Electronic supplementary information

A series of 1D, 2D and 3D coordination polymers based on a 5-(benzonic-4-ylmethoxy)isophthalic acid: syntheses, structures and photoluminescence

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Table S1. Selected bond distances (Å) and angles (°) for compounds **1**-**7**.

1			
Zn(1)-O(7)	1.9275(16)	Zn(1)-O(5)$^{\#1}$	1.9451(15)
Zn(1)-O(4)$^{\#2}$	1.9494(15)	Zn(1)-O(1W)	2.105(2)
Zn(1)-O(2)$^{\#3}$	2.4591(15)		
O(7)-Zn(1)-O(5)$^{\#1}$	110.13(8)	O(7)-Zn(1)-O(4)$^{\#2}$	141.42(7)
O(5)$^{\#1}$-Zn(1)-O(4)$^{\#2}$	105.41(7)	O(7)-Zn(1)-O(1W)	97.93(7)
O(5)$^{\#1}$-Zn(1)-O(1W)	91.09(7)	O(4)$^{\#2}$-Zn(1)-O(1W)	95.89(7)
O(7)-Zn(1)-O(2)$^{\#3}$	93.53(7)	O(5)$^{\#1}$-Zn(1)-O(2)$^{\#3}$	85.50(6)
O(4)$^{\#2}$-Zn(1)-O(2)$^{\#3}$	74.54(6)	O(1W)-Zn(1)-O(2)$^{\#3}$	168.52(7)
2			
Zn(1)-O(4)$^{\#1}$	1.9911(14)	Zn(1)-N(1)	2.0948(14)
Zn(1)-N(2)	2.1428(18)	Zn(1)-O(2)	2.1674(18)
Zn(1)-O(1)	2.2924(16)	Zn(1)-O(6)$^{\#2}$	2.3044(15)
O(4)$^{\#1}$-Zn(1)-N(1)	123.25(5)	O(4)$^{\#1}$-Zn(1)-N(2)	95.27(5)
N(1)-Zn(1)-N(2)	78.83(6)	O(4)$^{\#1}$-Zn(1)-O(2)	142.71(6)
N(1)-Zn(1)-O(2)	93.06(6)	N(2)-Zn(1)-O(2)	100.42(6)
O(4)$^{\#1}$-Zn(1)-O(1)	87.67(5)	N(1)-Zn(1)-O(1)	148.27(5)
N(2)-Zn(1)-O(1)	92.51(6)	O(2)-Zn(1)-O(1)	58.22(5)
O(4)$^{\#1}$-Zn(1)-O(6)$^{\#2}$	88.63(5)	N(1)-Zn(1)-O(6)$^{\#2}$	89.75(6)
N(2)-Zn(1)-O(6)$^{\#2}$	168.24(5)	O(2)-Zn(1)-O(6)$^{\#2}$	82.81(5)
O(1)-Zn(1)-O(6)$^{\#2}$	98.74(6)		
3			
Zn(1)-O(7)	1.9683(15)	Zn(1)-N(5)	2.0129(19)
Zn(1)-O(2)$^{\#1}$	2.029(2)	Zn(1)-N(1)	2.0763(19)
Zn(1)-O(1)$^{\#1}$	2.461(2)		
O(7)-Zn(1)-N(5)	120.74(8)	O(7)-Zn(1)-O(2)$^{\#1}$	113.26(7)
N(5)-Zn(1)-O(2)$^{\#1}$	115.42(9)	O(7)-Zn(1)-N(1)	102.69(7)
N(5)-Zn(1)-N(1)	106.56(7)	O(2)$^{\#1}$-Zn(1)-N(1)	92.76(9)
O(7)-Zn(1)-O(1)$^{\#1}$	95.07 (7)	N(5)-Zn(1)-O(1)$^{\#1}$	86.25(8)
O(2)$^{\#1}$-Zn(1)-O(1)$^{\#1}$	55.43(9)	N(1)-Zn(1)-O(1)$^{\#1}$	147.89(9)
4			
Zn(1)-O(6)	1.9695(15)	Zn(1)-O(11)$^{\#1}$	1.9790(14)
Zn(1)-N(1)	2.010(2)	Zn(1)-N(12)	2.0409(16)
Zn(2)-O(8)	1.9793(15)	Zn(2)-O(4)$^{\#2}$	2.0052(14)

Zn(2)-N(8)	2.012(2)	Zn(2)-N(6)	2.0536(17)
O(6)-Zn(1)-O(11)$^{\#1}$	95.98(7)	O(6)-Zn(1)-N(1)	120.29(7)
O(11)$^{\#1}$-Zn(1)-N(1)	109.65(7)	O(6)-Zn(1)-N(12)	113.25(7)
O(11)$^{\#1}$-Zn(1)-N(12)	112.24(7)	N(1)-Zn(1)-N(12)	105.33(8)
O(8)-Zn(2)-O(4)$^{\#2}$	99.02(6)	O(8)-Zn(2)-N(8)	115.98(7)
O(4)$^{\#2}$-Zn(2)-N(8)	111.03(7)	O(8)-Zn(2)-N(6)	109.15(7)
O(4)$^{\#2}$-Zn(2)-N(6)	116.15(7)	N(8)-Zn(2)-N(6)	105.84(7)

