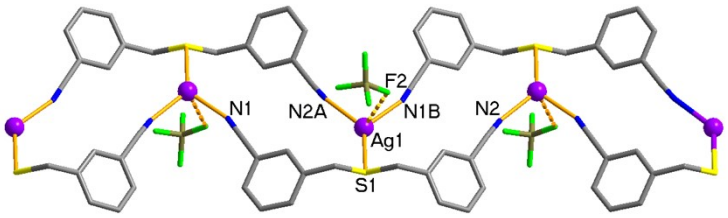


(a)

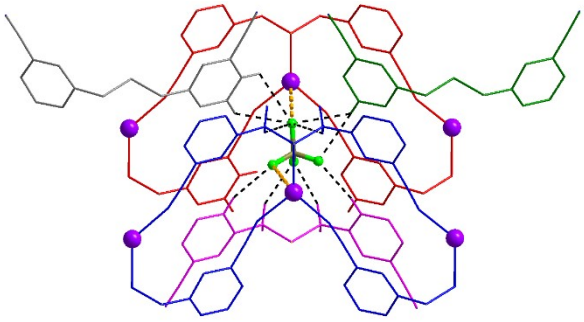


(b)

Fig. S2 Crystal structure of **1**, [Ag(*o*-**L**)BF_4]$_n$ showing non-coordinated anions with weak Ag···F interactions (Ag1···F1 = 3.004 Å) and (b) Partial packing view of **1** showing multiple C-H···F H-bonds (H···F = 2.299–2.782 Å).

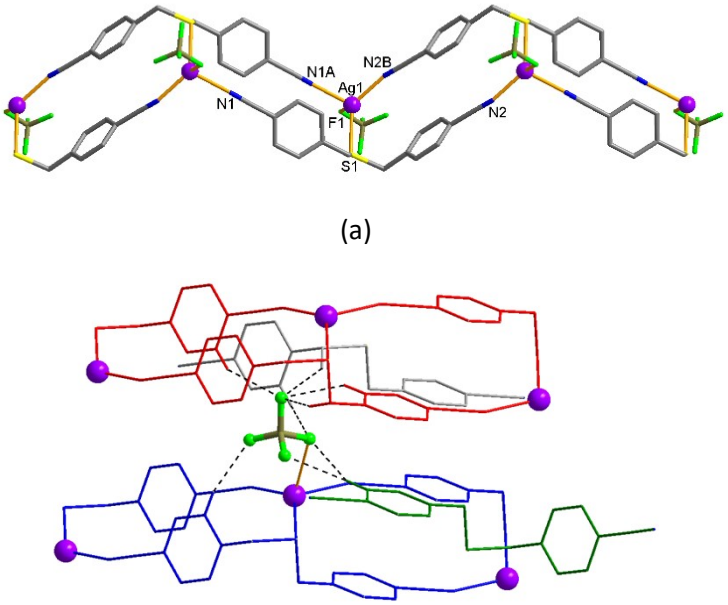


(a)



(b)

