Electronic Supplementary Information

Construction of a 2D Interwoven and 3D Interpenetrated Metal-Organic Frameworks of Zn(II) by Varying N,N'-Donor Spacers

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Table S1. Selected bond lengths (Å) and bond angles (°) in compound **1**.

Zn1-O1	1.953(5)	O1-Zn1-O2	100.3(2)
Zn1-O2	1.969(5)	O1-Zn1-N1	107.8(2)
Zn1-N1	2.017(6)	O1-Zn1-N2	115.7(2)
Zn1-N2	2.022(6)	O2-Zn1-N1	112.23(19)
Zn2-O3	1.974(4)	O2-Zn1-N2	107.1(2)
Zn2-N3	2.010(6)	N1-Zn1-N2	113.2(2)
Zn2-N4	2.018(6)	O3-Zn2-N3	109.33(19)
Zn2-O4^{i}	1.959(5)	O3-Zn2-N4	110.23(19)
O4^{i}-Zn2-N4	111.2(2)	O3-Zn2-O4^{i}	97.73(19)
Zn1-O1-C1	112.8(4)	N3-Zn2-N4	113.2(2)
Zn1-O2-C7	118.6(5)	O4^{i}-Zn2-N3	114.1(2)
Zn2-O3-C6	118.2(4)	Zn2-N3-C23^{iii}	123.2(4)
Zn2^{ii}-O4-C12	111.9(2)	Zn2-N3-C27^{iii}	120.8(4)
Zn1-N1-C13	122.5(4)	Zn2-N4-C28	121.6(4)
Zn1-N1-C17	122.0(4)	Zn2-N4-C32	122.3(4)
Zn1-N2-C18	121.1(4)	Zn1-N2-C22	121.3(4)

Symmetry codes: (i) x, -1+y, z; (ii) x,1+y,z; (iii) 1+x, y, z

Table S2. Selected bond lengths (Å) and bond angles (°) in compound **2**.

Zn1-O1	1.9696(9)	O1-Zn1-O1^{i}	104.29(4)
Zn1-N1	2.0438(11)	O1-Zn1-N1^{i}	98.93(4)
Zn1-O1^{i}	1.9696(9)	O1^{i} -Zn1-N1	98.93(4)
Zn1-N1^{i}	2.0438(11)	N1-Zn1-N1^{i}	108.02(4)
O1W-H1A	0.81(3)	O1^{i}-Zn1-N1^{i}	124.48(4)
O1W-H1B	0.80(3)	Zn1-O1-C1	110.77(7)
O2W-H2A	0.88(3)	Zn1-N1-C4	121.52(8)
O2W-H2B	0.84(3)	Zn1-N1-C8	120.50(8)
O1-Zn1-N1	124.48(4)		

Symmetry codes: (i) 1-x, y, ½-z

Table S3. Selected bond lengths (Å) and bond angles (°) in compound **3**.

Zn1-O1	1.933(2)	O1-Zn1-N1^{i}	103.93(4)
Zn1-N1	2.052(2)	O1^{i}-Zn1-N1	103.93(4)
Zn1-O1^{i}	1.933(2)	N1-Zn1-N1^{i}	99.95(4)
Zn1-N1^{i}	2.052(2)	O1^{i}-Zn1-N1^{i}	123.95(4)
O1-Zn1-N1	123.95(4)	Zn1-O1-C1	120.00(8)
O1-Zn1-O1^{i}	103.19(4)	Zn1-N1-C4	120.77(9)
		Zn1-N1-C8	119.69(9)

Symmetry codes: (i) 1-x, y, 3/2-z

Table S4. Selected bond lengths (Å) and bond angles (°) for compound **4**.

