Electronic Supplementary Material (ESI) for RSC Advances.

A series of coordination polymers based on terphenyl tetracarboxylates and bis-pyridyl ligands with water vapor sorption properties

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Table S1. Selected bond distances (Å) and angles (°) for complexes **1**–**6**.

Complex **1**			
Mn(1)-O(2)#1	2.093(3)	Mn(1)-O(1)	2.168(3)
Mn(1)-N(1)	2.208(4)	Mn(1)-O(6)	2.225(4)
Mn(1)-O(3)#2	2.227(3)	Mn(1)-O(4)#2	2.265(3)
O(2)#1-Mn(1)-O(1)	92.39(13)	O(2)#1-Mn(1)-N(1)	95.85(15)
O(1)-Mn(1)-N(1)	87.35(15)	O(2)#1-Mn(1)-O(6)	84.95(15)
O(1)-Mn(1)-O(6)	175.91(13)	N(1)-Mn(1)-O(6)	89.83(16)
O(2)#1-Mn(1)-O(3)#2	112.05(13)	O(1)-Mn(1)-O(3)#2	96.09(13)
N(1)#1-Mn(1)-O(3)#2	151.65(15)	O(2)#1-Mn(1)-O(4)#2	168.57(13)
O(6)-Mn(1)-O(3)#2	87.79(14)	N(1)-Mn(1)-O(4)#2	93.34(14)
O(1)-Mn(1)-O(4)#2	94.82(12)	O(3)#2-Mn(1)-O(4)#2	58.36(12)
O(6)-Mn(1)-O(4)#2	88.30(14)		
Complex **2**			
Mn(1)-O(9)	2.095(9)	Mn(1)-O(7)	2.141(10)
Mn(1)-O(3)	2.152(10)	Mn(1)-O(1)	2.156(9)
Mn(1)-O(10)	2.287(9)	Mn(1)-O(5)	2.501(9)
Mn(2)-O(4)#1	2.149(10)	Mn(2)-O(9)	2.183(10)
Mn(2)-O(8)#1	2.184(9)	Mn(2)-O(9)#1	2.193(9)
Mn(2)-O(5)	2.323(9)	Mn(2)-N(1)	2.342(12)
O(9)-Mn(1)-O(7)	94.1(4)	O(9)-Mn(1)-O(3)	111.2(3)
O(7)-Mn(1)-O(3)	87.7(4)	O(9)-Mn(1)-O(1)	83.2(3)
O(7)-Mn(2)-O(1)	93.5(4)	O(9)-Mn(2)-O(10)	158.6(3)
O(7)-Mn(2)-O(10)	104.5(3)	O(3)-Mn(2)-O(10)	80.5(3)
O(1)-Mn(2)-O(10)	85.1(3)	O(9)-Mn(2)-O(5)	76.7(3)

