

Supporting Information File

Assembly of four d¹⁰-metal inorganic–organic hybrid coordination polymers based on bipyrazine imine-based ligand: synthesis, crystal structures and luminescent properties

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Table S1. Selected Bond Distances (Å) and Bond Angles (°) for **1–4**.

Polymer 1			
Ag(1)–N(3B)	2.266(4)	Ag(1)–N(1)	2.333(4)
Ag(1)–N(2)	2.467(4)	Ag(1)–O(1)	2.559(5)
N(3B)–Ag(1)–N(1)	167.83(16)	N(3B)–Ag(1)–N(2)	115.70(15)
N(1)–Ag(1)–N(2)	68.12(14)	N(3B)–Ag(1)–O(1)	100.71(16)
N(1)–Ag(1)–O(1)	85.82(16)	N(2)–Ag(1)–O(1)	121.28(16)
Polymer 2			
Ag(1)–N(1)	2.270(3)	Ag(1)–N(3)	2.386(3)
Ag(1)–S(1C)	2.507(1)	Ag(1)–S(1B)	2.644(1)
N(1)–Ag(1)–N(3)	97.25(14)	N(1)–Ag(1)–S(1C)	121.68(14)
N(3)–Ag(1)–S(1C)	113.67(7)	N(1)–Ag(1)–S(1B)	96.76(11)
N(3)–Ag(1)–S(1B)	116.10(7)	S(1C)–Ag(1)–S(1B)	110.25(4)
Polymer 3			
Cd(1)–N(1C)	2.275(2)	Cd(1)–N(3)	2.402(2)
Cd(1)–S(1)	2.751(5)		
N(1C)–Cd(1)–N(3)	89.97(7)	N(1D)–Cd(1)–N(3)	90.03(7)
N(1C)–Cd(1)–S(1)	87.59(5)	N(1D)–Cd(1)–S(1)	92.41(5)
N(3B)–Cd(1)–S(1)	89.70(5)	N(3)–Cd(1)–S(1)	90.30(5)
Polymer 4			
Cd(1)–N(1)	2.436(2)	Cd(1)–I(1)	2.894(1)
Cd(1)–I(1B)	3.013(1)		
N(1)–Cd(1)–I(1)	89.61(5)	N(1)–Cd(1)–I(1C)	89.69(5)
I(1)–Cd(1)–I(1 C)	91.60(1)	N(1)–Cd(1)–I(1 B)	90.31(5)
I(1)–Cd(1)–I(1 B)	88.40(1)	N(1)–Cd(1)–I(1D)	90.39(5)

Symmetry transformations used to generate equivalent atoms: **1**: B $-1/2 + x, 1/2 + y, z$; **2**: B $-1 - x, -1/2 - y, -1/2 + z$; C $1/2 + x, -1/2 - y, z$; **3**: B $-x, 1 - y, 1 - z$; C $1 + x, y, z$; D $-1 - x, 1 - y, 1 - z$; **4**: B $1 + x, y, z$; C $-1 - x, -1 - y, -z$; D $-x, -1 - y, -z$.

Table S2. Hydrogen Bonding Interactions (Å° and °) of **1–4**.

D–H...A	D–H	H...A	D...A	∠DHA	Symmetry Codes
Polymer 1					
O(1W)–H(1WA)···O(2)	0.85	2.08	2.929(8)	179	
C(2)–H(2A)···O(1)	0.93	2.54	3.447(7)	166	$5/2 - x, 1/2 - y, 1 - z$
C(6)–H(6A)···O(2)	0.96	2.51	3.238(9)	133	$2 - x, -1 + y, 3/2 - z$
C(6)–H(6A)···N(2)	0.96	2.34	2.770(8)	107	$2 - x, y, 3/2 - z$
C(6)–H(6B)···O(1)	0.96	2.38	3.282(9)	157	$5/2 - x, -1/2 + y, 3/2 - z$
Polymer 2					
C(7)–H(7A)···N(4)	0.96	2.31	2.733(5)	106	$-1 - x, -y, z$
Polymer 3					
C(7)–H(7A)···N(4)	0.96	2.31	2.728(4)	105	$-1 - x, 1 - y, -z$
Polymer 4					
C(6)–H(6A)···N(3)	0.96	2.34	2.731(4)	103	$1 - x, -1 - y, 1 - z$

