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Fluorescent and photochromic properties of a series of new Zn(II)/Cd(II) coordination compounds with a flexible semi-rigid tetrazole-viologen derivative

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Table S1 The selected bond distances (Å) and angles (°) for **1**–**4**.

		1	
Zn1–N26	2.039(4)	Zn2–N16	2.071(4)
Zn1–Cl1	2.304(3)	Zn2–N21	2.030(4)
Zn1–N11	2.014(4)	Zn2–N27	2.034(4)
Zn1–N17	1.9005(15)	Zn2–Cl2	2.2328(15)
N17–Zn1–N11	106.45(10)	N21–Zn2–N27	107.60(17)
N17–Zn1–N26	113.50(12)	N21–Zn2–N16	106.85(15)
N11–Zn1–N26	105.49(15)	N27–Zn2–N16	110.40(18)
N17–Zn1–Cl1	113.23(8)	N21–Zn2–Cl2	108.16(12)
N11–Zn1–Cl1	108.21(12)	N27–Zn2–Cl2	117.91(13)
N26–Zn1–Cl1	109.50(11)	N16–Zn2–Cl2	105.41(10)
		2	
Zn(1)–N(7)	2.001(4)	Zn(1)–N(3)#1	2.024(3)
Zn(1)–N(1)	2.033(3)	Zn(1)–Cl(1)	2.2094(14)
N(7)–Zn(1)–N(3)#1	106.96(13)	N(7)–Zn(1)–N(1)	111.80(14)
N(3)#1–Zn(1)–N(1)	102.16(11)	N(7)–Zn(1)–Cl(1)	112.02(11)
N(3)#1–Zn(1)–Cl(1)	112.75(9)	N(1)–Zn(1)–Cl(1)	110.72(8)
Symmetry transformations used to generate equivalent atoms: #1 x, –y + 1/2, z – 1/2; #2 x, –y + 1/2, z + 1/2.			
		3	
Zn(1)–O(1)	1.915(3)	Zn(1)–N(1)	2.028(4)
Zn(1)–N(6)#1	2.065(4)	Zn(1)-Cl(1)	2.2298(16)
Zn(2)–O(1)	1.946(3)	Zn(2)-N(4)#2	2.077(4)
Zn(2)–Cl(2)	2.2289(15)	Zn(2)-Cl(3)	2.2512(15)

O(1)–Zn(1)–N(1)	112.38(16)	O(1)-Zn(1)-N(6)#1	110.05(16)
N(1)–Zn(1)–N(6)#1	104.79(17)	O(1)-Zn(1)-Cl(1)	117.55(11)
N(1)–Zn(1)–Cl(1)	108.18(12)	N(6)#1-Zn(1)-Cl(1)	102.76(12)
O(1)–Zn(2)–N(4)#2	105.96(15)	O(1)-Zn(2)-Cl(2)	118.90(12)
N(4)#2–Zn(2)–Cl(2)	105.69(12)	O(1)-Zn(2)-Cl(3)	104.49(11)
N(4)#2–Zn(2)–Cl(3)	102.86(12)	Cl(2)-Zn(2)-Cl(3)	117.28(6)

Symmetry transformations used to generate equivalent atoms:
#1 –x + 1, –y + 2, –z + 1; #2 x – 1, y, z; #3 x + 1, y, z.

