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Effect of organic anions on the self-assembly of Zn(II)-containing coordination polymers based on trigonal N-donor ligands

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Table S1a. Selected bond distances and angles for compound **1**.

Zn(1)-O(1)	1.988(19)	Zn(1)-O(3)#1	1.999(2)
Zn(1)-N(1)	2.091(2)	Zn(1)-O(1W)	2.179(2)
Zn(1)-N(7)#2	2.215(2)		
O(1)-Zn(1)-O(3)#1	117.89(9)	O(1)-Zn(1)-N(1)	138.73(10)
O(3)#1-Zn(1)-N(1)	103.31(9)	O(1)-Zn(1)-O(1W)	86.21(8)
O(3)#1-Zn(1)-O(1W)	94.68(8)	N(1)-Zn(1)-O(1W)	88.30(9)
O(1)-Zn(1)-N(7)#2	89.42(9)	O(3)#1-Zn(1)-N(7)#2	90.17(9)
N(1)-Zn(1)-N(7)#2	92.92(9)	O(1W)-Zn(1)-N(7)#2	174.60(9)

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

Table S1b. Hydrogen bonds for **1** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(2)#3	0.86	1.89	2.697(3)	156.9
O(1W)-H(1B)···O(4)#1	0.86	1.75	2.595(3)	166.2

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

Table S2. Selected bond distances and angles for compound **2**.

Zn(1)-O(4)#1	1.9418(17)	Zn(1)-O(1)	1.9842(18)
Zn(1)-N(1)	2.0418(19)	Zn(1)-N(8)#2	2.044(2)
O(4)#1-Zn(1)-O(1)	120.49(8)	O(4)#1-Zn(1)-N(1)	109.29(8)
O(1)-Zn(1)-N(1)	96.52(8)	O(4)#1-Zn(1)-N(8)#2	116.43(8)
O(1)-Zn(1)-N(8)#2	106.97(8)	N(1)-Zn(1)-N(8)#2	104.18(8)

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

Table S3a. Selected bond distances and angles for compound **3**.

Zn(1)-O(3)	1.941(2)	Zn(1)-O(1)	1.954(3)
Zn(1)-N(1)	2.026(3)	Zn(1)-N(7)#1	2.059(3)
O(3)-Zn(1)-O(1)	117.25(12)	O(3)-Zn(1)-N(1)	112.94(12)
O(1)-Zn(1)-N(1)	97.88(12)	O(3)-Zn(1)-N(7)#1	100.77(11)

O(1)-Zn(1)-N(7)#1	118.52(12)	N(1)-Zn(1)-N(7)#1	109.91(12)

Symmetry transformations used to generate equivalent atoms: [#1] x, y + 1, z + 1.

Table S3b. Hydrogen bonds for **3** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(2)	0.85	1.91	2.730(6)	161.8

Table S4. Selected bond distances and angles for compound **4**.

Zn(1)-O(7)	1.925(3)	Zn(1)-O(3)#1	1.959(2)
Zn(1)-O(6)#2	2.017(3)	Zn(1)-N(1)	2.018(3)
Zn(2)-O(7)	1.920(3)	Zn(2)-O(1)	1.925(3)
Zn(2)-O(5)#2	1.928(3)	Zn(2)-N(7)#3	2.070(3)
O(7)-Zn(1)-O(3)#1	125.26(13)	O(7)-Zn(1)-O(6)#2	103.21(13)
O(3)#1-Zn(1)-O(6)#2	101.65(11)	O(7)-Zn(1)-N(1)	110.30(14)
O(3)#1-Zn(1)-N(1)	112.04(12)	O(6)#2-Zn(1)-N(1)	100.33(13)
O(7)-Zn(2)-O(1)	111.51(13)	O(7)-Zn(2)-O(5)#2	98.95(13)
O(1)-Zn(2)-O(5)#2	134.29(16)	O(7)-Zn(2)-N(7)#3	109.46(14)
O(1)-Zn(2)-N(7)#3	99.87(14)	O(5)#2-Zn(2)-N(7)#3	101.07(16)

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

Table S4b. Hydrogen bonds for **4** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(1)#6	0.85	2.23	2.820(15)	125.9
O(1W)-H(1B)···O(2)#7	0.84	2.39	2.811(15)	111.9

Symmetry transformations used to generate equivalent atoms: [#6] x, -y + 1, z - 1/2; [#7] -x, y, -z - 1/2.