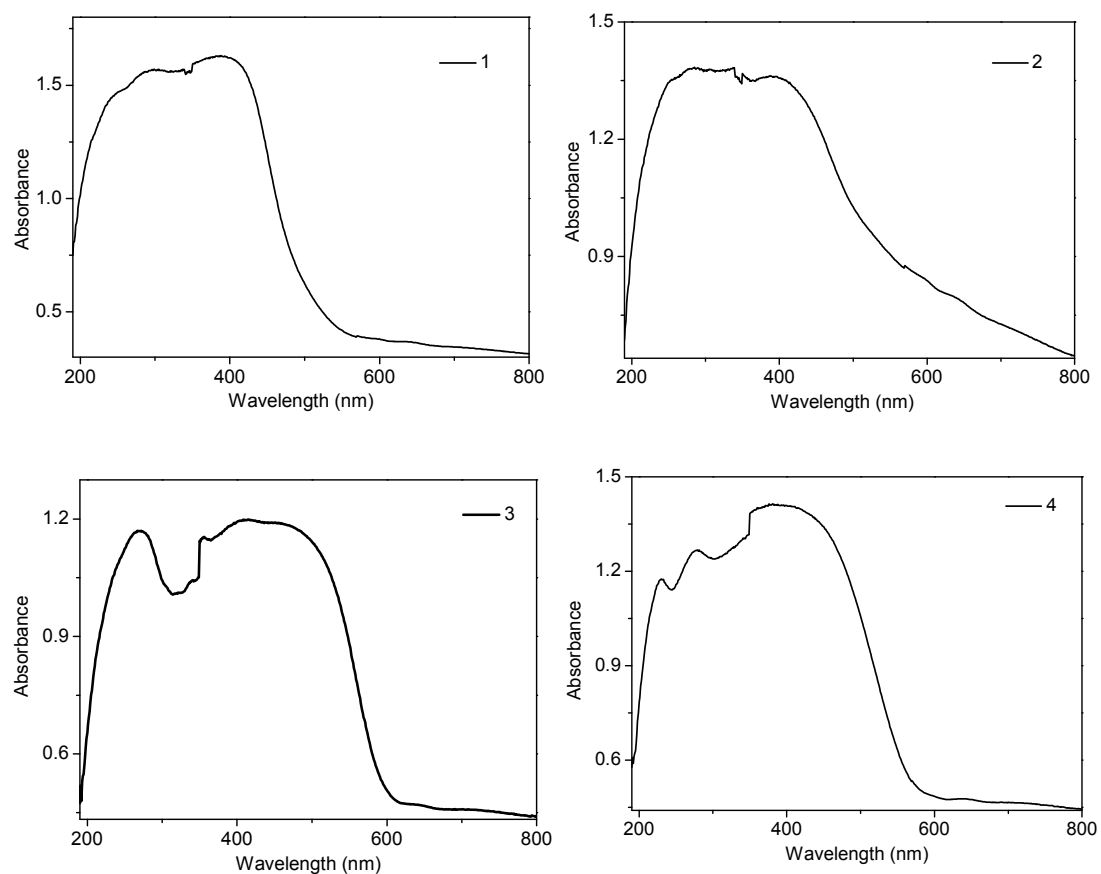


Figure S1. The electronic absorption spectra of **1-4** at room temperature in the solid state.

