10.1071/CH15110_AC

Australian Journal of Chemistry 2015, 68(10), 1550-1561

SUPPLEMENTARY MATERIAL

Assembly and properties of four new metal-organic complexes based on 1,4-naphthalenedicarboxylate: effect of four bis-pyridyl-bis-amide ligands with diverse spacers on the structures

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

Cu(1)–O(3)#1	1.967(3)	Cu(1)–N(1)	2.015(4)
Cu(1)–O(4)#2	1.979(3)	Cu(1)–O(1W)	2.3030(10)
Cu(1)–O(1)	1.984(3)		
O(3)#1–Cu(1)–O(4)#2	155.83(14)	O(1)–Cu(1)–N(1)	175.40(14)
O(3)#1–Cu(1)–O(1)	88.94(14)	O(3)#1–Cu(1)–O(1W)	103.59(13)
O(4)#2–Cu(1)–O(1)	87.27(14)	O(4)#2–Cu(1)–O(1W)	100.45(12)
O(3)#1–Cu(1)–N(1)	92.82(15)	O(1)–Cu(1)–O(1W)	92.95(12)
O(4)#2–Cu(1)–N(1)	92.82(15)	N(1)–Cu(1)–O(1W)	82.51(13)
Symmetry code: #1 x+1/2,–y+1/2,–z+1; #2 –x+1/2,y–1/2,z			

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

Cu(1)–O(4)#1	1.957(3)	Cu(1)–O(3)	1.969(4)
Cu(1)–O(1)	1.972(4)	Cu(1)–O(2)#2	1.974(4)
Cu(1)–N(1)	2.133(5)		
O(4)#1–Cu(1)–O(3)	166.64(16)	O(4)#1–Cu(1)–O(1)	92.09(16)
O(3)–Cu(1)–O(1)	87.19(16)	O(4)#1–Cu(1)–O(2)#2	89.62(16)
O(3)–Cu(1)–O(2)#2	87.98(16)	O(1)–Cu(1)–O(2)#2	166.14(16)
O(4)#1–Cu(1)–N(1)	94.93(18)	O(3)–Cu(1)–N(1)	98.28(18)
O(1)–Cu(1)–N(1)	101.97(18)		
Symmetry code: #1 x,y+1,z; #2 –x,y,–z+3/2			

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

Cu(1)–O(1)	1.909(4)	Cu(2)–O(3)#2	1.961(4)
Cu(1)–O(5)	1.968(4)	Cu(2)–O(3)	1.961(4)
Cu(1)–N(1)	2.025(5)	Cu(2)–N(5)#2	1.994(5)
Cu(1)–N(2)#1	2.043(5)	Cu(2)–N(5)	1.994(5)
Cu(1)–O(1W)	2.392(5)		
O(1)–Cu(1)–O(5)	176.77(19)	N(1)–Cu(1)–O(1W)	98.96(18)
O(1)–Cu(1)–N(1)	94.51(19)	N(2)#1–Cu(1)–O(1W)	94.94(19)
O(5)–Cu(1)–N(1)	87.63(18)	O(3)#2–Cu(2)–O(3)	179.999(2)
O(1)–Cu(1)–N(2)#1	89.52(18)	O(3)#2–Cu(2)–N(5)#2	89.1(2)
O(5)–Cu(1)–N(2)#1	88.99(17)	O(3)–Cu(2)–N(5)#2	90.9(2)
N(1)–Cu(1)–N(2)#1	165.63(18)	O(3)#2–Cu(2)–N(5)	90.9(2)
O(1)–Cu(1)–O(1W)	88.2(2)	O(3)–Cu(2)–N(5)	89.1(2)
O(5)–Cu(1)–O(1W)	89.03(17)	N(5)#2–Cu(2)–N(5)	180.0(2)
Symmetry code: #1 x,y,z+1; #2 –x+1,–y+2,–z+2			