5

Zn(1)-O(7)	1.9358(12)	Zn(1)-O(2)$^{\#1}$	1.9491(11)
Zn(1)-O(1)$^{\#2}$	1.9957(13)	Zn(1)-N(1)	2.0004(15)
O(7)-Zn(1)-O(2)$^{\#1}$	115.30(5)	O(7)-Zn(1)-O(1)$^{\#2}$	104.90(5)
O(2)$^{\#1}$-Zn(1)-O(1)$^{\#2}$	114.22(6)	O(7)-Zn(1)-N(1)	120.50(6)
O(2)$^{\#1}$-Zn(1)-N(1)	101.16(6)	O(1)$^{\#2}$-Zn(1)-N(1)	100.19(6)

6

Zn(1)-O(1)	1.9732(17)	Zn(1)-N(2)	2.021(2)
Zn(1)-N(6)$^{\#1}$	2.023(2)	Zn(1)-O(3)$^{\#2}$	2.1178(19)
Zn(1)-O(4)$^{\#2}$	2.2648(19)		
O(1)-Zn(1)-N(2)	93.47(8)	O(1)-Zn(1)-N(6)$^{\#1}$	101.68(8)
N(2)-Zn(1)-N(6)$^{\#1}$	106.60(9)	O(1)-Zn(1)-O(3)$^{\#2}$	102.92(8)
N(2)-Zn(1)-O(3)$^{\#2}$	88.53(9)	N(6)$^{\#1}$-Zn(1)-O(3)$^{\#2}$	150.16(8)
O(1)-Zn(1)-O(4)$^{\#2}$	131.50(8)	N(2)-Zn(1)-O(4)$^{\#2}$	126.74(8)
N(6)$^{\#1}$-Zn(1)-O(4)$^{\#2}$	92.21(8)	O(3)$^{\#2}$-Zn(1)-O(4)$^{\#2}$	58.64(7)

7

Cu(1)-O(8)$^{\#1}$	1.9324(17)	Cu(1)-O(5)$^{\#2}$	1.9480(15)
Cu(1)-O(1)	1.9600(16)	Cu(1)-O(2)	1.9718(15)
Cu(1)-O(1W)	2.287(3)	Cu(2)-O(4)$^{\#3}$	1.9156(15)
Cu(2)-O(3)	1.9550(15)	Cu(2)-O(1)	1.9686(15)
Cu(2)-O(1)$^{\#4}$	1.9935(15)	Cu(2)-O(7)$^{\#5}$	2.374(2)
Cu(2)...Cu(2)$^{\#4}$	3.0274(5)		
O(8)$^{\#1}$-Cu(1)-O(5)$^{\#2}$	84.63(7)	O(8)$^{\#1}$-Cu(1)-O(1)	174.81(8)
O(5)$^{\#2}$-Cu(1)-O(1)	92.41(6)	O(8)$^{\#1}$-Cu(1)-O(2)	92.91(7)
O(5)$^{\#2}$-Cu(1)-O(2)	151.81(8)	O(1)-Cu(1)-O(2)	91.71(7)
O(8)$^{\#1}$-Cu(1)-O(1W)	91.33(10)	O(5)$^{\#2}$-Cu(1)-O(1W)	114.03(9)
O(1)-Cu(1)-O(1W)	85.98(9)	O(2)-Cu(1)-O(1W)	94.06(8)
O(4)$^{\#3}$-Cu(2)-O(3)	84.57(6)	O(4)$^{\#3}$-Cu(2)-O(1)	174.10(7)

O(3)-Cu(2)-O(1)	99.76(6)	$O(4)^{\#3}$-Cu(2)-$O(1)^{\#4}$	97.11(6)
O(3)-Cu(2)-$O(1)^{\#4}$	158.32(9)	O(1)-Cu(2)-$O(1)^{\#4}$	80.35(7)
$O(4)^{\#3}$-Cu(2)-$O(7)^{\#5}$	93.29(8)	O(3)-Cu(2)-$O(7)^{\#5}$	97.46(9)
O(1)-Cu(2)-$O(7)^{\#5}$	82.23(8)	$O(1)^{\#4}$-Cu(2)-$O(7)^{\#5}$	103.99(8)
$O(4)^{\#3}$-Cu(2)-$Cu(2)^{\#4}$	136.75(5)	O(3)-Cu(2)-$Cu(2)^{\#4}$	136.24(5)
O(1)-Cu(2)-$Cu(2)^{\#4}$	40.48(5)	$O(1)^{\#4}$-Cu(2)-$Cu(2)^{\#4}$	39.87(4)
$O(7)^{\#5}$-Cu(2)-$Cu(2)^{\#4}$	94.09(6)		

Symmetry codes for **1**: $^{\#1}$ -x+2, -y, -z+2; $^{\#2}$ x, -y-1/2, z-1/2; $^{\#3}$ -x+1, y+3/2, -z+3/2. For **2**: $^{\#1}$ x-1, y, z; $^{\#2}$ -x,-y+2,-z+2. For **3**: $^{\#1}$ x, y+1, z+1. For **4**: $^{\#1}$ -x+1, -y+1, -z+1; $^{\#2}$ -x+2, -y+1, -z. For **5**: $^{\#1}$ -x+2, y+1/2, -z+3/2; $^{\#2}$ -x+2,-y,-z+2. For **6**: $^{\#1}$ -x+3/2, y+1/2, -z+1; $^{\#2}$ x+1/2, -y+1/2, -z-1. For **7**: $^{\#1}$ -x+4, -y+1, -z+3; $^{\#2}$ x, y-1, z; $^{\#3}$ -x+2, -y+2, -z+2; $^{\#4}$ -x+2, -y+1, -z+2; $^{\#5}$ x-1, y, z-1.

