Supporting Information for

Architectures and DFT calculations of polyrotaxane MOFs with nanoscale macrocycles†

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Table S1 Selected bond lengths (Å) and angles (º) by X-ray and theoretical calculations for complexes **1** and **2**

Bond lengths (Å) for **1**[a]			
N(1)-Ni(1)	2.030(3)	Ni(1)-O(3)	2.213(2)
Ni(1)-N(2)#1	2.062(3)	Ni(1)-O(4)	2.063(2)
Ni(1)-O(1)	2.084(2)	Ni(1)-O(2)	2.143(2)
Bond lengths (Å) for **2**[b]			
N(1)-Zn(1)	2.087(4)	Zn(1)-N(2)#1	2.051(4)
O(2)-Zn(1)	2.006(3)	O(4)-Zn(1)	1.956(3)
Bond angles (º) for **1**[a]			
N(1)-Ni(1)-N(2)#1	96.00(10)	N(1)-Ni(1)-O(4)	100.65(10)
N(2)#1-Ni(1)-O(4)	95.22(9)	N(1)-Ni(1)-O(1)	162.35(10)
N(2)#1-Ni(1)-O(1)	89.76(10)	O(4)-Ni(1)-O(1)	95.40(8)
N(1)-Ni(1)-O(2)	100.19(10)	N(2)#1-Ni(1)-O(2)	98.13(10)
O(4)-Ni(1)-O(2)	153.84(8)	O(1)-Ni(1)-O(2)	62.40(8)
N(1)-Ni(1)-O(3)	93.23(9)	N(2)#1-Ni(1)-O(3)	156.21(9)
O(4)-Ni(1)-O(3)	61.46(8)	O(1)-Ni(1)-O(3)	87.99(9)
O(2)-Ni(1)-O(3)	101.75(8)		
Bond angles (º) for **2**[b]			
O(4)-Zn(1)-O(2)	135.02(15)	O(4)-Zn(1)-N(2)#1	117.83(15)
O(2)-Zn(1)-N(2)#1	97.82(15)	O(4)-Zn(1)-N(1)	101.55(15)
O(2)-Zn(1)-N(1)	95.74(15)	N(2)#1-Zn(1)-N(1)	102.82(15)

[a] Symmetry codes for **1**: #1 = $-x + 2, -y + 1, -z + 1$; [b] Symmetry codes for **2**: #1 = $x + 3, -y + 1, -z + 1$.

Table S2. Hydrogen-bonding geometry (Å, °) for complex **1**.

D-H···A	d(H···A)	d(D···A)	∠D-H···A
O1W-H1WB···O2	2.13	2.898(4)	150
O1W-H1WC···O3	2.42	2.899(4)	115
O2W-H2WA···O1W	2.33	2.775(5)	113
O2W-H2WB···O1W	2.49	2.775(5)	101