O(7)-Mn(2)-O(5)	161.6(3)	O(3)-Mn(2)-O(5)	81.0(3)
O(1)-Mn(2)-O(5)	101.1(3)	O(10)-Mn(2)-O(5)	88(3)
O(4)-Mn(2)-O(9)	86.8(4)	O(4)#1-Mn(2)-O(8)#1	89.2(4)
O(9)-Mn(2)-O(1)	164.7(3)	O(4)#1-Mn(2)-O(9)#1	102.5(3)
O(9)-Mn(2)-O(1)	77.5(4)	O(8)#1-Mn(2)-O(9)#1	89.0(3)
O(4)#1-Mn(2)-O(5)	151.3(3)	O(9)-Mn(2)-O(5)	79.1(3)
O(8)#1-Mn(2)-O(5)	110.4(4)	O(9)#1-Mn(2)-O(5)	98.7(3)
O(4)#1-Mn(2)-N(1)	79.6(4)	O(9)-Mn(2)-N(1)	109.0(4)
O(8)#1-Mn(2)-N(1)	84.7(4)	O(9)#1-Mn(2)-N(1)	173.4(4)
O(5)-Mn(2)-N(1)	81.6(4)		
Complex **3**			
Ni(1)-O(1)	2.023(2)	Ni(1)-O(10)	2.0237(19)
Ni(1)-O(5)#1	2.0503(19)	Ni(1)-N(3)	2.111(2)
Ni(1)-N(4)	2.118(8)	Ni(1)-O(9)	2.146(2)
O(1)-Ni(1)-O(10)	97.07(8)	O(1)-Ni(1)-O(5)#1	170.51(18)
O(10)-Ni(1)-O(5)#1	92.43(8)	O(1)-Ni(1)-N(3)	91.29(9)
O(10)-Ni(1)-N(3)	97.40(9)	O(5)#1-Ni(1)-N(3)	87.51(9)
O(1)-Ni(1)-N(4)	87.28(9)	O(10)-Ni(1)-N(4)	90.48(9)
O(5)#1-Ni(1)-N(4)	92.62(9)	N(3)-Ni(1)-N(4)	172.11(9)
O(1)-Ni(1)-O(9)	85.80(8)	O(10)-Ni(1)-O(9)	174.79(9)
O(5)#1-Ni(1)-O(9)	84.73(8)	N(3)-Ni(1)-O(9)	86.85(9)
N(4)-Ni(1)-O(9)	85.30(9)		
Complex **4**			
Co(1)-O(3)	2.068(8)	Co(1)-O(10)	2.084(9)
Co(1)-O(7)	2.095(9)	Co(1)-O(11)	2.121(9)
Co(1)-N(1)	2.221(10)	Co(1)-O(9)	2.298(8)
Co(1)-O(13)	2.056(8)	Co(2)-O(4)	2.091(8)
Co(2)-O(6)#1	2.122(8)	Co(2)-O(12)	2.140(9)
Co(2)-N(3)	2.153(9)	Co(2)-O(9)	2.201(7)
O(3)-Co(1)-O(10)	177.3(4)	O(3)-Co(1)-O(7)	95.5(3)
O(10)-Co(1)-O(7)	86.8(4)	O(3)-Co(1)-O(11)	85.6(4)
O(10)-Co(1)-O(11)	92.1(4)	O(7)-Co(1)-O(11)	177.7(4)
O(3)-Co(1)-N(1)	92.4(3)	O(10)-Co(1)-N(1)	88.9(4)
O(7)-Co(1)-N(1)	96.0(4)	O(11)-Co(1)-N(1)	86.0(4)
O(3)-Co(1)-O(9)	93.8(3)	O(10)-Co(1)-O(9)	84.5(3)

O(7)-Co(1)-O(9)	95.8(3)	O(11)-Co(1)-O(9)	82.1(3)
N(1)-Co(1)-O(9)	166.1(3)	O(13)-Co(2)-O(4)	176.0(3)
O(13)-Co(2)-O(6)#1	92.1(4)	O(4)-Co(2)-O(6)#1	85.5(3)
O(13)-Co(2)-O(12)	92.1(4)	O(4)-Co(2)-O(12)	90.3(3)
O(6)#1-Co(2)-O(12)	175.4(3)	O(13)-Co(2)-N(3)	94.7(4)
O(4)-Co(2)-N(3)	88.7(3)	O(6)#1-Co(2)-N(3)	92.3(4)
O(12)-Co(2)-N(3)	85.6(4)	O(13)-Co(2)-O(9)	91.0(3)
O(4)-Co(2)-O(9)	86.0(3)	O(6)#1-Co(2)-O(9)	95.8(3)
O(12)-Co(2)-O(9)	85.9(3)	N(3)-Co(2)-O(9)	169.9(3)
Complex **5**			
Co(1)-O(1)#2	2.071(5)	Co(1)-N(1)	2.099(6)
Co(1)-O(4)#1	2.108(5)	Co(1)-O(6)	2.125(5)
Co(1)-O(3)#1	2.293(5)	Co(1)-O(1)#2	2.306(5)
O(1)-Co(1)-O(9)	102.8(2)	O(1)-Co(1)-O(4)#1	105.67(19)
N(1)-Co(1)-O(9)	150.1(2)	O(1)-Co(1)-O(6)	93.1(2)
N(1)-Co(1)-O(9)	95.7(2)	O(4)#1-Co(1)-O(6)	91.8(2)
O(1)-Co(1)-O(9)	165.05(18)	N(1)-Co(1)-O(3)#1	91.5(2)
O(4)#1-Co(2)-O(9)	59.50(19)	O(6)-Co(1)-O(3)#1	89.5(2)
O(1)-Co(1)-O(9)	77.70(19)	N(1)-Co(1)-O(1)#2	91.6(2)
O(4)#1-Co(1)-O(9)	85.76(18)	O(6)-Co(1)-O(1)#2	169.41(19)
O(3)#1-Co(1)-O(9)	98.08(18)		
Complex **6**			
Co(1)-O(7)#1	2.006(9)	Co(1)-O(1)	2.114(9)
Co(1)-N(2)	2.133(11)	Co(1)-N(1)	2.146(13)
Co(1)-O(9)	2.178(9)	Co(1)-O(2)	2.304(9)
O(7)#1-Co(1)-O(1)	169.0(4)	O(7)#1-Co(1)-N(2)	96.4(4)
O(1)-Co(1)-O(2)	93.8(4)	O(7)#1-Co(1)-N(1)	93.4(4)
O(1)-Co(1)-O(1)	90.6(4)	N(2)-Co(1)-N(1)	91.4(5)
O(7)#1-Co(1)-O(9)	88.5(4)	O(1)-Co(1)-O(9)	87.7(3)
O(2)-Co(1)-O(9)	87.5(4)	N(1)-Co(1)-O(9)	177.9(4)
O(7)#1-Co(1)-O(2)	111.2(4)	O(1)-Co(1)-O(2)	58.5(4)
O(2)-Co(1)-O(2)	152.2(4)	N(1)-Co(1)-O(2)	90.4(4)
O(9)-Co(1)-O(2)	89.8(3)		