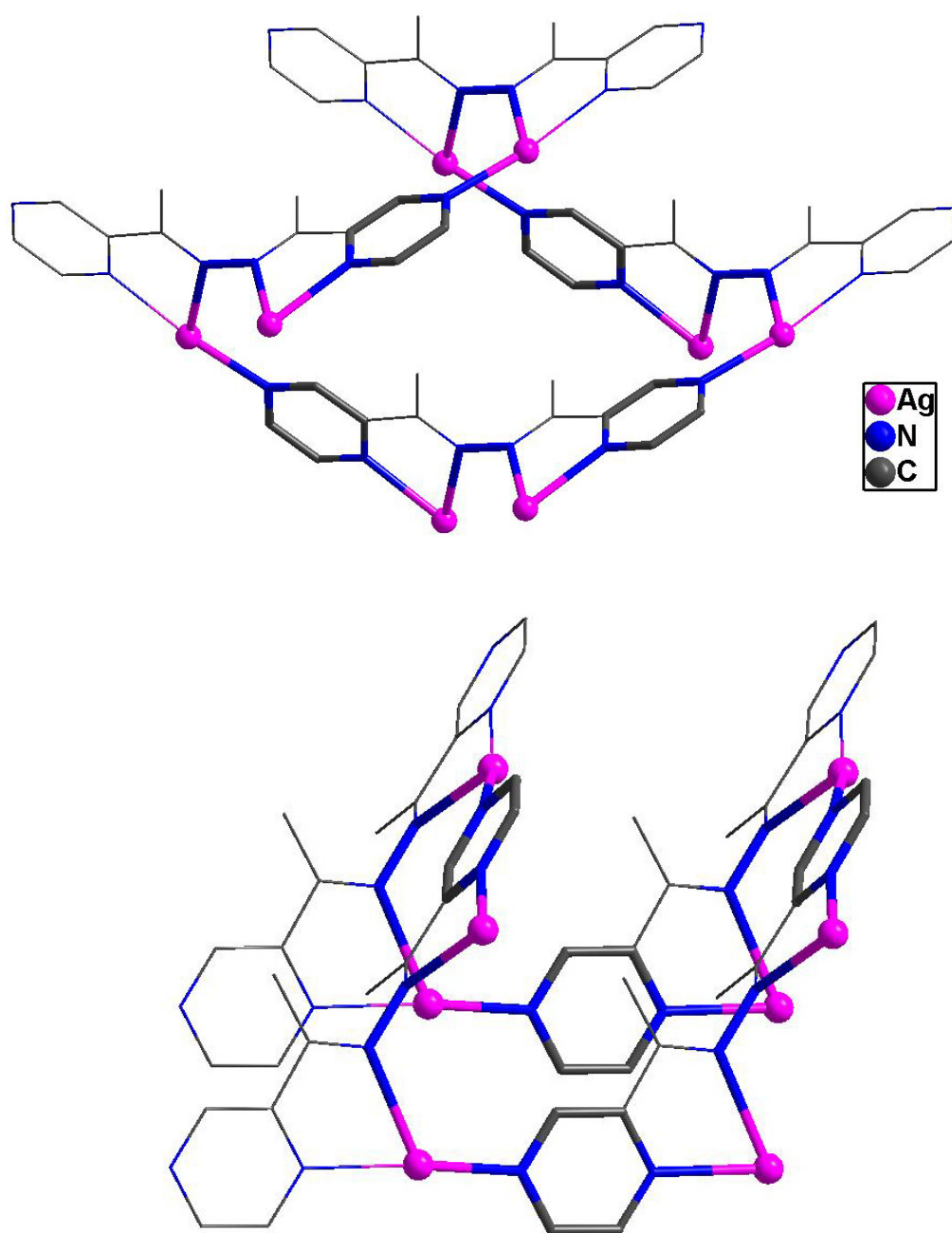


Figure S2. An U-type macrometallacyclic unit with H atoms omitted for clarity in polymer **1**