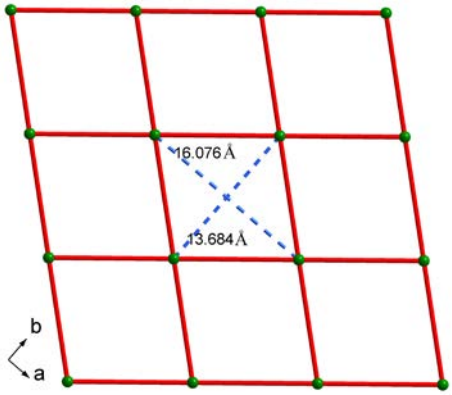
Table S4. Selected bond distances (Å) and angles (deg) for complex **4**

Cu(1)–O(1)	1.9442(17)	Cu(1)–N(1)	2.008(2)
Cu(1)–N(2)	2.019(2)	Cu(1)–O(4)#1	2.083(3)
Cu(1)–O(3)#1	2.423(3)		
O(1)–Cu(1)–N(1)	90.34(8)	O(1)–Cu(1)–N(2)	89.10(8)
N(1)–Cu(1)–N(2)	167.25(9)	O(1)–Cu(1)–O(4)#1	146.87(10)
N(1)–Cu(1)–O(4)#1	93.85(9)	N(2)–Cu(1)–O(4)#1	93.58(9)
O(1)–Cu(1)–O(3)#1	155.64(9)	N(1)–Cu(1)–O(3)#1	82.77(9)
N(2)–Cu(1)–O(3)#1	92.57(9)	O(4)#1–Cu(1)–O(3)#1	57.29(10)
Symmetry code: #1 x,y–1,z			

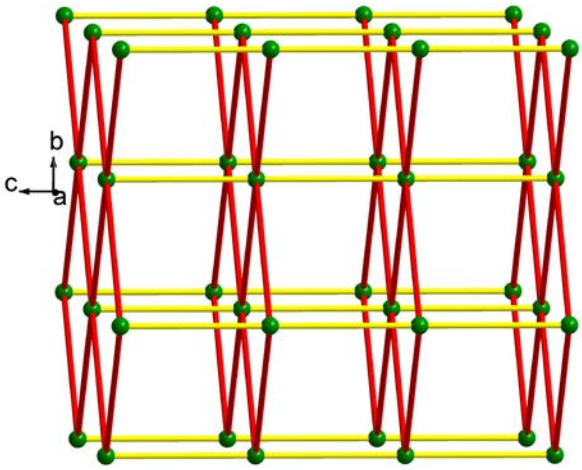
Table S5. Hydrogen-bonding geometry (Å, °) for complexes **3** and **4**

D–H···A	D–H	H···A	D···A	D–H···A
		3		
N4–H4A···O4[a]	0.86	2.08	2.906(7)	161
N6–H6A···O6[b]	0.86	1.98	2.818(7)	163
		4		
N3–H3B···O2[a]	0.86	2.10	2.910(4)	157
N4–H4A···O5[b]	0.86	2.47	3.061(3)	127

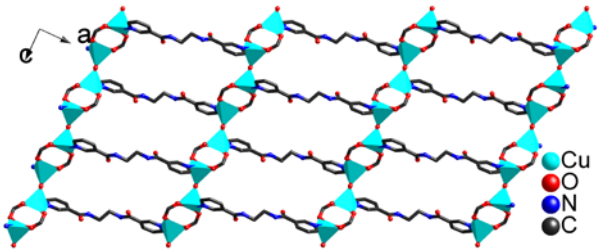
Symmetry code for **3**: (a) -x,1-y,1-z; (b) x,1+y,z; for **4**: (a) 1-x,1-y,1-z; (b) 2-x,1-y,-z.



