Supplementary Material (ESI) for CrystEngComm

Syntheses, structures and photoluminescent properties of a series of metal-organic frameworks based on a flexible tetracarboxylic acid and different bis(imidazole) Ligands

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

Co(1)-O(9)#1	1.981(4)	Co(1)-O(7)#2	2.000(4)
Co(1)-O(1)	2.085(4)	Co(1)-O(4)#3	2.097(4)
Co(1)-O(2)	2.273(5)	Co(1)-O(3)#3	2.313(4)
Co(2)-O(10)#4	2.056(5)	Co(2)-O(8)	2.073(4)
Co(2)-O(2W)	2.083(4)	Co(2)-O(1W)	2.092(5)
Co(2)-O(3W)	2.094(5)	Co(2)-O(4)#5	2.182(3)
O(9)#1-Co(1)-O(7)#2	101.25(17)	O(9)#1-Co(1)-O(1)	143.58(18)
O(7)#2-Co(1)-O(1)	97.31(17)	O(9)#1-Co(1)-O(4)#3	106.89(16)
O(7)#2-Co(1)-O(4)#3	102.26(16)	O(1)-Co(1)-O(4)#3	99.31(18)
O(9)#1-Co(1)-O(2)	90.25(18)	O(7)#2-Co(1)-O(2)	91.37(17)
O(1)-Co(1)-O(2)	58.08(19)	O(4)#3-Co(1)-O(2)	155.26(16)
O(9)#1-Co(1)-O(3)#3	88.50(17)	O(7)#2-Co(1)-O(3)#3	160.65(18)
O(1)-Co(1)-O(3)#3	83.90(16)	O(4)#3-Co(1)-O(3)#3	58.64(15)
O(2)-Co(1)-O(3)#3	105.40(16)	O(10)#4-Co(2)-O(8)	98.25(17)
O(10)#4-Co(2)-O(2W)	84.40(18)	O(8)-Co(2)-O(2W)	91.60(16)
O(10)#4-Co(2)-O(1W)	174.81(17)	O(8)-Co(2)-O(1W)	85.66(17)
O(2W)-Co(2)-O(1W)	92.11(17)	O(10)#4-Co(2)-O(3W)	88.90(19)
O(8)-Co(2)-O(3W)	172.8(2)	O(2W)-Co(2)-O(3W)	89.95(17)
O(1W)-Co(2)-O(3W)	87.25(19)	O(10)#4-Co(2)-O(4)#5	94.66(15)
O(8)-Co(2)-O(4)#5	86.85(14)	O(2W)-Co(2)-O(4)#5	178.06(17)
O(1W)-Co(2)-O(4)#5	88.94(16)	O(3W)-Co(2)-O(4)#5	91.74(15)

Symmetry codes for **1**: #1 -x+3/2, y-1/2, -z+3/2; #2 x-1, y, z-1; #3 -x+3/2, y-1/2,

-z+1/2; #4 -x+5/2, y-1/2, -z+5/2; #5 -x+5/2, y-1/2, -z+3/2.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Co(1)-O(3)#1	1.957(2)	Co(1)-O(1)	2.000(3)
Co(1)-N(4)	2.006(3)	Co(1)-N(1)#2	2.035(3)
O(3)#1-Co(1)-O(1)	107.02(11)	O(3)#1-Co(1)-N(4)	107.71(11)
O(1)-Co(1)-N(4)	120.64(12)	O(3)#1-Co(1)-N(1)#2	95.53(12)
O(1)-Co(1)-N(1)#2	111.37(12)	N(4)-Co(1)-N(1)#2	111.38(12)

Symmetry codes for **2**: #1 x-1/2, -y+1/2, z-1/2; #2 -x+5/2, y+1/2, -z+1/2.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Co(1)-O(3)#1	1.9556(18)	Co(1)-O(1)	1.9951(19)
Co(1)-N(4)	2.012(2)	Co(1)-N(1)#2	2.025(3)
O(3)#1-Co(1)-O(1)	106.35(8)	O(3)#1-Co(1)-N(4)	109.48(8)
O(1)-Co(1)-N(4)	118.64(9)	O(3)#1-Co(1)-N(1)#2	95.47(9)
O(1)-Co(1)-N(1)#2	115.94(9)	N(4)-Co(1)-N(1)#2	108.29(10)

