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Construction of Several New *s*-/*p*-Block Complexes Containing Binuclear Metal-Terpyridine Building Blocks: Dependence of Structural Diversity on Number of Coordinated Water Molecules

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Supporting information

Table S1 Selected bond lengths [Å] and angles[°] for the compounds.[a]

Complex **1**			
Mg(1)-O(1W)	2.018(2)	Mg(1)-O(2W)	2.058(2)
Mg(1)-O(6)#1	2.096(2)	Mg(1)-N(2)	2.133(2)
Mg(1)-N(3)	2.189(3)	Mg(1)-N(1)	2.231(3)
O(1W)-Mg(1)-O(2W)	88.91(11)	O(1W)-Mg(1)-O(6)#1	86.08(10)
O(2W)-Mg(1)-O(6)#1	172.12(11)	O(1W)-Mg(1)-N(2)	174.74(11)
O(2W)-Mg(1)-N(2)	94.58(10)	O(6)#1-Mg(1)-N(2)	90.86(9)
O(1W)-Mg(1)-N(3)	101.33(10)	O(2W)-Mg(1)-N(3)	93.70(11)
O(6)#1-Mg(1)-N(3)	93.24(9)	N(2)-Mg(1)-N(3)	74.55(9)
O(1W)-Mg(1)-N(1)	110.55(10)	O(2W)-Mg(1)-N(1)	86.69(11)
O(6)#1-Mg(1)-N(1)	89.39(9)	N(2)-Mg(1)-N(1)	73.64(9)
N(3)-Mg(1)-N(1)	148.11(10)		
Complex **2**			
Ca(1)-O(4)	2.307(4)	Ca(1)-N(2)#2	2.521(4)
Ca(1)-O(1)#1	2.326(4)	Ca(1)-N(3)#2	2.558(5)
Ca(1)-O(1W)	2.399(4)	Ca(1)-N(1)#2	2.548(5)
Ca(1)-O(2W)	2.441(4)	O(4)-Ca(1)-N(3)#2	97.32(16)
O(4)-Ca(1)-O(1)#1	167.89(16)	O(1)#1-Ca(1)-N(3)#2	94.45(14)
O(4)-Ca(1)-O(1W)	90.43(17)	O(1W)-Ca(1)-N(3)#2	75.85(15)
O(1)#1-Ca(1)-O(1W)	95.23(16)	O(2W)-Ca(1)-N(3)#2	149.49(14)
O(4)-Ca(1)-O(2W)	89.96(14)	N(2)#2-Ca(1)-N(3)#2	64.27(14)
O(1)#1-Ca(1)-O(2W)	81.29(12)	O(4)-Ca(1)-N(1)#2	86.59(16)
O(1W)-Ca(1)-O(2W)	74.51(15)	O(1)#1-Ca(1)-N(1)#2	84.04(14)
O(4)-Ca(1)-N(2)#2	80.17(12)	O(1W)-Ca(1)-N(1)#2	157.16(14)
O(1)#1-Ca(1)-N(2)#2	102.53(12)	O(2W)-Ca(1)-N(1)#2	82.85(14)
O(1W)-Ca(1)-N(2)#2	137.16(15)	N(2)#2-Ca(1)-N(1)#2	64.48(13)
O(2W)-Ca(1)-N(2)#2	146.21(14)	N(3)#2-Ca(1)-N(1)#2	126.99(14)
Complex **3**			
N(2)-Pb(1)	2.495(5)	N(1)-Pb(1)	2.530(6)
N(3)-Pb(1)	2.533(7)	Pb(1)-O(1)#1	2.622(6)
O(1W)-Pb(1)	2.400(7)		
O(1W)-Pb(1)-N(2)	87.3(2)	N(1)-Pb(1)-N(3)	128.0(2)
O(1W)-Pb(1)-N(1)	86.7(2)	O(1W)-Pb(1)-O(1)#1	160.5(2)
N(2)-Pb(1)-N(1)	65.1(2)	N(2)-Pb(1)-O(1)#1	73.59(19)
O(1W)-Pb(1)-N(3)	78.9(3)	N(1)-Pb(1)-O(1)#1	82.2(2)

