Supplementary Material

Structural Diversity and Magnetic Properties of Five Cu(II) Complexes with Mixed Naphthalene-based Dicarboxyl Tecton and Different *N*-Donor Co-Ligands

Jiong Wen,[A] *Jing-Yun Hu,*[A] *E. Carolina Sañudo,*[B] *Min Chen,*[A,C] *and Chun-Sen Liu*[A,C]

[A] Zhengzhou University of Light Industry, Henan Provincial Key Laboratory of Surface & Interface Science, Zhengzhou, Henan 450002, P. R. China.

[B] Institut de Nanociència i Nanotecnologia i Departament de Química Inorgànica, Universitat de Barcelona, Diagonal, 647, 08028 Barcelona, Spain.

[C] Corresponding author E-mails: chenmin@zzuli.edu.cn (M. C.); chunsenliu@zzuli.edu.cn (C.S.L.)

Table S1 Selected bond lengths (Å) and angles (°) for **1–5**.[a]

1			
Cu1–O3$^{\#1}$	1.9289(19)	Cu1–O1	1.9406(19)
Cu1–O5	2.5431(18)	Cu2–O5	1.945(2)
Cu2–O2$^{\#3}$	1.9635(19)	Cu2–O1	2.4257(19)
O3$^{\#1}$–Cu1–O3$^{\#2}$	85.61(12)	O3$^{\#1}$–Cu1–O1	168.17(8)
O3$^{\#2}$–Cu1–O1	92.25(8)	O1$^{\#3}$–Cu1–O1	92.14(12)
O5$^{\#4}$–Cu2–O2$^{\#3}$	89.12(9)	O5–Cu2–O2$^{\#3}$	90.88(8)
O5–Cu2–O1$^{\#4}$	94.81(7)	O5–Cu2–O2$^{\#5}$	89.12(8)
O2$^{\#3}$–Cu2–O1$^{\#4}$	87.55(7)	O2$^{\#3}$–Cu2–O1	92.45(7)
O5–Cu2–O1	85.19(7)		
2			
Cu1–O1	1.958(2)	Cu1–O6	1.966(2)
Cu1–O3$^{\#1}$	1.969(2)	Cu1–O5	1.994(3)
Cu1–O4$^{\#2}$	2.206(3)		
O3$^{\#1}$–Cu1–O5	170.43(11)	O1–Cu1–O6	177.87(13)
O6–Cu1–O5	86.35(10)	O1–Cu1–O3$^{\#1}$	86.42(10)
O1–Cu1–O4$^{\#2}$	88.18(12)	O3$^{\#1}$–Cu1–O4$^{\#2}$	90.23(10)
O1–Cu1–O5	91.56(10)	O6–Cu1–O4$^{\#2}$	92.56(12)
O6–Cu1–O3$^{\#1}$	95.57(9)	O5–Cu1–O4$^{\#2}$	99.06(10)
3			
Cu1–O6	1.9332(19)	Cu1–O4$^{\#1}$	1.953(2)
Cu1–O1	1.981(2)	Cu1–O9	1.9934(18)
Cu1–O5	2.332(2)	Cu2–O3$^{\#1}$	1.935(2)
Cu2–O9	1.958(3)	Cu2–O8	2.009(3)
Cu2–O7	2.244(3)		
O1–Cu1–O9	164.10(12)	O6–Cu1–O4$^{\#1}$	173.23(11)
O6–Cu1–O9	81.81(9)	O4$^{\#1}$–Cu1–O5	87.67(9)
O4$^{\#1}$–Cu1–O1	89.02(10)	O4$^{\#1}$–Cu1–O9	93.04(9)
O6–Cu1–O1	94.74(10)	O9–Cu1–O5	99.85(10)
O1–Cu1–O5	95.98(10)	O6–Cu1–O5	97.52(11)
O9–Cu2–O7	92.49(12)	O3$^{\#1}$–Cu2–O8	83.53(7)
O8–Cu2–O7	94.86(12)	O3$^{\#1}$–Cu2–O7	95.78(7)
O3$^{\#1}$–Cu2–O9	95.74(7)	O3$^{\#1}$–Cu2–O3$^{\#2}$	163.31(14)
O9–Cu2–O8	172.65(12)		
4			
Cu1–O1	1.9273(17)	Cu1–N1	2.012(2)
Cu1–O3	2.406(3)		
O1–Cu1–N1$^{\#1}$	176.61(9)	N1$^{\#1}$–Cu1–N1	81.78(12)
O1–Cu1–O1$^{\#1}$	87.10(11)	N1–Cu1–O3	90.90(8)
O1–Cu1–O3	91.20(8)	O1–Cu1–N1	95.52(8)
5			