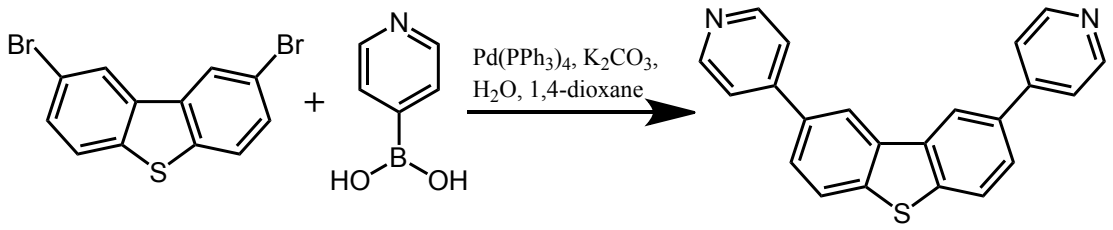

Fig. S1. Synthetic reaction of DPDBT

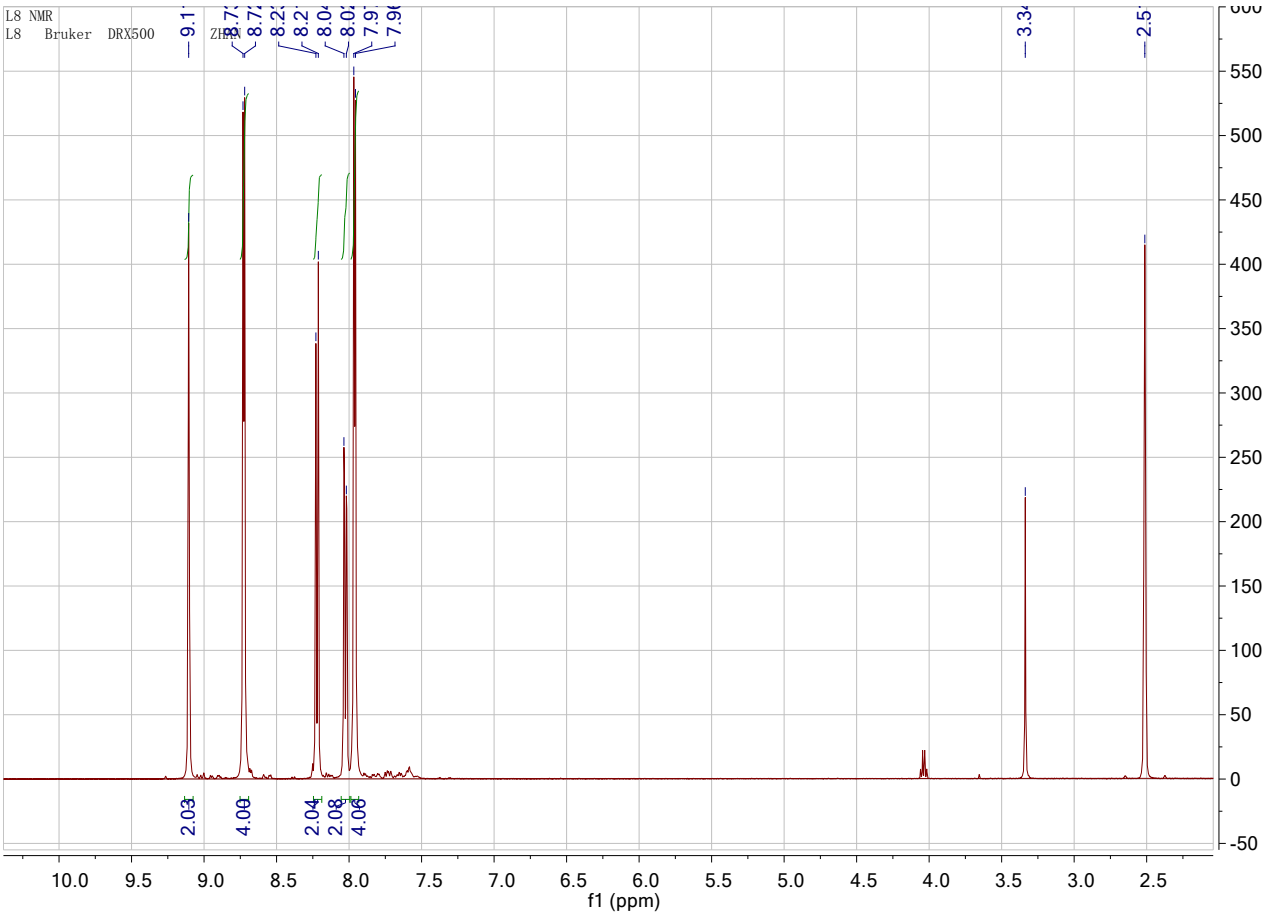

Fig. S2. ^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of DPDBT.