N(2)-Pb(1)-N(3)	64.5(2)	N(3)-Pb(1)-O(1)#1	95.4(2)
Complex **4**			
Pb(1)-O(2)#1	2.457(16)	Pb(1)-N(1)	2.589(19)
Pb(1)-N(2)	2.542(17)	Pb(1)-O(6)#2	2.684(15)
Pb(1)-N(3)	2.58(2)	O(6)-Pb(1)#2	2.684(15
O(2)-Pb(1)#1	2.457(16		
N(2)-Pb(1)-N(1)	64.1(5)	N(3)-Pb(1)-N(1)	122.7(6)
O(2)#1-Pb(1)-N(2)	102.4(6)	O(2)#1-Pb(1)-O(6)#2	167.0(7)
O(2)#1-Pb(1)-N(3)	87.9(7)	N(2)-Pb(1)-O(6)#2	72.4(5)
N(2)-Pb(1)-N(3)	62.7(5)	N(3)-Pb(1)-O(6)#2	79.1(5)
O(2)#1-Pb(1)-N(1)	83.6(6)	N(1)-Pb(1)-O(6)#2	103.9(5)
Complex **5**			
Pb(1)-N(8)#1	2.497(7)	Pb(2)-N(1)	2.519(9)
Pb(1)-O(10)#1	2.507(7)	Pb(2)-O(7)	2.656(6)
Pb(1)-N(7)#1	2.514(8)	Pb(3)-N(4)	2.507(7)
Pb(1)-N(9)#1	2.523(8)	Pb(3)-O(17)	2.514(12)
Pb(1)-O(6)	2.574(7)	Pb(3)-N(04)	2.510(9)
Pb(2)-O(1W)	2.478(8)	Pb(3)-N(6)	2.515(9)
Pb(2)-N(2)	2.502(8)	Pb(3)-O(17')	2.757(19)
Pb(2)-N(3)	2.516(8)	Pb(3)-O(3)	2.631(7)
N(8)#1-Pb(1)-O(10)#1	75.8(2)	N(3)-Pb(2)-O(7)	87.1(2)
N(8)#1-Pb(1)-N(7)#1	64.9(3)	N(1)-Pb(2)-O(7)	79.3(2)
O(10)#1-Pb(1)-N(7)#1	79.0(3)	N(4)-Pb(3)-O(17)	75.3(3)
N(8)#1-Pb(1)-N(9)#1	65.3(3)	N(4)-Pb(3)-N(04)	64.8(3)
O(10)#1-Pb(1)-N(9)#1	90.3(3)	O(17)-Pb(3)-N(04)	101.2(4)
N(7)#1-Pb(1)-N(9)#1	130.2(3)	N(4)-Pb(3)-N(6)	64.8(3)
N(8)#1-Pb(1)-O(6)	84.9(2)	O(17)-Pb(3)-N(6)	66.9(4)
O(10)#1-Pb(1)-O(6)	160.6(2)	N(04)-Pb(3)-N(6)	129.6(3)
N(7)#1-Pb(1)-O(6)	94.3(3)	N(4)-Pb(3)-O(17')	72.5(4)
N(9)#1-Pb(1)-O(6)	80.1(3)	O(17)-Pb(3)-O(17')	34.4(5)
O(1W)-Pb(2)-N(2)	77.6(2)	N(04)-Pb(3)-O(17')	69.0(5)
O(1W)-Pb(2)-N(3)	85.1(3)	N(6)-Pb(3)-O(17')	97.0(5)
N(2)-Pb(2)-N(3)	64.9(3)	N(4)-Pb(3)-O(3)	69.8(2)
O(1W)-Pb(2)-N(1)	82.2(3)	O(17)-Pb(3)-O(3)	143.9(3)
N(2)-Pb(2)-N(1)	65.4(3)	N(04)-Pb(3)-O(3)	71.9(2)
N(3)-Pb(2)-N(1)	130.2(3)	N(6)-Pb(3)-O(3)	89.8(3)
O(1W)-Pb(2)-O(7)	147.8(2)	O(17')-Pb(3)-O(3)	134.1(4)
N(2)-Pb(2)-O(7)	70.7(2)	N(3)-Pb(2)-O(7)	87.1(2)