Cu1–O2	1.992(3)	Cu1–N2	2.022(3)
Cu1–O1	2.025(3)	Cu1–N1	2.033(3)
Cu1–N3	2.121(3)		
O2–Cu1–N2	90.64(13)	O2–Cu1–O1	146.33(11)
N2–Cu1–O1	88.87(13)	O2–Cu1–N1	89.73(14)
N2–Cu1–N1	178.33(14)	O1–Cu1–N1	91.73(14)
O2–Cu1–N3	111.18(13)	N2–Cu1–N3	91.87(14)
O1–Cu1–N3	102.48(13)	N1–Cu1–N3	86.47(14)

[a] Symmetry codes: #1 = –x + 1, y – 1, –z + 1/2; #2 = x, y – 1, z; #3 = –x + 1, y, –z + 1/2; #4 = –x + 1, –y + 1, –z + 1; #5 = x, –y + 1, z + 1/2 for **1**; #1 = x + 1, y, z; #2 = –x + 2, y – 1/2, –z + 1 for **2**; #1 = x – 1/2, y, –z + 3/2; #2 = x – 1/2, –y + 3/2, –z + 3/2 for **3**; #1 = –x + 1, y, z for **4**.

Table S2 Hydrogen bond lengths /Å and angles /º for complexes **1–4**[a].