4

Cd(1)-N(7)	2.282(2)	Cd(1)-O(2)#1	2.2896(18)
Cd(1)-O(1)	2.3086(17)	Cd(1)-N(1)	2.376(2)
Cd(1)-N(6)#2	2.399(2)	Cd(1)-N(4)#3	2.452(2)
N(7)-Cd(1)-O(2)#1	175.31(7)	N(7)-Cd(1)-O(1)	104.02(7)
O(2)#1-Cd(1)-O(1)	72.49(6)	N(7)-Cd(1)-N(1)	98.02(8)
O(2)#1-Cd(1)-N(1)	85.53(6)	O(1)-Cd(1)-N(1)	157.95(6)
N(7)-Cd(1)-N(6)#2	92.36(8)	O(2)#1-Cd(1)-N(6)#2	90.54(7)
O(1)-Cd(1)-N(6)#2	86.10(7)	N(1)-Cd(1)-N(6)#2	92.61(7)
N(7)-Cd(1)-N(4)#3	89.56(8)	O(2)#1-Cd(1)-N(4)#3	86.84(7)
O(1)-Cd(1)-N(4)#3	81.83(7)	N(1)-Cd(1)-N(4)#3	98.97(7)
N(6)#2-Cd(1)-N(4)#3	167.88(7)		

Symmetry transformations used to generate equivalent atoms:
#1 –x + 1, –y + 1, –z; #2 –x + 2, –y, –z; #3 –x + 1, y + 1/2, –z + 1/2.

Fig. S1 The IR spectra of (cmb)Cl, (Htzmb)Cl and **1**–**4**.

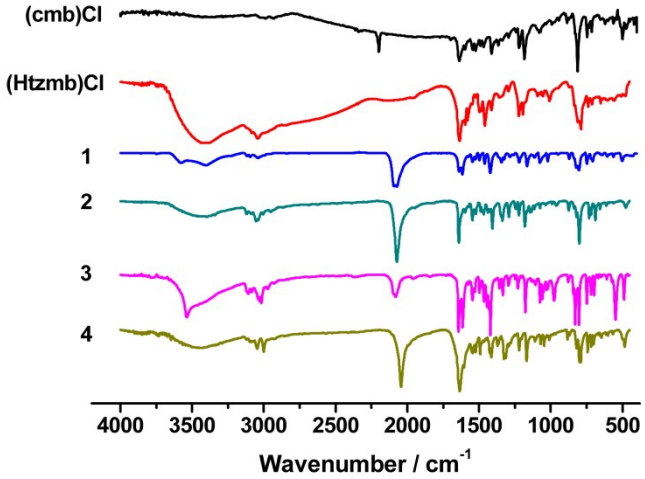

Fig. S2 The TGA curves of **1**–**4**.

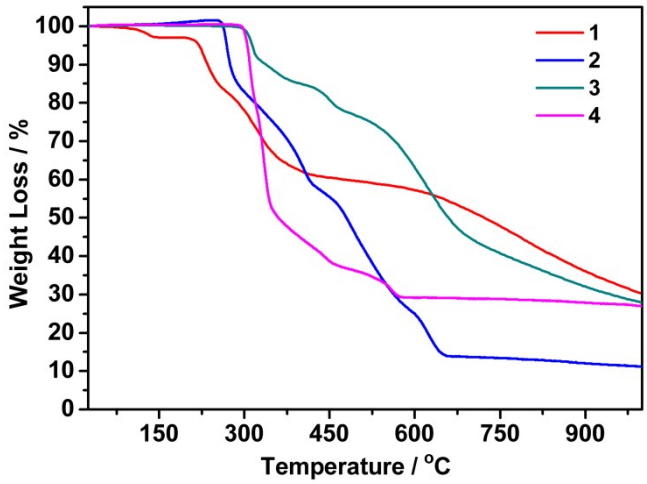

Fig. S3 Powdered *X*-ray diffraction (PXRD) patterns of **1**–**4**.

