

Supporting Information for CrystEngComm

Syntheses, Structures and Characteristics of Four Metal Organic Coordination Polymers Based on 5-Hydroxyisophthalic Acid and N-containing Auxiliary Ligands

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(1) Table S1 Selected bond lengths (Å) and angles (°) for 1-4.

Compound 1					
Zn1-O1	2.047 (2)	Zn1-O2 ⁱ	1.991 (2)	Zn1-O3 ⁱⁱ	1.975 (2)
Zn1-N1	2.127 (3)	Zn1-N2	2.159 (3)	O1-Zn1-N1	88.54 (10)
O1-Zn1-N2	143.28 (10)	O2 ⁱ -Zn1-O1	92.53 (10)	O2 ⁱ -Zn1-N1	159.42 (11)
O2 ⁱ -Zn1-N2	91.40 (12)	O3 ⁱⁱ -Zn1-O1	94.33 (10)	O3 ⁱⁱ -Zn1-O2 ⁱ	100.78 (10)
O3 ⁱⁱ -Zn1-N1	99.63 (11)	O3 ⁱⁱ -Zn1-N2	120.68 (10)	N1-Zn1-N2	75.84 (11)
Symmetry codes: (i) -x, +y, 1/2-z; (ii) 1/2-x, 1/2-y, 1-z.					
Compound 2					
Ni1-O1 ⁱ	2.098 (3)	Ni1-O1W	2.055 (3)	Ni1-O2 ⁱ	2.179 (3)
Ni1-O5	2.024 (3)	Ni1-N1	2.100 (3)	Ni1-N2 ⁱⁱ	2.132 (3)
O1 ⁱ -Ni1-O2 ⁱ	61.80 (10)	O1 ⁱ -Ni1-N1	89.97 (12)	O1 ⁱ -Ni1-N2 ⁱⁱ	91.14 (12)
O1W-Ni1-O1 ⁱ	164.41 (10)	O1W-Ni1-O2 ⁱ	102.61 (11)	O1W-Ni1-N1	89.96 (12)
O1W-Ni1-N2 ⁱⁱ	89.03 (12)	O5-Ni1-O1W	96.54 (12)	O5-Ni1-O1 ⁱ	99.05 (11)
Symmetry codes: (i) x+1, y, z; (ii) x, y, z+1; (iii) x-1, y, z; (iv) x, y, z-1.					
Compound 3					
Zn1-O2	1.929 (2)	Zn1-O3 ⁱ	1.948 (2)	Zn1-N1 ⁱⁱ	2.027 (3)
Zn1-N6	2.022 (3)	O2-Zn1-O3 ⁱ	122.41 (9)	O2-Zn1-N1 ⁱⁱ	116.47 (10)
O3 ⁱ -Zn1-N1 ⁱⁱ	98.00 (10)	O2-Zn1-N6	115.30 (10)		
Symmetry codes: (i) 1+x,+y,+z; (ii) +x,1/2-y,1/2+z; (iii) -1+x,+y,+z; (iv) +x,1/2-y,-1/2+z.					
Compound 4					
Zn1-O2	1.941 (5)	Zn1-O6	1.953 (5)	Zn1-O8 ⁱ	1.931 (5)
Zn1-O10 ⁱⁱ	1.995 (4)	Zn2-O3 ⁱⁱⁱ	1.940 (4)	Zn2-O4 ⁱ	1.942 (5)
Zn2-O10	1.971 (4)	Zn2-O1 ⁱⁱ	1.977 (5)	O8 ⁱ -Zn1-O2	121.1 (2)
O8 ⁱ -Zn1-O6	100.7 (2)	O2-Zn1-O6	109.7 (2)	O8 ⁱ -Zn1-O10 ⁱⁱ	108.5 (2)
O2-Zn1-O10 ⁱⁱ	104.46 (19)	O6-Zn1-O10 ⁱⁱ	112.52 (19)	O3 ⁱⁱⁱ -Zn2-O4 ⁱ	109.2 (2)
O3 ⁱⁱⁱ -Zn2-O10	108.44 (19)	O4 ⁱ -Zn2-O10	122.2 (2)	O3 ⁱⁱⁱ -Zn2-O1 ⁱⁱ	104.4 (2)
O4 ⁱ -Zn2-O1 ⁱⁱ	105.7 (3)	O10-Zn2-O1 ⁱⁱ	105.4 (2)		
Symmetry codes: (i) -x, y-1/2, -z+1/2; (ii) -x, -y+1, -z; (iii) x-1, -y+3/2, z-1/2; (iv) x+1, -y+3/2, z+1/2; (v) -x, y+1/2, -z+1/2.					

(2) Table S2 The hydrogen bond geometries for 1-4.

Compound 1				
<i>D-H...A</i>	<i>D-H</i>	<i>H...A</i>	<i>D...A</i>	<i>D-H...A</i>
O(5)-H(5)···O(4) ⁱⁱⁱ	0.82	1.95	2.690 (4)	151
C(12)-H(12)···O(4) ^{iv}	0.93	2.40	3.309 (5)	166
C(15)-H(15)···O(4) ^{iv}	0.93	2.51	3.413 (5)	165
Symmetry codes: (iii) $-x+1, y, -z+1/2$; (iv) $x-1/2, y-1/2, z$.				
Compound 2				
<i>D-H...A</i>	<i>D-H</i>	<i>H...A</i>	<i>D...A</i>	<i>D-H...A</i>
O1W-H1WA···O4	0.88	1.87	2.617 (4)	141
O3-H3A···O2W	0.82	1.90	2.713 (5)	171
O1W-H1WB···O2 ^v	0.88	1.93	2.744 (4)	153
Symmetry code: (v) $-x+2, -y+1, -z$.				
Compound 3				
<i>D-H...A</i>	<i>D-H</i>	<i>H...A</i>	<i>D...A</i>	<i>D-H...A</i>
O5-H5A···O1 ^v	0.82	1.93	2.752 (3)	177
C20-H20···O1 ^v	0.93	2.57	3.274 (4)	132
C23-H23···O5 ^{vi}	0.93	2.57	3.246 (4)	130
Symmetry codes: (v) $-x+3, y+1/2, -z+3/2$; (vi) $-x+3, y-1/2, -z+3/2$.				
Compound 4				
No Classic Hydrogen Bonds Found				

(3) Figure S1 The powder XRD patterns and the simulated one from the single-crystal diffraction data for compounds 1-4