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

for **1**; #1 –x+1, –y+1, –z+1 for **2**; #1 x, –y+1/2, z+1/2 for **3**; #1 x, y+1, z for **4**; #1 x, y+1, z; #2 –x+1, –y+1, –z+1 for **5**; #1 x–1, y+1, z+1 for **6**.

Table S2. Hydrogen-bonding geometry (Å, °) for complex **2**–**4** and **6**.

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠D–H···A	Symmetry codes
Complex **2**					
O(10)–H(10D)···O(2)	0.850	1.938	2.767	164.78	–x+1, –y+1, –z+1
O(10)–H(10E)···N(2)	0.850	1.968	2.797	164.85	–x+2, –y+2, –z
O(11)–H(11C)···O(2)	0.850	2.197	3.029	166.17	–x+1, –y+1, –z+1
O(11)–H(11D)···O(6)	0.850	2.075	2.906	165.74	x+1, y–1, z
Complex **3**					
O(10)–H(10D)···O(7)	0.850	1.988	2.741	147.19	–x+2, y+1/2, –z+1/2
Complex **4**					
O(9)–H(9A)···O(1)	0.850	1.959	2.751	154.72	x, y, z–1
Complex **6**					
O(9)–H(9D)···O(8)	0.850	1.949	2.771	162.59	–x+1, –y+1, –z

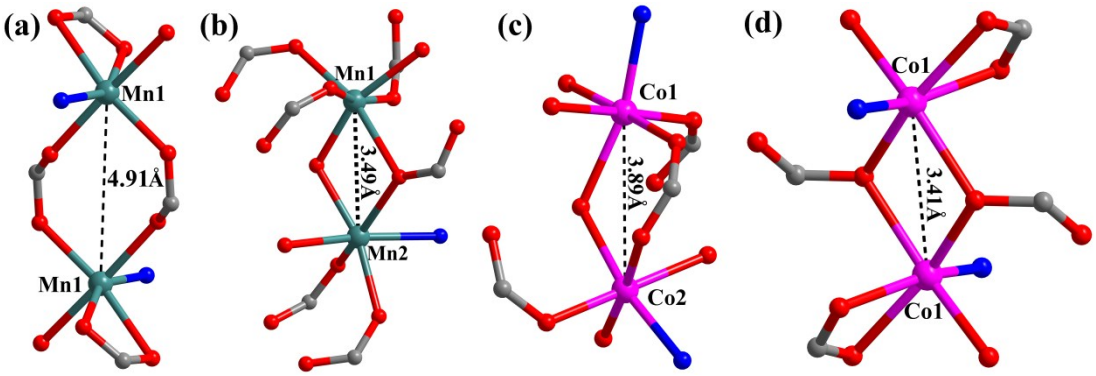

Fig. S1. The dinuclear (a) Mn^{II} unit in complex **1**; (b) Mn^{II} unit in complex **2**; (c) Co^{II} unit in complex **4**; (d) Co^{II} unit in complex **5**. Color legend: teal, Mn; pink, Co; gray, C; blue, N; red, O.