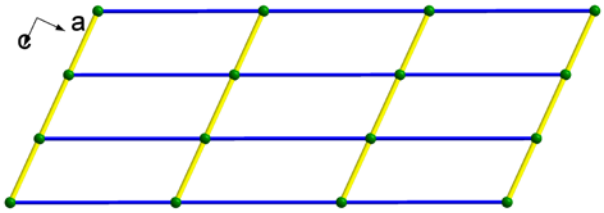
(a)



(b)

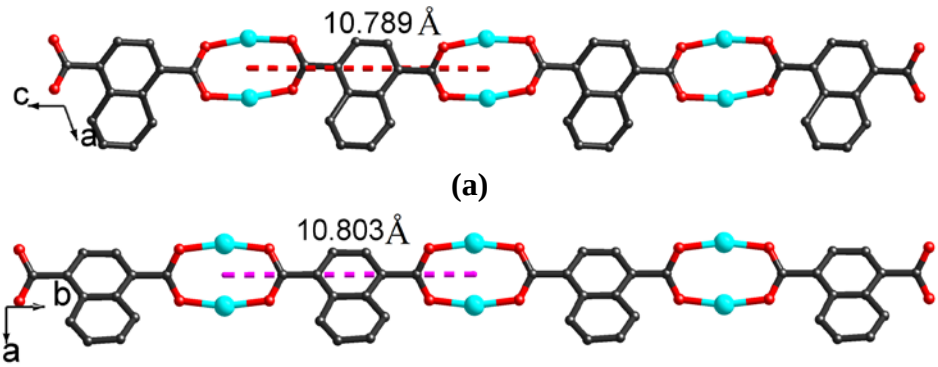


(c)



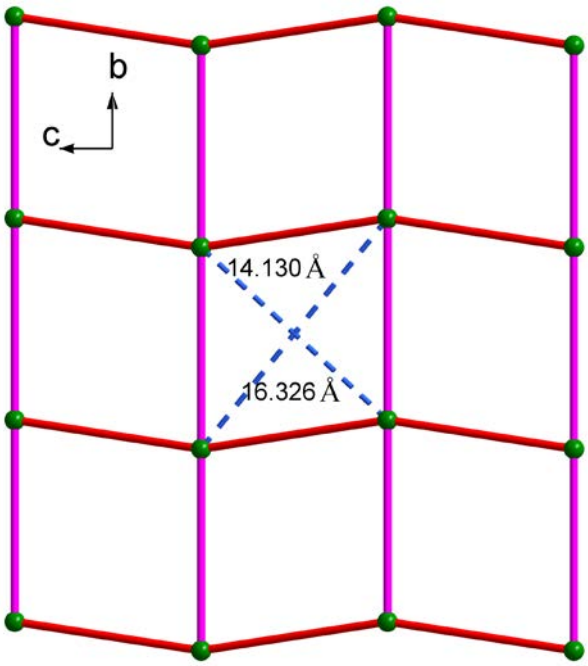
(d)

Fig. S1. (a) The schematic of 2D $[Cu_2(1,4\text{-NDC})_2]_n$ layer along *c*-axis in complex **1**; (b) The simplified representation of 3D $[Cu_2(1,4\text{-NDC})_2(H_2O)]_n$ framework in **1**; (c) The 2D $[Cu_2(H_2O)(3\text{-bpye})]_n$ framework constructed by the coordinated water molecules and two bridging ligands 3-bpye in **1**; (d) The schematic of 2D $[Cu_2(H_2O)(3\text{-bpye})]_n$ structure of **1**.

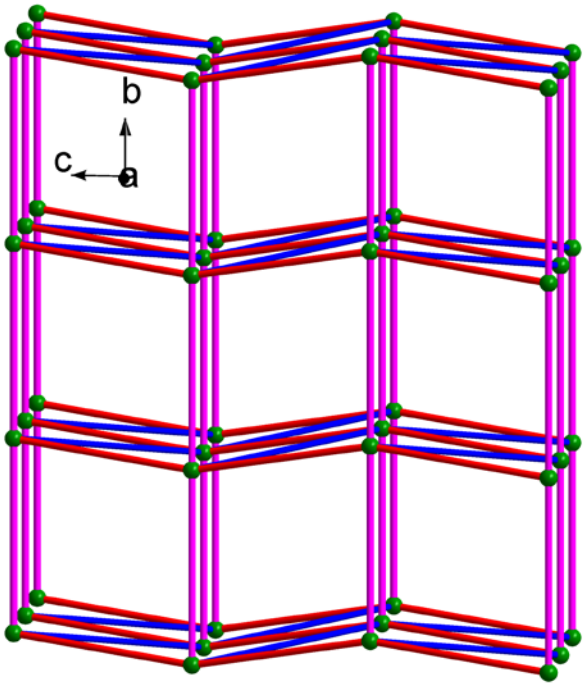


(a)

