Supporting Information

Combined influence of hydrogen bonds and π-π interactions in the assembly of five manganese coordination polymers with magnetic properties

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Outlines

Table S1 Selected bond distances (Å) and bond angles (°).

Compound **1**			
Mn(1)-O(16)	2.114(3)	Mn(1)-O(1W)	2.131(3)
Mn(1)-O(2W)	2.170(3)	Mn(1)-O(7)	2.177(3)
Mn(1)-O(2)	2.204(3)	Mn(1)-O(1)	2.510(3)
Mn(2)-O(14)#1	2.100(2)	Mn(2)-O(9)#2	2.162(2)
Mn(2)-O(4)#3	2.169(2)	Mn(2)-O(6)	2.194(2)
Mn(2)-O(1)	2.247(2)	Mn(3)-O(3)#3	2.118(3)
Mn(3)-O(8)#2	2.121(3)	Mn(3)-O(13)#1	2.186(3)
Mn(3)-O(11)	2.198(2)	Mn(3)-O(5)	2.266(2)
Mn(3)-O(12)	2.398(3)	O(3)-Mn(3)#4	2.118(3)
O(8)-Mn(3)#1	2.121(3)	O(4)-Mn(2)#4	2.169(2)
O(9)-Mn(2)#1	2.165(2)	O(13)-Mn(3)#2	2.186(3)
O(14)-Mn(2)#2	2.100(2)		
O(16)-Mn(1)-O(1W)	83.52(12)	O(16)-Mn(1)-O(2W)	167.07(12)
O(1W)-Mn(1)-O(2W)	83.66(11)	O(16)-Mn(1)-O(7)	94.52(10)
O(1W)-Mn(1)-O(7)	116.71(13)	O(2W)-Mn(1)-O(7)	89.69(10)
O(16)-Mn(1)-O(2)	98.34(11)	O(1W)-Mn(1)-O(2)	112.15(13)
O(7)-Mn(1)-O(2)	130.49(10)	O(2W)-Mn(1)-O(2)	88.11(11)
O(16)-Mn(1)-O(1)	108.79(11)	O(1W)-Mn(1)-O(1)	162.69(11)
O(7)-Mn(1)-O(1)	75.39(9)	O(2W)-Mn(1)-O(1)	84.11(10)
O(14)#1-Mn(2)-O(9)#2	123.34(10)	O(2)-Mn(1)-O(1)	55.18(9)
O(14)#1-Mn(2)-O(4)#3	93.32(10)	O(14)#1-Mn(2)-O(6)	95.21(11)
O(9)#2-Mn(2)-O(4)#3	94.00(10)	O(9)#2-Mn(2)-O(6)	141.38(11)
O(4)#3-Mn(2)-O(6)	85.21(10)	O(14)#1-Mn(2)-O(1)	90.99(10)
O(9)#2-Mn(2)-O(1)	86.50(10)	O(4)#3-Mn(2)-O(1)	174.47(10)
O(6)-Mn(2)-O(1)	90.99(10)	O(3)#3-Mn(3)-O(8)#2	93.44(11)
O(3)#3-Mn(3)-O(13)#1	84.81(11)	O(8)#2-Mn(3)-O(13)#1	135.75(10)
O(3)#3-Mn(3)-O(11)	106.11(12)	O(8)#2-Mn(3)-O(11)	134.76(11)
O(13)#1-Mn(3)-O(11)	87.25(10)	O(3)#3-Mn(3)-O(5)	157.27(10)
O(8)#2-Mn(3)-O(5)	84.01(10)	O(13)#1-Mn(3)-O(5)	81.47(10)
O(11)-Mn(3)-O(5)	91.28(11)	O(3)#3-Mn(3)-O(12)	92.79(11)
O(8)#2-Mn(3)-O(12)	82.70()	O(13)#1-Mn(3)-O(12)	141.52(10)
O(11)-Mn(3)-O(12)	56.51(10)	O(5)-Mn(3)-O(12)	109.20(11)
Mn(2)-O(1)-Mn(1)	102.75(9)		
Compound **2**			
Mn(1)-O(1)	2.185(2)	Mn(1)-O(1W)	2.198(2)
Mn(1)-O(4)#1	2.203(3)	Mn(1)-N(2)	2.259(3)
Mn(1)-N(1)	2.282(3)	Mn(1)-O(3)#1	2.450(3)
Mn(1)-O(2)	2.488(2)	O(4)-Mn(1)#2	2.203(3)

O(3)-Mn(1)#2	2.450(3)		
O(1)-Mn(1)-O(1W)	100.86(10)	O(1)-Mn(1)-O(4)#1	81.06(10)
O(1W)-Mn(1)-O(4)#1	91.71(11)	O(1)-Mn(1)-N(2)	138.13(11)
O(1W)-Mn(1)-N(2)	92.01(10)	O(4)#1-Mn(1)-N(2)	138.67(11)
O(1)-Mn(1)-N(1)	93.67(11)	O(1W)-Mn(1)-N(1)	163.45(10)
O(4)#1-Mn(1)-N(1)	98.39(12)	N(2)-Mn(1)-N(1)	71.76(11)
O(1)-Mn(1)-O(3)#1	136.21(10)	O(1W)-Mn(1)-O(3)#1	84.74(10)
O(4)#1-Mn(1)-O(3)#1	55.24(10)	N(2)-Mn(1)-O(3)#1	84.18(11)
N(1)-Mn(1)-O(3)#1	90.26(11)	O(1)-Mn(1)-O(2)	55.37(8)
O(1W)-Mn(1)-O(2)	84.36(9)	O(4)#1-Mn(1)-O(2)	134.26(9)
N(2)-Mn(1)-O(2)	87.07(10)	N(1)-Mn(1)-O(2)	97.66(10)