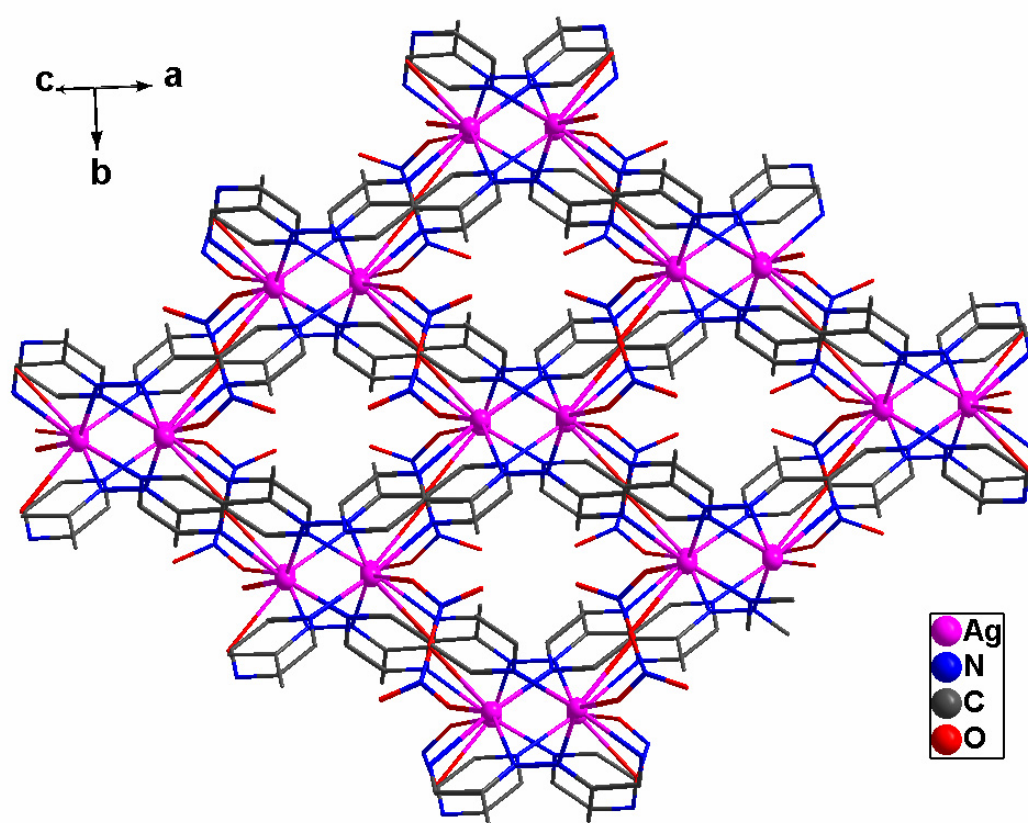


Figure S3. View of 3D structure of **1** with solvent molecules omitted for clarity.

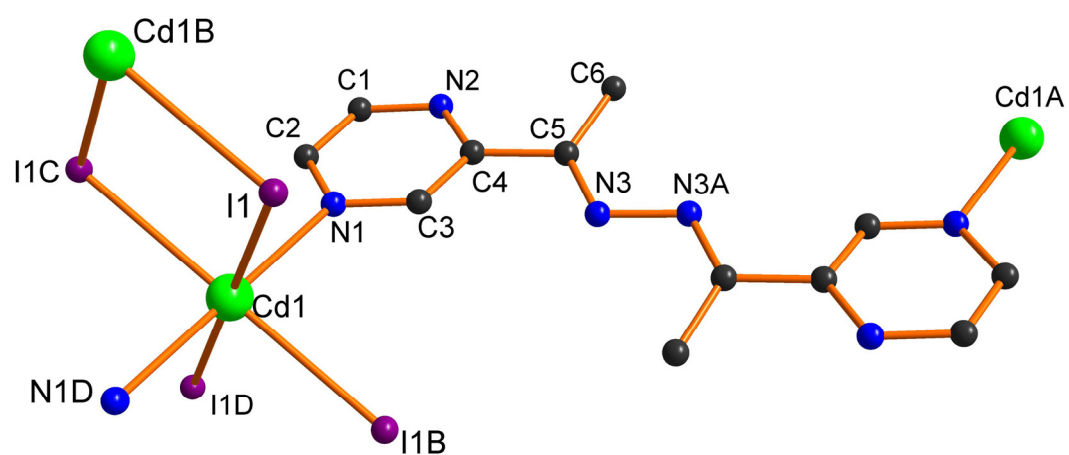


Figure S4. The coordination environments for Cd atom in **4** with H atoms omitted for clarity.