(b)

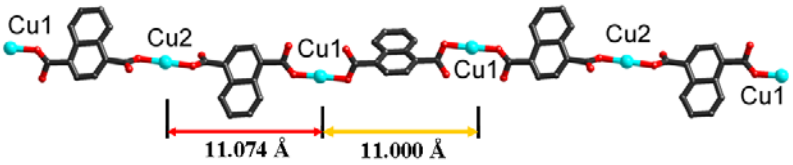


(c)

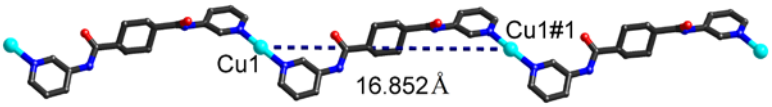


(d)

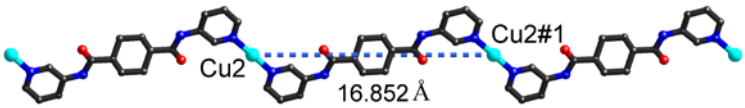
Fig. S2. (a) The 1D $[Cu(1,4\text{-}NDC^1)]_n$ chain with the distance of adjacent $\{Cu_2\}$ cores of 10.789 Å; (b) The 1D $[Cu(1,4\text{-}NDC^2)]_n$ chain with the distance of adjacent $\{Cu_2\}$ cores of 10.803 Å; (c) The schematic of 2D $[Cu_2(1,4\text{-}NDC)_2]_n$ layer along *a*-axis in **2**; (d) The topology of 3D network for complex **2** constructed by ligands 1,4-NDC and 3-bpfp (Red bonds: $1,4\text{-}NDC^1$, Pink bonds: $1,4\text{-}NDC^2$, Blue bonds; 3-bpfp).



(a)



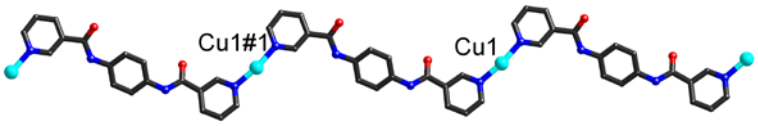
(b)



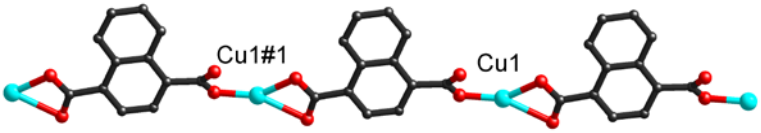
(c)

Fig. S3. (a) The 1D $[Cu(1,4\text{-}NDC)]_n$ chain formed by $1,4\text{-}NDC^1$ and $1,4\text{-}NDC^2$ anions alternately connected Cu1 and Cu2 ions in complex **3**; (b) The 1D $[Cu1(3\text{-}bpcd^1)]_n$

chain; (c) The 1D $[Cu2(3\text{-}bpcd^2)]_n$ chain in **3**.



(a)



(b)

Fig. S4. (a) The 1D $[Cu1(3\text{-}bpcb)]_n$ chain in complex **4**; (b) The 1 D $[Cu(1,4\text{-}NDC)]_n$ chain in **4**.