Table S2. Hydrogen-bonding parameters for **1**-**7** (in Å and deg)

D-H···A	d(D-H)	d(D···A)	∠(D-H···A)
1			
O(1W)-H(1A)...$O(4)^{\#4}$	0.841(18)	2.33(2)	3.110(2)	154(3)
O(1W)-H(1B)...$O(6)^{\#5}$	0.82(3)	2.02(3)	2.808(3)	161(3)
2			
O(7)-H(7A)...$O(3)^{\#5}$	0.82	1.84	2.5806(18)	150.2
O(1W)-H(1A)...O(1)	0.936(18)	2.047(19)	2.968(3)	168(3)
O(1W)-H(1B)...$O(1)^{\#6}$	0.915(18)	2.110(19)	3.017(3)	171(3)
O(2W)-H(2A)...$O(2)^{\#4}$	0.904(19)	2.09(2)	2.932(6)	155(5)
4			
O(1W)-H(1B)...$O(2W)^{\#3}$	0.835(17)	2.192(18)	3.025(3)	176(4)
O(1W)-H(1A)...O(2)	0.875(17)	2.20(2)	3.052(4)	163(5)
O(2W)-H(2A)...O(9)	0.893(18)	1.99(2)	2.838(3)	158(7)
O(1)-H(1)...$O(5)^{\#4}$	0.82	1.81	2.588(2)	157.7
O(14)-H(14)...$O(10)^{\#5}$	0.82	1.78	2.566(2)	160.1
5			
O(5)-H(5A)...$O(6)^{\#3}$	0.82	1.85	2.6421(18)	162.7
6			
O(6)-H(6A)...$O(4)^{\#3}$	0.82	1.86	2.679(3)	174.2
7			

O(1W)-H(1A)...O(6)$^{\#6}$	0.842(19)	2.38(3)	3.141(3)	150(4)
O(1W)-H(1B)...O(7)$^{\#7}$	0.851(19)	2.09(2)	2.895(3)	158(4)
O(1)-H(1)...O(2)$^{\#8}$	0.79(3)	2.05(3)	2.790(3)	156(3)
O(2W)-H(2A)...O(1W)	0.92(2)	2.56(10)	3.119(17)	119(9)

Symmetry code for **1**: $^{\#4}$ -x+2, -y-1, -z+2; $^{\#5}$ -x+2, y+1/2, -z+3/2. For **2**: $^{\#4}$ -x+1, -y+1, -z+1; $^{\#5}$ x-1, y+1, z+1; $^{\#6}$ -x, -y+1, -z+2. For **4**: $^{\#3}$ -x+2, -y, -z; $^{\#4}$ x, y-1, z; $^{\#5}$ x, y+1, z. For **5**: $^{\#3}$ -x+1, y-1/2, -z+5/2. For **6**: $^{\#3}$ -x+1, -y, z+1. For **7**: $^{\#6}$ x-1, y, z; $^{\#7}$ -x+3, -y+1, -z+3; $^{\#8}$ -x+3, -y+1, -z+2.

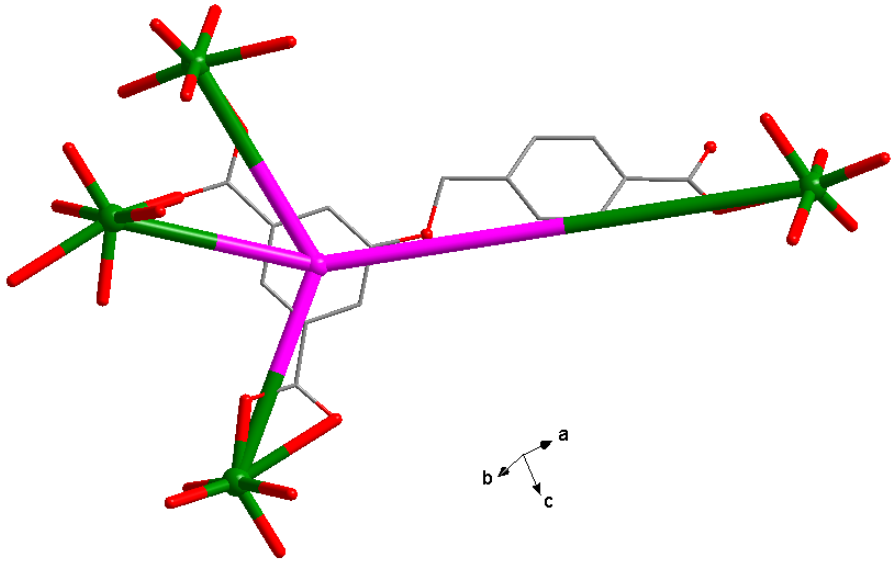


Fig. S1. View of the four-connected node of HL anion in **1**.