Symmetry codes: A $1 - x, -1 - y, 1 - z$; B $1 + x, y, z$; C $-1 - x, -1 - y, -z$; D $-x, -1 - y, -z$.

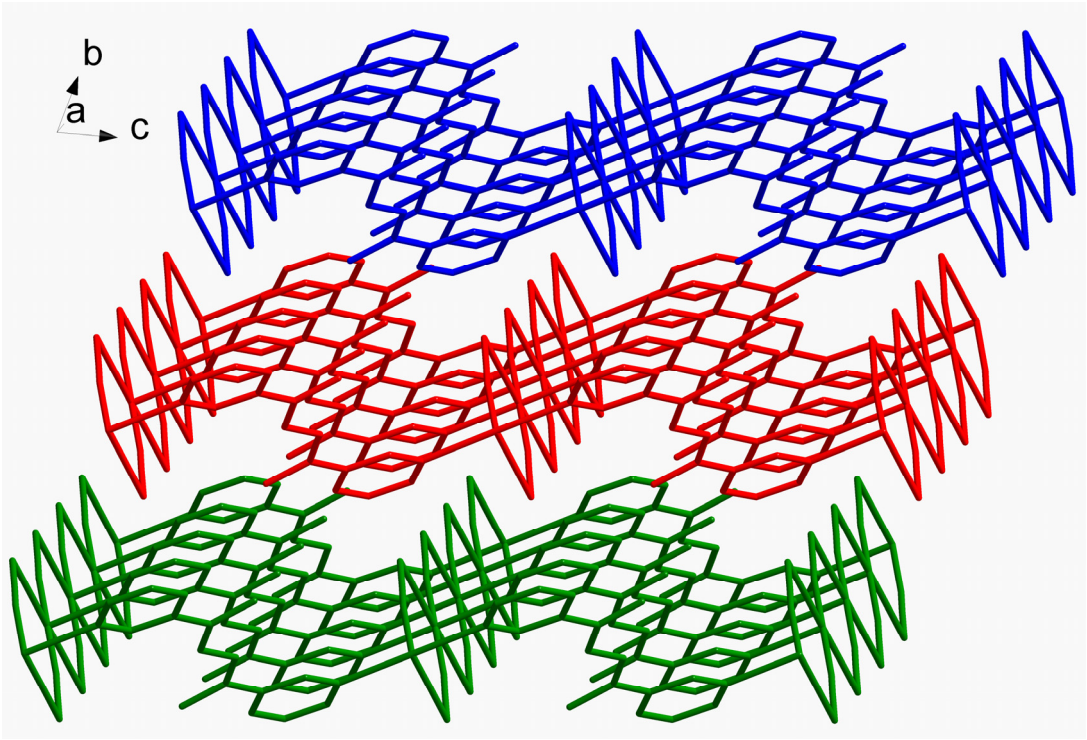


Figure S5. View of 3D supramolecular structure of **3**.