Compound **3**

Mn(1)-O(1)	2.076(3)	Mn(1)-O(4)#1	2.083(2)
Mn(1)-O(1W)	2.108(2)	Mn(1)-N(2)	2.251(3)
Mn(1)-N(1)	2.263(3)	O(4)-Mn(1)#2	2.083(2)
O(1)-Mn(1)-O(4)#1	95.23(10)	O(1)-Mn(1)-O(1W)	138.04(11)
O(4)#1-Mn(1)-O(1W)	97.32(10)	O(1)-Mn(1)-N(2)	115.76(11)
O(4)#1-Mn(1)-N(2)	88.09(10)	O(1)-Mn(1)-N(1)	93.93(11)
O(1W)-Mn(1)-N(2)	104.55(9)	O(4)#1-Mn(1)-N(1)	161.61(11)
O(1W)-Mn(1)-N(1)	86.35(10)	N(2)-Mn(1)-N(1)	73.57(10)

Compound **4**

Mn(1)-O(1W)	2.1619(13)	Mn(1)-O(2W)	2.2038(13)
Mn(1)-O(1)	2.2079(12)	Mn(1)-N(1)	2.2404(13)
Mn(1)-O(4)#1	2.2484(12)	Mn(1)-O(3)#1	2.4779(15)
O(3)-Mn(1)#2	2.4779(15)	O(4)-Mn(1)#2	2.2484(12)
O(1W)-Mn(1)-O(2W)	172.65(5)	O(1W)-Mn(1)-O(1)	97.82(5)
O(2W)-Mn(1)-O(1)	88.78(5)	O(1W)-Mn(1)-N(1)	92.32(5)
O(2W)-Mn(1)-N(1)	85.10(5)	O(1)-Mn(1)-N(1)	135.89(5)
O(1W)-Mn(1)-O(4)#1	85.70(5)	O(2W)-Mn(1)-O(4)#1	91.83(5)
O(1)-Mn(1)-O(4)#1	83.82(5)	N(1)-Mn(1)-O(4)#1	139.92(5)
O(1W)-Mn(1)-O(3)#1	89.82(5)	O(2W)-Mn(1)-O(3)#1	83.11(5)
O(1)-Mn(1)-O(3)#1	137.23(4)	N(1)-Mn(1)-O(3)#1	85.27(5)
O(4)#1-Mn(1)-O(3)#1	54.73(4)		

Compound **5**

Mn(1)-O(2)	2.1805(15)	Mn(1)-N(1)	2.1867(18)
Mn(1)-O(4)#1	2.2974(15)	Mn(1)-O(4)#2	2.2999(15)
Mn(1)-O(5)#3	2.3061(15)	Mn(1)-O(1)	2.4027(16)
Mn(1)-O(3)#2	2.4379(17)	O(3)-Mn(1)#4	2.4379(17)
O(4)-Mn(1)#1	2.2974(15)	O(4)-Mn(1)#4	2.2999(15)

O(5)-Mn(1)#5	2.3061(15)		
O(2)-Mn(1)-N(1)	145.58(6)	O(2)-Mn(1)-O(4)#1	88.94(6)
N(1)-Mn(1)-O(4)#1	81.01(6)	O(2)-Mn(1)-O(4)#2	82.72(6)
N(1)-Mn(1)-O(4)#2	127.61(6)	O(4)#1-Mn(1)-O(4)#2	82.03(6)
O(2)-Mn(1)-O(5)#3	97.26(6)	N(1)-Mn(1)-O(5)#3	87.10(6)
O(4)#1-Mn(1)-O(5)#3	166.36(5)	O(4)#2-Mn(1)-O(5)#3	110.73(5)
O(2)-Mn(1)-O(1)	56.87(5)	N(1)-Mn(1)-O(1)	89.50(6)
O(4)#1-Mn(1)-O(1)	86.20(6)	O(4)#2-Mn(1)-O(1)	138.08(5)
O(5)#3-Mn(1)-O(1)	87.05(6)	O(2)-Mn(1)-O(3)#2	128.88(6)
N(1)-Mn(1)-O(3)#2	85.37(6)	O(4)#1-Mn(1)-O(3)#2	109.42(6)
O(4)#2-Mn(1)-O(3)#2	55.00(5)	O(5)#3-Mn(1)-O(3)#2	76.00(6)
O(1)-Mn(1)-O(3)#2	162.50(6)	Mn(1)#1-O(4)-Mn(1)#4	97.97(6)

Symmetry codes for compounds **1-5**. For **1**, #1 x-1/2, -y-1/2, z; #2 x+1/2, -y-1/2, z; #3 x, y-1, z; #4 x, y+1, z. For **2**, #1 x, y-1, z; #2 x, y+1, z. For **3**, #1 -x+1, y+1/2, -z+3/2; #2 -x+1, y-1/2, -z+3/2. For **4**, #1 x-1, y, z; #2 x+1, y, z. For **5**, #1, -x+2, -y+2, -z+1; #2 x-1, y, z; #3 -x+3/2, y-1/2, -z+3/2; #4 x+1, y, z; #5 -x+3/2, y+1/2, -z+3/2.

Table S2 Hydrogen bond distances (Å) and bond angles (°).