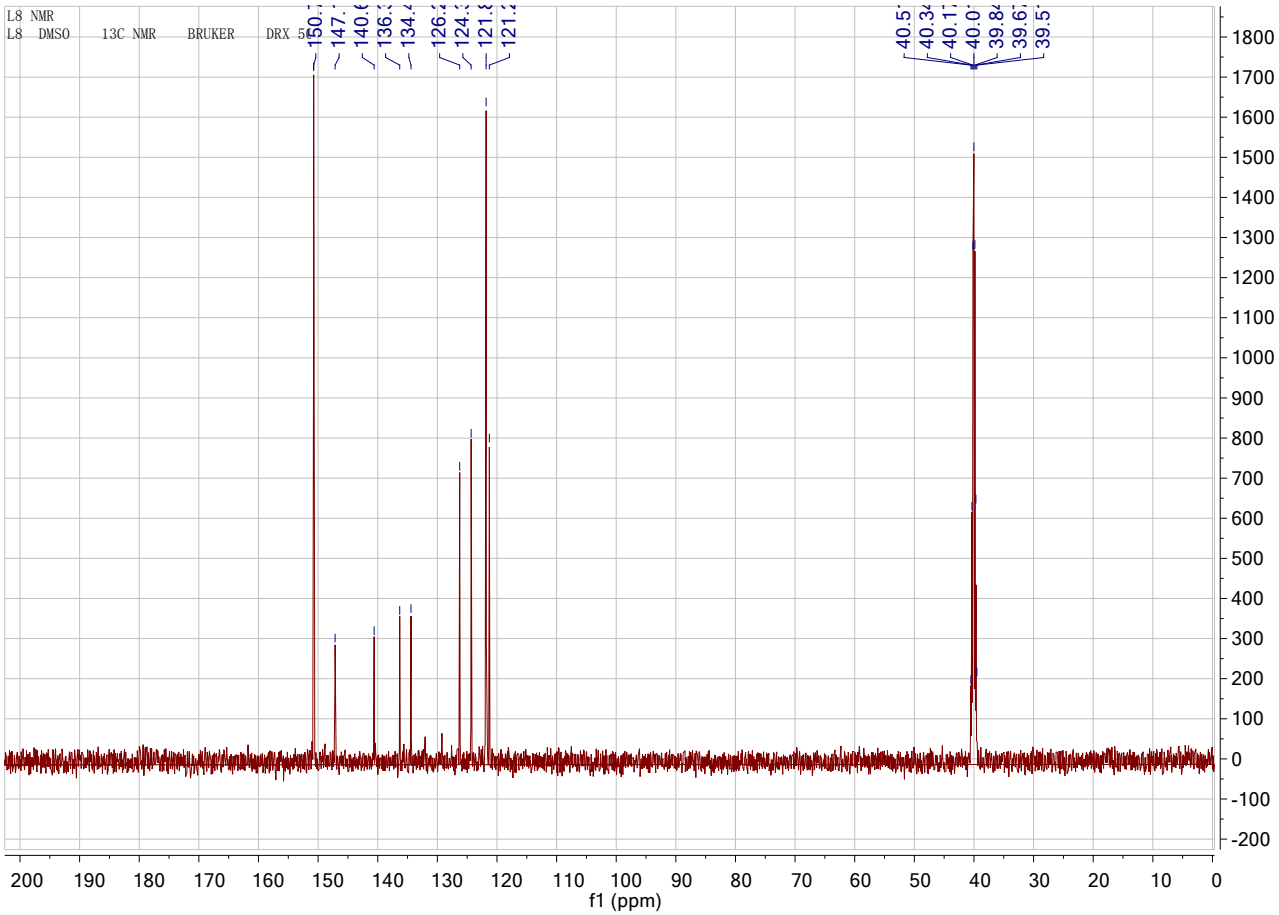

Fig. S3. ^{13}C NMR (DMSO-d_6, 125 MHz) spectrum of DPDBT.