| D–H⋯A	d(H⋯A) (Å)	d(D⋯A) (Å)	∠D–H⋯A (°)	Symmetry codes
1				
O5–H1W⋯O3	2.01	2.719(3)	140	$-x + 1, -y + 1, -z + 1$
O5–H2W⋯O4	1.75	2.576(3)	163	$-x + 1, y - 1, -z + 1/2$
2				
O5–H1W⋯O2	1.91	2.746(4)	169	$-x + 2, y - 1/2, -z + 1$
O5–H2W⋯O1	2.04	2.812(4)	151	$-x + 2, y + 1/2, -z + 1$
O6–H3W⋯O3	1.95	2.757(4)	159	$-x + 3, y - 1/2, -z + 1$
O6–H4W⋯O2	1.97	2.805(4)	167	$-x + 3, y - 1/2, -z + 1$
3				
O7–H3W⋯O2	1.85	2.668(3)	161	
O6–H6⋯O8	2.17	2.949(3)	153	$x + 1/2, -y + 3/2, -z + 3/2$
O5–H1W⋯O12	1.89	2.724(5)	165	$x - 1, y, z + 1$
O5–H2W⋯O10	1.84	2.693(4)	178	$x, y, z + 1$
O8–H4W⋯O5	1.99	2.777(3)	155	$x, y, z - 1$
O11–H5W⋯O7	1.98	2.826(5)	171	
O11–H6W⋯O6	1.91	2.758(5)	180	$x, y, z - 1$
O10–H7W⋯O2	1.88	2.690(4)	159	
O10–H8W⋯O11	2.33	3.060(4)	145	
O9–H9⋯O11	1.89	2.735(4)	173	$x - 1/2, -y + 3/2, -z + 3/2$
O12–H9W⋯O1	2.22	2.962(4)	146	$x + 1/2, y, -z + 3/2$
O12–H10W⋯O4	2.43	2.960(5)	121	$x + 1/2, y, -z + 1/2$
4				
O3–H3⋯O2	1.96	2.767(6)	167	$-x, -y + 1/2, z + 1/2$
O4–H4⋯O3	2.12	2.930(6)	169	$x + 1, y, z$
5				