Symmetry codes for **3**: #1 x+1/2, -y+1/2, z+1/2; #2 -x-1/2, y+1/2, -z+1/2.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Co(1)-O(1)	1.9638(17)	Co(1)-O(4)#1	1.985(2)
Co(1)-N(4)	2.012(2)	Co(1)-N(1)#2	2.033(2)
O(1)-Co(1)-O(4)#1	107.15(8)	O(1)-Co(1)-N(4)	108.20(9)
O(4)#1-Co(1)-N(4)	120.10(10)	O(1)-Co(1)-N(1)#2	96.58(9)
O(4)#1-Co(1)-N(1)#2	115.11(9)	N(4)-Co(1)-N(1)#2	106.95(10)

Symmetry codes for **4**: #1 x-1/2, -y+1/2, z-1/2; #2 -x-1/2, y+1/2, -z+1/2.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Co(1)-O(3)	2.010(3)	Co(1)-O(4)#1	2.036(3)
Co(1)-N(1)	2.042(3)	Co(1)-O(10)#2	2.045(3)
Co(1)-O(9)#3	2.251(2)	Co(1)-O(9)#2	2.400(3)
Co(2)-N(4)	2.029(5)	Co(2)-N(5)	2.052(4)
Co(2)-O(6)#4	2.055(3)	Co(2)-O(11)#5	2.101(2)

Co(2)-O(12)#5	2.218(3)	Co(2)-O(5)#4	2.369(3)
O(3)-Co(1)-O(4)#1	159.46(9)	O(3)-Co(1)-N(1)	98.87(11)
O(4)#1-Co(1)-N(1)	95.37(11)	O(3)-Co(1)-O(10)#2	95.55(11)
O(4)#1-Co(1)-O(10)#2	94.28(11)	N(1)-Co(1)-O(10)#2	107.21(11)
O(3)-Co(1)-O(9)#3	83.09(11)	O(4)#1-Co(1)-O(9)#3	81.59(10)
N(1)-Co(1)-O(9)#3	92.41(11)	O(10)#2-Co(1)-O(9)#3	160.27(10)
O(3)-Co(1)-O(9)#2	83.47(10)	O(4)#1-Co(1)-O(9)#2	86.35(10)
N(1)-Co(1)-O(9)#2	165.79(10)	O(10)#2-Co(1)-O(9)#2	58.57(9)
O(9)#3-Co(1)-O(9)#2	101.80(8)	N(4)-Co(2)-N(5)	100.04(19)
N(4)-Co(2)-O(6)#4	96.65(18)	N(5)-Co(2)-O(6)#4	95.97(15)
N(4)-Co(2)-O(11)#5	102.08(17)	N(5)-Co(2)-O(11)#5	105.36(13)
O(6)#4-Co(2)-O(11)#5	148.45(13)	N(4)-Co(2)-O(12)#5	161.71(18)
N(5)-Co(2)-O(12)#5	90.70(14)	O(6)#4-Co(2)-O(12)#5	96.90(13)
O(11)#5-Co(2)-O(12)#5	60.51(9)	N(4)-Co(2)-O(5)#4	90.72(15)
N(5)-Co(2)-O(5)#4	152.96(14)	O(6)#4-Co(2)-O(5)#4	57.92(12)
O(11)#5-Co(2)-O(5)#4	96.39(11)	O(12)#5-Co(2)-O(5)#4	86.13(11)

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

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Co(1)-O(1)	1.965(3)	Co(1)-O(4)#1	2.041(3)
Co(1)-N(4)	2.052(4)	Co(1)-N(5)	2.052(4)
Co(1)-O(3)#1	2.354(4)	Co(2)-O(8)#2	1.980(3)
Co(2)-N(8)	2.035(4)	Co(2)-N(1)#3	2.067(4)
Co(2)-N(1)#3	2.067(4)	Co(2)-O(9)#4	2.131(3)
Co(2)-O(10)#4	2.245(4)		
O(1)-Co(1)-O(4)#1	133.35(15)	O(1)-Co(1)-N(4)	112.09(18)
O(4)#1-Co(1)-N(4)	106.00(17)	O(1)-Co(1)-N(5)	99.21(17)
O(4)#1-Co(1)-N(5)	99.00(18)	N(4)-Co(1)-N(5)	100.91(17)
O(1)-Co(1)-O(3)#1	92.44(14)	O(4)#1-Co(1)-O(3)#1	58.98(13)