Donor---H···Acceptor	d(D---H)	d(H···A)	d(D···A)	∠D---H···A
Compound **1**				
O1W---H1WA···O3W	0.86	2.03	2.730(4)	138
O2W---H2WA···O10#1	0.87	2.59	3.243(4)	133
O2W---H2WB···O9#1	0.87	1.86	2.717(4)	171
O3W---H3WA···O10#1	0.85	2.13	2.949(4)	163
O3W---H3WB···O13#2	0.85	2.06	2.882(4)	161
O17---H17···O1W#3	0.82	2.03	2.729(3)	142
C10---H10A···O10#4 (intra)	0.97	2.45	3.279(5)	143
C16---H16···O11 (intra)	0.93	2.35	3.197(5)	151
C40---H40···O15 (intra)	0.93	2.28	2.904(5)	124
Compound **2**				
O1W---H1WA···O2W#1	0.88	1.92	2.732(5)	154
O1W---H1WB···O2#1	0.88	1.99	2.781(4)	149
C6---H6···O4 (intra)	0.93	2.48	2.787(5)	100
C6---H6···O5A (intra)	0.93	2.25	2.855(10)	123
C8---H8···O5B (intra)	0.93	2.27	2.879(8)	122
Compound **3**				
O1W---H1WA···O3#1	0.88	1.78	2.613(4)	156
O1W---H1WB···O2#2	0.88	1.94	2.736(3)	149
C8---H8···O4 (intra)	0.93	2.44	2.751(4)	100
C8---H8···O5(intra)	0.93	2.25	2.857(5)	122
C17---H17···O2(intra)	0.93	2.54	3.257(5)	134
C28---H28···O4(intra)#3	0.93	2.59	3.145(4	119
Compound **4**				
O1W---H1WA···O3W	0.86	1.88	2.717(3)	162
O1W---H1WB···O2	0.86	1.95	2.716(2)	146
O2W---H2WB···O1#1	0.86	1.91	2.721(2)	155
O3W---H3WA···O3#2	0.85	1.99	2.764(3)	152
C5---H5···O5(intra)	0.93	2.35	2.893(2)	117
Compound **5**				
C8---H8···O5(intra)	0.93	2.34	2.920(3)	120
C13---H13···O2(intra)#1	0.93	2.43	3.320(3)	161

Symmetry codes for compounds **1-5**. For **1**, #1 1/2+x, -1/2-y, z; #2 -x, -y, -1/2+z; #3 -1/2-x, -1/2+y, 1/2+z; #4 -1-x, -y, 1/2+z. For **2**, #1 1-x, 2-y, 1-z. For **3**, #1 x, 1/2-y, -1/2+z; #2 1-x, 1-y, 1-z; #3 1-x, 1/2+y, 3/2-z. For **4**, #1 2-x, 2-y, -z; #2 2-x, 1-y, -z. For **5**, 3/2-x, 1/2+y, 3/2-z.

Table S3 Intermolecular π-π interaction distances (Å).

π-π interactions	**Plane A**	**Plane B**	**Distance**
Compound **1**			
Cg(A)•••Cg(B)	N2···C25···C28···C27···C26	C35···C36···C37···C38···C39··· C40	3.958(2)
Cg(A)•••Cg(B)	C19···C20···C21···C22···C23··· C24	C43···C44···C45···C46···C47··· C48	3.743(2)
Compound **2**			
Cg(A)•••Cg(B)	N3···C9···C16···C11···C10	C2···C3···C4···C6···C7··· C8	3.639(2)
Cg(A)•••Cg(B)	N3···C9···C16···C11···C10	C11···C12···C13···C14···C15··· C16	3.480(3)
Cg(A)•••Cg(B)	N2···C22···C23···C24···C25···C26	N2···C22···C23···C24···C25···C26	3.612(3)
Cg(A)•••Cg(B)	C2···C3···C4···C6···C7··· C8	C11···C12···C13···C14···C15··· C16	3.560(3)
Compound **5**			
Cg(A)•••Cg(B)	N2···C9···C12···C11···C10	C11···C12···C13···C14···C15··· C16	3.7515(14)
Cg(A)•••Cg(B)	C2···C3···C4···C6···C7··· C8	C11···C12···C13···C14···C15··· C16	3.8909(13)