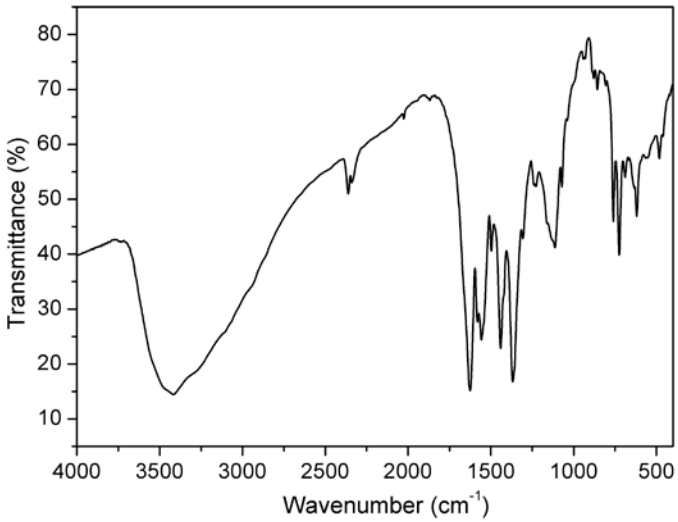


Fig. S5. The IR spectrum of complex **1.**

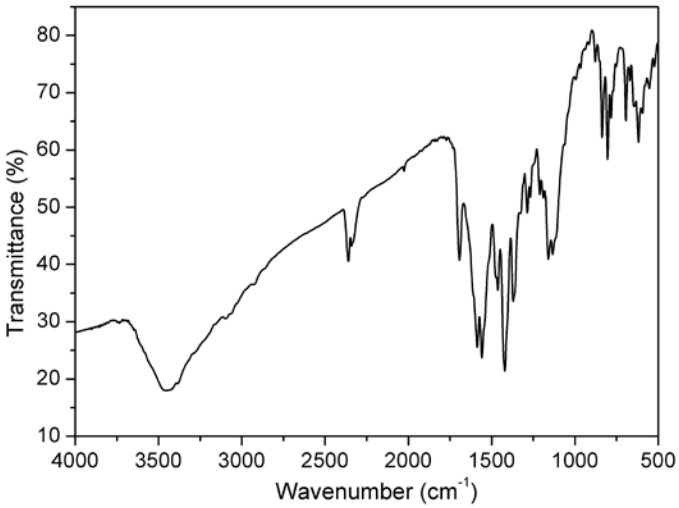


Fig. S5. The IR spectrum of complex **2.**

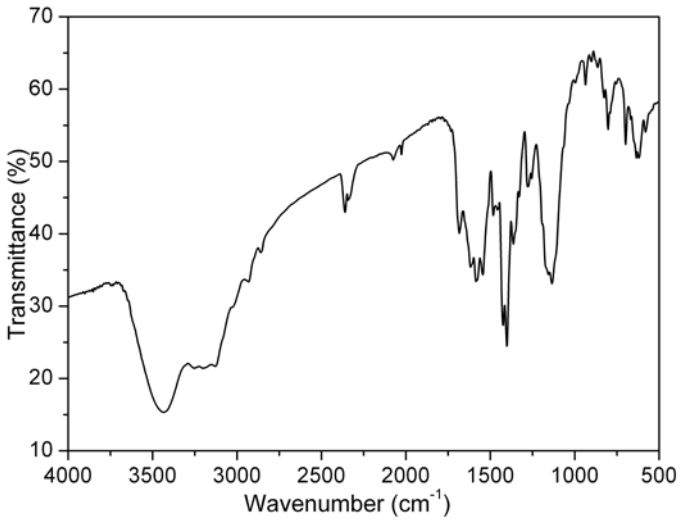


Fig. S5. The IR spectrum of complex **3.**

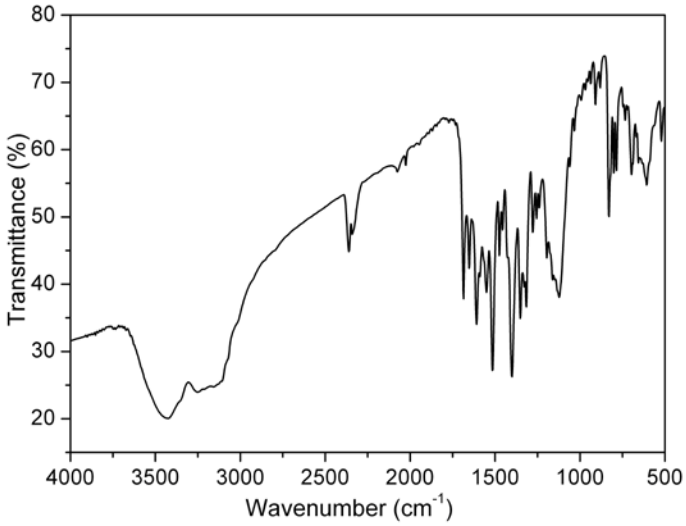