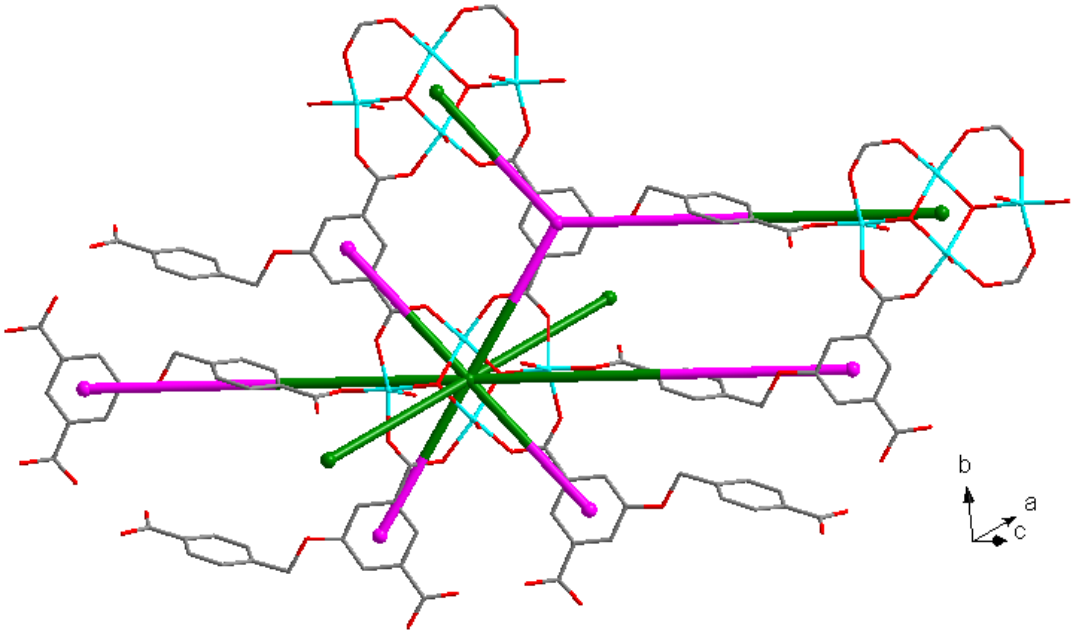


Fig. S2. View of the eight-connected and three-connected nodes of **7**.