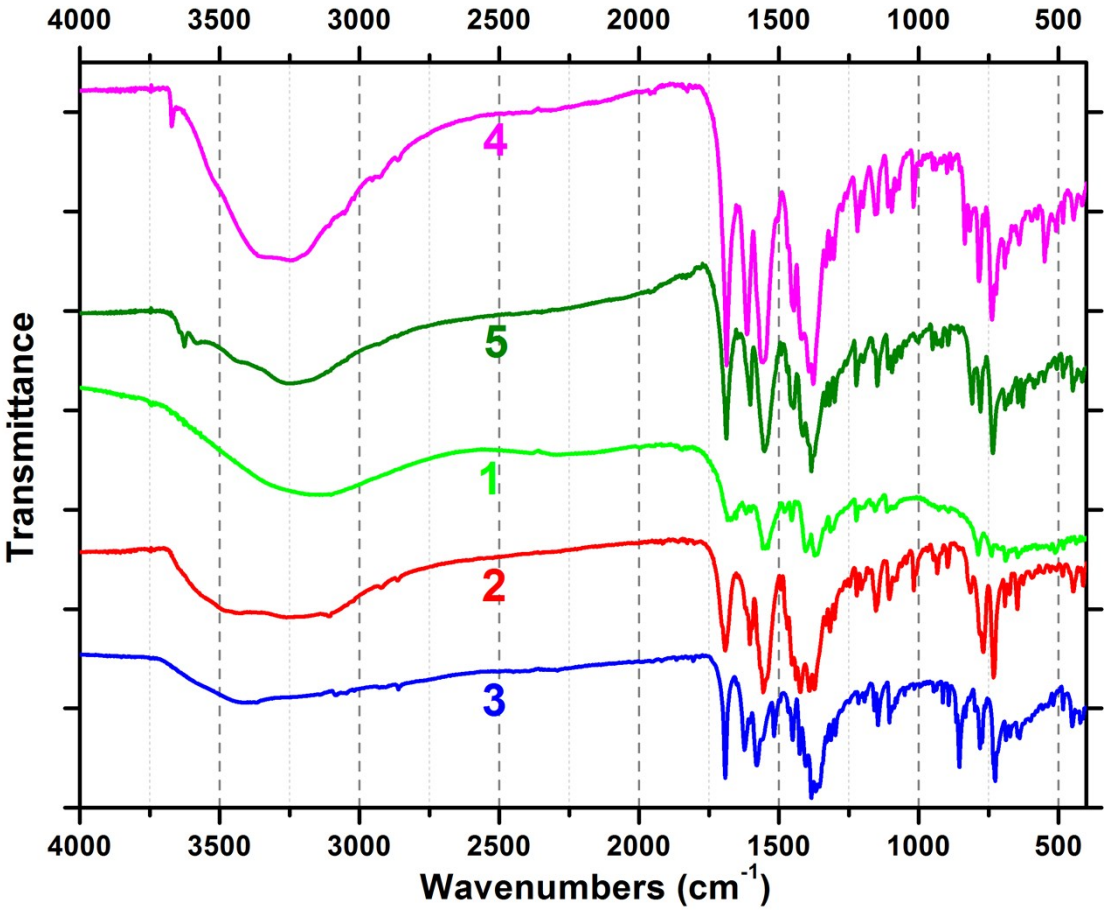

Fig. S1 The FT-IR spectra of **1-5**.

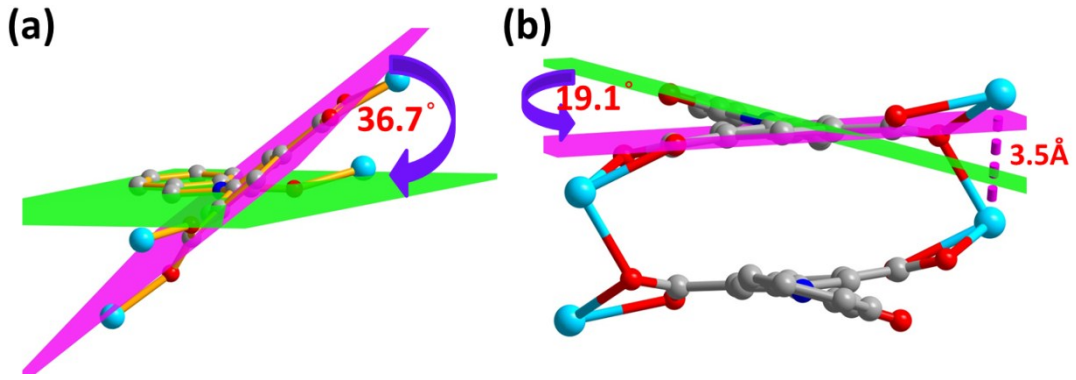

Fig. S2 The torsion angle in $IDPA^{2-}$ ligand between the pink plane of C3···C4···C5···C6···C7···C8 and the green plane of N1···C9···C11···C12···C10. (a) for compound **1** and (b) for compound **5**.