Fig. S5. The IR spectrum of complex **4.**

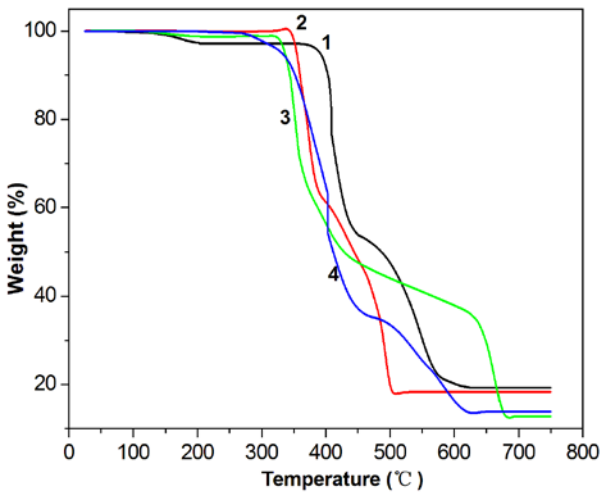


Fig. S6. TG curves for complexes **1–4.**

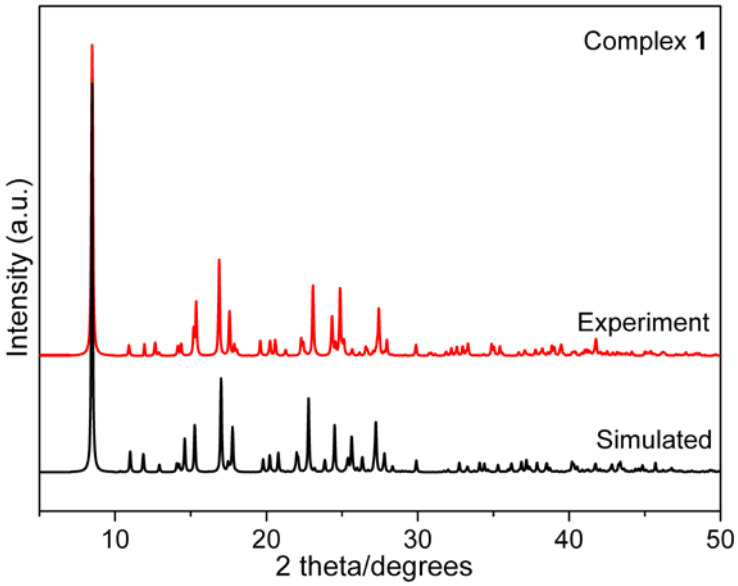


Fig. S7. PXRD patterns: (a) simulated from single crystal X-ray data; (b) as-synthesized complex **1**.