Table S5. Selected bond distances and angles for compound **5**.

Zn(1)-O(1)	1.931(2)	Zn(1)-O(3)#1	1.959(2)
Zn(1)-N(1)	2.040(3)	Zn(1)-N(8)#2	2.050(3)

O(1)-Zn(1)-O(3)#1	98.10(10)	O(1)-Zn(1)-N(1)	111.95(11)
O(3)#1-Zn(1)-N(1)	116.52(10)	O(1)-Zn(1)-N(8)#2	113.65(11)
O(3)#1-Zn(1)-N(8)#2	116.80(10)	N(1)-Zn(1)-N(8)#2	100.52(11)

Symmetry transformations used to generate equivalent atoms: [#1] x, -y + 1/2, z - 1/2; [#2] -x + 1, -y, -z.

Table S5b. Hydrogen bonds for **5** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···N(5)#5	0.85	2.51	3.160(5)	133.9
O(1W)-H(1B)···O(2W)#4	0.86	2.22	3.025(8)	155.4
O(2W)-H(2A)···O(1)	0.85	2.35	3.203(7)	178.2
O(2W)-H(2B)···O(4)#3	0.85	2.32	3.093(7)	151.6

Symmetry transformations used to generate equivalent atoms: [#3] -x + 2, -y + 1, -z; [#4] x, -y + 1/2, z + 1/2; [#5] -x + 2, y + 1/2, -z + 1/2.

Table S6a. Selected bond distances and angles for compound **6**.

Zn(1)-O(2)	1.956(3)	Zn(1)-O(3)#1	1.959(3)
Zn(1)-N(1)	2.050(3)	Zn(1)-N(8)#2	2.116(3)
O(2)-Zn(1)-O(3)#1	106.44(12)	O(2)-Zn(1)-N(1)	111.09(12)
O(3)#1-Zn(1)-N(1)	128.71(13)	O(2)-Zn(1)-N(8)#2	94.88(13)
O(3)#1-Zn(1)-N(8)#2	115.40(13)	N(1)-Zn(1)-N(8)#2	95.06(13)

Symmetry transformations used to generate equivalent atoms: [#1] -x + 1, -y, -z; [#2] -x + 2, -y + 1, -z - 1.

Table S6b. Hydrogen bonds for **6** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(4)	0.85	2.15	2.867(5)	141.2
O(1W)-H(1B)···N(2)#1	0.85	2.19	3.030(5)	168.8

Symmetry transformations used to generate equivalent atoms: [#1] -x + 1, -y, -z.

Table S7a. Selected bond distances and angles for compound **7**.

Zn(1)-O(2)	2.042(2)	Zn(1)-O(4)#1	2.057(2)

Zn(1)-O(1W)	2.082(2)	Zn(1)-N(1)	2.157(2)
Zn(1)-N(8)#2	2.217(3)		
O(2)-Zn(1)-O(4)#1	97.03(10)	O(2)-Zn(1)-O(1W)	91.13(9)
O(4)#1-Zn(1)-O(1W)	92.13(8)	O(2)-Zn(1)-N(1)	135.91(10)
O(4)#1-Zn(1)-N(1)	127.00(10)	O(1W)-Zn(1)-N(1)	89.65(9)
O(2)-Zn(1)-N(8)#2	91.04(10)	O(4)#1-Zn(1)-N(8)#2	90.92(9)
O(1W)-Zn(1)-N(8)#2	176.02(9)	N(1)-Zn(1)-N(8)#2	86.47(10)

Symmetry transformations used to generate equivalent atoms: [#1] x, y, z+1; [#2] x - 1/2, -y + 1/2, z + 1/2.