C22–H22A⋯O6	2.50	3.430(11)	173	$x - 1, -y, z - 1/2$
C9–H9A⋯O8	2.55	3.257(14)	133	$x, -y + 1, z - 1/2$
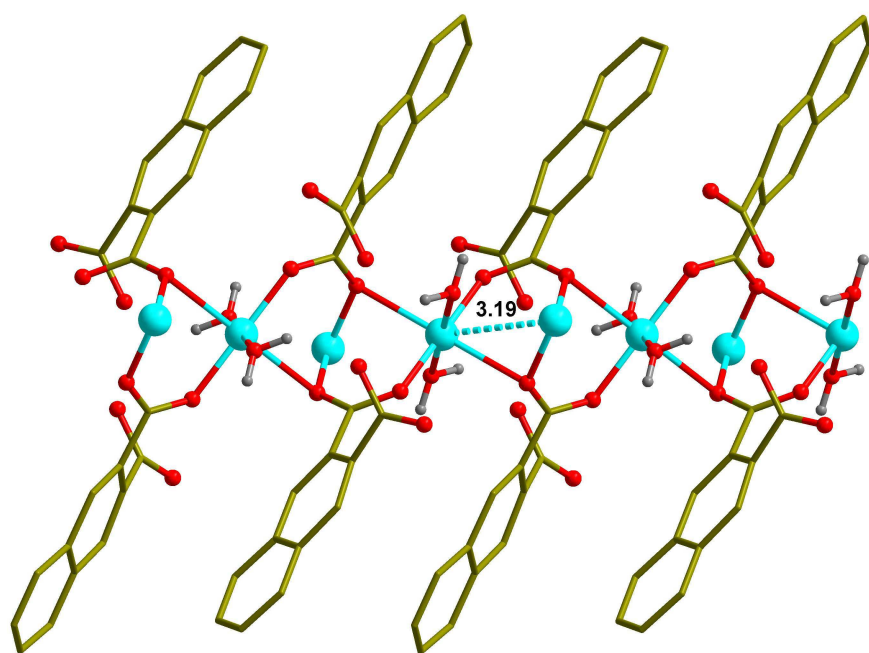
Fig. S1 View of the 1D chain in **1**.
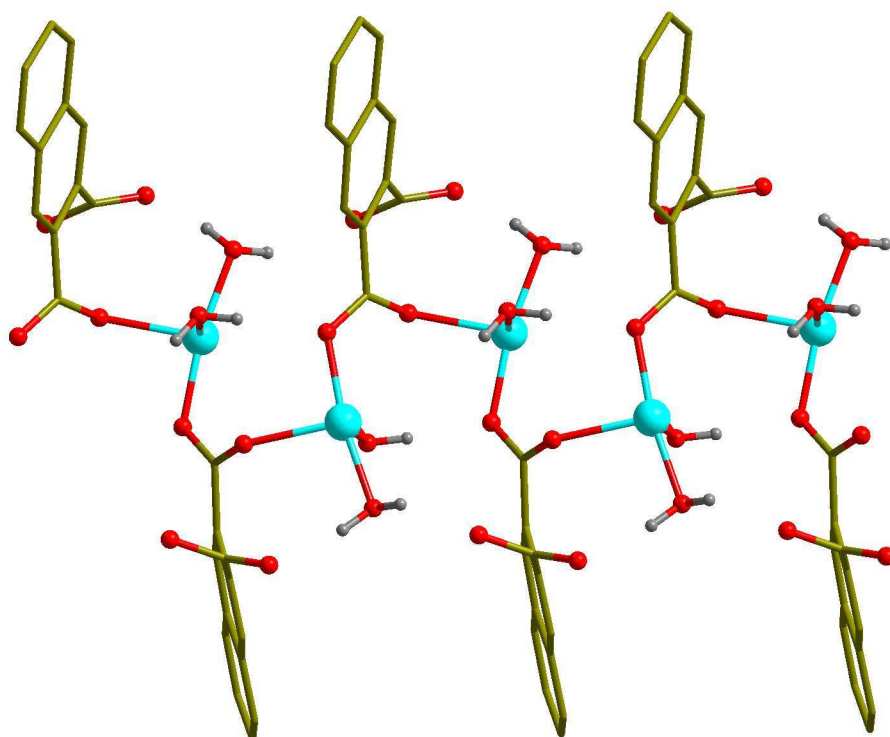
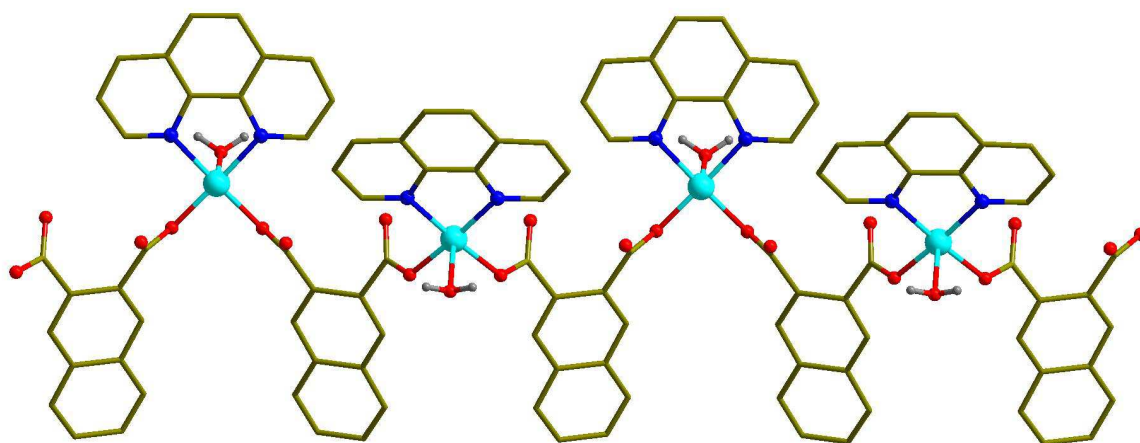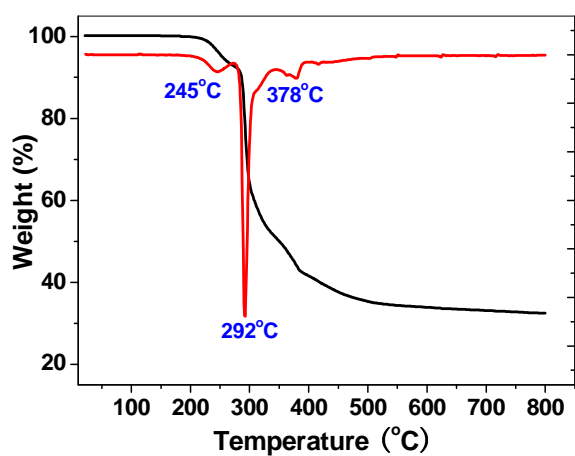**Fig. S2** View of the 1D chain in **2**.
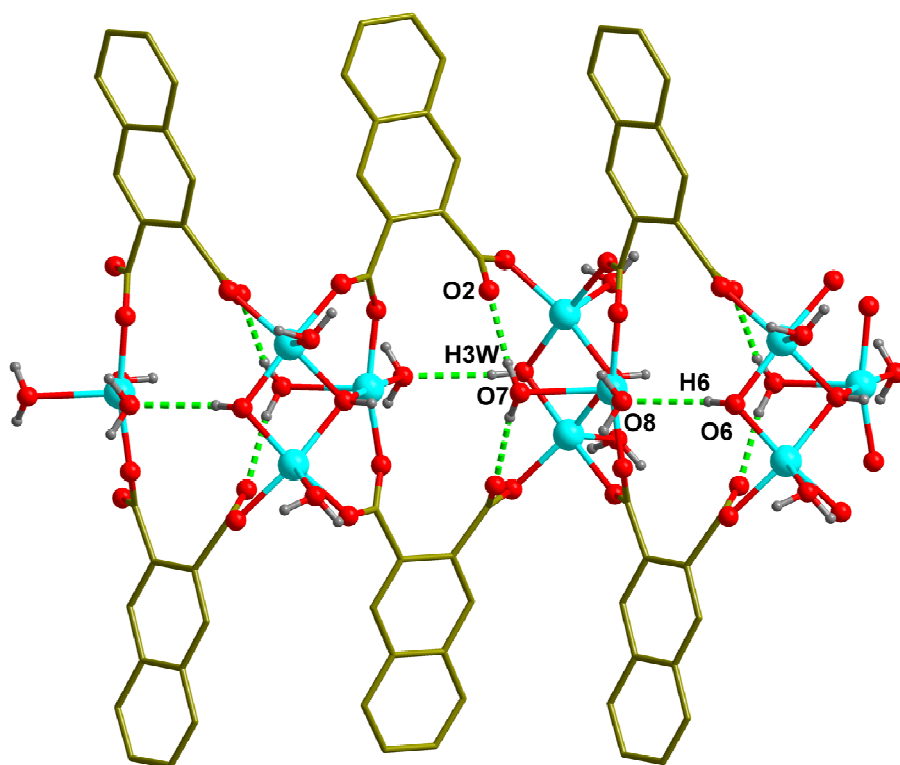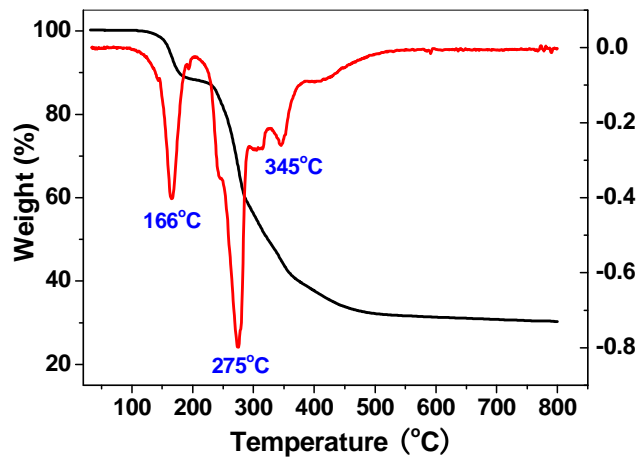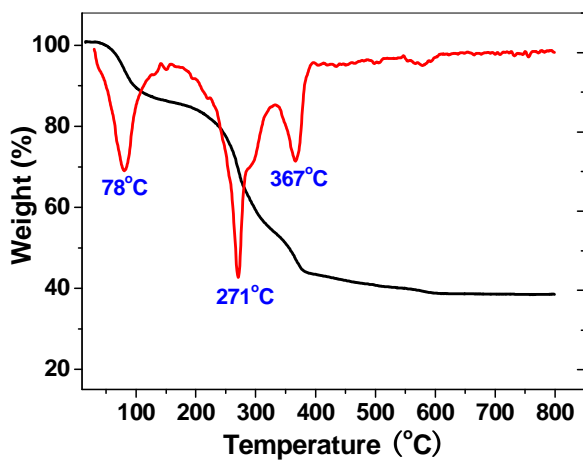
Fig. S3 View of the 1D chain in **3**.