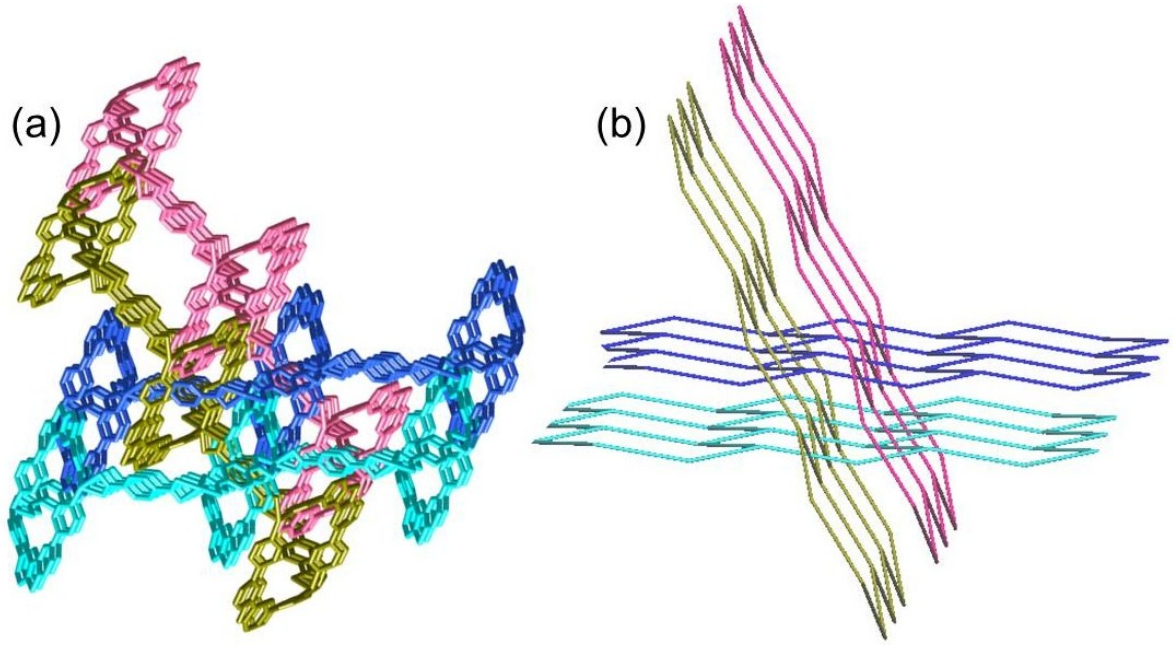

Fig. S4. (a) A view of the packing drawing of **1** along the direction parallel to the two sets of networks. (b) Simplified networks (6, 3) nets with ***hcb*** topology of **1**.

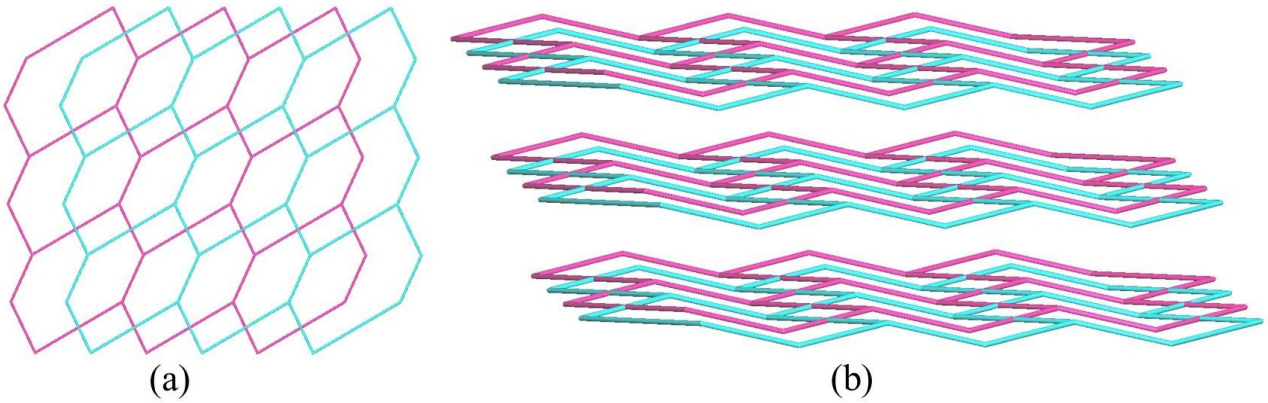

Fig. S5. (a) Simplified 2-fold interpenetrating 2D hcb network. (b) Packing drawing of the (6, 3) nets with ***hcb*** topology of **2**.