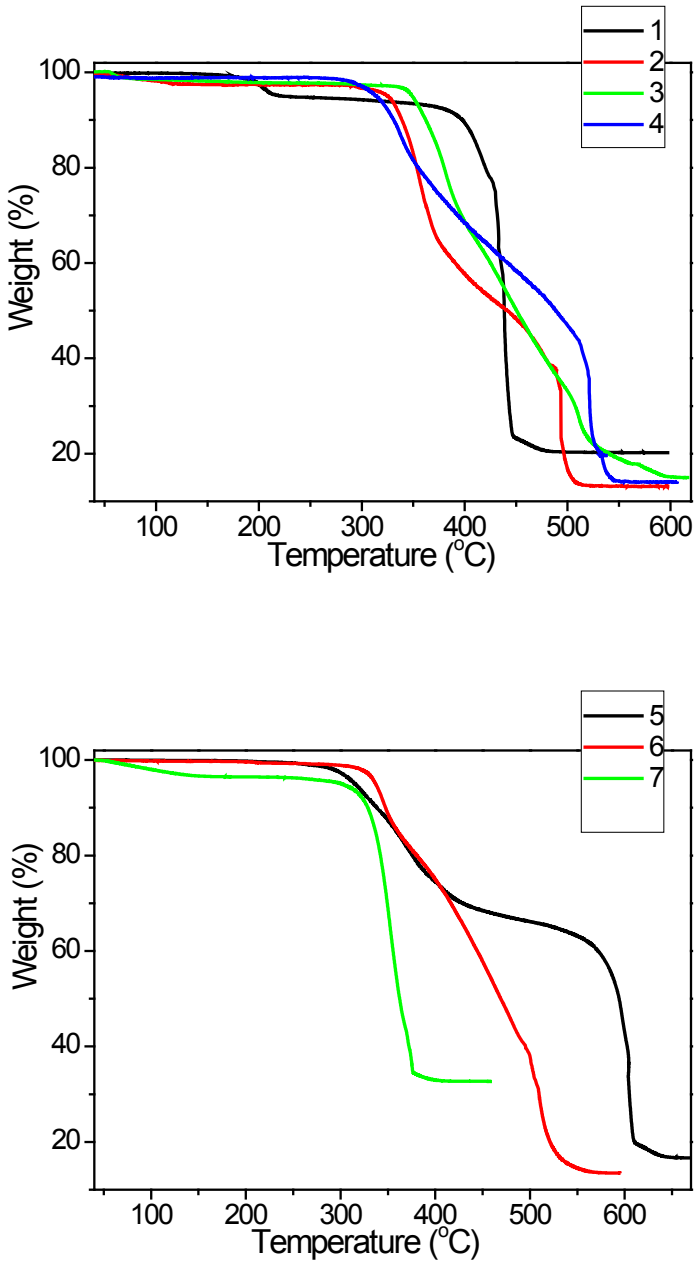
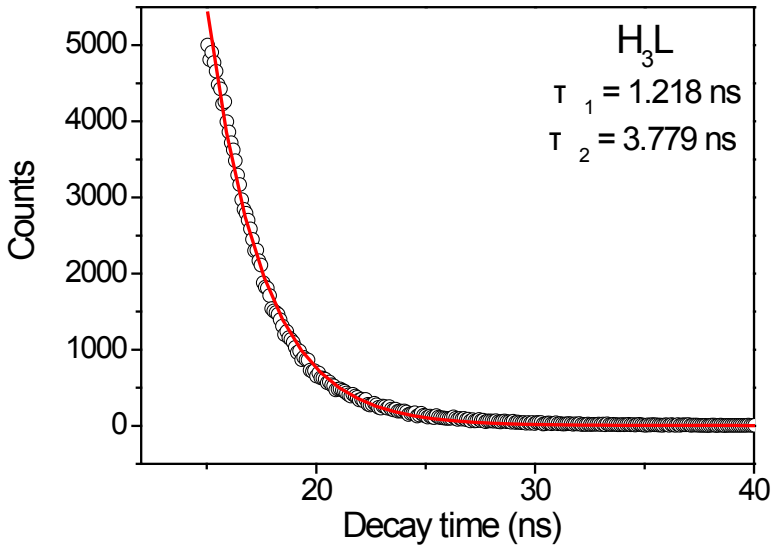
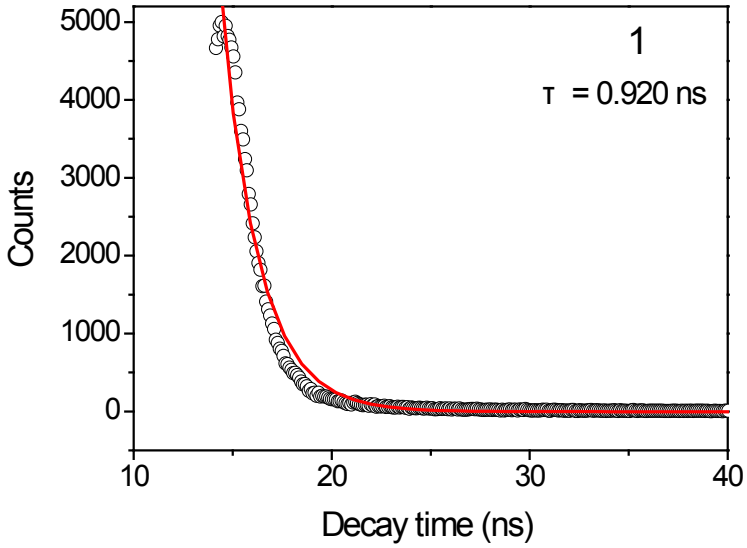
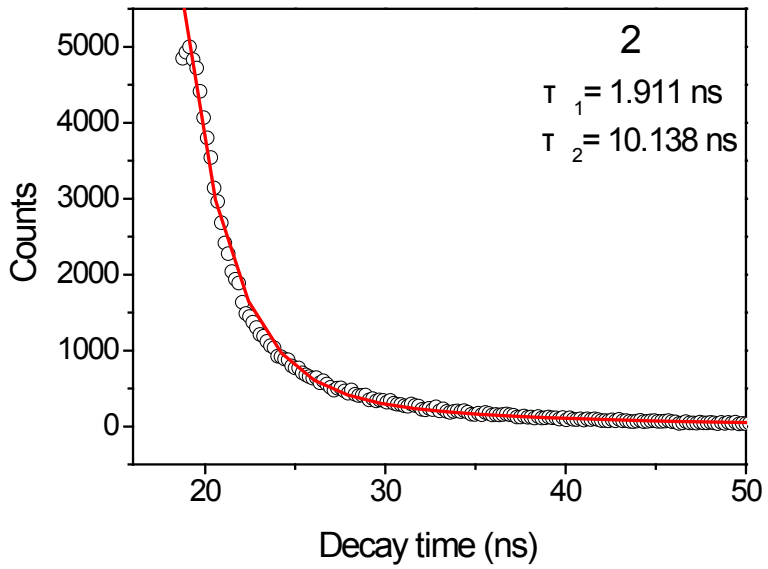
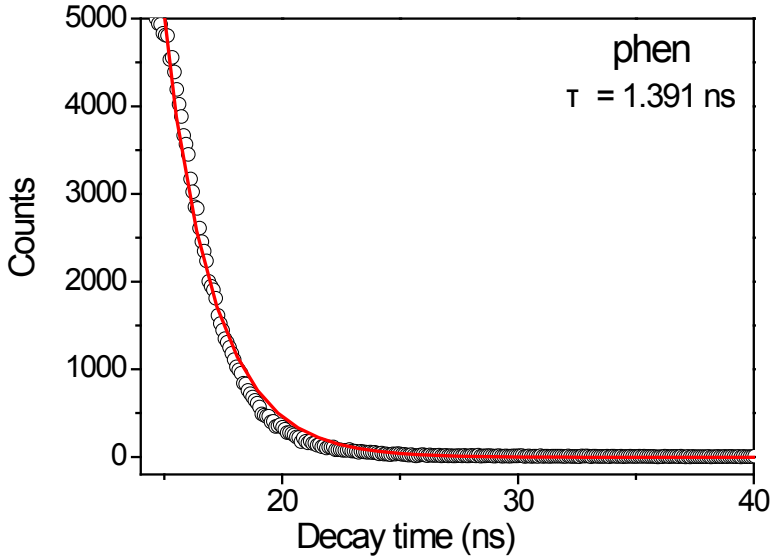