Zn1-O1	2.360(2)	O5-Zn2-O8^{i}	153.82(8)
Zn1-O2	2.116(2)	O6-Zn2-O7	138.02(9)
Zn1-O3	2.019(2)	O6-Zn2-N3	88.86(8)
Zn1-O4	2.012(2)	O6-Zn2-N4	90.88(8)
Zn1-N1	2.151(3)	O6-Zn2-O8^{i}	82.14(8)
Zn1-N2	2.177(3)	O7-Zn2-N3	86.89(9)
Zn2-O5	2.035(2)	O7-Zn2-N4	90.85(10)
Zn2-O6	2.015(2)	O7-Zn2-O8^{i}	55.89(8)
Zn2-O7	2.060(2)	N3-Zn2-N4	176.32(10)
Zn2-N3	2.154(3)	O8^{i}-Zn2-N3	84.73(9)
Zn2-N4	2.151(3)	O8^{i}-Zn2-N4	91.59(9)
Zn2-O8^{i}	2.545(2)	O9-Zn3-O10	58.35(8)
Zn3-O9	2.374(2)	O9-Zn3-O11	153.11(8)
Zn3-O10	2.105(2)	O9-Zn3-O12	92.18(9)
Zn3-O11	2.021(2)	O9-Zn3-N5	92.77(9)
Zn3-O12	2.015(2)	O9-Zn3-N6^{ii}	83.61(9)
Zn3-N5	2.133(3)	O10-Zn3-O11	94.84(9)
Zn3-N6^{ii}	2.182(3)	O10-Zn3-O12	149.90(9)
Zn4-O13	2.024(2)	O10-Zn3-N5	93.92(9)
Zn4-O14	2.072(2)	O10-Zn3-N6^{ii}	85.86(9)
Zn4-O15	2.365(2)	O11-Zn3-O12	114.16(9)
Zn4-O16	2.133(2)	O11-Zn3-N5	90.99(9)
Zn4-N7	2.143(3)	O11-Zn3-N6^{ii}	93.13(9)
Zn4-N8	2.140(3)	O12-Zn3-N5	93.48(9)
O1-Zn1-O2	58.36(8)	O12-Zn3-N6^{ii}	84.72(9)
O1-Zn1-O3	87.43(8)	N5-Zn3-N6^{ii}	175.88(9)
O1-Zn1-O4	148.81(8)	O13-Zn4-O14	115.03(9)
O1-Zn1-N1	94.64(9)	O13-Zn4-O15	150.30(8)
O1-Zn1-N2	82.49(9)	O13-Zn4-O16	92.44(8)
O2-Zn1-O3	145.79(9)	O13-Zn4-N7	95.34(9)
O2-Zn1-O4	91.77(9)	O13-Zn4-N8	92.48(9)
O2-Zn1-N1	93.63(9)	O14-Zn4-O15	94.09(8)
O2-Zn1-N2	87.70(9)	O14-Zn4-O16	152.05(9)
O3-Zn1-O4	121.96(9)	O14-Zn4-N7	89.23(9)
O3-Zn1-N1	88.54(9)	O14-Zn4-N8	85.04(9)
O5-Zn2-N3	88.84(9)	O15-Zn4-O16	58.10(8)
O5-Zn2-N4	94.37(9)	O15-Zn4-N7	90.55(9)
O3-Zn1-N2	88.02(9)	O15-Zn4-N8	83.93(9)
O4-Zn1-N1	96.18(9)	O16-Zn4-N7	93.47(9)
O4-Zn1-N2	87.96(9)	O16-Zn4-N8	88.85(9)
N1-Zn1-N2	175.61(9)	N7-Zn4-N8	171.74(8)
O5-Zn2-O6	123.16(9)		
O5-Zn2-O7	98.50(9)		

Symmetry codes: (i) x, -1+y, z; (ii) x, 1+y,-1+z

Table S5. Hydrogen bonding interactions (Å,°) in compound **1**

D–H···A	H···A	D···A	D–H···A
C13–H13···O7	2.4700	3.175(9)	133.00
C16–H16···O8^{i}	2.5100	3.392(8)	159.00
C18–H18···O2w^{ii}	2.5500	3.332(13)	142.00
C22–H22···O8	2.3300	3.075(8)	137.00
C23–H23···O5^{iii}	2.5800	3.248(8)	129.00
C27–H27···O6^{i}	2.3400	3.097(8)	139.00
C28–H28···O5	2.4600	3.175(8)	133.00
C29–H29···O2w^{iv}	2.4900	3.101(12)	123.00
C31–H31···O6^{v}	2.5300	3.416(7)	160.00
C34–H34B ···O2^{v}	2.5400	3.358(11)	143.00
C39–H39B ···O2w	2.1200	3.07(3)	170.00