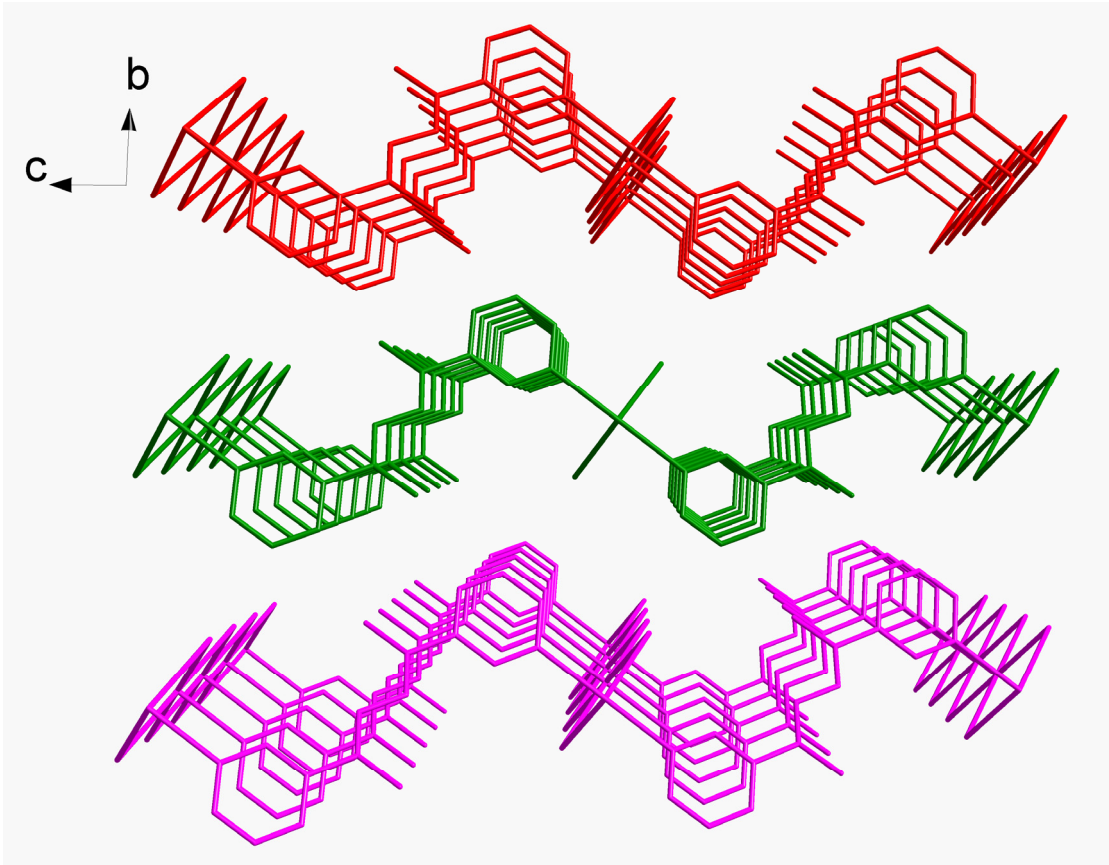


Figure S6. View of 3D supramolecular structure of **4**.