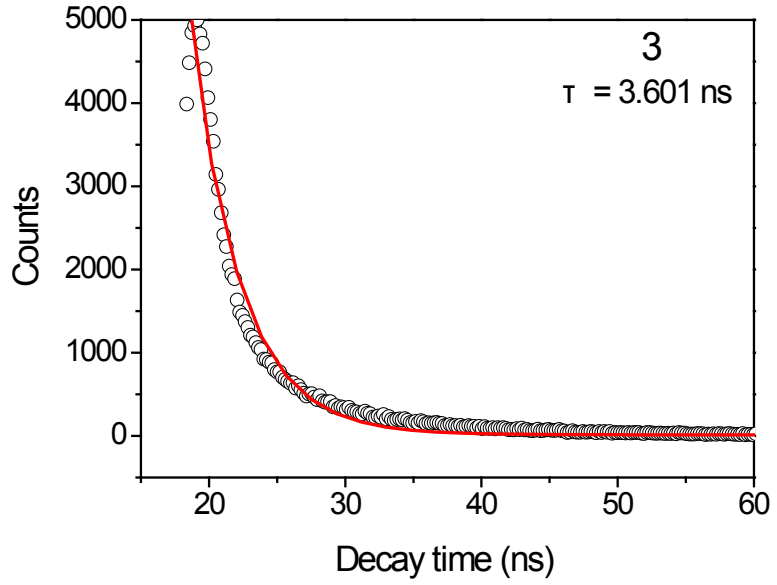
Fig. S3. TGA curves of compounds **1-7**.