Table S7b. Hydrogen bonds for **7** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(2W)#5	0.83	1.89	2.691(3)	160.0
O(1W)-H(1B)···O(3)#5	0.84	1.89	2.720(3)	169.0
O(2W)-H(2A)···N(5)	0.85	2.53	3.235(4)	140.8
O(2W)-H(2B)···O(1)	0.85	2.21	2.785(4)	125.2
O(2W)-H(2B)···N(7)#6	0.85	2.36	3.060(4)	139.4

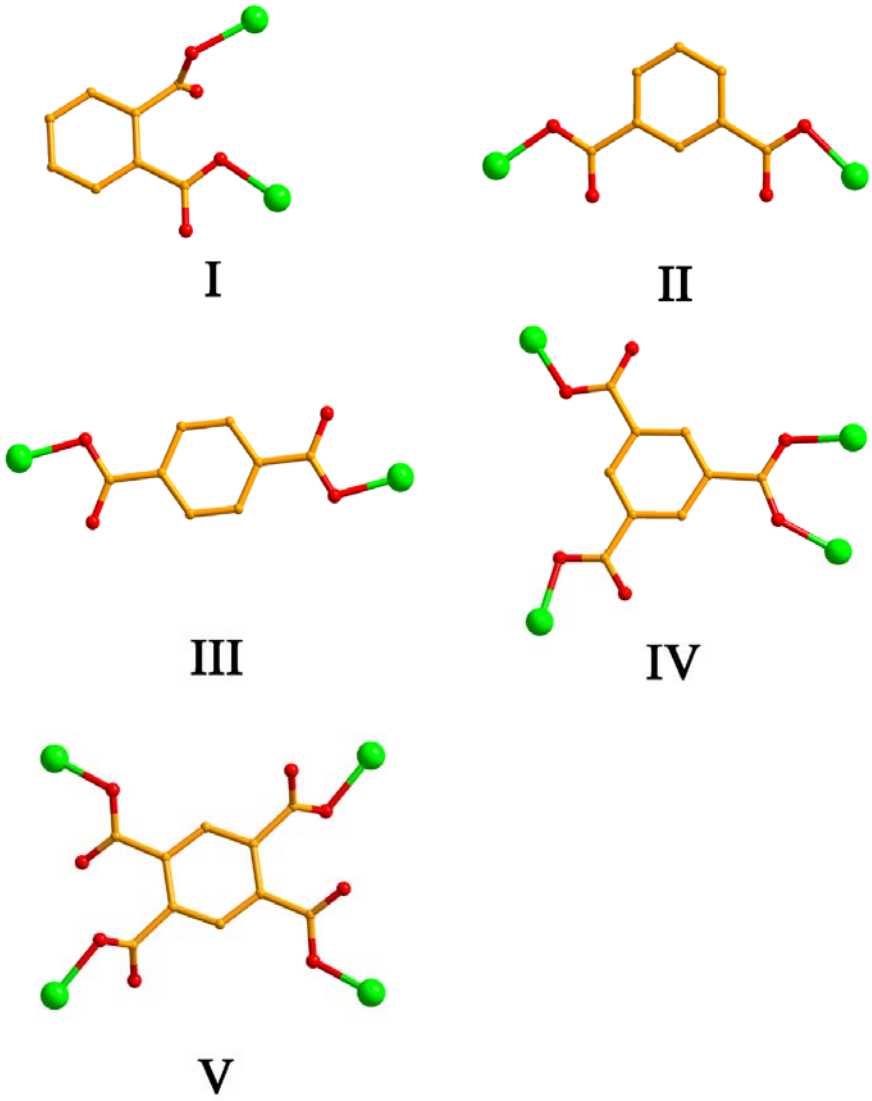
Symmetry transformations used to generate equivalent atoms: [#5] -x, -y, -z + 1; [#6] x - 1/2, -y + 1/2, z - 1/2.

Table S8. Selected bond distances and angles for compound **8**.