N(4)-Co(1)-O(3)#1	93.14(16)	N(5)-Co(1)-O(3)#1	156.73(16)
O(8)#2-Co(2)-N(8)	106.10(17)	O(8)#2-Co(2)-N(1)#3	103.90(17)
N(8)-Co(2)-N(1)#3	102.83(17)	O(8)#2-Co(2)-O(9)#4	140.98(15)
N(8)-Co(2)-O(9)#4	99.68(16)	N(1)#3-Co(2)-O(9)#4	98.20(17)
O(8)#2-Co(2)-O(10)#4	89.36(15)	N(8)-Co(2)-O(10)#4	94.56(17)
N(1)#3-Co(2)-O(10)#4	154.01(16)	O(9)#4-Co(2)-O(10)#4	59.46(14)

Symmetry codes for **6**: #1 x-1/2, -y-3/2, z; #2 x-1/2, -y-1/2, z-1; #3 x, y+1, z; #4 x, y, z-1.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Ni(1)-O(1)	1.992(3)	Ni(1)-N(5)	2.042(4)
Ni(1)-O(3)#1	2.051(3)	Ni(1)-N(4)	2.060(4)
Ni(1)-N(1)#2	2.103(4)		
O(1)-Ni(1)-N(5)	105.35(16)	O(1)-Ni(1)-O(3)#1	160.07(16)
N(5)-Ni(1)-O(3)#1	94.18(16)	O(1)-Ni(1)-N(4)	90.51(14)
N(5)-Ni(1)-N(4)	97.78(16)	O(3)#1-Ni(1)-N(4)	90.73(14)
O(1)-Ni(1)-N(1)#2	84.96(14)	N(5)-Ni(1)-N(1)#2	92.01(17)
O(3)#1-Ni(1)-N(1)#2	90.53(14)	N(4)-Ni(1)-N(1)#2	170.01(17)

Symmetry codes for **7**: #1 x, y-1, z; #2 x, y, z+1.

Table S8. Selected bond distances (Å) and angles (°) for **8**.

Ni(1)-N(4)	2.035(5)	Ni(1)-N(5)	2.043(5)
Ni(1)-O(9)#1	2.083(3)	Ni(1)-O(3)#2	2.120(3)
Ni(1)-O(4)#2	2.132(4)	Ni(1)-O(10)#1	2.188(4)
Ni(2)-N(1)#3	2.009(6)	Ni(2)-N(8)	2.042(5)
Ni(2)-O(8)#4	2.072(3)	Ni(2)-O(1)	2.086(3)
Ni(2)-O(7)#4	2.160(4)	Ni(2)-O(2)	2.180(4)
N(4)-Ni(1)-N(5)	93.51(19)	N(4)-Ni(1)-O(9)#1	90.74(17)
N(5)-Ni(1)-O(9)#1	102.25(17)	N(4)-Ni(1)-O(3)#2	100.68(18)
N(5)-Ni(1)-O(3)#2	94.48(17)	O(9)#1-Ni(1)-O(3)#2	159.14(15)
N(4)-Ni(1)-O(4)#2	162.66(17)	N(5)-Ni(1)-O(4)#2	89.68(17)
O(9)#1-Ni(1)-O(4)#2	105.25(14)	O(3)#2-Ni(1)-O(4)#2	62.05(14)

N(4)-Ni(1)-O(10)#1	90.73(16)	N(5)-Ni(1)-O(10)#1	163.43(16)
O(9)#1-Ni(1)-O(10)#1	61.65(13)	O(3)#2-Ni(1)-O(10)#1	100.46(14)
O(4)#2-Ni(1)-O(10)#1	91.02(14)	N(1)#3-Ni(2)-N(8)	100.3(2)
N(1)#3-Ni(2)-O(8)#4	97.36(19)	N(8)-Ni(2)-O(8)#4	95.14(17)
N(1)#3-Ni(2)-O(1)	95.9(2)	N(8)-Ni(2)-O(1)	98.50(18)
O(8)#4-Ni(2)-O(1)	158.94(17)	N(1)#3-Ni(2)-O(7)#4	89.17(19)
N(8)-Ni(2)-O(7)#4	156.29(18)	O(8)#4-Ni(2)-O(7)#4	61.89(14)
O(1)-Ni(2)-O(7)#4	102.12(16)	N(1)#3-Ni(2)-O(2)	156.65(19)
N(8)-Ni(2)-O(2)	89.07(19)	O(8)#4-Ni(2)-O(2)	103.10(15)
O(1)-Ni(2)-O(2)	61.34(15)	O(7)#4-Ni(2)-O(2)	90.60(15)