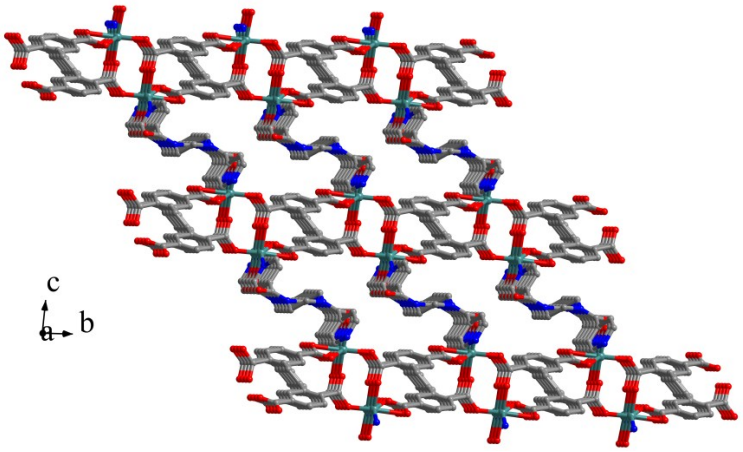

Fig. S2. The 3D framework of complex **1**. Color legend: teal, Mn; gray, C; blue, N; red, O. All hydrogen atoms, the lattice H_2O and CH_3OH are omitted for clarity.

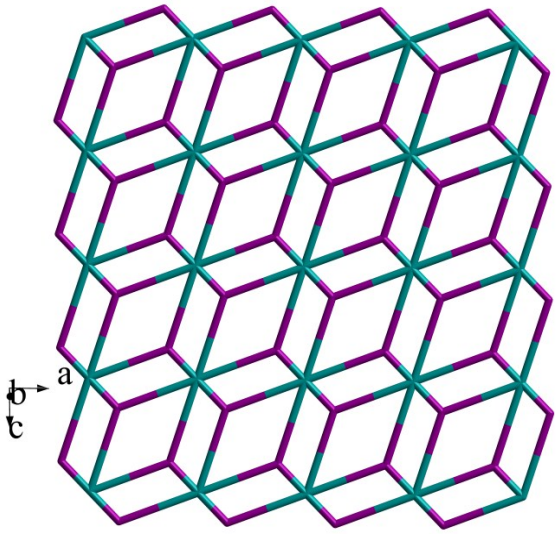

Fig. S3. The (3,6)-connected 2D grid in complex **2**.

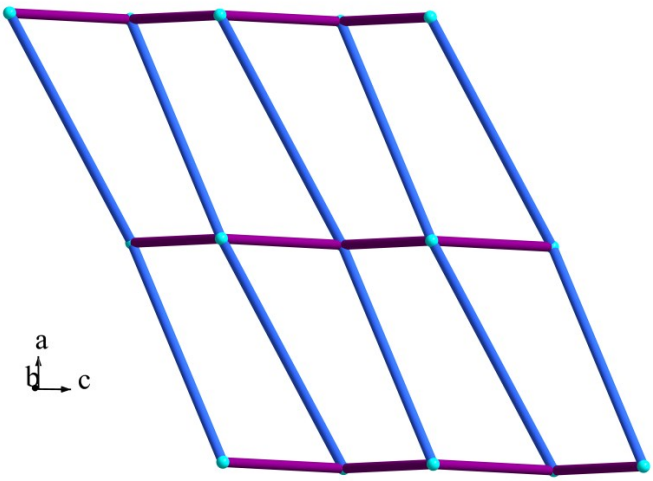

Fig. S4. The 4-connected 2D grid in complex **3**.