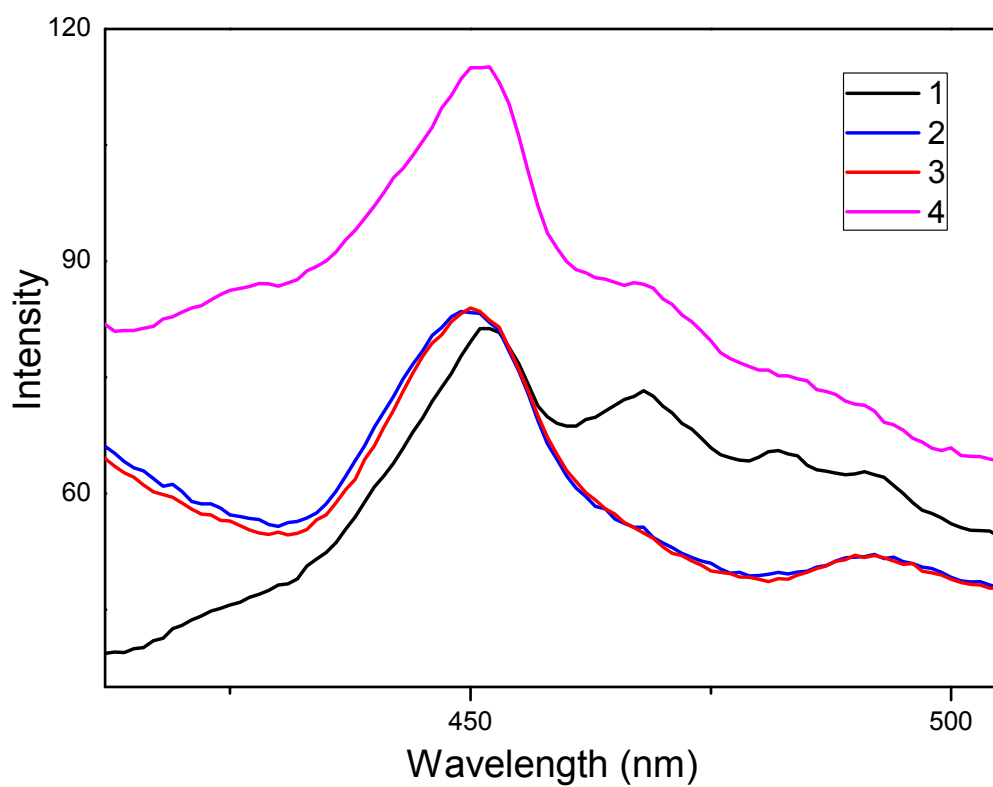


Figure S7 Photoinduced emission spectra of **1–4** in the solid state at room temperature.

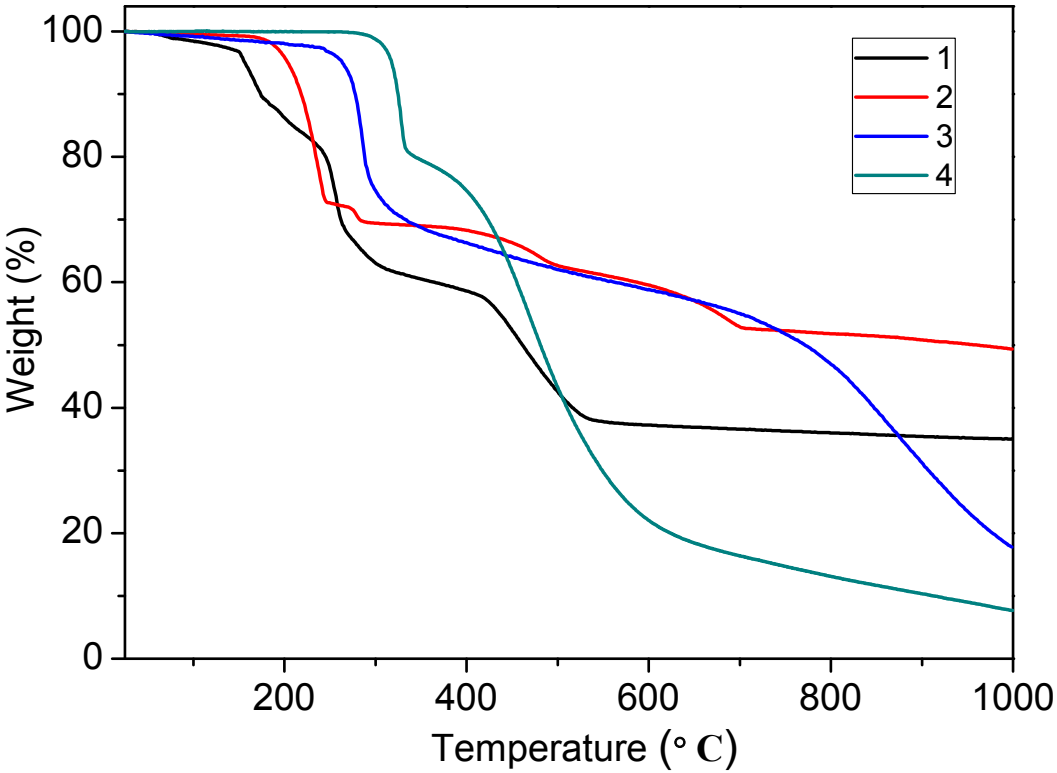


Figure S8. TGA curves for **1–4** polymers.