Symmetry codes: (i)1/2+x, 1-y, z; (ii)1/2-x, 1+y, 1/2+z; (iii)-1+x, y, z; (iv)1/2+x, -y, z; (v) -1/2+x, 1-y, z

Fig. S1 Space-fill model of the 3D framework, **3**

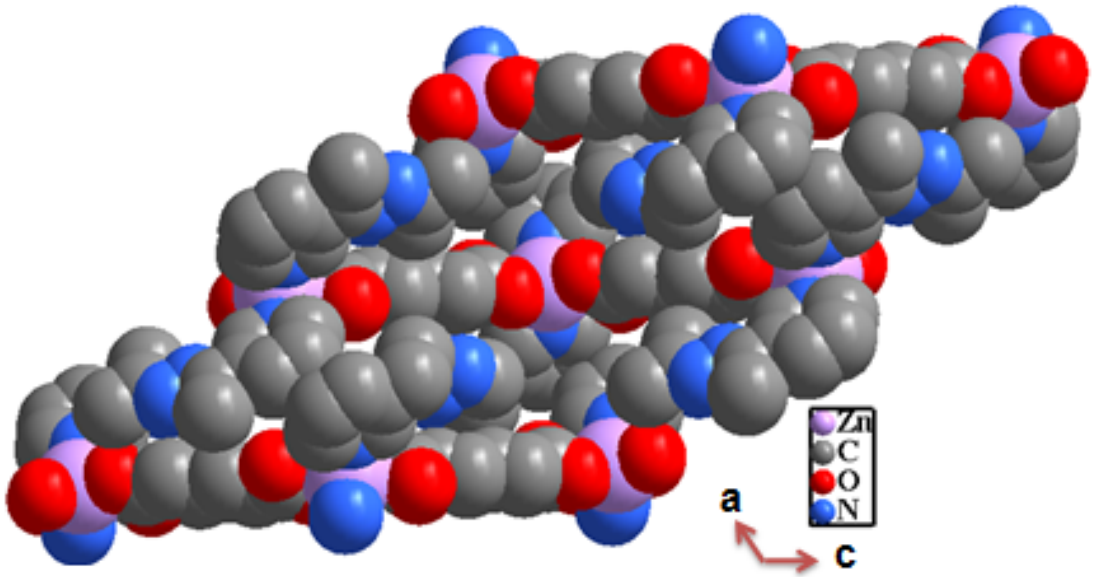

Table S6. Selected hydrogen bonding interactions (Å,°) in compound **2**

D–H···A	H···A	D···A	D–H···A
O1W–H1A···O2W	2.06(3)	2.866(2)	171(3)
O1W – H1B···O2W^{i}	2.18(3)	2.966(2)	169(3)
O2W – H2A···O2	1.84(3)	2.706(2)	171(3)
O2W – H2B···O1W^{i}	2.08(3)	2.873(2)	159(2)

Symmetry code: (i) 3/2-x,1/2+y, 1/2-z

Fig. S2 View of the 3D framework in compound **4** showing the guest 4bpdh molecule inside the open channel involved in C-H…O and C-H…N hydrogen bonding interaction.

