Electronic Supplementary Information (ESI)

Zinc(II) coordination compounds based on *in situ* generated 3-(5*H*-tetrazol)benzaldehyde with diverse modes: hydrothermal syntheses, crystal structures and photoluminescent properties

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Table S1 The selected bond distances and angles for **1**–**4**.

		1	
Zn(1)-N(11)	1.992(3)	Zn(1)-N(22)	2.020(2)
Zn(2)-N(14)#2	1.998(2)	Zn(2)-N(23)	2.015(2)
N(11)-Zn(1)-N(11)#1	121.70(15)	N(11)-Zn(1)-N(22)#1	104.51(10)
N(11)-Zn(1)-N(22)	111.84(10)	N(22)#1-Zn(1)-N(22)	100.57(13)
N(14)#2-Zn(2)-N(14)#3	105.53(14)	N(14)#2-Zn(2)-N(23)#1	113.62(10)
N(14)#2-Zn(2)-N(23)	111.03(10)	N(23)#1-Zn(2)-N(23)	102.25(14)
		2	
Zn(1)-O(1)	1.992(2)	Zn(1)-O(1)#1	2.018(2)
Zn(1)-N(21)	2.204(4)	Zn(1)-N(13)#1	2.168(3)
Zn(1)-N(12)	2.247(3)	Zn(1)-O(1)#2	2.540(2)
O(1)-Zn(1)-O(1)#1	154.01 (11)	O(1)-Zn(1)-O(1)#2	77.74(9)
N(21)-Zn(1)-N(12)	86.64(11)	O(1)-Zn(1)-N(13)#1	108.60(9)
O(1)#1-Zn(1)-N(13)#1	85.13(9)	O(1)-Zn(1)-N(21)	98.99(13)
O(1)#1-Zn(1)-N(21)	103.30(11)	N(13)#1-Zn(1)-N(21)	88.97(11)
O(1)-Zn(1)-N(12)	80.81(13)	O(1)#1-Zn(1)-N(12)	87.26(9)

N(13)#1-Zn(1)-N(12)	170.17(13)	N(12)-Zn(1)-O(1)#2	104.28(8)
O(1)#1-Zn(1)-O(1)#2	83.01(8)	N(13)#1-Zn(1)-O(1)#2	80.97(8)
N(21)-Zn(1)-O(1)#2	167.77(9)		
		3	
Zn(1)-N(61)	2.150(3)	Zn(1)-N(61)#1	2.174(3)
Zn(1)-N(51)#2	2.174(3)	Zn(1)-N(32)	2.216(3)
Zn(1)-N(52)	2.217(3)	Zn(1)-N(13)	2.268(3)
Zn(2)-N(23)	2.013(3)	Zn(2)-N(33)	2.037(3)
Zn(2)-N(12)	2.045(3)	Zn(2)-N(42)	2.207(3)
Zn(2)-N(41)#1	2.211 (3)	N(61)-Zn(1)-N(51)#2	94.99(12)
N(61)-Zn(1)-N(61)#1	78.87(13)	N(61)-Zn(1)-N(51)#2	94.99(12)
N(61)#1-Zn(1)-N(51)#2	93.54(12)	N(61)-Zn(1)-N(32)	171.40(11)
N(61)#1-Zn(1)-N(32)	93.57(12)	N(51)#2-Zn(1)-N(32)	89.53(12)
N(61)-Zn(1)-N(52)	91.14(12)	N(61)#1-Zn(1)-N(52)	94.14(12)
N(51)#2-Zn(1)-N(52)	170.97(12)	N(32)-Zn(1)-N(52)	85.28(12)
N(61)-Zn(1)-N(13)	93.33(12)	N(61)#1-Zn(1)-N(13)	172.20(12)
N(51)#2-Zn(1)-N(13)	86.92(12)	N(32)-Zn(1)-N(13)	94.22(12)
N(52)-Zn(1)-N(13)	86.10(12)	N(23)-Zn(2)-N(33)	124.58(13)
N(23)-Zn(2)-N(12)	126.96(13)	N(33)-Zn(2)-N(12)	108.46(13)
N(23)-Zn(2)-N(42)	87.91(13)	N(33)-Zn(2)-N(42)	91.85(12)
N(12)-Zn(2)-N(42)	90.98(13)	N(23)-Zn(2)-N(41)#2	92.39(13)
N(33)-Zn(2)-N(41)#2	88.51(12)	N(12)-Zn(2)-N(41)#2	88.33(12)
N(42)-Zn(2)-N(41)#2	179.29(12)		
		4	
Zn(1)-N(23)#1	2.059(2)	Zn(1)-N(13)	2.080(3)
Zn(1)-N(22)	2.136(2)	Zn(1)-N(31)	2.134(2)
Zn(1)-N(32)	2.163(3)	N(31)-Zn(1)-N(32)	77.32(10)
N(13)-Zn(1)-N(22)	88.61(10)	N(23)#1-Zn(1)-N(31)	101.12(9)
N(13)-Zn(1)-N(31)	99.36(10)	N(22)-Zn(1)-N(31)	152.94(10)
N(23)#1-Zn(1)-N(32)	102.29(10)	N(13)-Zn(1)-N(32)	160.88(11)
N(22)-Zn(1)-N(32)	86.70(10)	N(23)#1-Zn(1)-N(13)	96.83(10)
N(23)#1-Zn(1)-N(22)	103.56(9)		