Symmetry codes for **8**: #1 -x+1, -y+1, -z+2; #2 x, y-1, z; #3 x-1/2, -y+3/2, z+1/2; #4 -x+1/2, y+1/2, -z+5/2.

Table S9. Selected bond distances (Å) and angles (°) for **9**.

Zn(1)-O(1)	1.942(2)	Zn(1)-O(4)#1	1.970(2)
Zn(1)-N(1)#2	1.992(3)	Zn(1)-N(4)	2.026(3)
O(1)-Zn(1)-O(4)#1	108.59(10)	O(1)-Zn(1)-N(1)#2	109.63(11)
O(4)#1-Zn(1)-N(1)#2	116.96(11)	O(1)-Zn(1)-N(4)	96.21(11)
O(4)#1-Zn(1)-N(4)	109.96(11)	N(1)#2-Zn(1)-N(4)	113.42(12)

Symmetry codes for **9**: #1 x+1/2, -y+1/2, z+1/2; #2 -x+3/2, y-1/2, -z+3/2.

Table S10. Selected bond distances (Å) and angles (°) for **10**.

Zn(1)-O(2)	1.9425(18)	Zn(1)-O(4)#1	1.9768(19)
Zn(1)-N(1)	1.996(2)	Zn(1)-N(4)#2	2.025(2)
O(2)-Zn(1)-O(4)#1	108.31(9)	O(2)-Zn(1)-N(1)	111.28(9)
O(4)#1-Zn(1)-N(1)	116.49(9)	O(2)-Zn(1)-N(4)#2	96.45(9)
O(4)#1-Zn(1)-N(4)#2	113.93(10)	N(1)-Zn(1)-N(4)#2	108.59(10)

Symmetry codes for **10**: #1 x-1/2, -y+1/2, z-1/2; #2 -x+1/2, y+1/2, -z+1/2.

Table S11. Selected bond distances (Å) and angles (°) for **11**.

Zn(1)-O(1)	1.952(3)	Zn(1)-O(4)#1	1.964(3)
Zn(1)-N(1)	1.996(4)	Zn(1)-N(4)#2	2.016(3)
O(1)-Zn(1)-O(4)#1	109.55(13)	O(1)-Zn(1)-N(1)	109.95(14)

O(4)#1-Zn(1)-N(1)	116.72(14)	O(1)-Zn(1)-N(4)#2	97.99(13)
O(4)#1-Zn(1)-N(4)#2	113.04(14)	N(1)-Zn(1)-N(4)#2	107.99(15)

Symmetry codes for **11**: #1 x-1/2, -y+1/2, z-1/2; #2 -x-1/2, y+1/2, -z+1/2.

Table S12. Selected bond distances (Å) and angles (°) for **12**.

Zn(1)-O(4)#1	1.950(2)	Zn(1)-O(10)#2	1.955(2)
Zn(1)-N(1)	1.985(3)	Zn(1)-O(11)#3	2.0084(19)
Zn(2)-O(9)#4	1.913(2)	Zn(2)-N(4)	1.973(3)
Zn(2)-O(2)	1.975(2)	Zn(2)-O(3)#5	2.018(2)
O(4)#1-Zn(1)-O(10)#2	109.73(10)	O(4)#1-Zn(1)-N(1)	119.66(11)
O(10)#2-Zn(1)-N(1)	117.31(11)	O(4)#1-Zn(1)-O(11)#3	98.55(9)
O(10)#2-Zn(1)-O(11)#3	104.42(9)	N(1)-Zn(1)-O(11)#3	103.83(10)
O(9)#4-Zn(2)-N(4)	122.93(10)	O(9)#4-Zn(2)-O(2)	106.54(10)
N(4)-Zn(2)-O(2)	110.14(11)	O(9)#4-Zn(2)-O(3)#5	98.63(10)
N(4)-Zn(2)-O(3)#5	112.36(10)	O(2)-Zn(2)-O(3)#5	104.34(9)

Symmetry codes for **12**: #1 x, y-1, z-1; #2 x, y-1, z; #3 -x+1, -y+2, -z+1; #4 -x, -y+2, -z+1; #5 -x+1, -y+2, -z+2.

