Supporting Information

Structural Transformation of Copper Coordination Complexes with Inducing Supramolecular Chirality

Zhongkui Li,[1, a] *Hao Su,*[1, a] *Yanhong Zhu,*[a] *Li Yan*[a, b] *and Hui Li*[a,]*

[a] Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, P. R. China

[b] Analytical and Test Center, Beijing institute of Technology, Liangxiang Campus, Liangxiang East Road, Beijing 102488, P. R. China

[1] Zhongkui Li and Hao Su contribute equally to the article.

*E-mail: lihui@bit.edu.cn

Contents

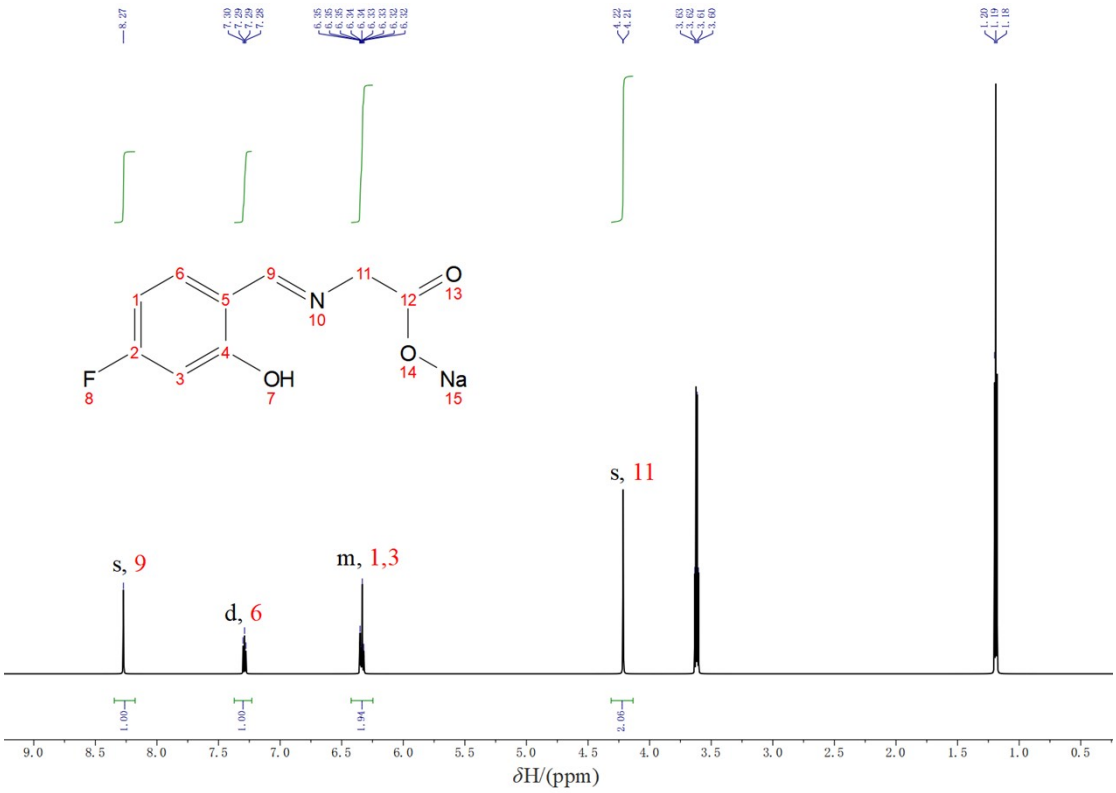

Fig. S1. [1]H-NMR spectra of **NaHL**.