Symmetry codes for **1**: (#1) 1 – x, y, –1.5 – z; (#2) 0.5 + x, 0.5 + y, –1.5 – z; (#3) 0.5 – x, 0.5 + y, z; for **2**: (#1) x, 2 – y, 0.5 + z; (#2) –x, y, 0.5 – z; for **3**: (#1) –x, 1 – y, –z; (#2) 1 + x, y, z; for **4**: (#1) 1 – x, 1 – y, 1 – z.

Table S2 Hydrogen-bonding geometries for **1**–**4**.

D-H···A	D-H/Å	H···A/Å	D···A/Å	∠D-H···A/º
		1		
O1W-H1WB···O11	0.85(2)	2.58(3)	3.193(10)	130(4)
C15-H15A···O1W_$1	0.93	2.57	3.290(8)	134
		2		
O1-H1···N11_$1	0.76(5)	2.56(5)	3.105(3)	130(4)
O1W-H1WA···N14	0.991(12)	1.925(12)	2.905(3)	169.1(10)
C17-H17A···O1W_$2	0.93	2.48	3.343(4)	154
C24-H24A···O11_$3	0.93	2.45	3.145(6)	132
C25-H25A···N12	0.93	2.53	3.063(5)	117
		3		
C41-H41A···N22_$1	0.93	2.59	3.196(6)	124
C45-H45A···N12_$2	0.93	2.62	3.125(5)	115
C47-H47A···O11_$3	0.93	2.57	3.155(6)	121
C48-H48A···O11_$3	0.93	2.52	3.141(6)	124
C48-H48A···N33	0.93	2.62	3.165(6)	118
		4		
C312-H31C···N22	0.93	2.61	3.119(5)	115
C31-H31D···14	0.93	2.44	3.222(6)	141
C32-H32A···O11_$1	0.93	2.56	3.372(7)	146
C37-H37A···N24_$1	0.93	2.57	3.457(5)	159

Symmetry code for **1**: $1 1 – x, –1 – y, –2 – z; for **2**: $1 x, 2 – y, –0.5 + z; $2 x, y, 1 + z; $3 0.5 – x, 2.5 – y, 1 – z; for **3**: $1 –1 – x, 1 – y, –1 – z; $2 –1 + x, y, z; $3 x, 1 + y, z; for **4**: $1 x, 1 + y, z.

Fig. S1 IR spectra of **1**–**4**.