Zn(1)-O(7)#1	1.954(2)	Zn(1)-O(1)	2.056(3)
Zn(1)-O(4)#2	2.095(2)	Zn(1)-N(1)	2.100(4)
Zn(1)-N(7)#3	2.167(4)	Zn(2)-O(7)	1.913(2)
Zn(2)-O(5)	1.939(3)	Zn(2)-O(3)#4	1.977(3)
Zn(2)-N(8)#5	2.280(4)	Zn(2)-O(1W)	2.288(3)
O(7)#1-Zn(1)-O(1)	105.06(10)	O(7)#1-Zn(1)-O(4)#2	96.94(10)
O(1)-Zn(1)-O(4)#2	157.98(10)	O(7)#1-Zn(1)-N(1)	100.45(13)
O(1)-Zn(1)-N(1)	86.91(12)	O(4)#2-Zn(1)-N(1)	88.43(12)
O(7)#1-Zn(1)-N(7)#3	97.49(12)	O(1)-Zn(1)-N(7)#3	89.96(12)
O(4)#2-Zn(1)-N(7)#3	87.86(12)	N(1)-Zn(1)-N(7)#3	161.99(12)

O(7)-Zn(2)-O(5)	111.63(11)	O(7)-Zn(2)-O(3)#4	110.07(11)
O(5)-Zn(2)-O(3)#4	137.94(12)	O(7)-Zn(2)-N(8)#5	92.23(12)
O(5)-Zn(2)-N(8)#5	89.10(13)	O(3)#4-Zn(2)-N(8)#5	94.53(12)
O(7)-Zn(2)-O(1W)	101.59(12)	O(5)-Zn(2)-O(1W)	82.43(12)
O(3)#4-Zn(2)-O(1W)	84.26(13)	N(8)#5-Zn(2)-O(1W)	165.70(12)

Symmetry transformations used to generate equivalent atoms: [#1] x, -y, z - 1/2; [#2] x, y + 1, z; [#3] x + 1/2, -y + 1/2, z + 1/2; [#4] x, -y - 1, z + 1/2; [#5] x + 1/2, -y - 1/2, z + 1/2.



Scheme S1 Coordination modes of the polycarboxylate anions.

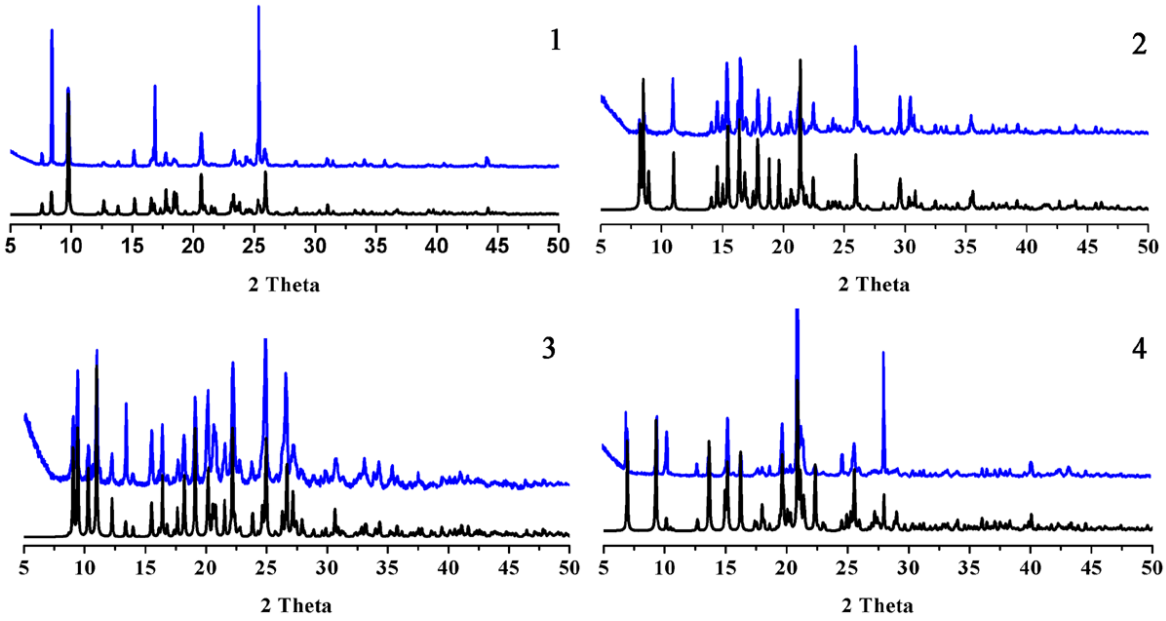


Fig. S1 The simulated (black) and experimental (blue) PXRD patterns for compounds **1**-**4**.