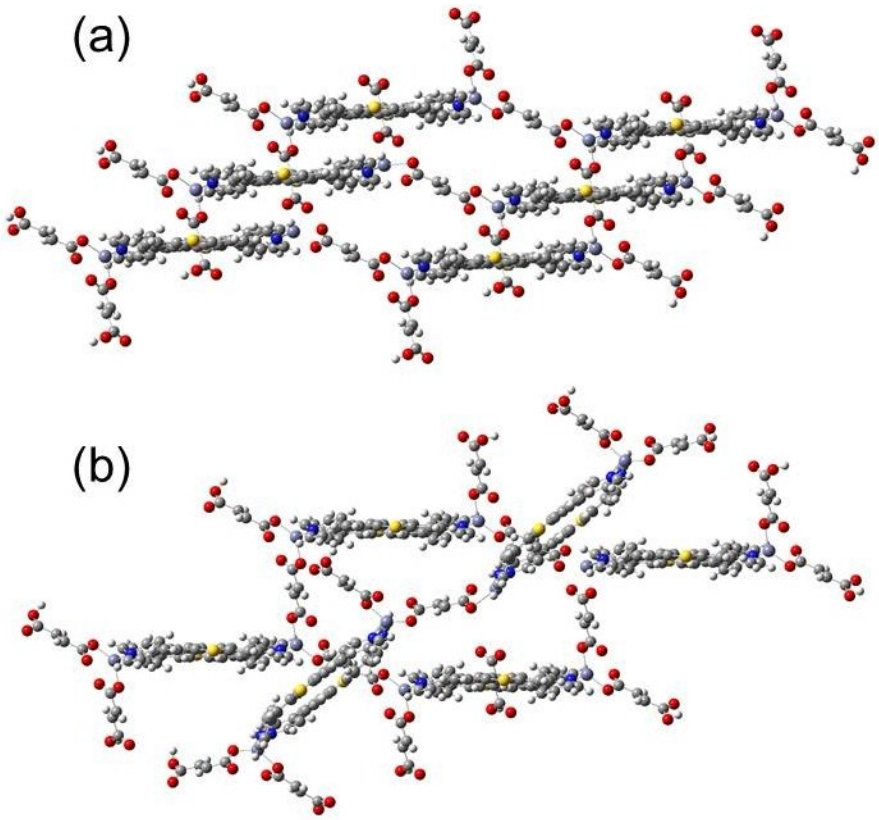

Fig. S6. (a) Parallel interlocking mode of complex **2**. (b) Inclined interlocking mode of complex **2**.