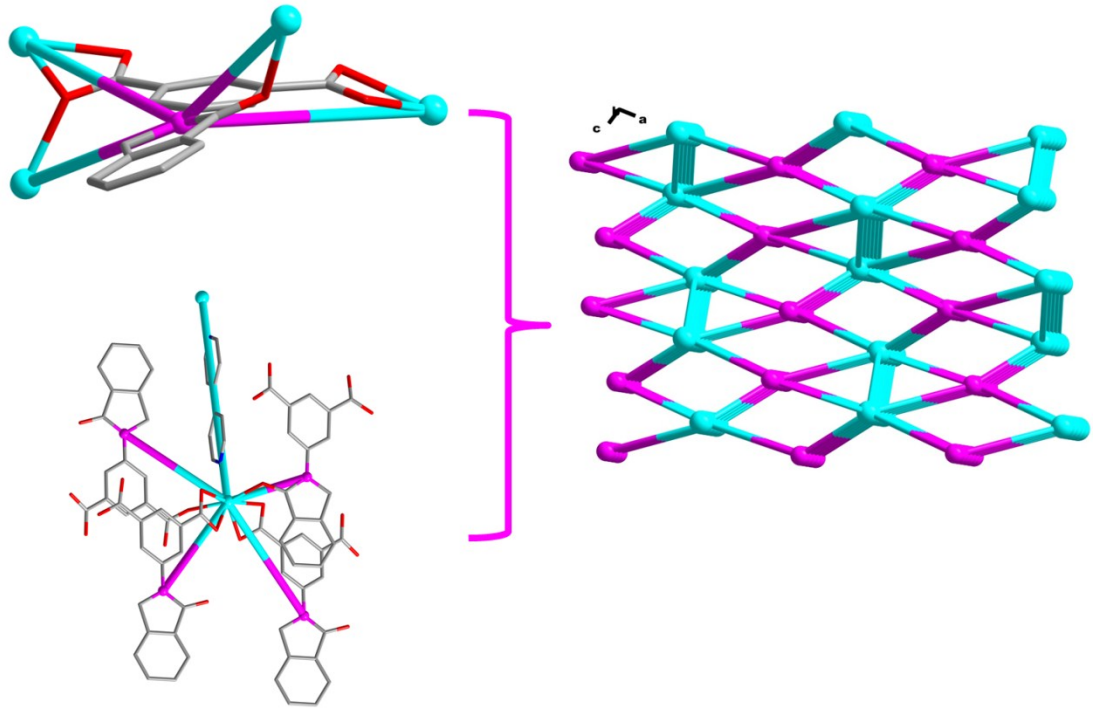

Fig. S3 Schematic representation of a binodal (4,5)-connected topology of **5** (the pink atom represents for H_2IDPA ligand and turquoise atom represents for Mn(II) ion).

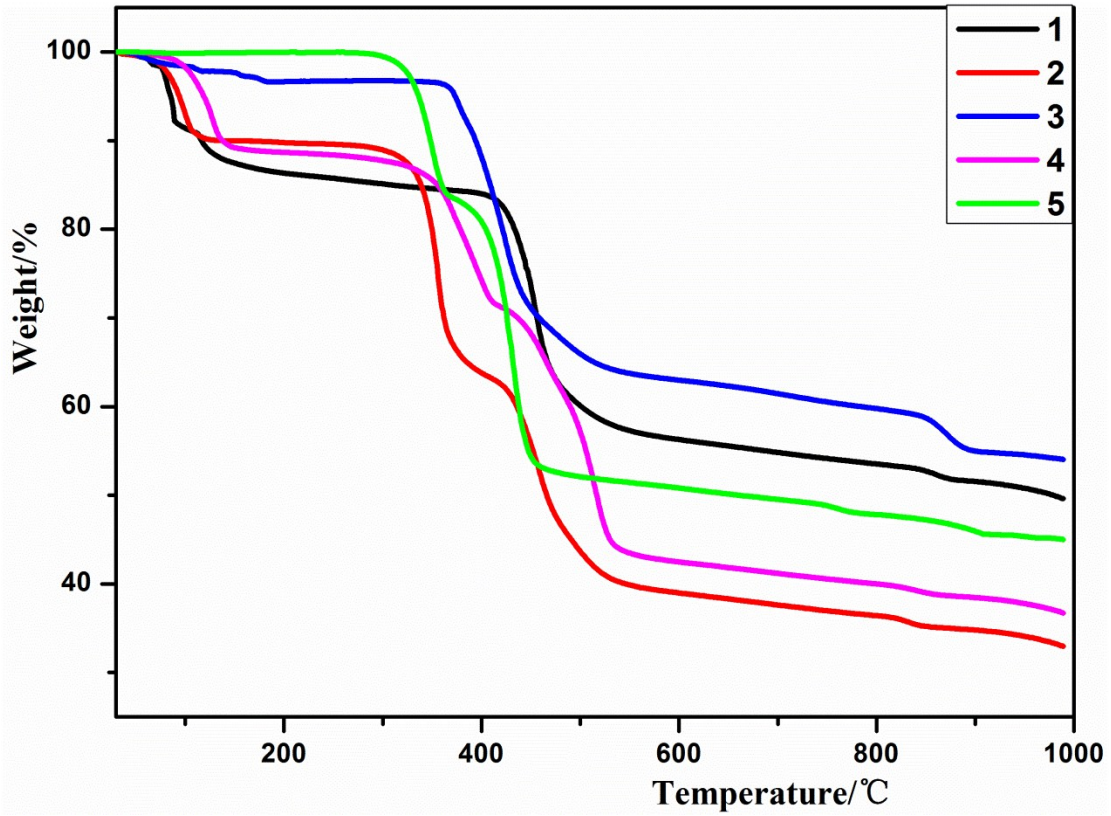

Fig. S4 The TGA curves for compounds **1–5**.