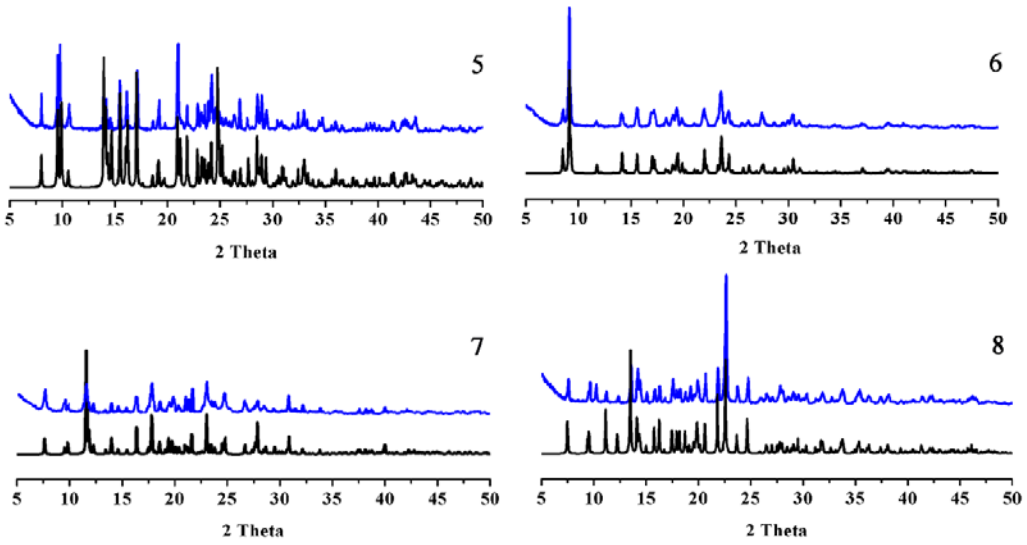


Fig. S2 The simulated (black) and experimental (blue) PXRD patterns for compounds **5**-**8**.

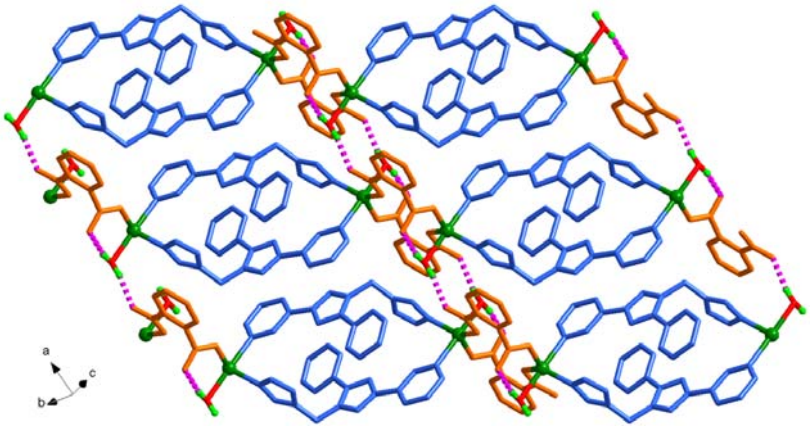


Fig. S3 View of the layer generated by the hydrogen bonding interactions in compound **1**.