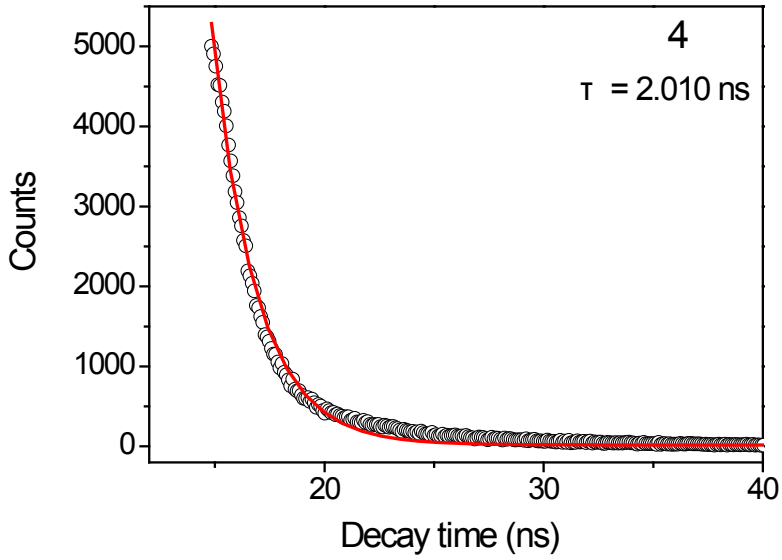


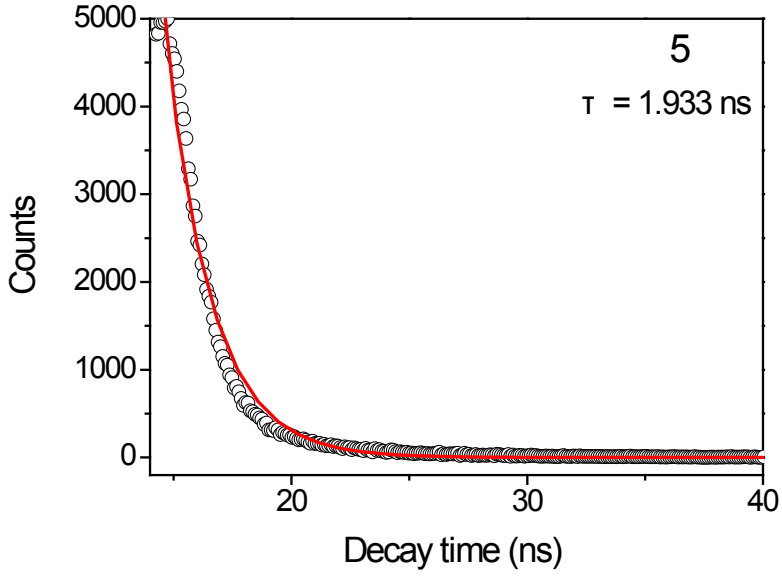












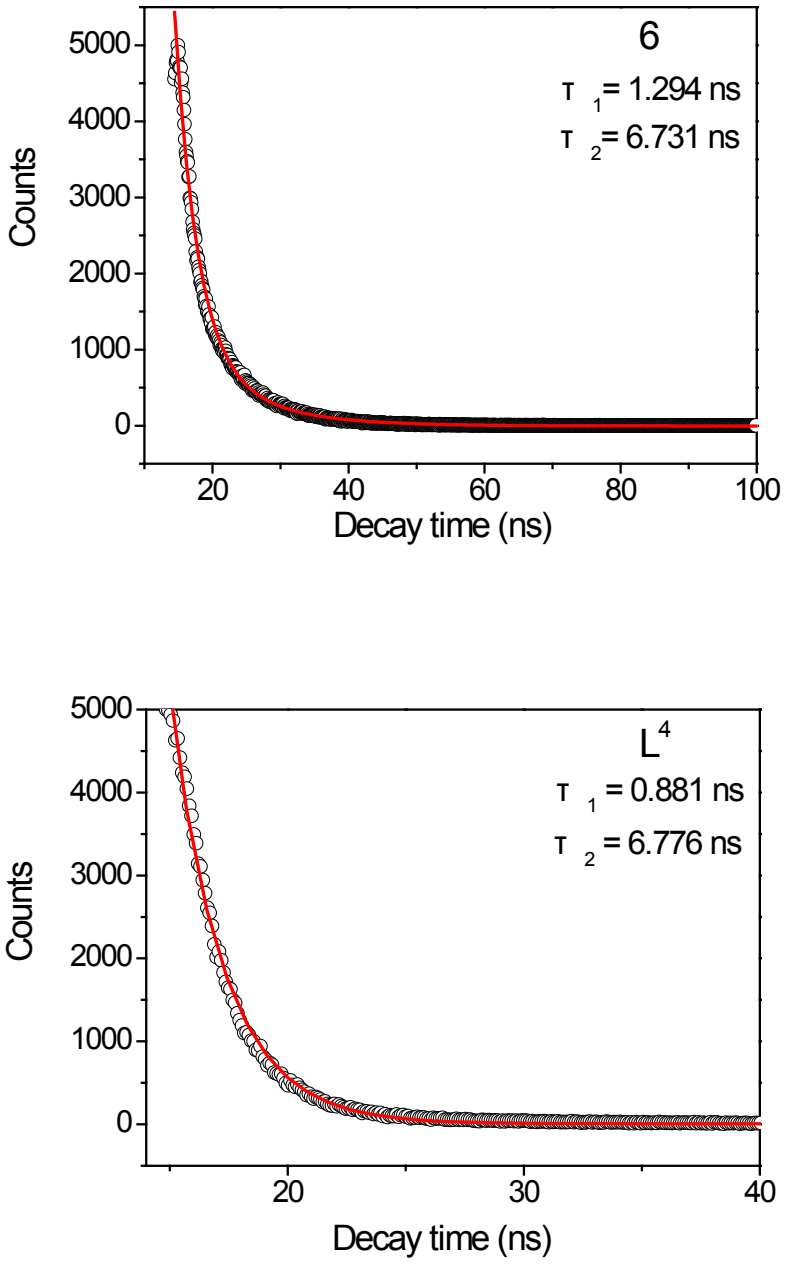
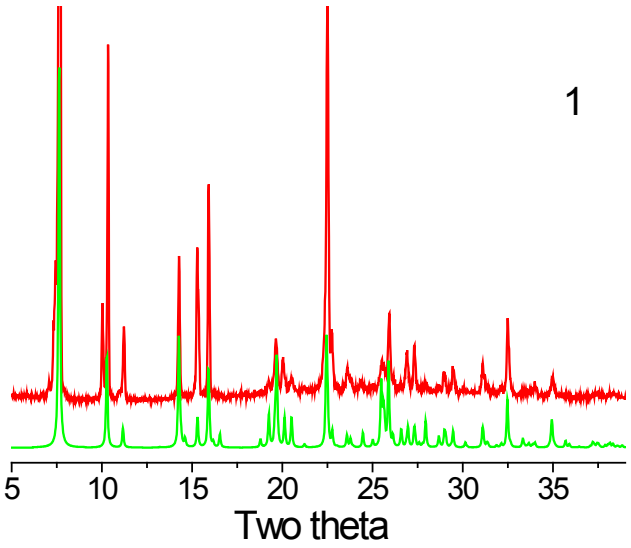
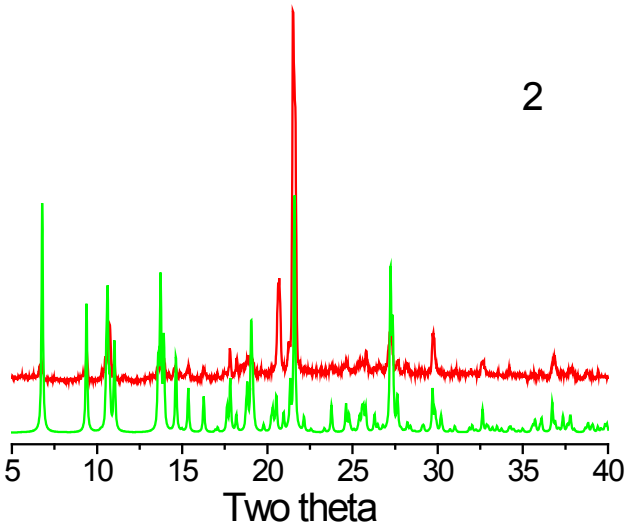
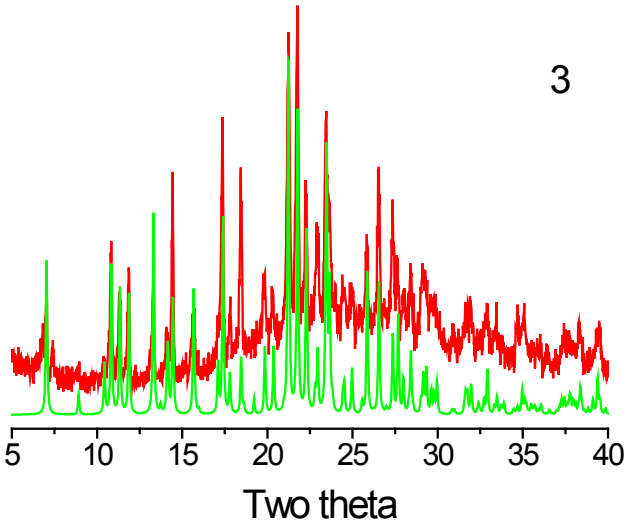
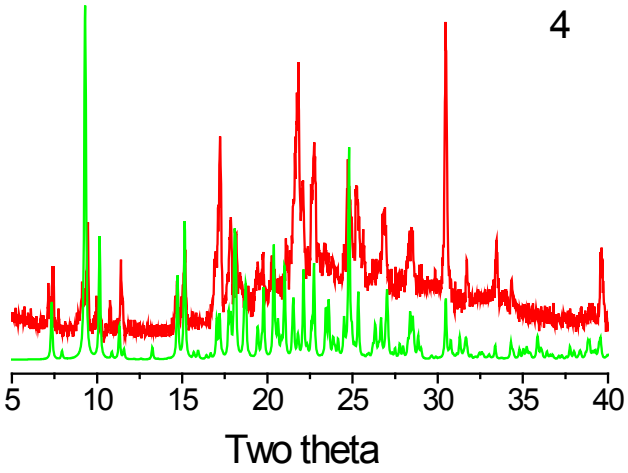