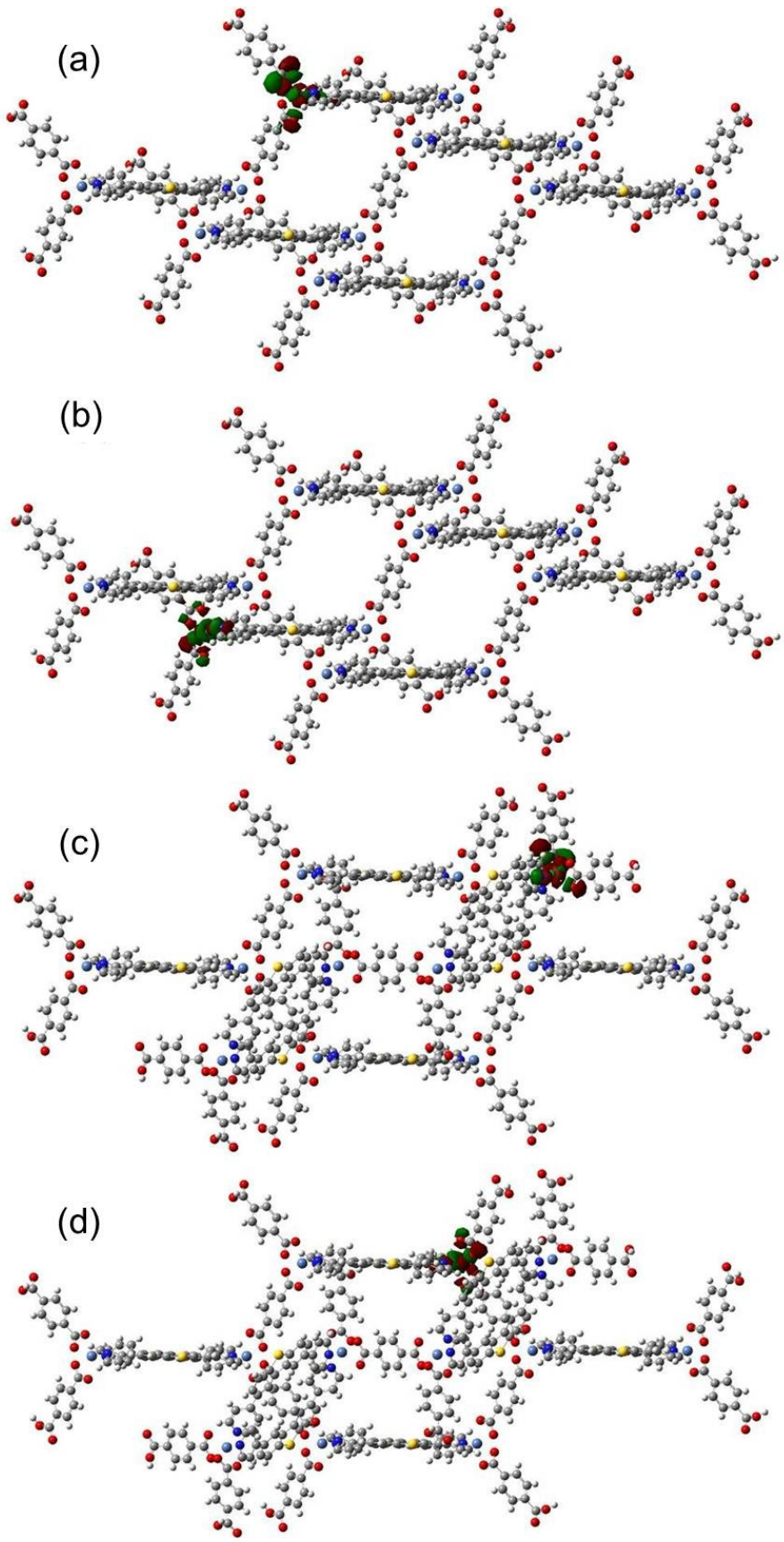

Fig. S7. Frontier molecular orbitals of networks **1**: HOMO (a) and LUMO (b) with simulative parallel interlocking mode, HOMO (c) and LUMO (d) with inclined interlocking mode.

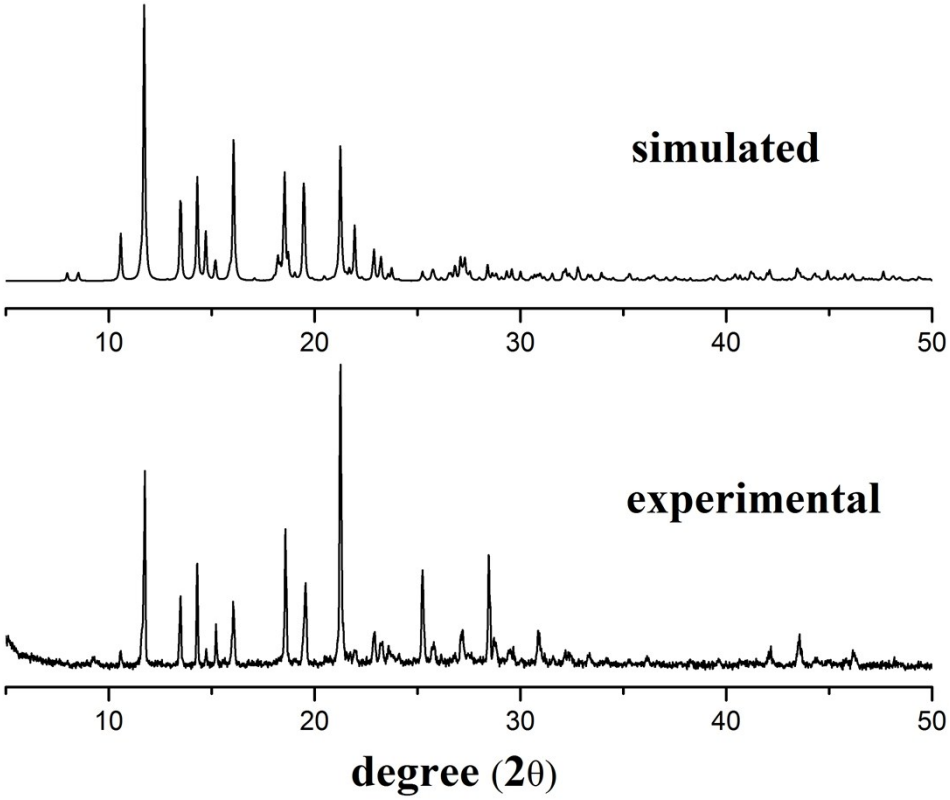

Fig. S8. Simulated and experimental PXRD plots of complex **1**.