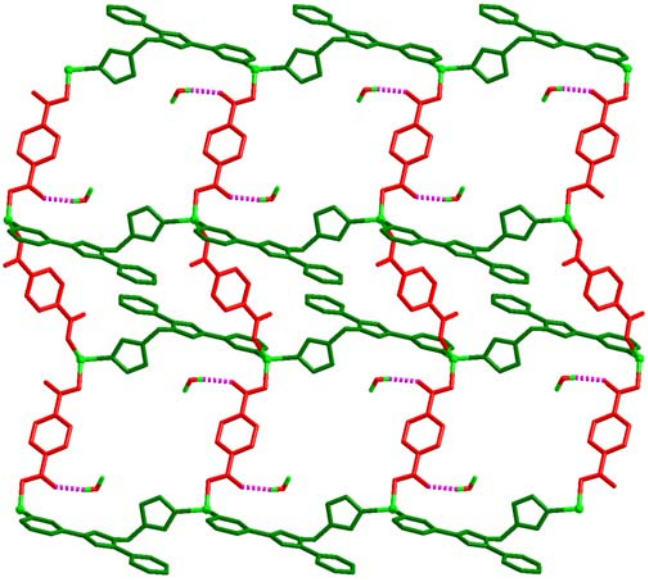


Fig. S4 View of the intramolecular hydrogen bonding interactions in compound **3**.

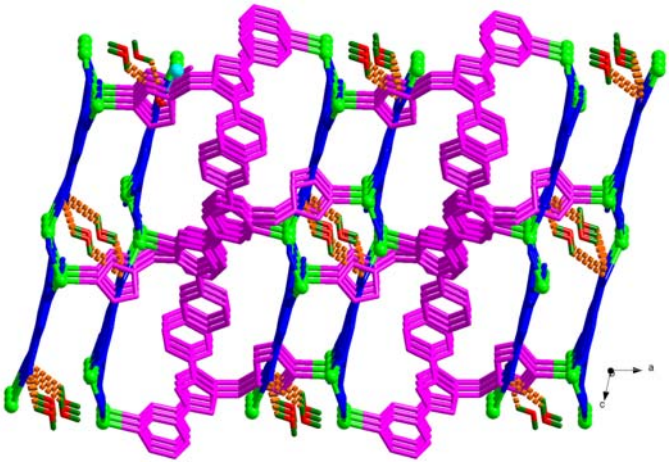


Fig. S5 View of the hydrogen bonding interactions in compound **4**.

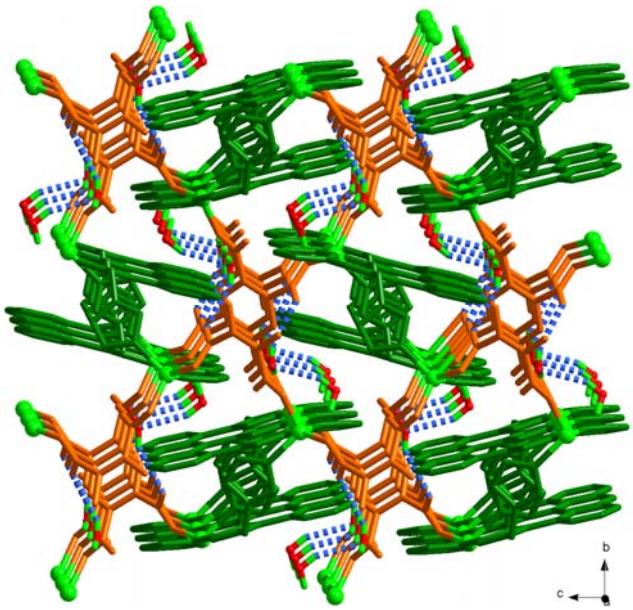


Fig. S6 View of the hydrogen bonding interactions in compound **5**.

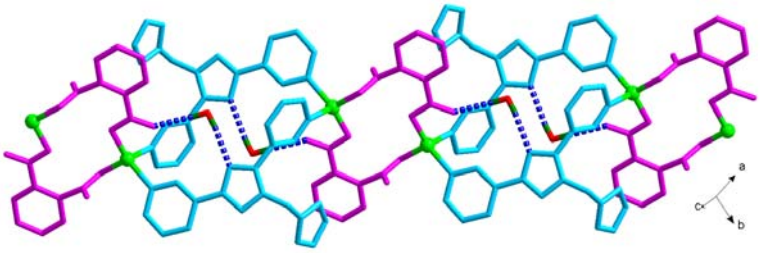


Fig. S7 View of the intramolecular hydrogen bonding interactions in **6**.

