Supporting Information

Structural Diversity of a series of coordination polymers built from 5-substituted isophthalic acid with or without methyl-functionalized N-donor ligand

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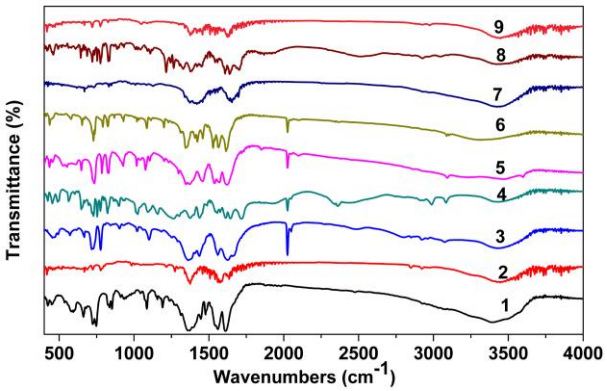

Figure S1. IR spectra of **1**-**9**.

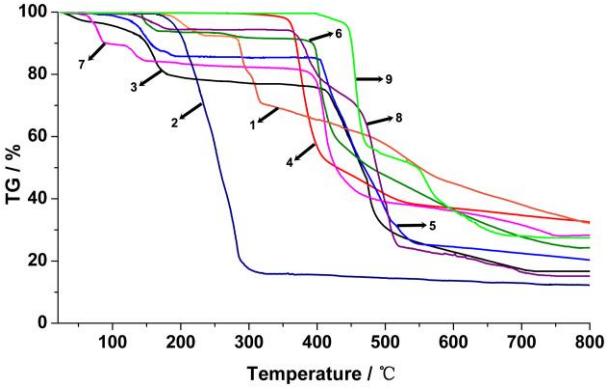

Figure S2. Themogravimetric curves for CPs **1**-**9**.

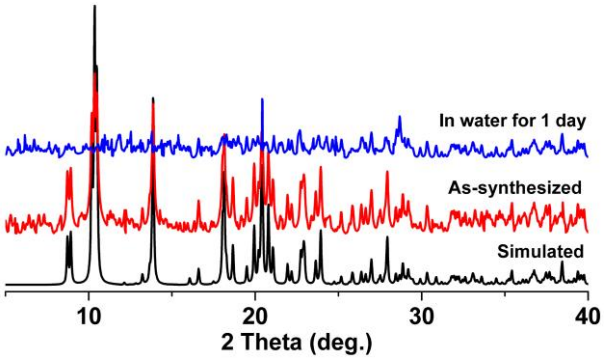

Figure S3. PXRD patterns of **1**.

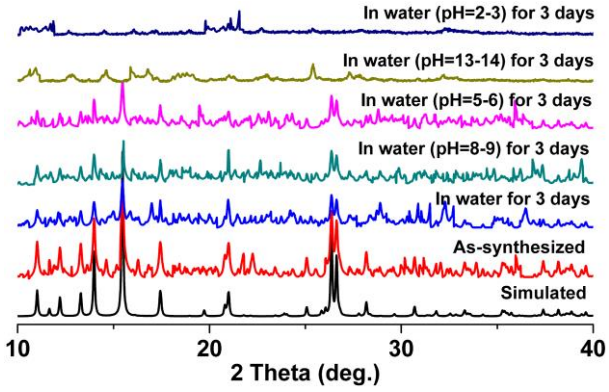

Figure S4. PXRD patterns of **2**.

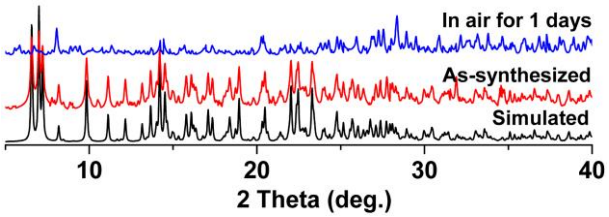

Figure S5. PXRD patterns of **3**.