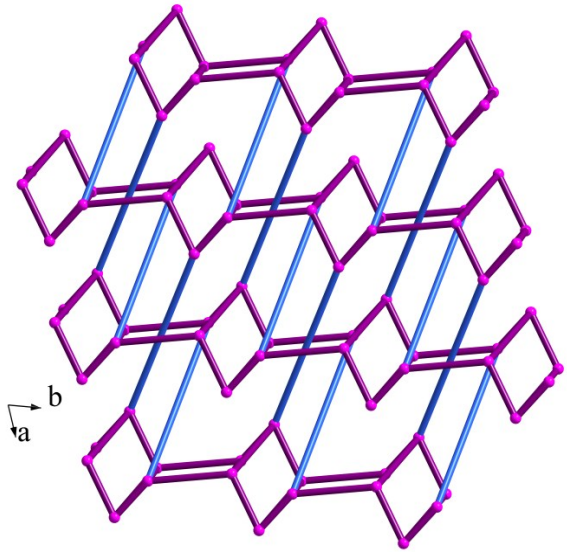

Fig. S5. The 4-connected 2D grid in complex **4**.

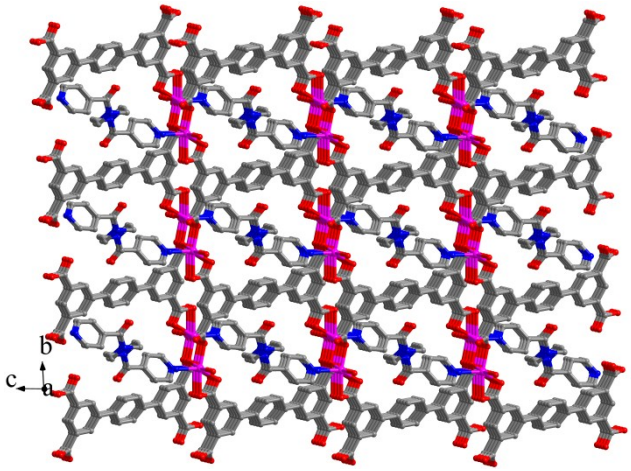

Fig. S6. The 3D framework of complex **5**. Color legend: pink, Co; gray, C; blue, N; red, O. All hydrogen atoms and the lattice H_2O are omitted for clarity.

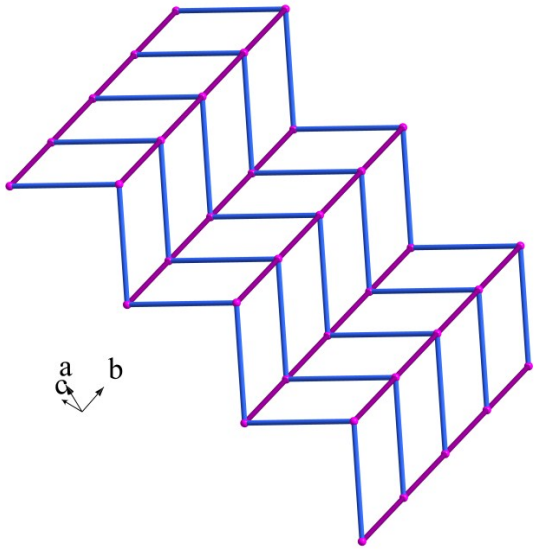

Fig. S7. The 4-connected 2D grid in complex **6**.