[a]Symmetry transformations used to generate equivalentatoms: #1 –x + 2, -y - 1, -z + 3 for complex **1**; #1 x - 1/2, -y + 1/2, z - 1/2, #2 –x + 1, y, -z + 3/2, #3 x + 1/2, -y + 1/2, z + 1/2, #4 –x + 1, y, -z + 1/2 for complex **2**; #1 –x + 2, -y + 3, -z + 3 for complex **3**; #1 –x - 1/2, -y + 3/2, -z + 2, #2 -x, y ,-z + 5/2 for complex **4**; #1 x - 1, y - 1, z, #2 x + 1, y + 1, z for complex **5**.

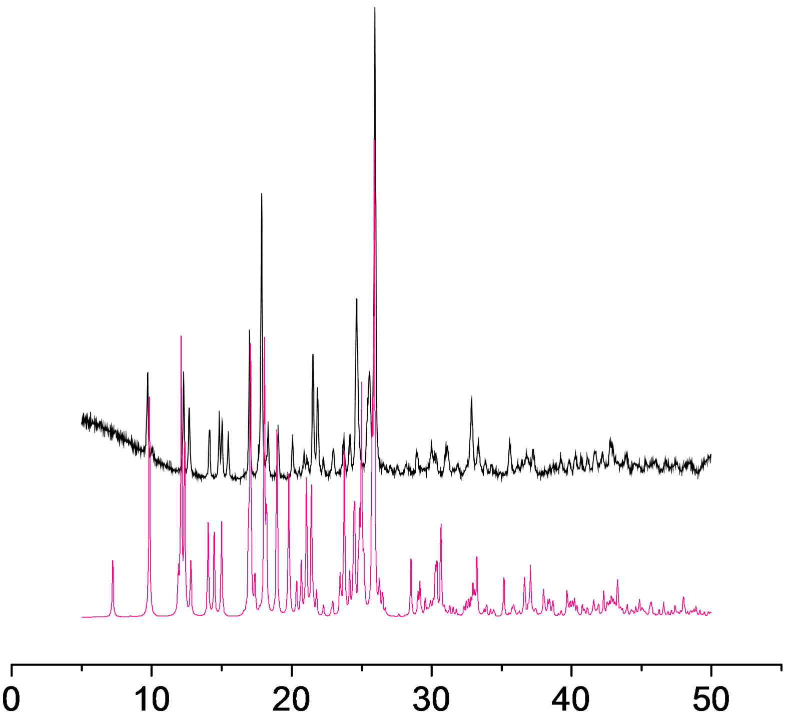