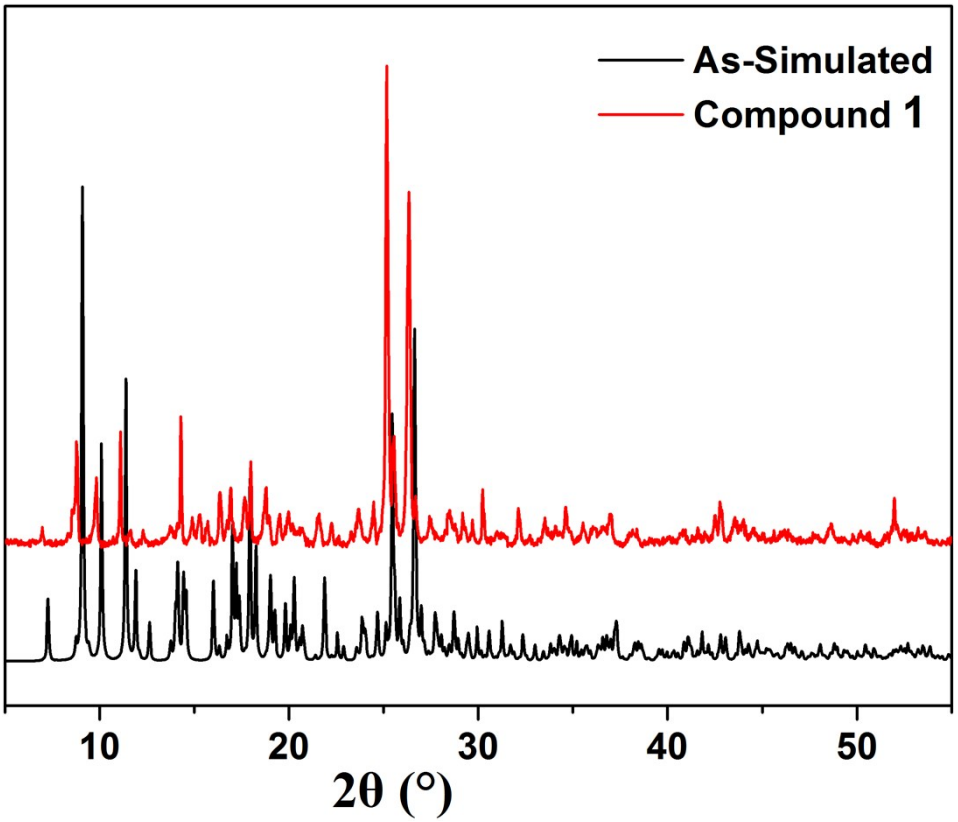

Fig. S5 The Powder X-ray diffraction (PXRD) patterns of **1** at room temperature.

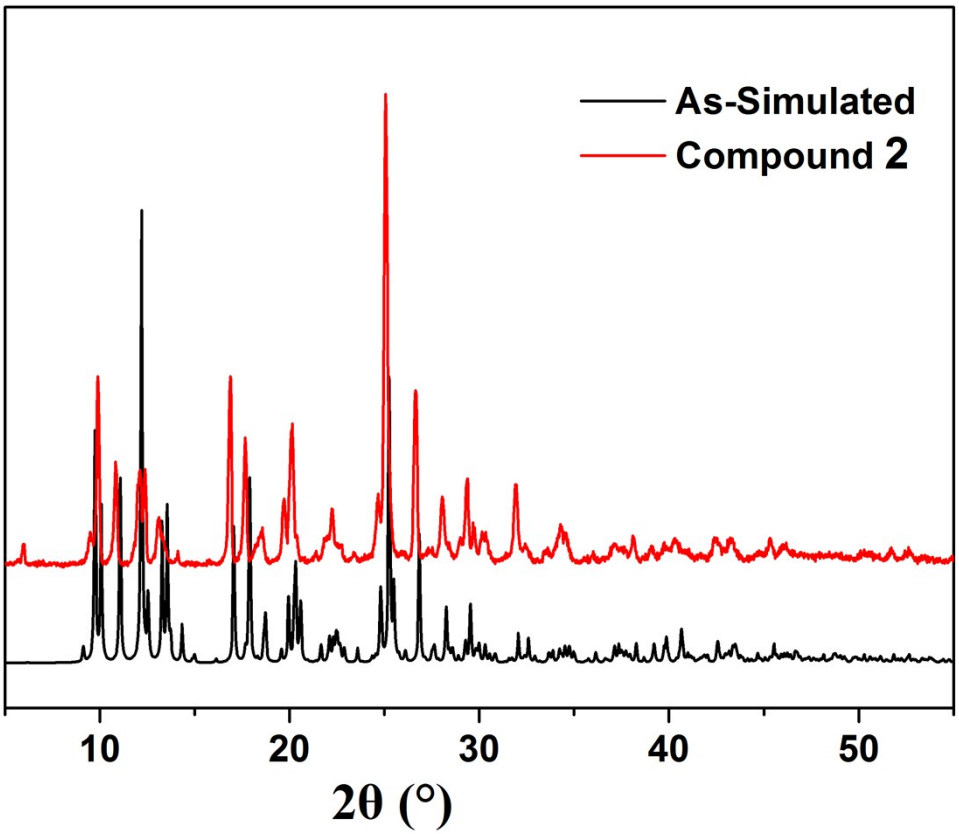

Fig. S6 The PXRD patterns of **2** at room temperature.