Fig. S4 View of the 1D chain in **4**.

(a)

(b)

(c)
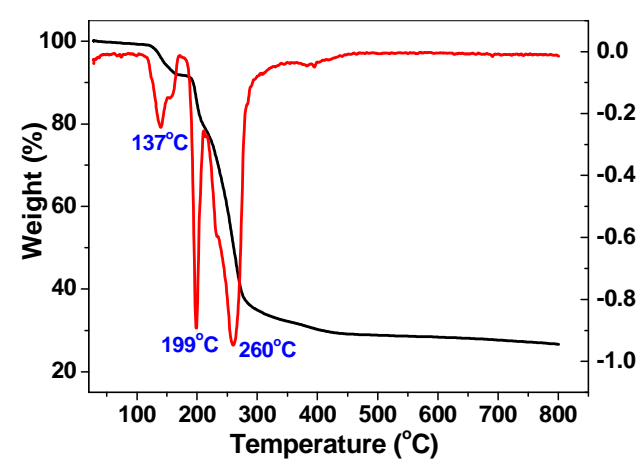
(d)
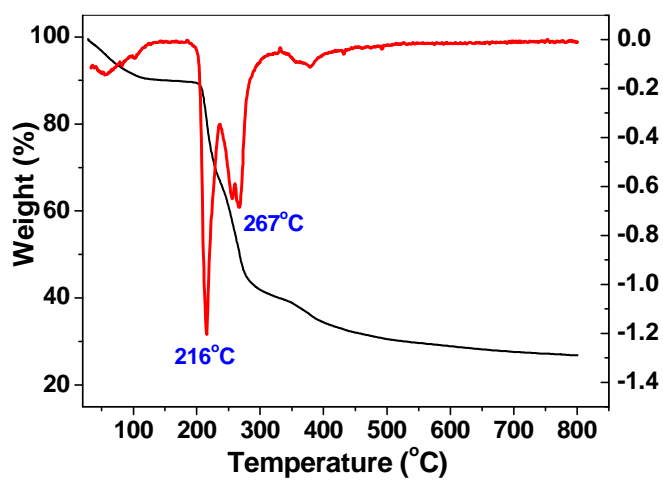
(e)