Fig. S1 The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of complex **1**

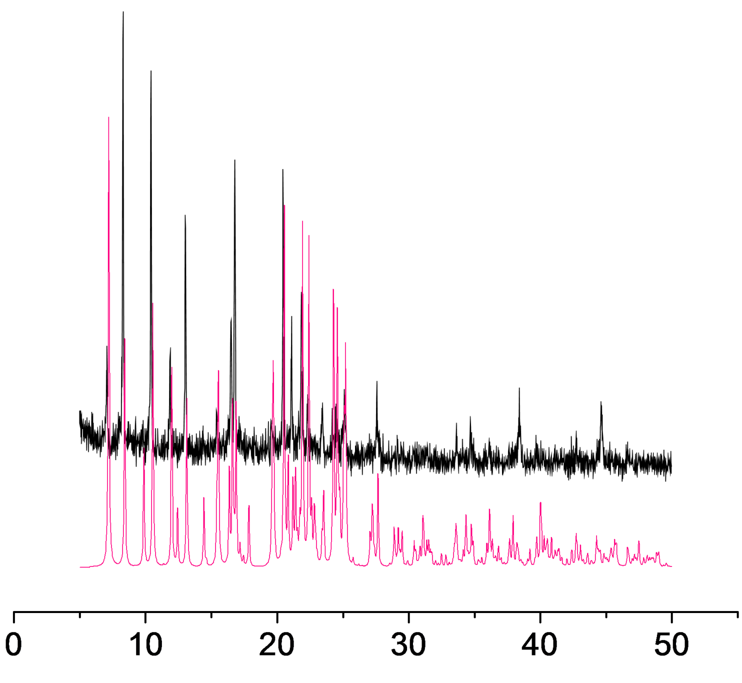

Fig. S2 The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of complex **2**

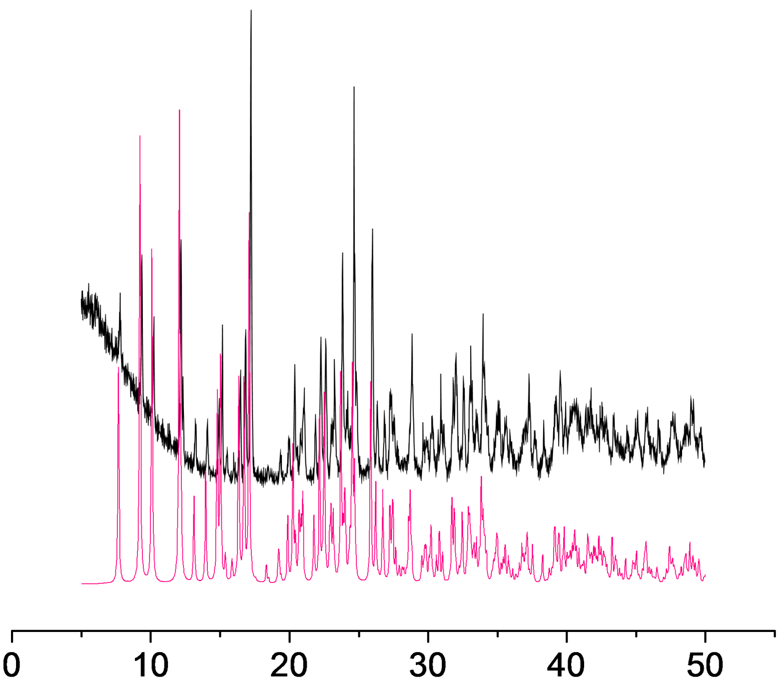

Fig. S3 The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of complex **3**

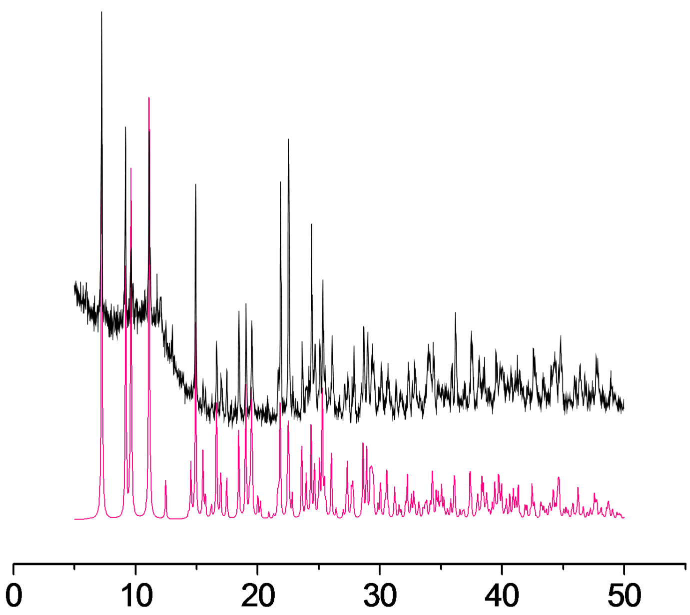

Fig. S4 The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of complex **4**

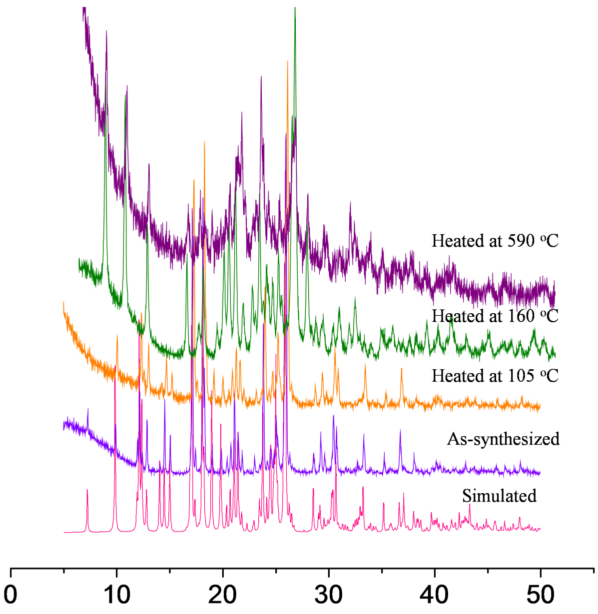