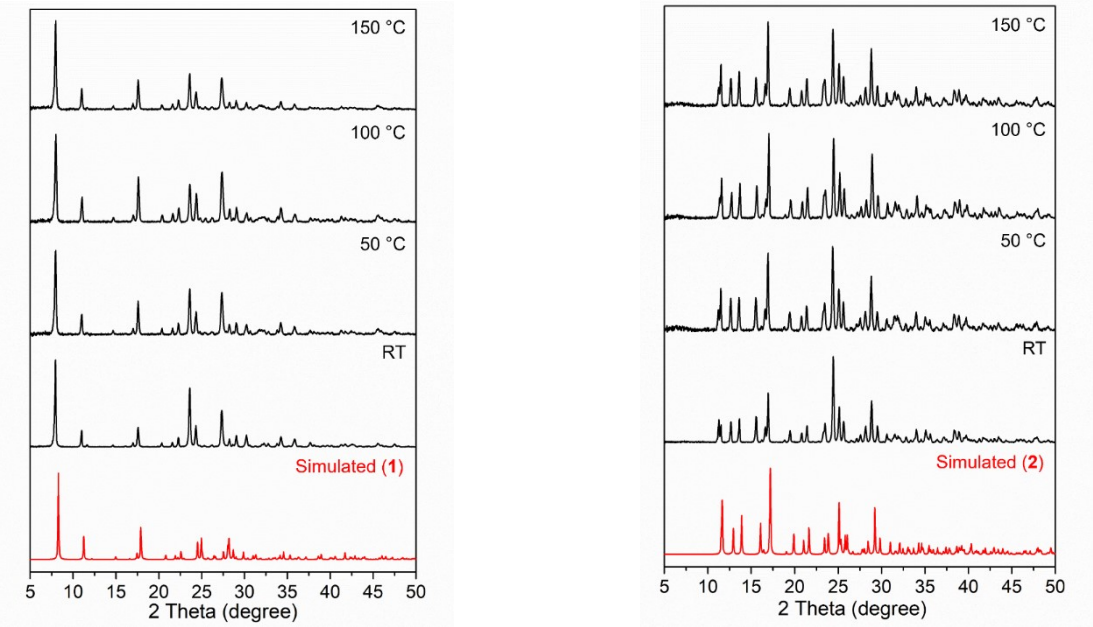
Fig. S3 (a) Crystal structure of **2**, [Ag(*m*-**L**)BF_4]$_n$ showing non-coordinated anions with weak Ag···F interactions (Ag1···F2 = 3.123 Å) and (b) Partial packing view of **2** showing multiple C-H···F H-bonds (H···F = 2.424–2.981 Å)



(a)

(b)

Fig. S4 (a) Crystal structure of **3** [Ag(*p*-**L**)BF_4]$_n$ showing non-coordinated anions with weak Ag–F bond distance (Ag1–F1 = 2.654(2) Å) and (b) Partial packing view of **3** showing multiple C-H···F H-bonds (H···F = 2.397–2.638 Å).



(a) (b)

Fig. S5 Variable-temperature PXRD patterns of (a) complex **1** ([Ag(*o*-**L**)BF_4]$_n$) and (b) complex **2** ([Ag(*m*-**L**) BF_4]$_n$) measured at room temperature after heating at 50, 100, and 150 °C for 1 h, compared with the pattern simulated from single-crystal X-ray data.

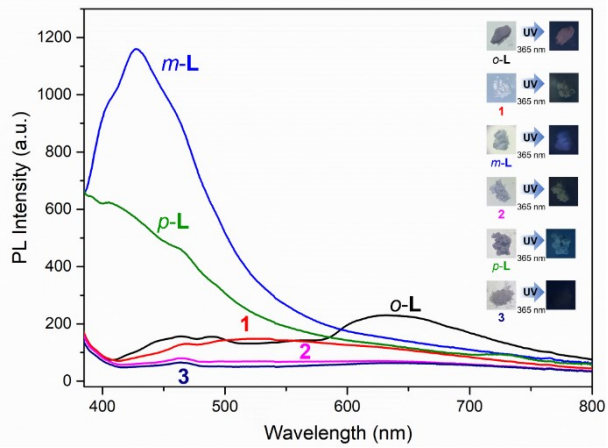


Fig. S6 Solid-state photoluminescence emission spectra of *o*-**L**, complex **1**, *m*-**L**, complex **2**, *p*-**L** and complex **3** (λ_{ex} = 360 nm).