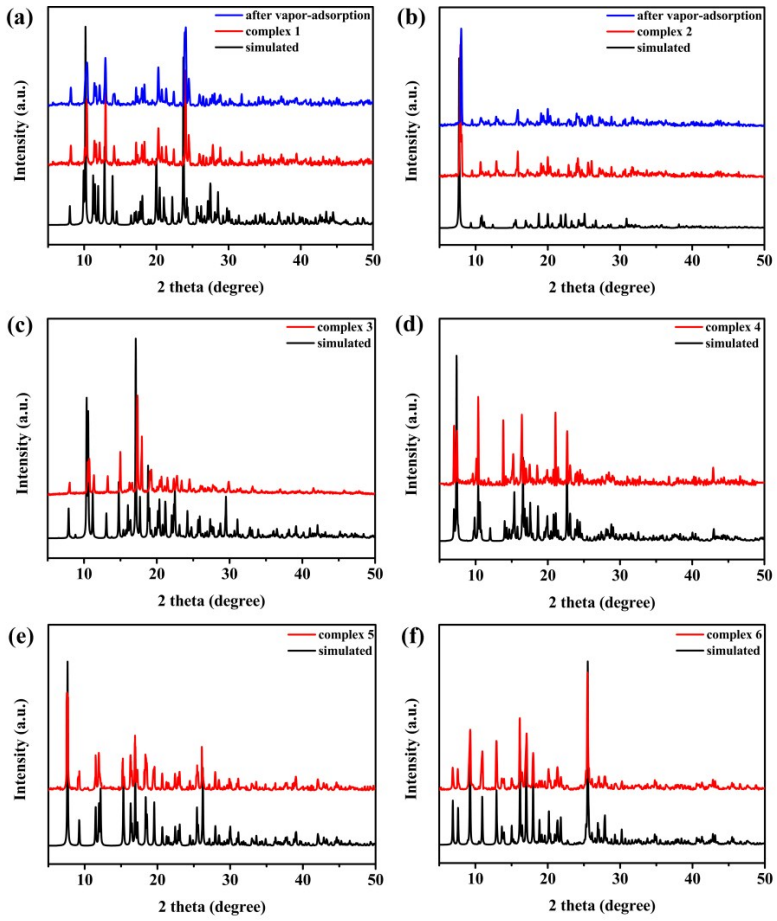

Fig. S8. The simulated (black line), experimental samples (red line) and samples after vapor-adsorption (blue line) powder X-ray diffraction patterns for complexes **1**–**6**.

Fig. S9. The TG curves of complexes **1**–**6**.

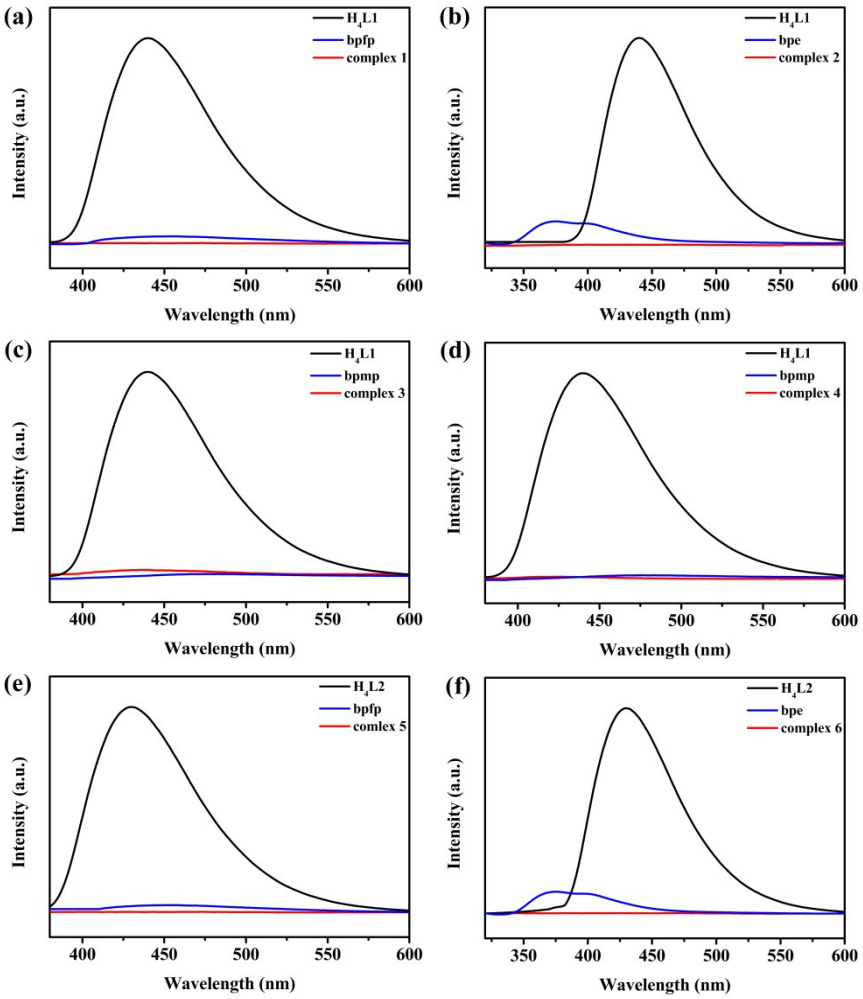

Fig. S10. Solid-state fluorescent emission spectra for ligands H_4L1 and H_4L2 (black); ligands bpfp, bpe and bpmp (blue); complexes **1**–**6** (red) in solid state at room temperature.