Fig. S5 The X-ray powder diffraction patterns of simulated, as-synthesized, and after heated at certain temperature of complex **1**.

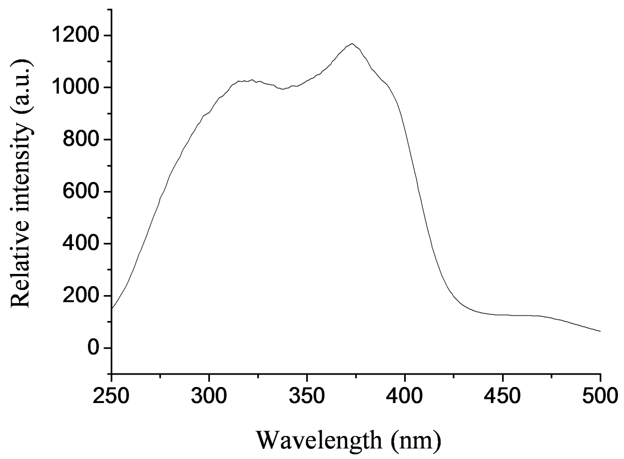

Fig. S6 Solid-state emission spectrum for H_2DSPT in the solid state at room temperature (fixing the emission wavelength at 518 nm).

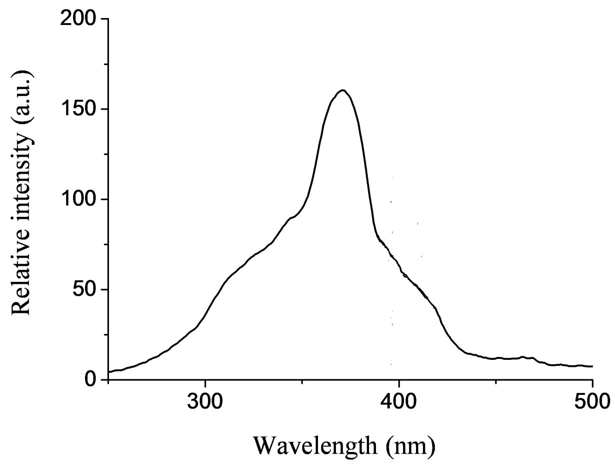

Fig. S7 Solid-state emission spectrum for complex **1** in the solid state at room temperature (fixing the emission wavelength at 520 nm).