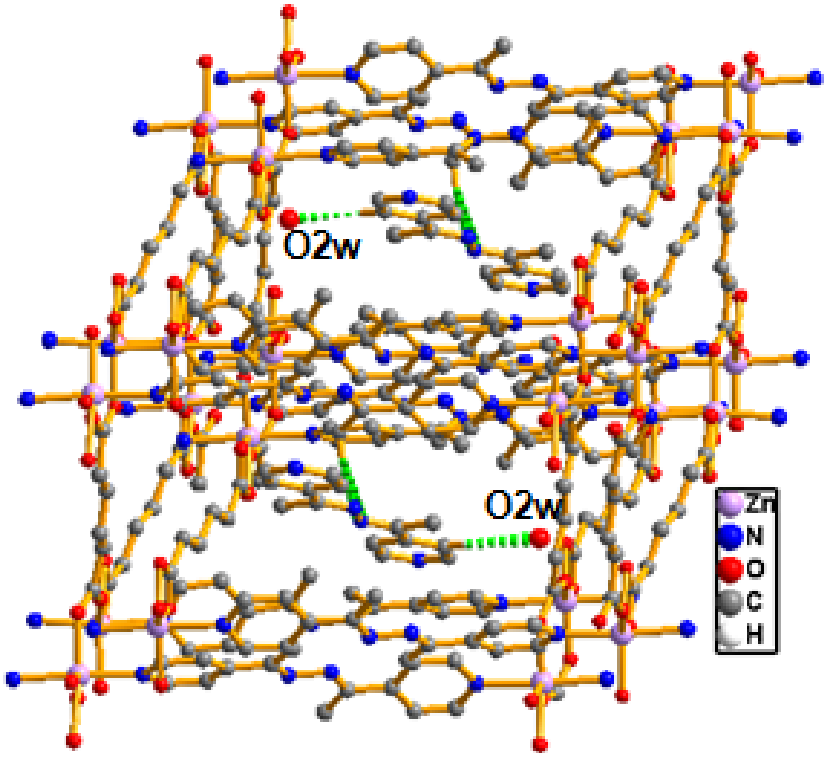

Table S7. Selected hydrogen bonding interactions (Å,°) in compound **4**

D–H···A	H···A	D···A	D–H···A
C33 – H33C…N19^{i}	2.6000	3.495(6)	156.00
C45 – H45A…N12	2.3100	2.710(5)	104.00
C83 – H83 …O1w^{ii}	2.4200	3.309(6)	160.00
C93 – H93 … O2w	2.4700	3.320(6)	152.00

Symmetry codes: (i) 1-x, 1-y, 2-z; (ii) 1-x, 2-y, 1-z.

Fig. S3 TGA plot for the compounds **1-4**.