Table S1 Crystal and experimental data for *o*-**L**, *m*-**L** and **1**-**3**

	o-**L**	*m*-**L**	**1**	**2**	**3**
Formula	$C_{16}H_{12}N_2S$	$C_{16}H_{12}N_2S$	$C_{16}H_{12}AgBF_4N_2S$	$C_{16}H_{12}AgBF_4N_2S$	$C_{16}H_{12}AgBF_4N_2S$
Formula weight	264.34	264.34	459.02	459.02	459.02
Temperature (K)	173(2)	173(2)	173(2)	173(2)	173(2)
Crystal system	Triclinic	Monoclinic	Orthorhombic	Monoclinic	Triclinic
Space group	*P-1*	*C*2/*c*	*Pnma*	$P2_1/m$	*P-1*
Z	2	4	4	2	2
a (Å)	7.7509(11)	15.5310(3)	7.101(16)	7.0638(2)	7.2026(3)
b (Å)	7.9064(10)	5.90210(10)	15.74(4)	15.1751(6)	8.0716(3)
c (Å)	11.7779(16)	14.9747(3)	14.51(3)	7.7137(3)	16.3023(7)
α (°)	73.163(6)	90	90	90	102.156(2)
β (°)	84.391(7)	109.4350(10)	90	96.851(2)	91.395(2)
γ (°)	71.470(7)°	90	90	90	114.742(2)
V (Å^3)	655.00(15)	1294.45(4)	1622(6)	820.96(5)	834.68(6)
D_x(g cm^{-3})	1.340	1.356	1.880	1.857	1.826
$2\vartheta_{max}$ (°)	54	56	50	57	56
R_1, wR_2 [$I > 2\sigma(I)$]	0.0651, 0.1547	0.0328, 0.0839	0.0415, 0.1105	0.0342, 0.0784	0.0244, 0.0639
R_1, wR_2 [all data]	0.1034, 0.1756	0.0365, 0.0869	0.0533, 0.1187	0.0417, 0.0823	0.0271, 0.0651
Data / restraints / parameters	2864 / 0 / 172	1558 / 0 / 87	2117 / 0 / 121	2133 / 0 / 131	4026 / 0 / 226
Goodness-of-fit on F^2	1.000	1.079	1.062	1.045	1.069
No. of reflection used [>2σ(*I*)]	2864 [R_{int} =0.0809]	1558 [R_{int} = 0.0297]	2117 [R_{int} = 0.0504]	2133 [R_{int} = 0.0399]	4026 [R_{int} = 0.0428]
Structure determination	SHELXTL	SHELXTL	SHELXTL	SHELXTL	SHELXTL
Refinement	full-matrix	full-matrix	full-matrix	full-matrix	full-matrix

Table S2 Selected bond lengths (Å) and bond angles (°) for **1**

Ag1-N1	2.276(5)	Ag1-S1B	2.446(5)
N1A-Ag1-N1	106.6(2)	N1-Ag1-S1B	126.1(1)

[a]Symmetry operations: (A) x, -y+1.5, z (B) x+1, y, z

Table S3 Selected bond lengths (Å) and bond angles (°) for **2**[a]

Ag1-N1A	2.249(2)	Ag1-N2B	2.249(2)
Ag1-S1	2.427(1)		
N1A-Ag1-N2B	97.0(1)	N2B-Ag1-S1	131.5(1)
N1A-Ag1-S1	131.5(1)		

[a]Symmetry operations: (A) x, -y+0.5, z (B) -x, -y+1, -z+1 (C) x, -y+1.5, z

Table S4 Selected bond lengths (Å) and bond angles (°) for **3**[a]

Ag1-N2A	2.216(2)	Ag1-S1	2.485(1)
Ag1-N1B	2.293(2)	Ag1-F1	2.654(2)
N2A-Ag1-N1B	109.7(1)	N2A-Ag1-F1	114.3(1)
N2A-Ag1-S1	128.1(1)	N1B-Ag1-F1	83.3(1)
N1B-Ag1-S1	115.2(1)	S1-Ag1-F1	95.8(1)

[a]Symmetry operations: (A) -x+2, -y+2, -z+2 (B) -x+2, -y+1, -z+1