Table S13. Selected bond distances (Å) and angles (°) for **13**.

Zn(1)-O(1)	1.9195(19)	Zn(1)-O(4)#1	1.941(2)
Zn(1)-O(3)#2	1.956(2)	Zn(1)-N(1)	2.003(3)
O(1)-Zn(1)-O(4)#1	119.63(9)	O(1)-Zn(1)-O(3)#2	96.12(9)
O(4)#1-Zn(1)-O(3)#2	114.72(9)	O(1)-Zn(1)-N(1)	113.70(10)
O(4)#1-Zn(1)-N(1)	101.66(11)	O(3)#2-Zn(1)-N(1)	111.53(12)

Symmetry codes for **13**: #1 x, y-1, z; #2 -x+1, -y+1, -z.

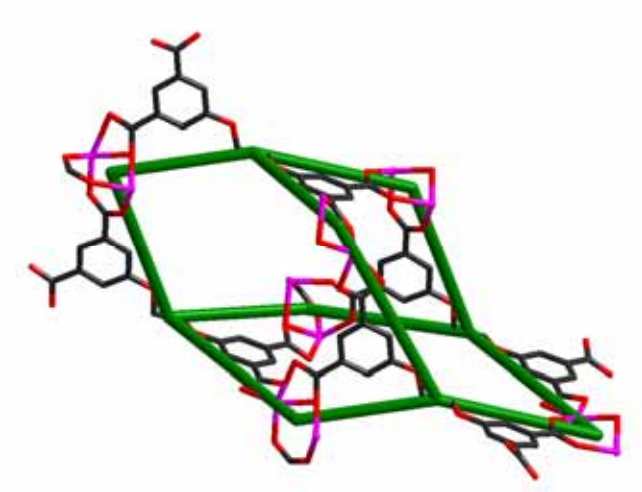

Fig. S1 Single adamantanoid cage in compound **1**.

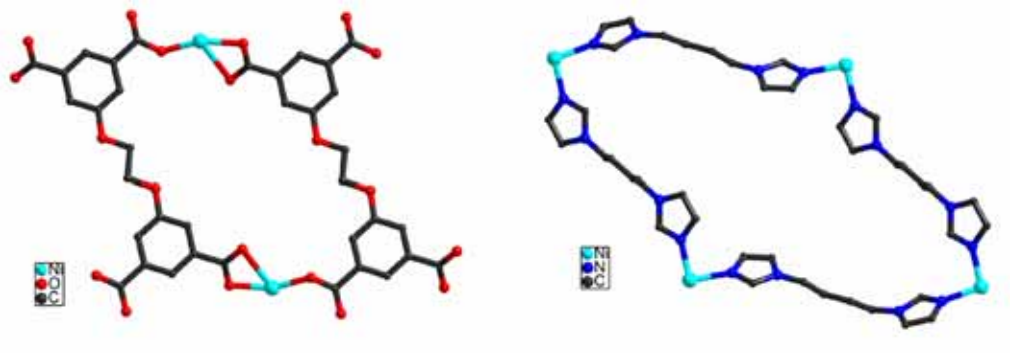

Fig. S2 Ring I (left) and Ring II (right) in compound **7**.