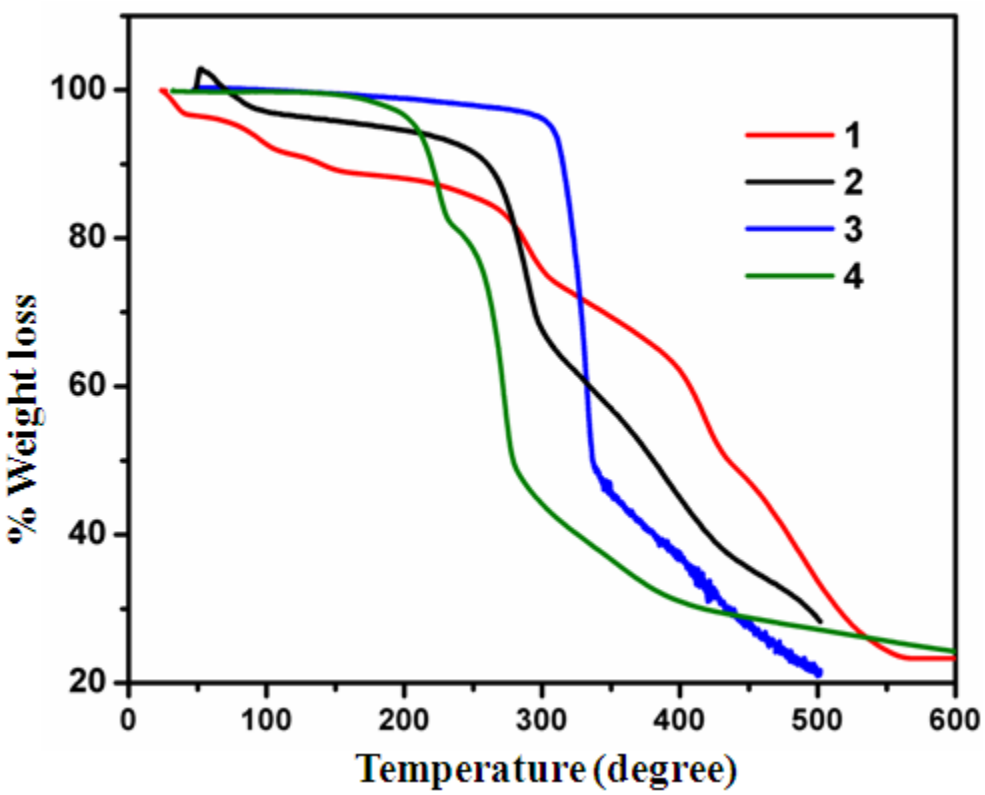

Fig. S4 PXRD patterns of compound **1**. (a) Simulated (b) as-synthesized.

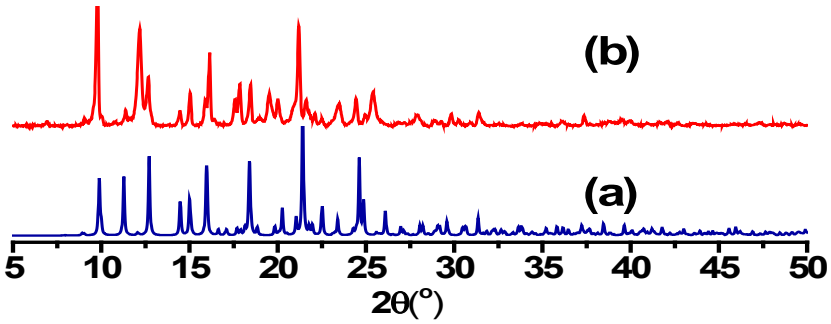

Fig. S5 PXRD patterns of compound **2**. (a) Simulated (b) as-synthesized;

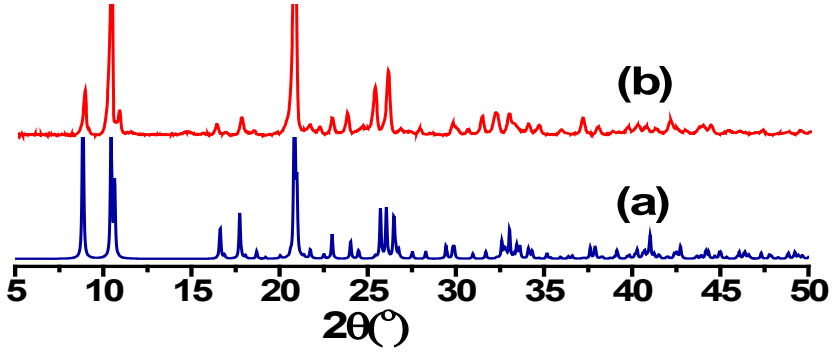

Fig. S6 PXRD patterns of compound **3**. (a) Simulated (b) as-synthesized.

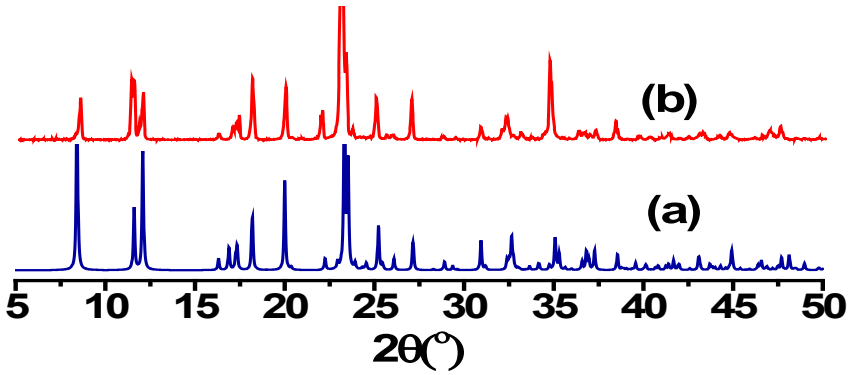

Fig. S7 PXRD patterns of compound **4**. (a) Simulated (b) as-synthesized;