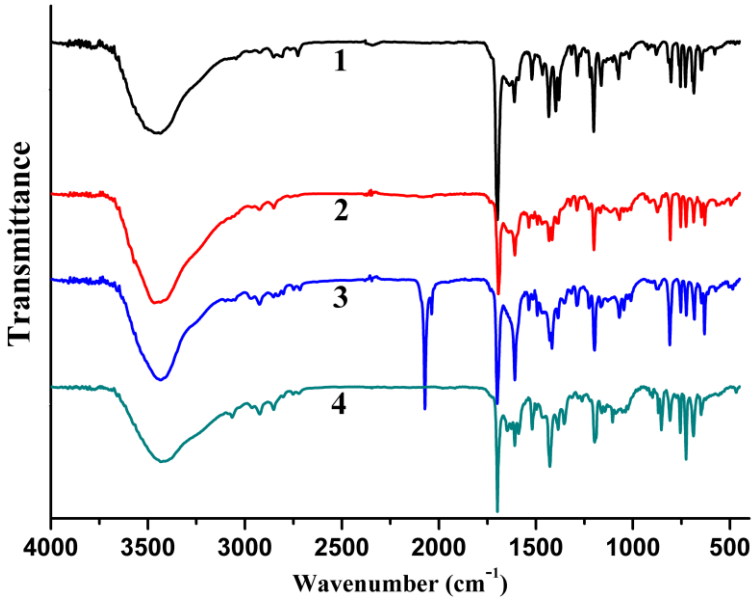

Fig. S2 Powdered *X*-ray diffraction (PXRD) patterns of **1**–**4**. The black and red lines represent simulated and experimental results, respectively.

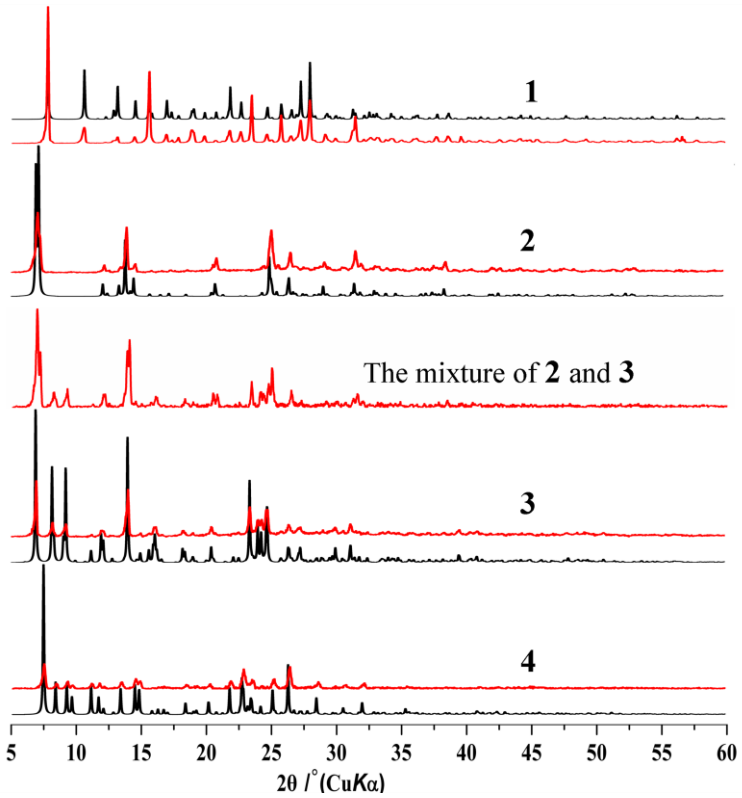

Fig. S3 Schematic representation of 2-D to 3-D supramolecular architecture *via* hydrogen bonds in **1**.

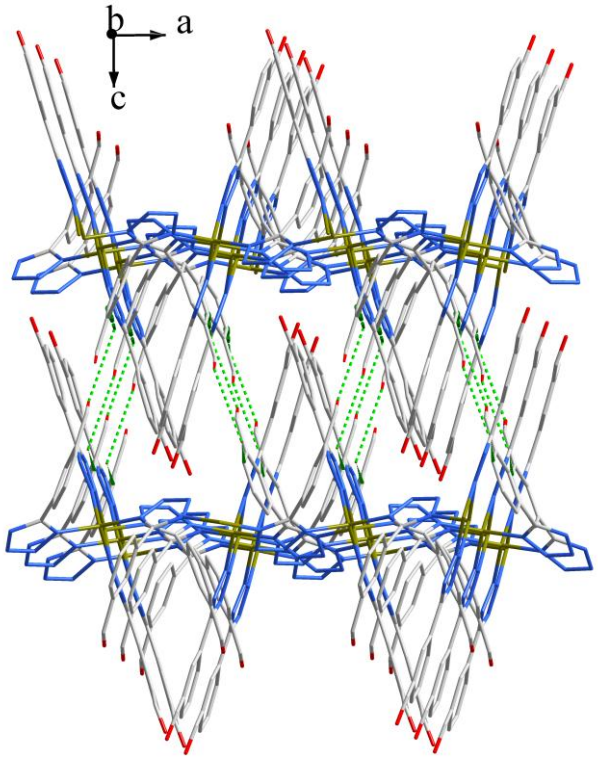

Fig. S4 Schematic representation of 2-D to 3-D supramolecular architecture *via* hydrogen bonds in **2**.