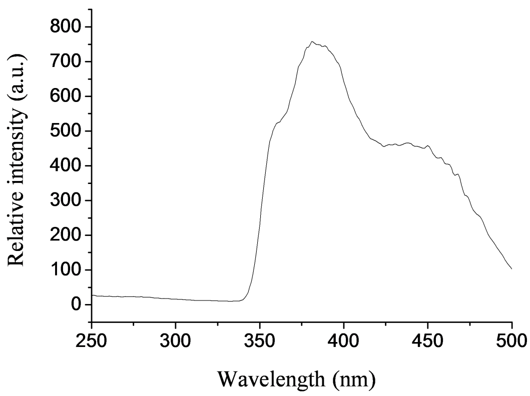

Fig. S8 Solid-state emission spectrum for complex **2** in the solid state at room temperature (fixing the emission wavelength at 514 nm).

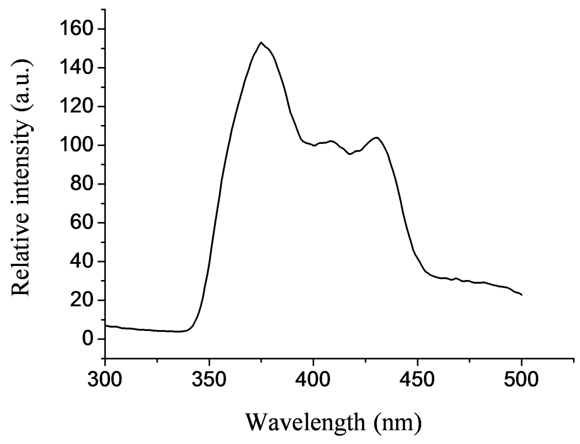

Fig. S9 Solid-state emission spectrum for complex **3** in the solid state at room temperature (fixing the emission wavelength at 548 nm).

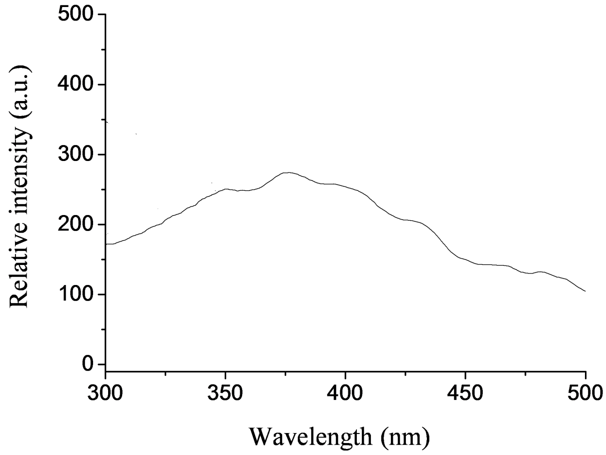

Fig. S10 Solid-state emission spectrum for complex **4** in the solid state at room temperature (fixing the emission wavelength at 545 nm).

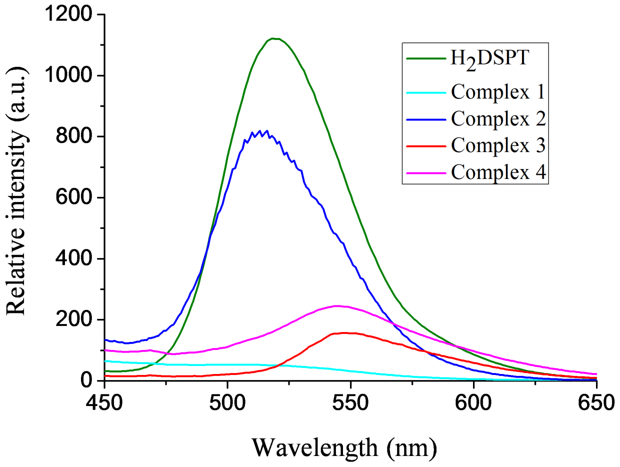

Fig. S11 Solid-state emission spectrum for H_2DSPT and **1-4** in the solid state at room temperature (excited at 373 nm).