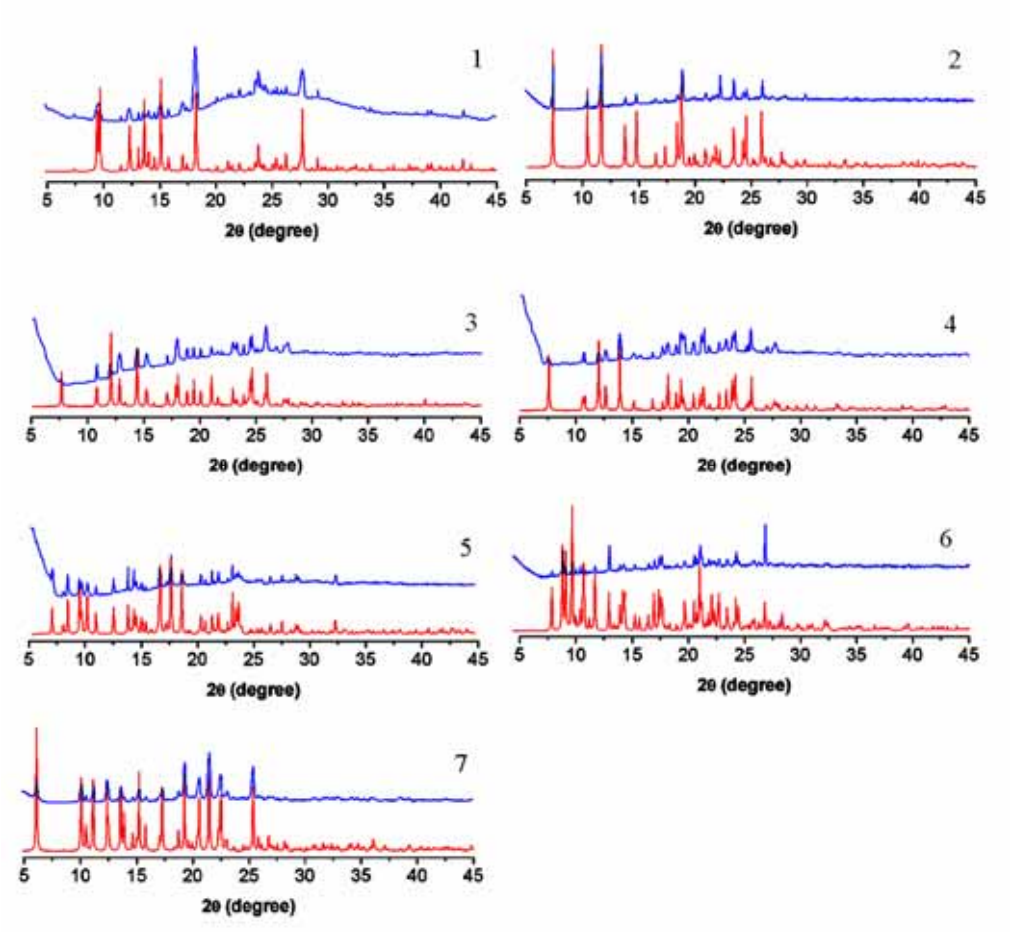

Fig. S3 Simulated (red) and experimental (blue) PXRD patterns of **1**-**7**.

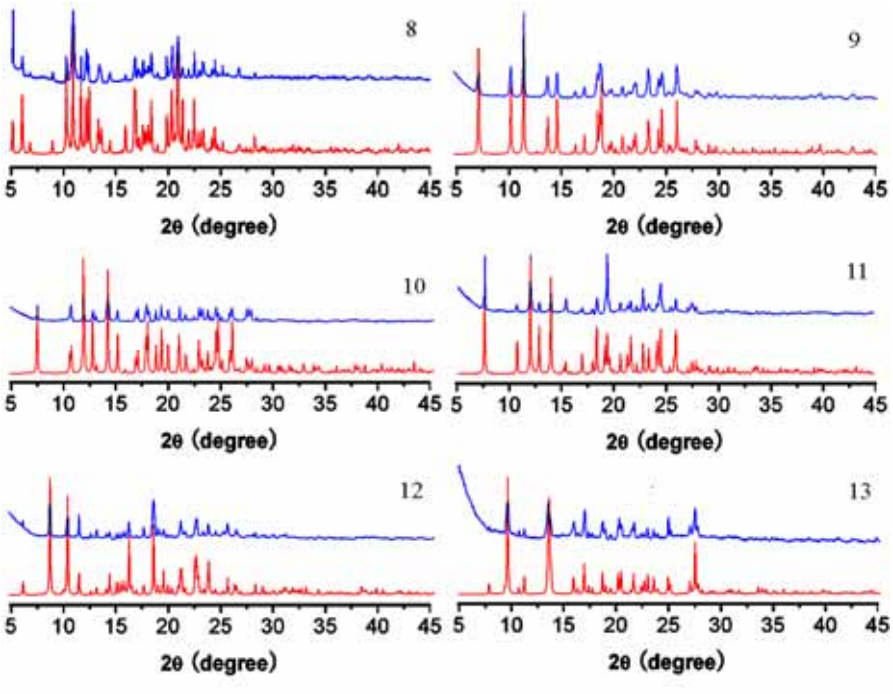

Fig. S4 Simulated (red) and experimental (blue) PXRD patterns of **8**-**13**.