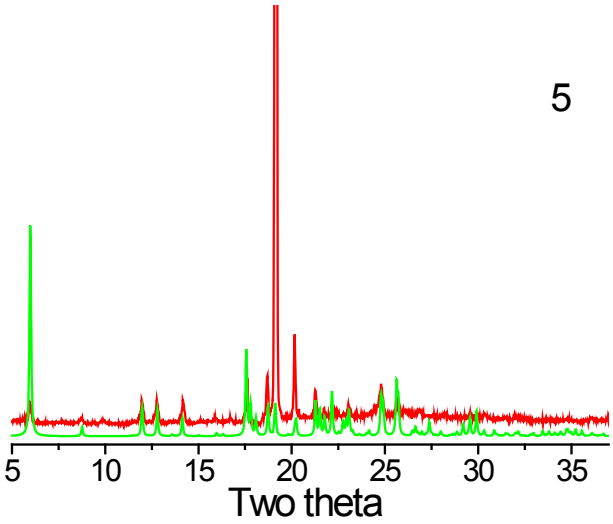
Fig. S4. Luminescence decay curves for compounds **1-6** (the black circles represent experimental data, and the solid red lines represent fitting results, H_3L: λ_{ex} = 364 nm, λ_{em} = 392 nm; **1**: λ_{ex} = 358 nm, λ_{em} = 413 nm; **2**: λ_{ex} = 372 nm, λ_{em} = 424 nm; phen: λ_{ex} = 325 nm, λ_{em} = 380 nm; **3**: λ_{ex} = 372 nm, λ_{em} = 426 nm; **4**: λ_{ex} = 352 nm, λ_{em} = 423 nm; **5**: λ_{ex} = 353 nm, λ_{em} = 395 nm; **6**: λ_{ex} = 353 nm, λ_{em} = 462 nm; L^4: λ_{ex} = 305 nm, λ_{em} = 443 nm).

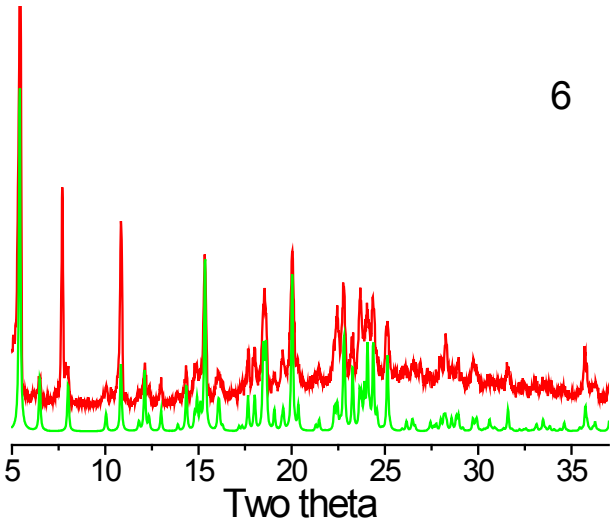












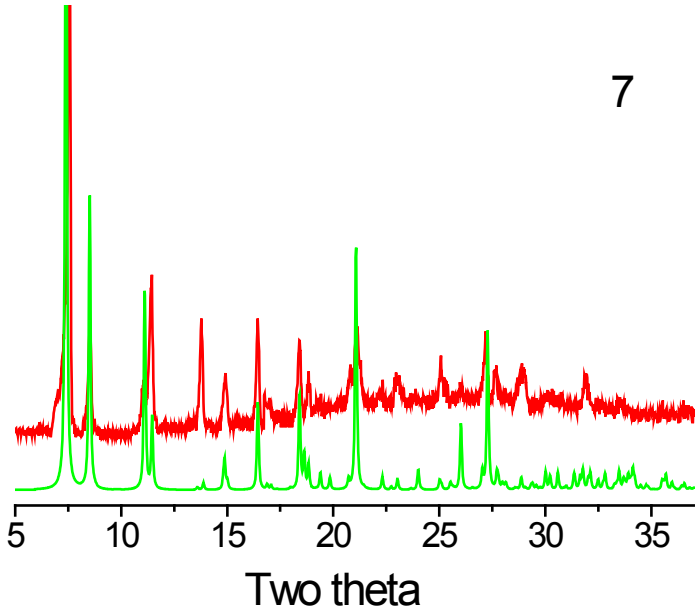


Fig. S5 The simulated (green) and experimental (red) XRPD patterns for the compounds **1-7** (the diffraction peaks of both simulated and experimental patterns match well in relevant positions, indicating that the phase purities of compounds **1-7** are good).