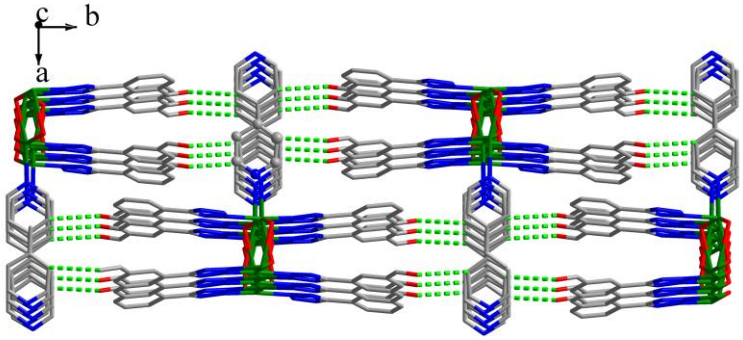

Fig. S5 Schematic representation of 1-D to 3-D supramolecular architecture *via* hydrogen bonds in **3**.

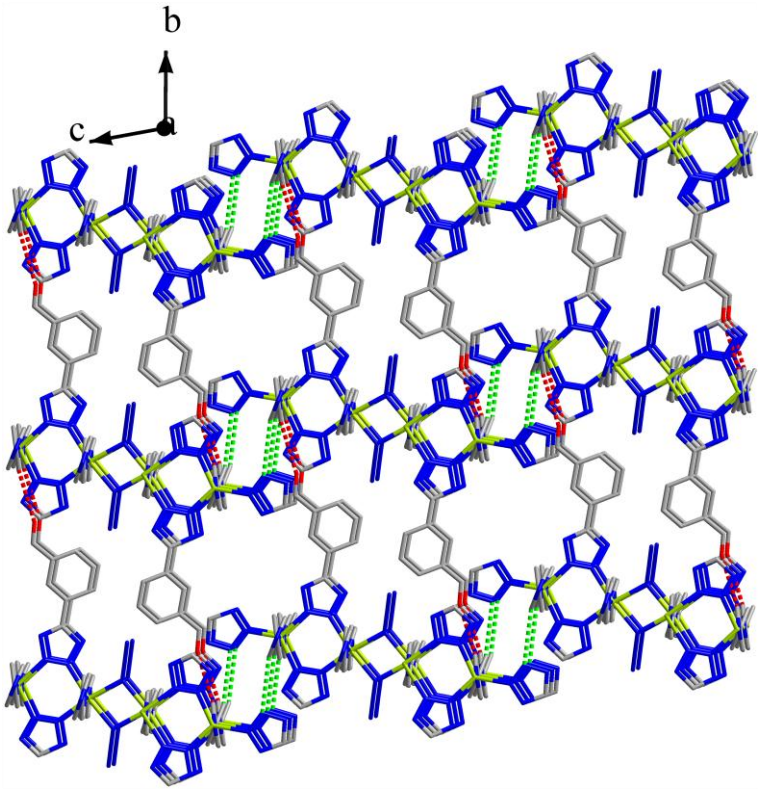

Fig. S6 Schematic representation of 0-D to 1-D supramolecular architecture *via* hydrogen bonds in **4**.

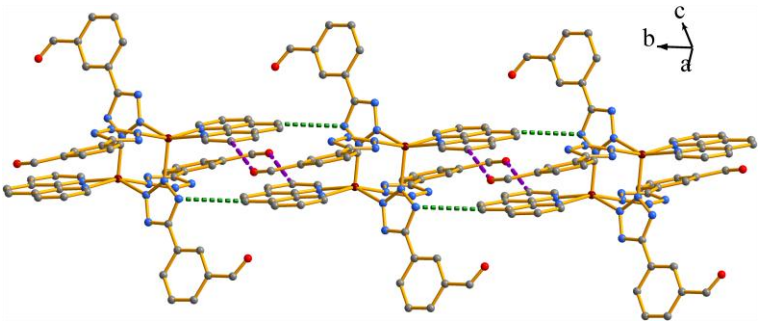

Fig. S7 The excitation spectra of **1**–**4** and free ligand 3-Htzbd.