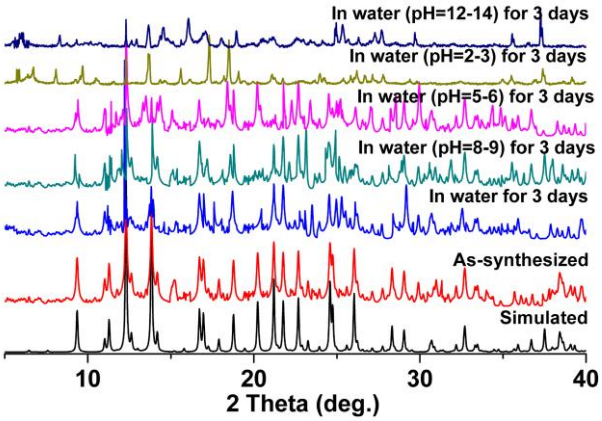

Figure S6. PXRD patterns of **4**.

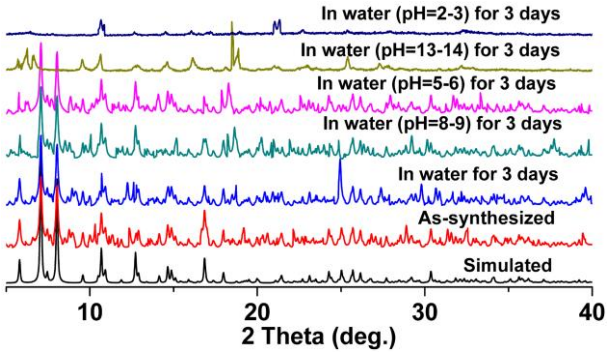

Figure S7. PXRD patterns of **5**.

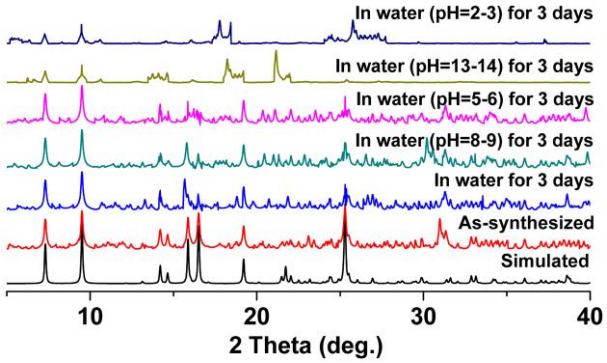

Figure S8. PXRD patterns of **6**.

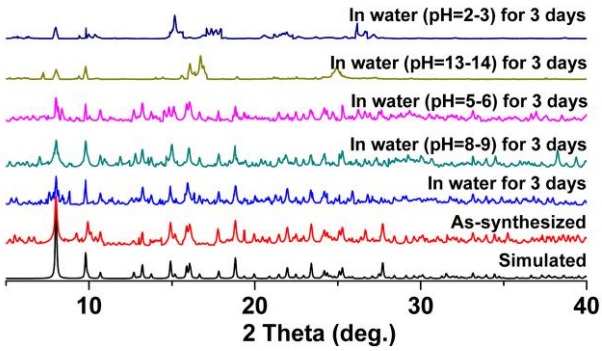

Figure S9. PXRD patterns of **7**.

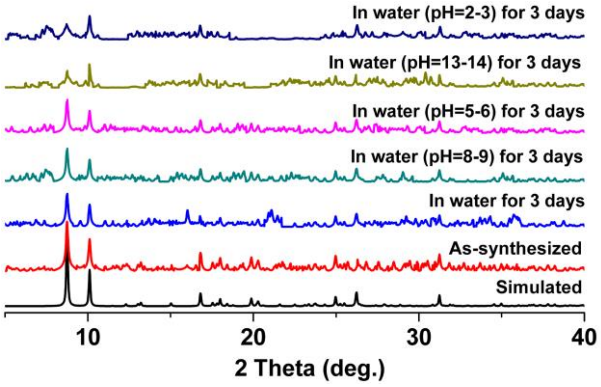

Figure S10. PXRD patterns of **8**.