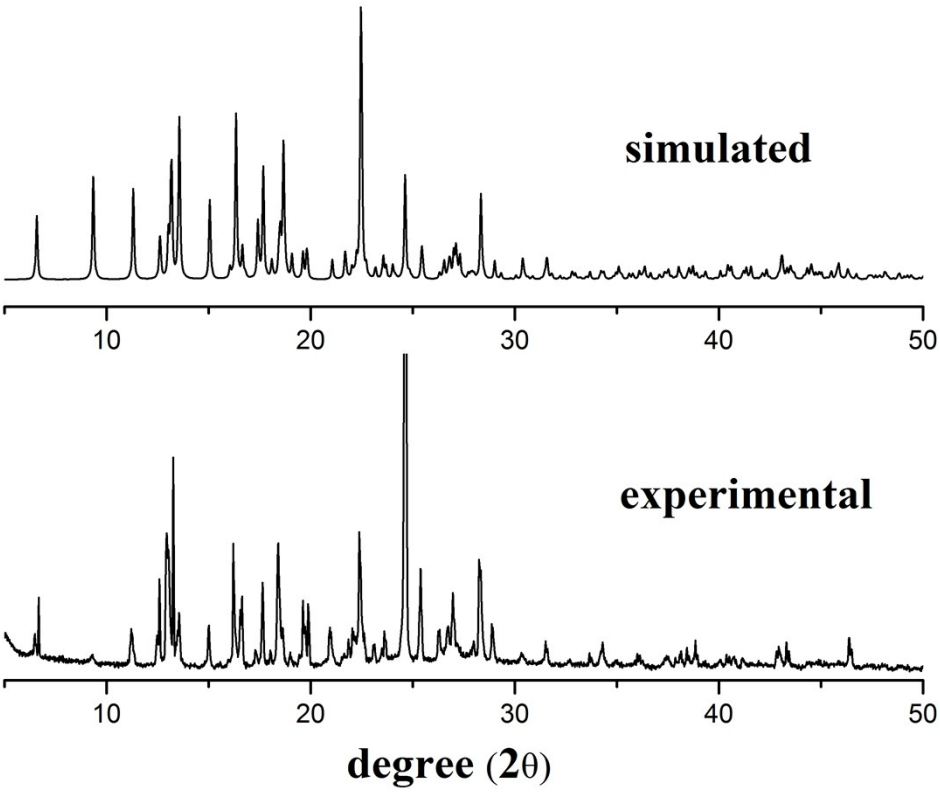

Fig. S9. Simulated and experimental PXRD plots of complex **2**.