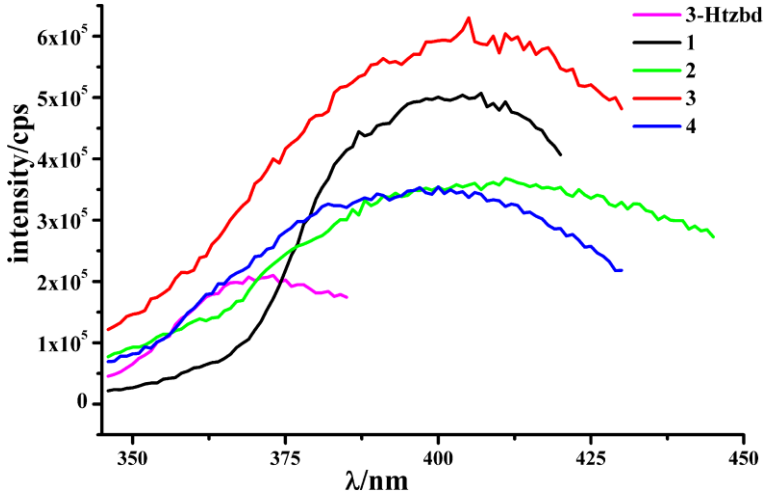

Fig. S8 Luminescent decay and IRF(instrument response function) curves of of **1**–**4**.

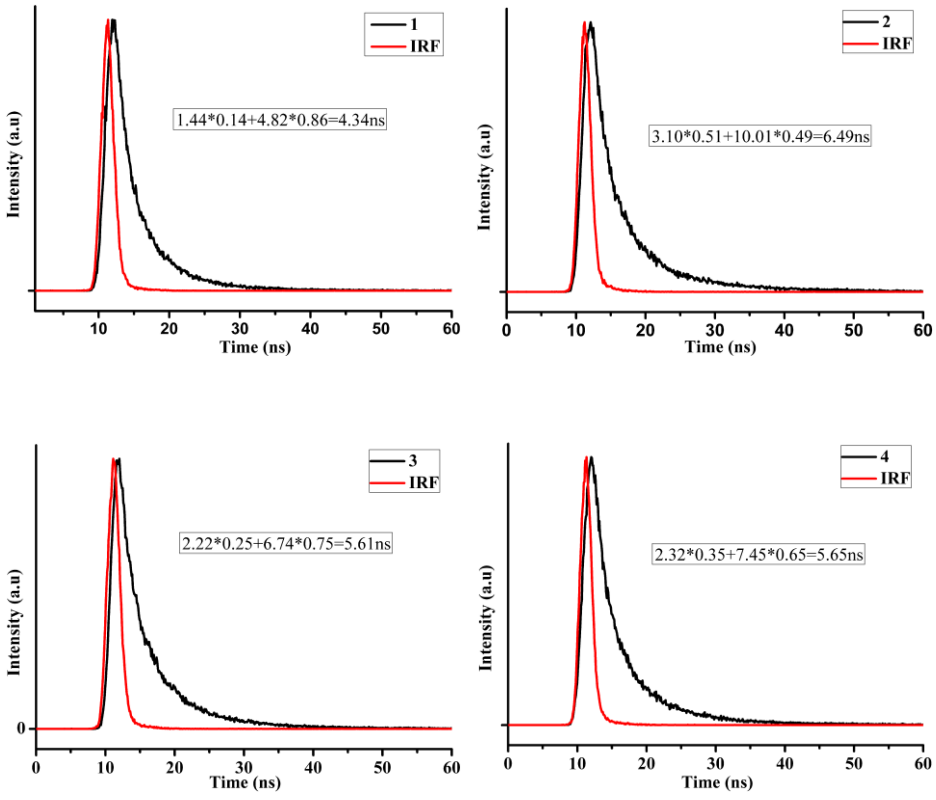

Fig. S9 Reflectance diffusion spectra of **1**–**4**.