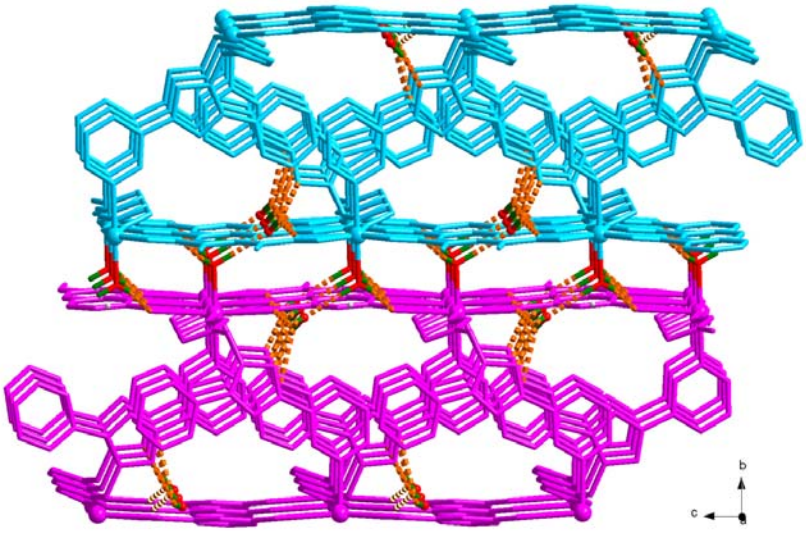


Fig. S8 3D supramolecular framework formed by the hydrogen bonding interactions in compound **7.**