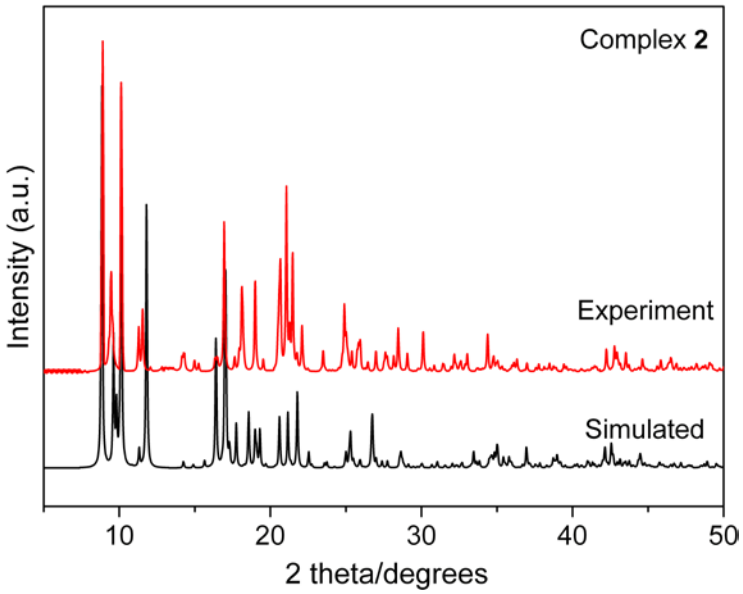


Fig. S8. PXRD patterns: (a) simulated from single crystal X-ray data; (b) as-synthesized complex **2**.

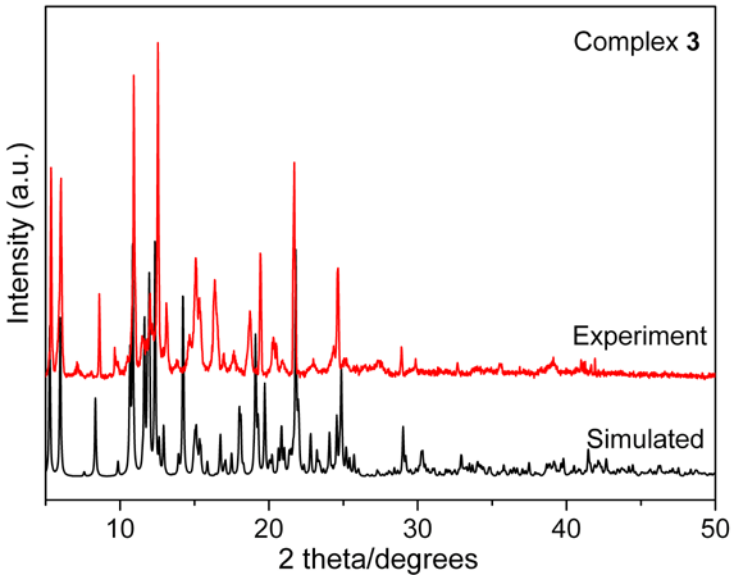


Fig. S9. PXRD patterns: (a) simulated from single crystal X-ray data; (b) as-synthesized complex **3**.

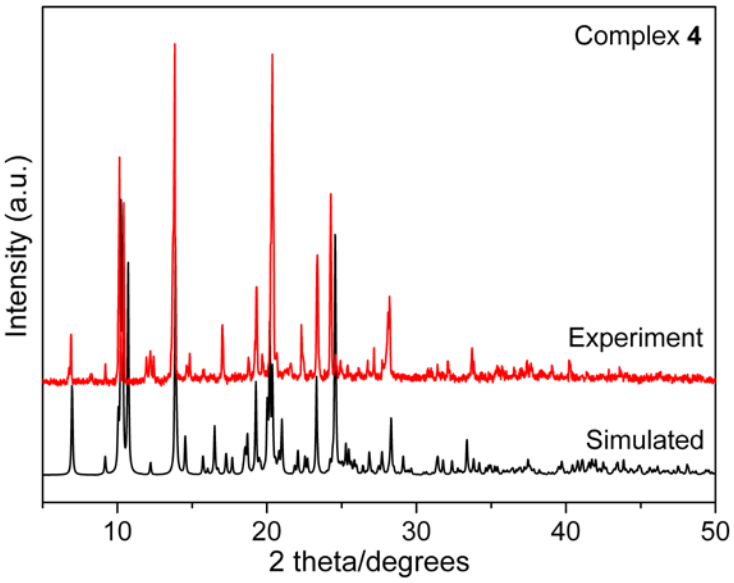


Fig. S10. PXRD patterns: (a) simulated from single crystal X-ray data; (b) as-synthesized complex **4**.