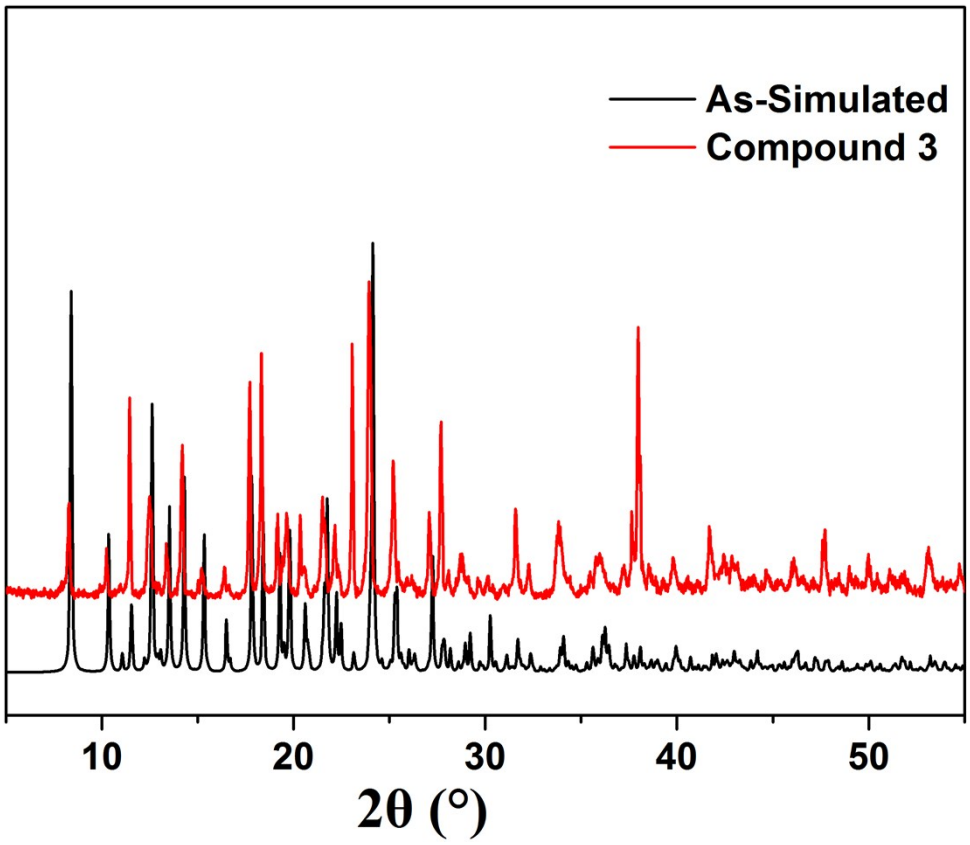

Fig. S7 The PXRD patterns of **3** at room temperature.

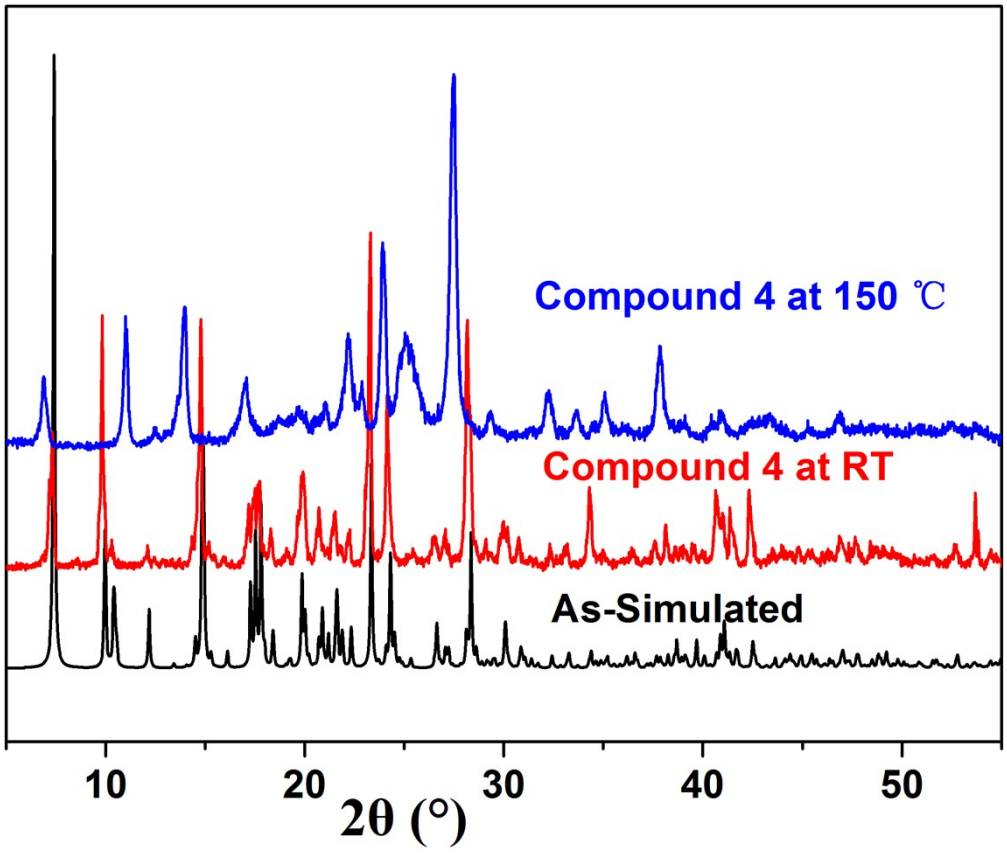

Fig. S8 The PXRD patterns of **4** at room temperature and 150 °C.