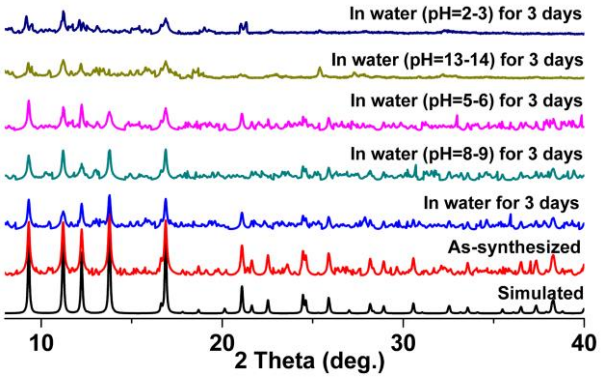

Figure S11. PXRD patterns of **9**.

Table S1 Selected bond length and angles of CPs **1-9**

		1	
Zn1-O1	2.141(9)	Zn1-O2	2.293(7)
Zn1-O3	2.068(8)	Zn1-O4^{i}	2.109(7)
Zn1-O5	2.278(8)	Zn2-O6	2.083(7)
Zn2-O7^{ii}	2.045(8)	Zn2-O9	2.060(8)
O4^{i}-Zn1-O8^{ii}	105.5(3)	O4^{i}-Zn1-O1	92.6(3)
O8^{ii}-Zn1-O5	148.0(3)	O4^{i}-Zn1-O2	150.5(3)
O4^{i}-Zn1-O6	103.3(3)	O7^{ii}-Zn2-O9	91.7(3)
O9-Zn2-O3^{i}	168.3(3)	O7^{ii}-Zn2-O11	179.3(3)

O7^{ii}-Zn2-O6	88.8(3)	O3^{i}-Zn2-O10	84.6(3)
		2	
Zn1-O1	1.9727(17)	Zn1-N1	2.097(2)
O1^{i}-Zn1-O1	127.96(11)	O1^{i}-Zn1-N1	100.62(8)
O1^{i}-Zn1-N1 ^{i}	108.75(7)		
		3	
Zn1-O1	2.112(4)	Zn1-O4^{i}	2.098(4)
Zn1-O5	2.064(4)	Zn1-O11^{ii}	2.049(5)
Zn2-O3^{i}	2.006(4)	Zn2-O6	1.977(4)
Zn2-O9	1.960(4)	Zn2-O13	1.989(4)
Zn3-O2	1.961(4)	Zn3-O7^{ii}	1.951(4)
Zn3-O12^{ii}	1.963(5)	Zn3-O16	1.942(4)
O11^{ii}-Zn1-O5	88.46(17)	O11^{ii}-Zn1-O15^{iii}	96.07(18)
O5-Zn1-O15^{iii}	91.05(18)	O11^{ii}-Zn1-O4^{i}	175.61(17)
O4^{i}-Zn1-O14	87.88(17)	O15^{iii}-Zn1-O1	91.84(17)
O9-Zn2-O6	91.06(17)	O9-Zn2-O13	111.00(19)
O9-Zn2-O3i	107.78(18)	O13-Zn2-O3^{i}	111.75(18)
O16^{iii}-Zn3-O7^{ii}	110.43(18)	O16^{iii}-Zn3-O2	122.18(18)
O7^{ii}-Zn3-O2	107.50(17)	O16^{iii}-Zn3-O12^{iii}	106.87(19)
		4	
Zn1-O13	1.964(13)	Zn1-O10	2.044(15)
Zn1-N1	2.055(9)	Zn1-O5	2.062(14)
Zn2-O9	1.977(14)	Zn2-N2^{i}	1.998(9)
Zn2-O1	2.000(13)	Zn2-O14	2.057(12)
Zn3-O8^{iv}	1.967(15)	Zn3-O3^{ii}	2.009(14)
Zn3-N3	2.022(5)	Zn3-O7	2.054(13)
Zn4-O12^{v}	1.982(14)	Zn4-N4	2.029(5)
Zn4-O11	2.086(13)	Zn4-O15^{vi}	2.091(12)
O13-Zn1-O10	91.3(6)	O13-Zn1-N1	101.3(5)
O10-Zn1-O5	87.6(6)	O2-Zn1-N1	103.2(5)
O9-Zn2-N2^{i}	95.9(6)	O9-Zn2-O1	162.0(6)
O9-Zn2-O14	88.3(6)	O9-Zn2-O6	102.7(5)
O8^{iv}-Zn3-O3^{ii}	89.4(6)	O8^{iv}-Zn3-O4^{iii}	161.7(6)
O3^{ii}-Zn3-N3	109.4(5)	O4^{iii}-Zn3-O7	89.4(6)
O12^{v}-Zn4-O16^{vii}	164.2(5)	O12^{v}-Zn4-N^{4}	97.0(4)
O16^{vii}-Zn4-O11	88.5(6)	N4-Zn4-O15^{vi}	100.3(4)
		5	
Zn1-O1	2.033(4)	Zn1-O14^{i}	1.999(5)
Zn1-O24^{ii}	1.938(4)	Zn2-O2	2.199(4)
Zn2-O7	2.135(5)	Zn2-O23^{ii}	2.116(4)
Zn3-O8	1.994(4)	Zn3-O13	1.968(4)
Zn3-O26	1.820(5)	Zn4-O17^{iii}	2.348(4)
Zn4-O19	1.998(5)	Zn4-O27	1.874(4)
Zn5-O18^{iii}	1.967(4)	Zn5-O20	1.981(5)