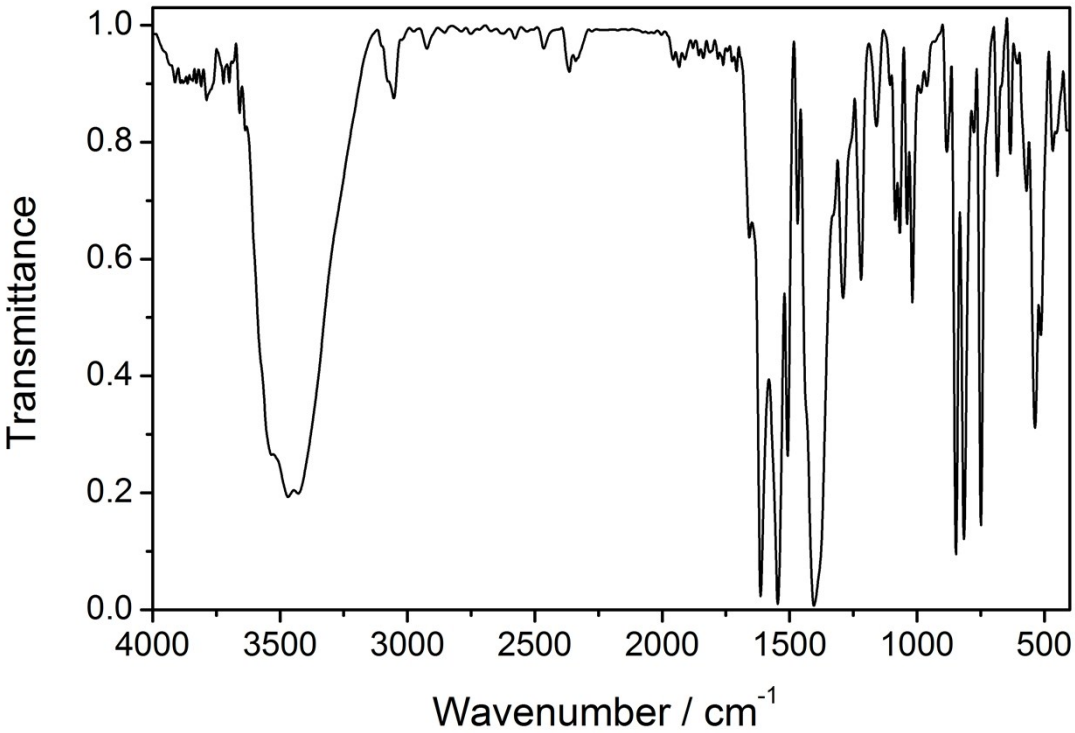

Fig. S10. IR spectrum of **1** at room temperature.

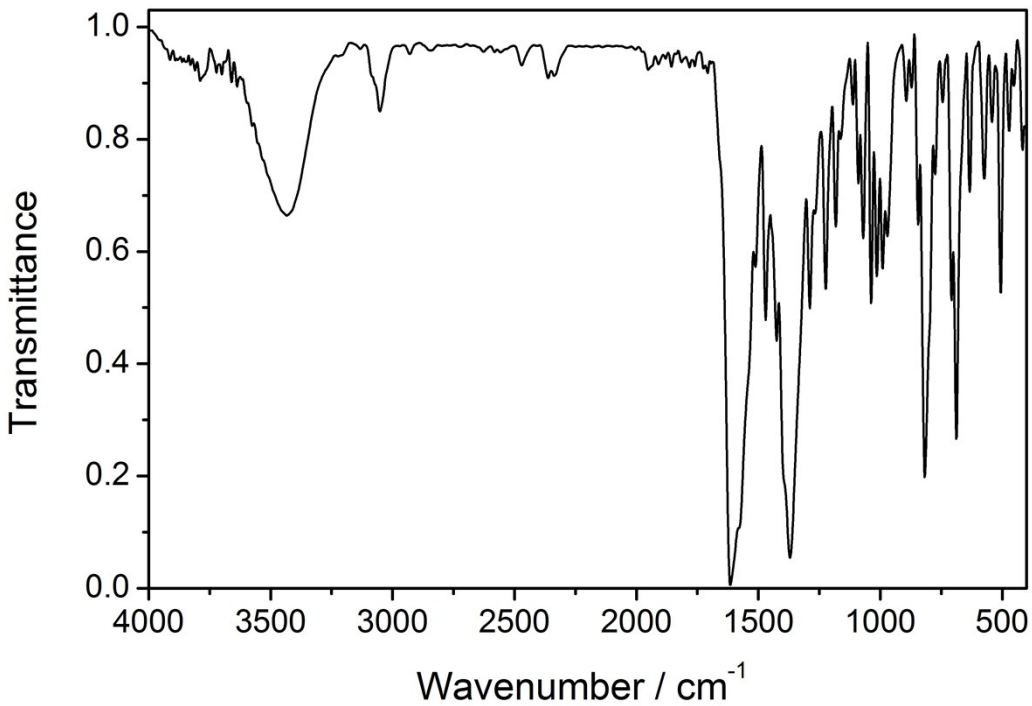

Fig. S11. IR spectrum of **2** at room temperature.