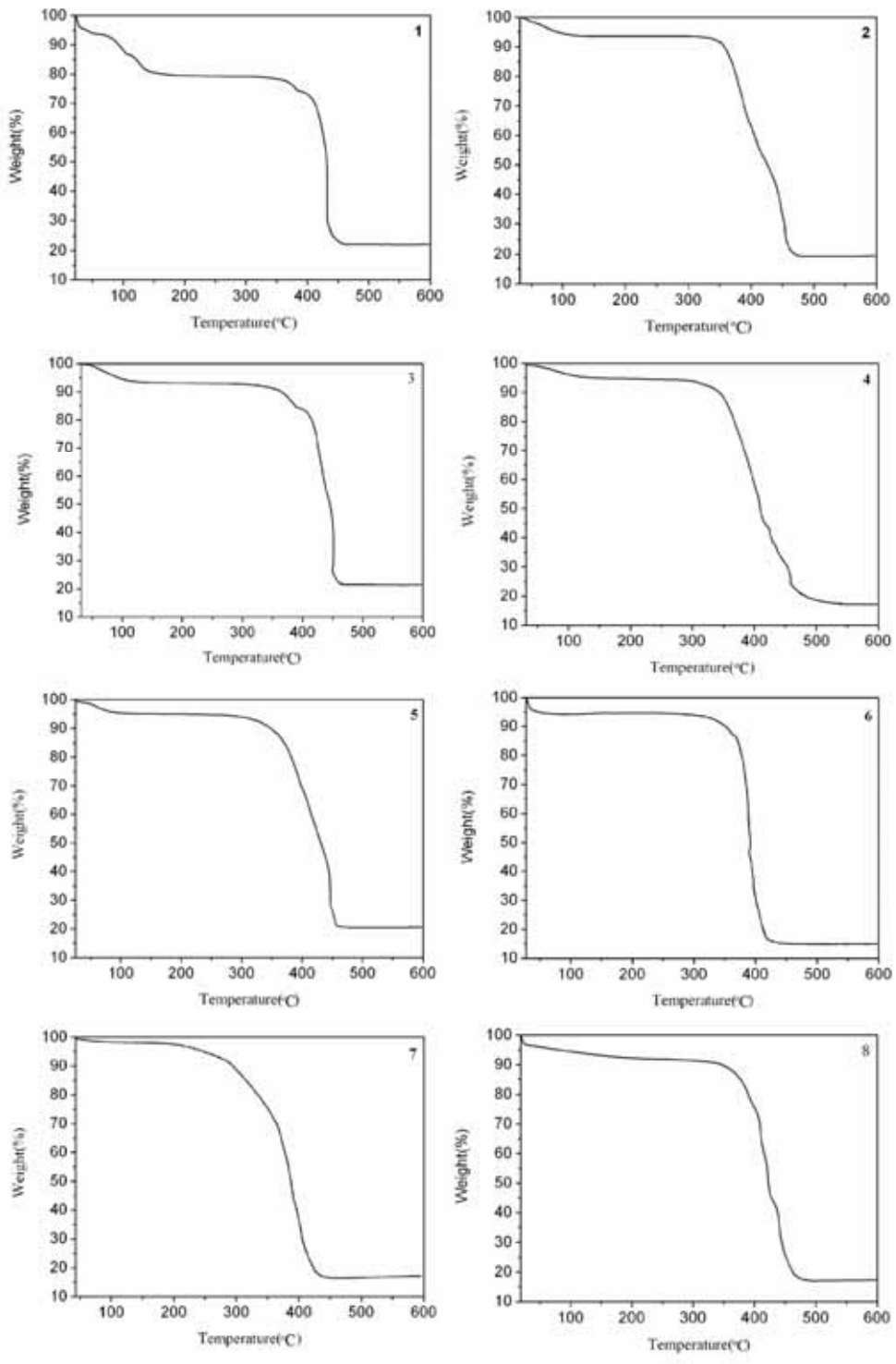

Fig. S5 The TGA curves of compounds **1**-**8**.