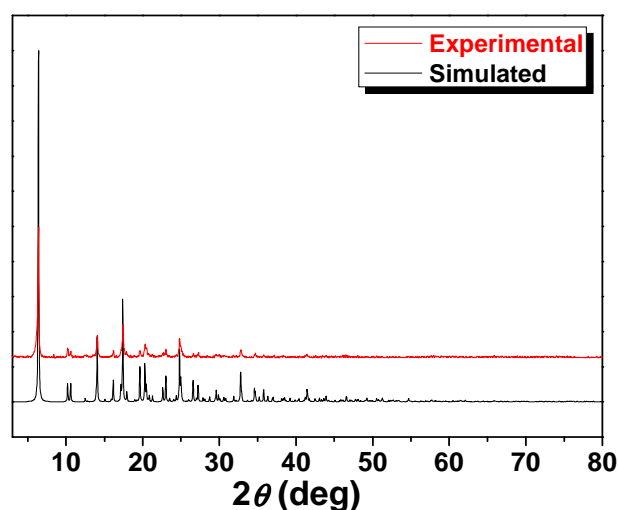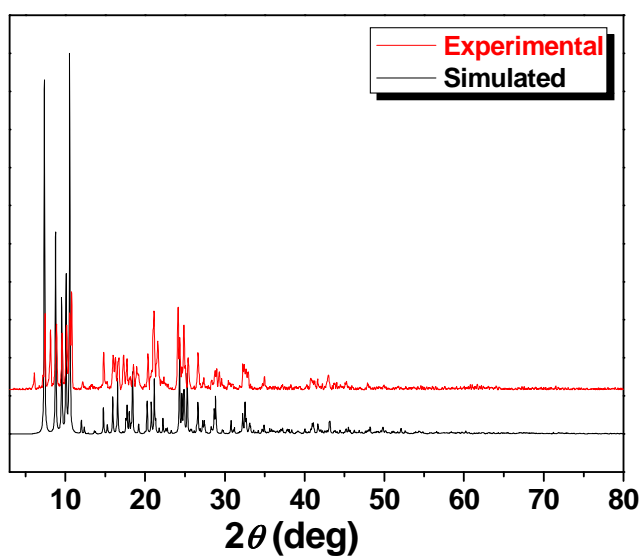**Fig. S5** TG-DTA curves of **1** (a), **2** (b), **3** (c), **4** (d), and **5** (e).
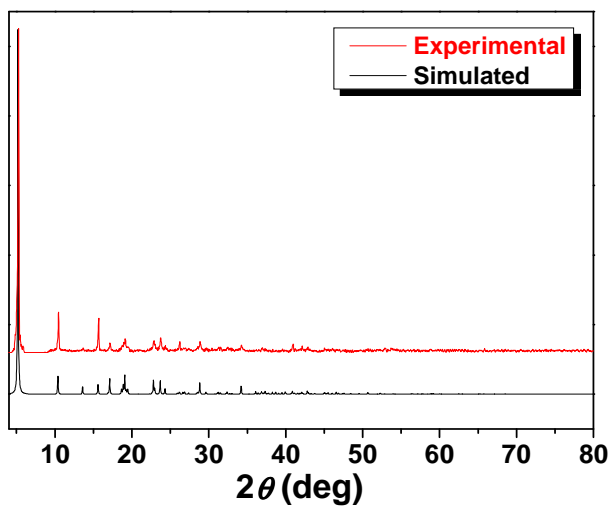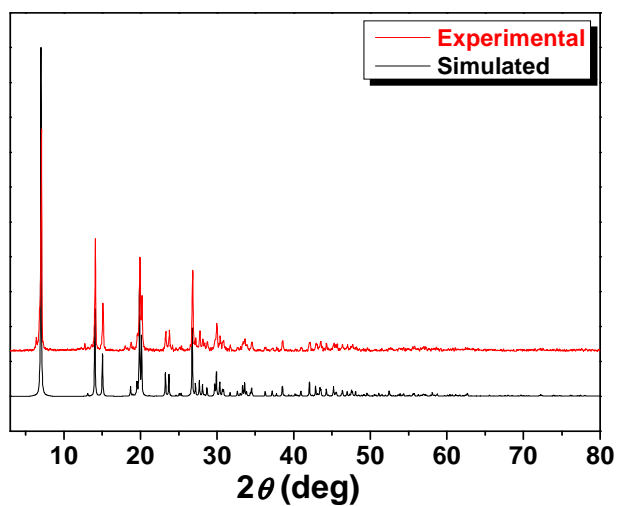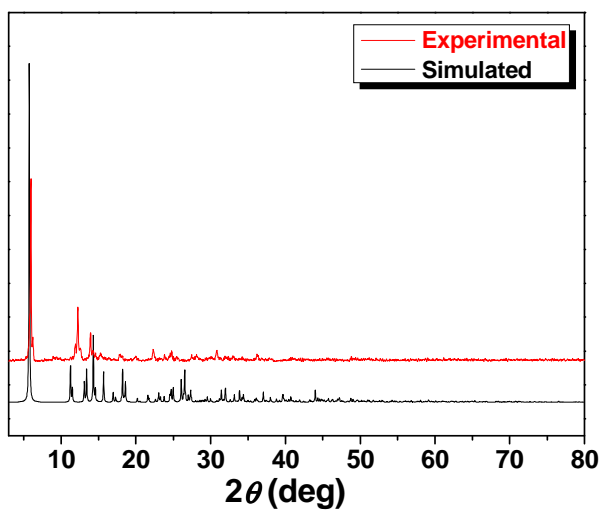
Fig. S6 PXRD patterns of **1** (a), **2** (b), **3** (c), **4** (d), and **5** (e).