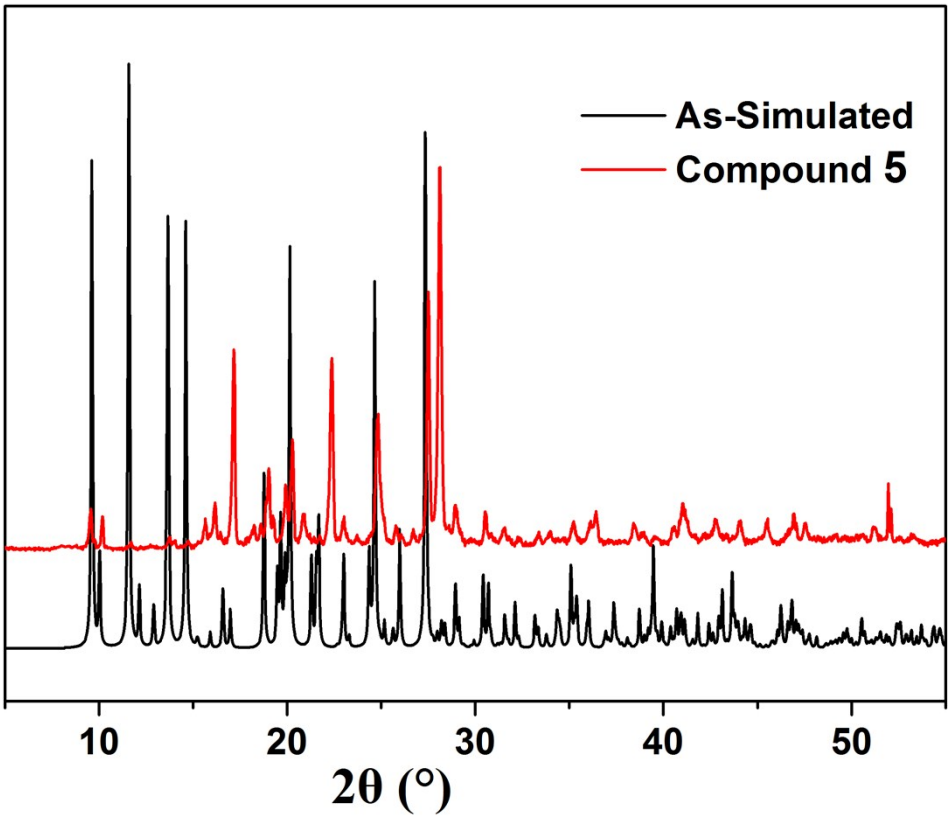

Fig. S9 The PXRD patterns of **5** at room temperature.

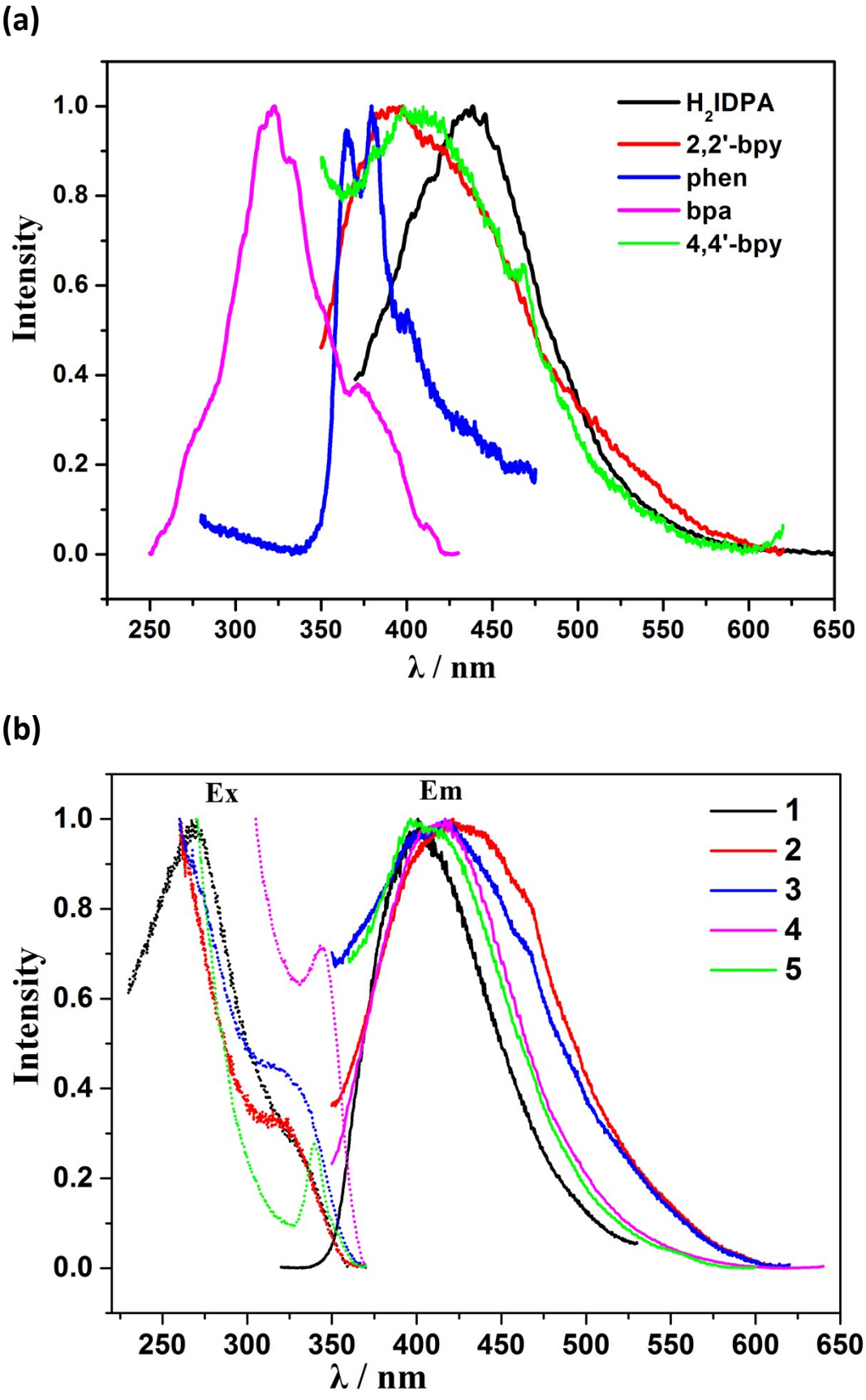

Fig. S10 (a) The emission spectra of organic ligands. (b) The excitation spectra (left) and emission spectra (right) of **1-5** in the solid state at room temperature.