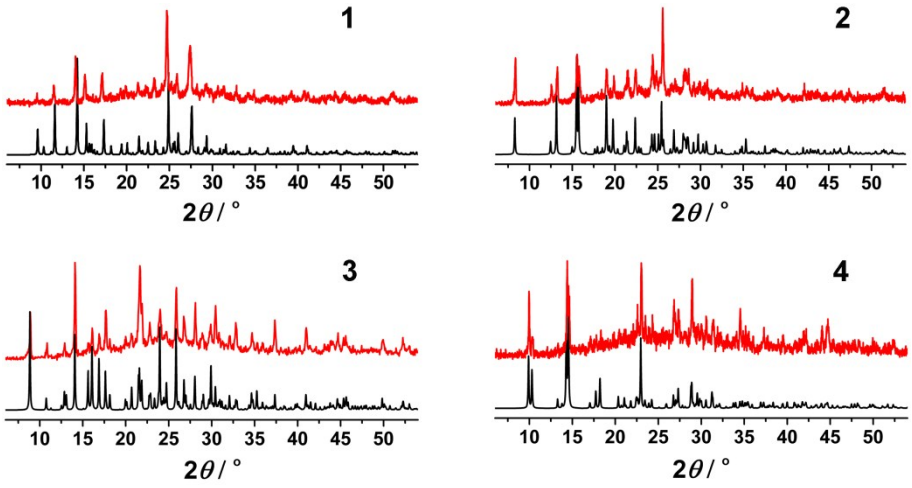

Fig. S4 Overlapping stack of adjacent zigzag chains in **2** with π···π interactions.

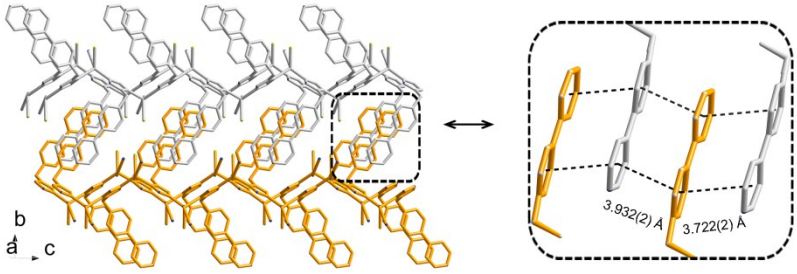

Fig. S5 An ···ABAB··· fashion along the *c* axis for **3**.

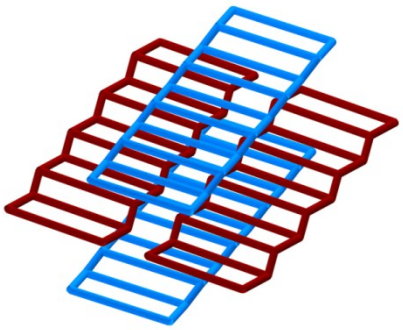

Fig. S6 The excitation (black line) and emission (red line) spectra of free ligand tzmb.

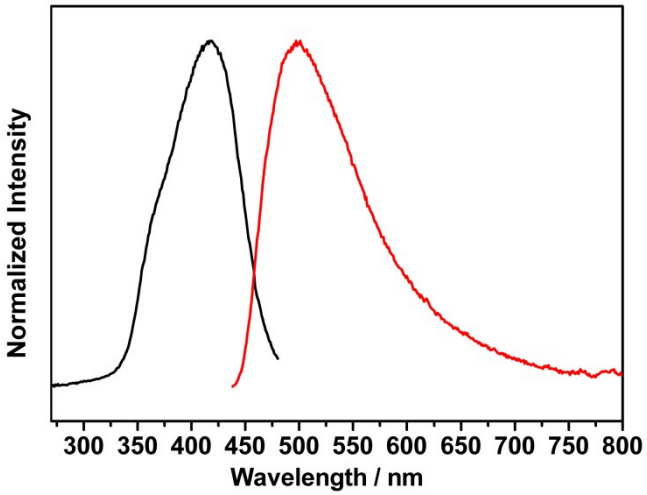

Fig. S7 Fluorescence lifetime investigation of **1**–**4**.