Zn6-O10^{v}	2.147(4)	Zn6-O28^{vii}	2.094(5)
Zn7-O5^{viii}	1.843(4)	Zn7-O9^{vi}	1.903(4)
O25-Zn1-O24^{ii}	112.7(2)	O24^{ii}-Zn1-O14^{i}	115.6(2)
O14^{i}-Zn1-O1	95.86(18)	O26-Zn2-O25	172.72(16)
O26-Zn2-O23^{ii}	89.43(18)	O25-Zn2-O25^{i}	80.2(2)
O26-Zn3-O13	123.8(2)	O13-Zn3-O27	105.30(18)
O27-Zn4-O17^{iii}	85.86(16)	O19-Zn4-O28	93.95(17)
O18^{iii}-Zn5-O20	101.07(17)	O18^{iii}-Zn5-O6^{iv}	94.26(17)
O20-Zn5-O1W	143.78(19)	O28^{vii}-Zn6-O10^{vi}	86.62(19)
O28^{vii}-Zn6-O10^{v}	93.38(19)	O10^{vi}-Zn6-O10^{v}	180.0
O5^{viii}-Zn7-O9^{vi}	119.55(17)	O5^{viii}-Zn7-O2W	102.58(17)
		6	
Zn1-O3^{ii}	1.9652(11)	Zn1-O2^{i}	1.9988(11)
Zn1-N2	2.0638(12)	Zn1-O1W	2.0997(12)
O3^{ii}-Zn1-O2^{i}	124.46(5)	O3^{ii}-Zn1-N2	121.01(5)
O2^{i}-Zn1-N2	113.63(5)	O3^{ii}-Zn1-O1W	92.27(5)
O2^{i}-Zn1-O1W	99.42(5)	N2-Zn1-O1W	87.60(5)
O3^{ii}-Zn1-O1	86.82(5)	O2^{i}-Zn1-O1	83.03(4)
		7	
Cd1-O1	2.234(2)	Cd1-O1W	2.299(2)
Cd1-O3^{i}	2.307(2)	Cd1-N1	2.309(2)
Cd1-O4^{ii}	2.375(2)	Cd1-O4^{i}	2.646(2)
O1-Cd1-O1W	87.84(9)	O1-Cd1-O3^{i}	125.01(8)
O1W-Cd1-O3^{i}	82.13(9)	O1-Cd1-N1	135.41(8)
O1W-Cd1-N1	90.60(9)	O3^{i}-Cd1-N1	98.79(8)
O1-Cd1-O4^{ii}	86.71(8)	O1-Cd1-O4^{i}	79.46(7)
		8	
Zn1-N1	2.356(6)	Zn1-O1^{ii}	2.324(5)
Zn1-O2	2.378(5)	Zn1-O3^{i}	2.309(6)
Zn1-O1W	2.351(6)	O3^{i}-Zn1-O1^{ii}	126.6(2)
O3^{i}-Zn1-O1W	81.0(2)	O1^{ii}-Zn1-O1W	82.9(2)
O3^{i}-Zn1-N1	104.4(2)	O1W-Zn1-N1	88.3(2)
O1^{ii}-Zn1-N1	125.6(2)	O1^{ii}-Zn1-O2	106.43(19)
		9	
Zn1-N1	2.057(4)	Zn1-O1	2.082(3)
Zn1-O2^{ii}	2.009(2)	Zn1-O2^{iii}	2.009(2)
O2^{ii}-Zn1-O2^{iii}	167.70(17)	O2^{ii}-Zn1-N1	96.15(8)
O2^{ii}-Zn1-O1^{i}	88.41(11)	O2^{iii}-Zn1-O1^{i}	88.30(11)
N1-Zn1-O1^{i}	105.50(7)	O1-Zn1-O1^{i}	148.99(14)