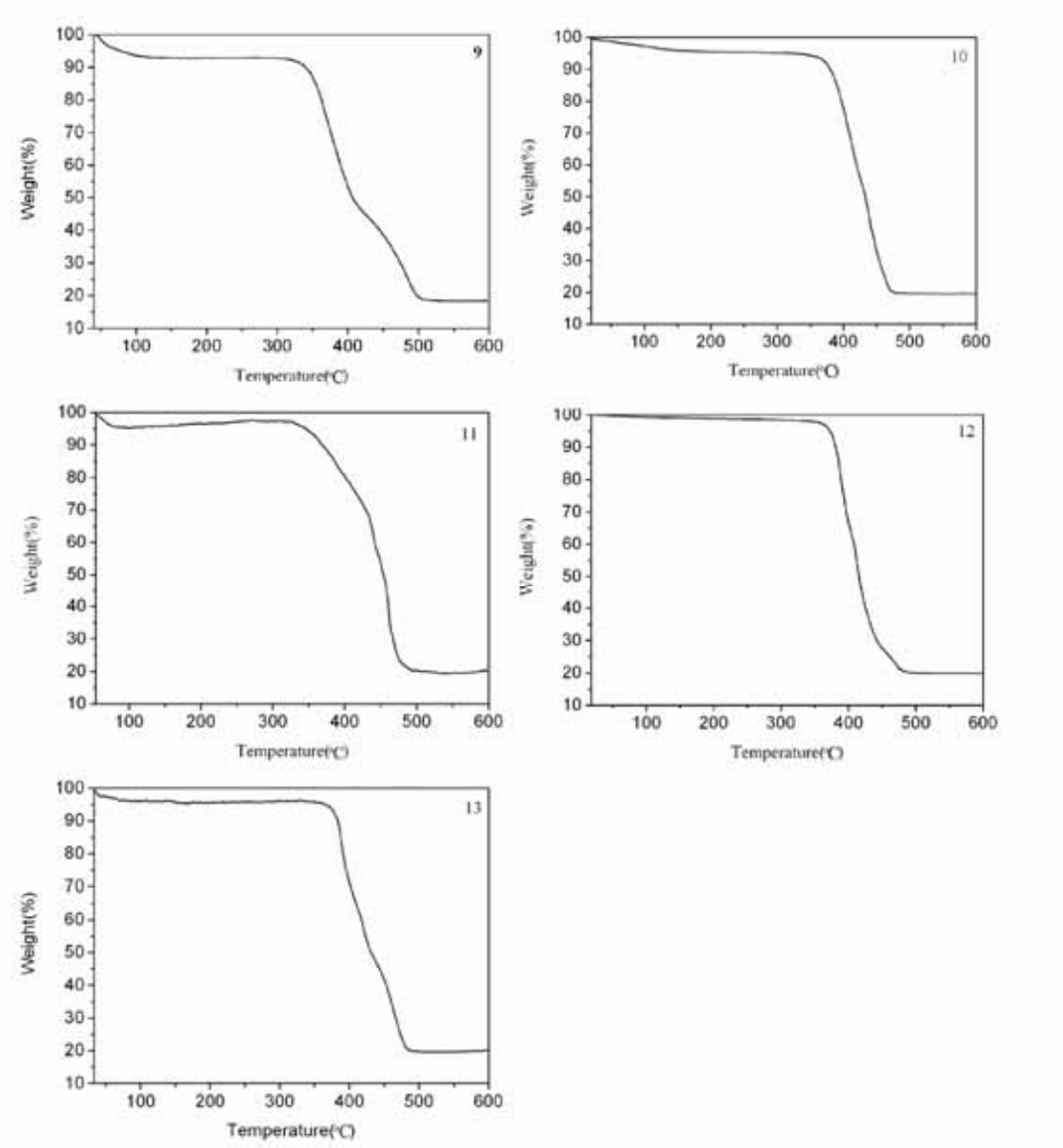

Fig. S6 The TGA curves of compounds **9-13**