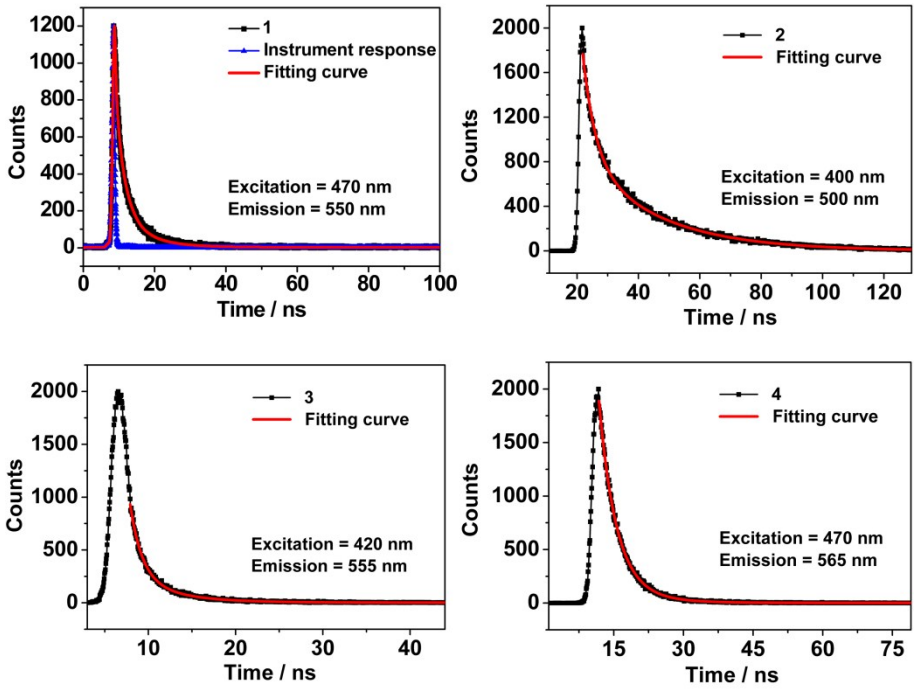

Fig. S8 The dinuclear SBU $[M_2(tzmb)_2]$ (M = Zn or Cd) in the structures of compounds **1**, **3** and **4**

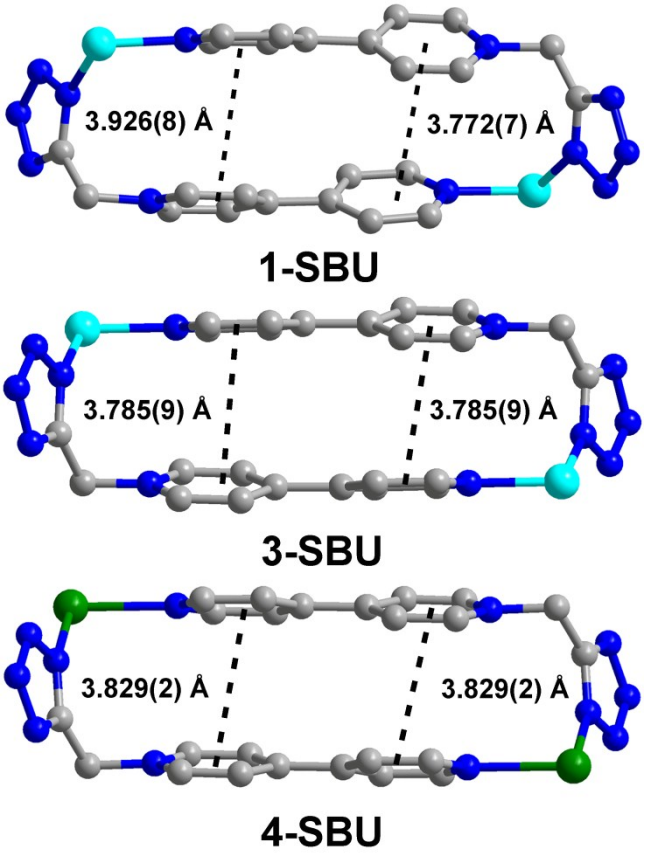

Fig. S9 Calculated spin density of the $[Zn_2Cl_2(N_3)_2(tzmb)_2]$ molecule of **1** in the triplet ground state.