Symmetry codes: **1**, i = x, y, 1+z; ii = 1-x, 0.5+y, -z; **2**, i = -x, y, 0.5-z; **3**, i = 2-x, 1-y, 2-z; ii = x, 0.5-y, 0.5+z; iii = 0.5+x, 0.5-y, 2-z; **4**, i = -1+x, y, z; ii = -0.5+x, -0.5+y, z; iii = 0.5-x, -0.5+y, 1.5-z; iv = -x, y, 1.5-z; v = x, 1-y, 2-z; vi = 0.5+x, -0.5+y, z; vii = 0.5+x, 1.5-y, 2-z; **5**, i = -x, 2-y, -z; ii = 1-x, 2-y, -z; iii = -x, 1-y, -z; iv = x, -1+y, z; v = 1+x, y, z; vi = -x, 2-y, 1-z; vii = 1-x, 2-y, 1-z; viii = 1-x, 3-y, 1-z; **6**, i = x, 1.5-y, 0.5+x; ii = 1-x, 1-y, 1-z; **7**, i = x, 1+y, z; ii = -x, 1-y, 1-z; **8**, i = -x, -y,

2-z; **9**, i = 1+y, -1+x, -z; ii = 2-x, -y, z; iii = 1-y, 1-x, -z.

Table S2 Hydrogen bond geometries for **2**, **6-8** (Å, °)

D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	∠D-H···A
		2		
O4-H4A···O2^{ii}	0.82	1.84	2.658	172
C12-H12···O3^{iii}	0.93	2.45	3.338	159
C13-H13···O1	0.93	2.59	3.194	123
		6		
O1W-H11···O2^{iii}	0.83	1.96	2.751	160
O1W-H12···O4^{iv}	0.83	1.91	2.706	159
C10-H10···O5^{v}	0.93	2.43	3.286	153
		7		
O1W-H1W···O3^{iii}	0.82	1.94	2.737	164
O1W-H2W···O2W^{iii}	0.82	1.89	2.702	169
O2W-H3W···N3	0.82	2.34	3.111	155
O2W-H4W···O2	0.82	1.91	2.732	175
C13-H13···O2	0.93	2.55	3.151	123
		8		
O1W-H1W···O4^{ii}	0.87	1.85	2.682	161
O1W-H2W···O1^{iii}	0.87	1.91	2.761	167
C14-H14···O2^{iv}	0.93	2.26	3.035	141
C15-H15A···O3^{i}	0.96	2.47	3.207	134

Symmetry codes: **2**, ii = 0.5-x, 0.5+y, 0.5-z; iii = -0.5+x, 1.5-y, -0.5+z; **6**, iii = x, y, 1+z; iv = 1-x, 0.5+y, 1.5-z; v = -x, 0.5+y, 1.5-z; **7**, iii = 1-x, 1-y, 1-z; 8, i = -x, -y, 2-z; ii = -1+x, 1+y, z; iii = -1+x, y, z; iv = -x, 1-y, 2-z.