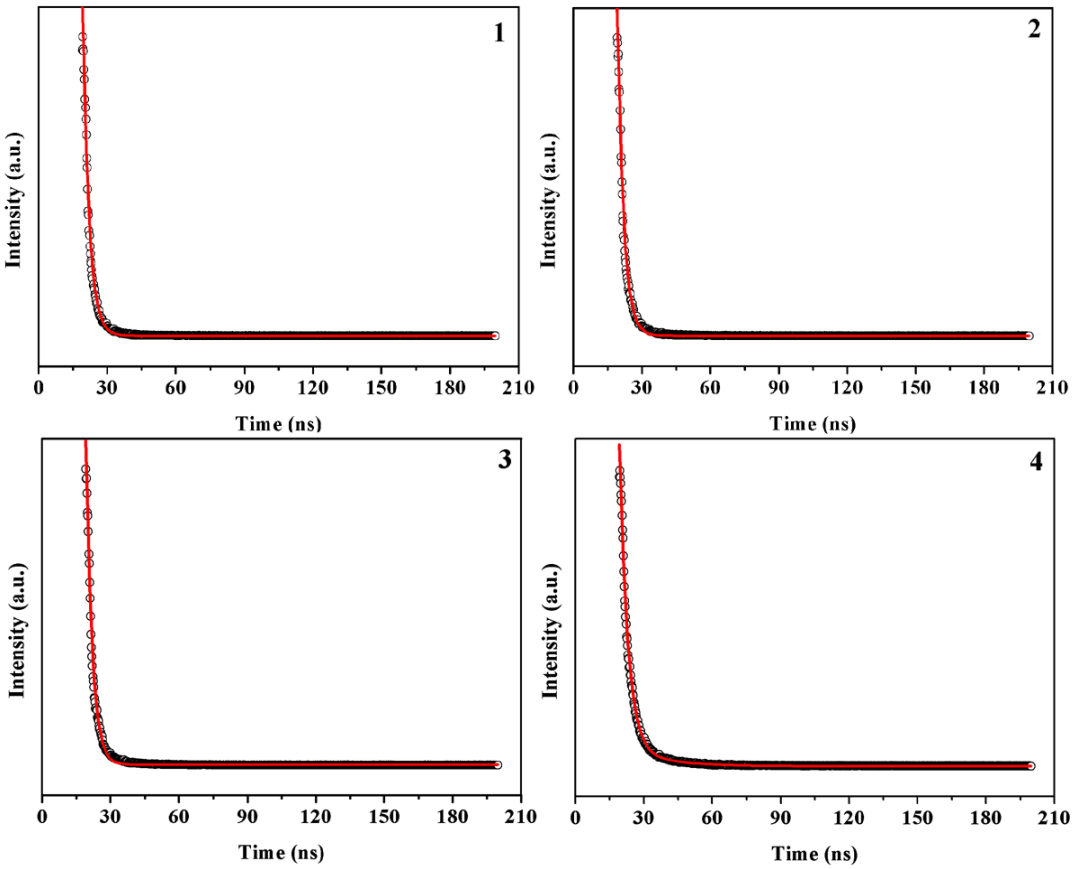


Fig. S9 Fitted decay curves for compounds **1**-**4** in the solid state at room temperature. (the black circles represent experimental data, and the solid red lines represent fitting results)**.**

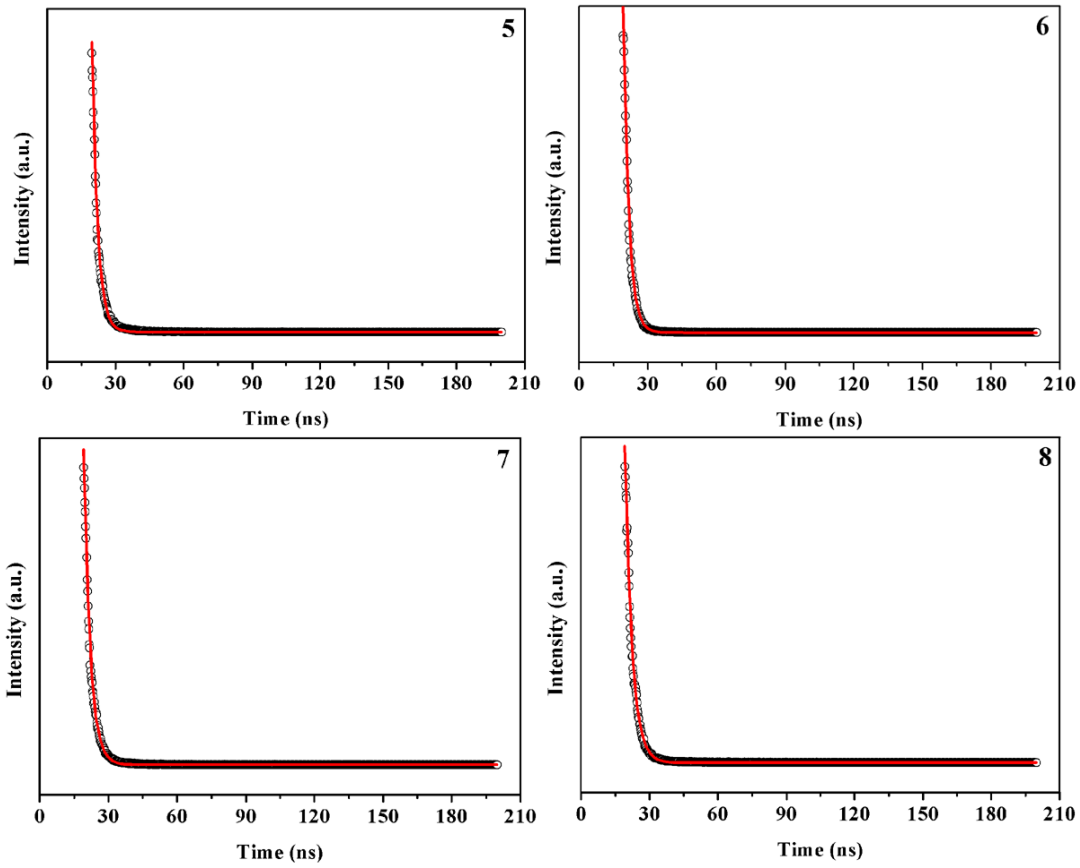


Fig. S10 Fitted decay curves for compounds **5-8** in the solid state at room temperature. (the black circles represent experimental data, and the solid red lines represent fitting results)**.**