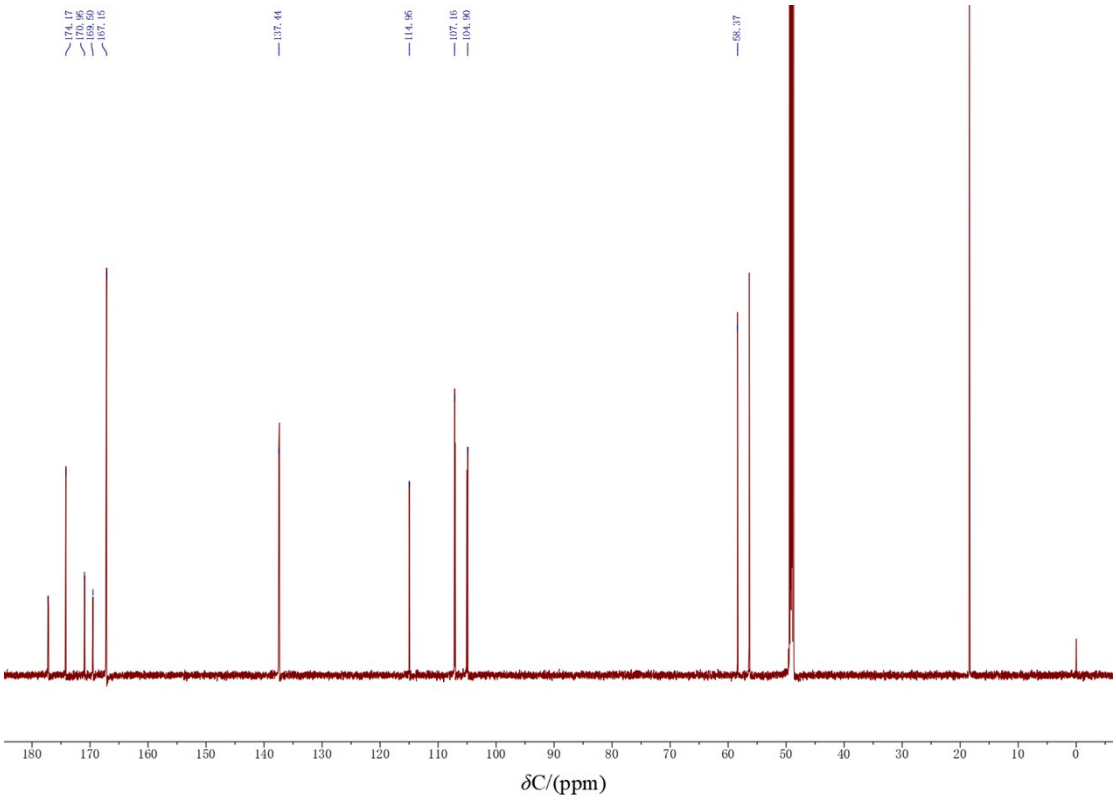

Fig. S2. [13]C-NMR spectra of **NaHL**.

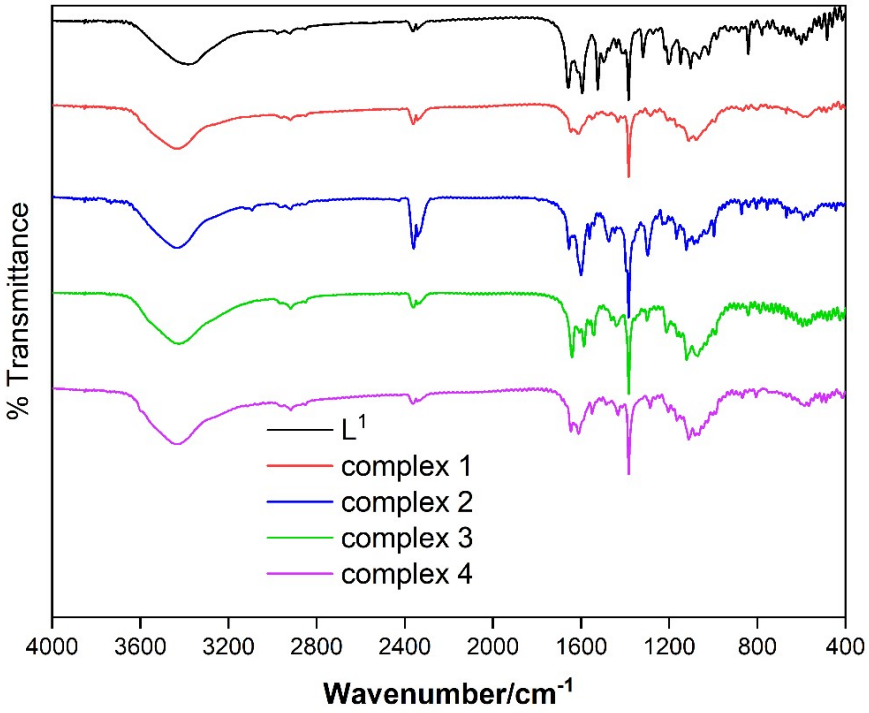

Fig. S3. FT-IR spectra of **NaHL**, complex **1**, complex **2**, complex **3** and complex **4**.

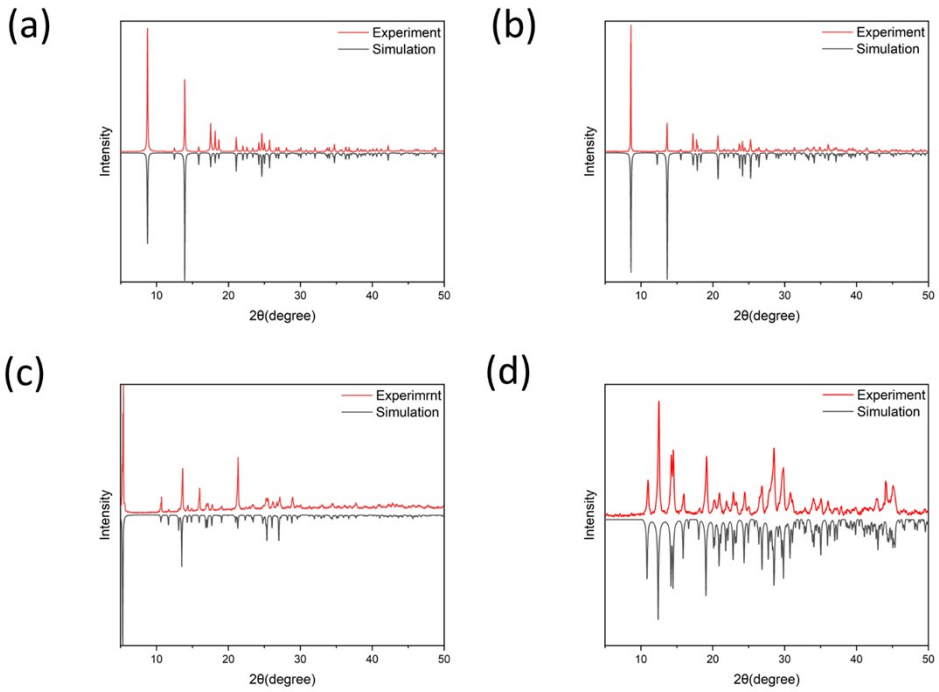

Fig. S4. PXRD spectra of complex **1** (a), complex **2** (b), complex **3** (c) and complex **4** (d) together.

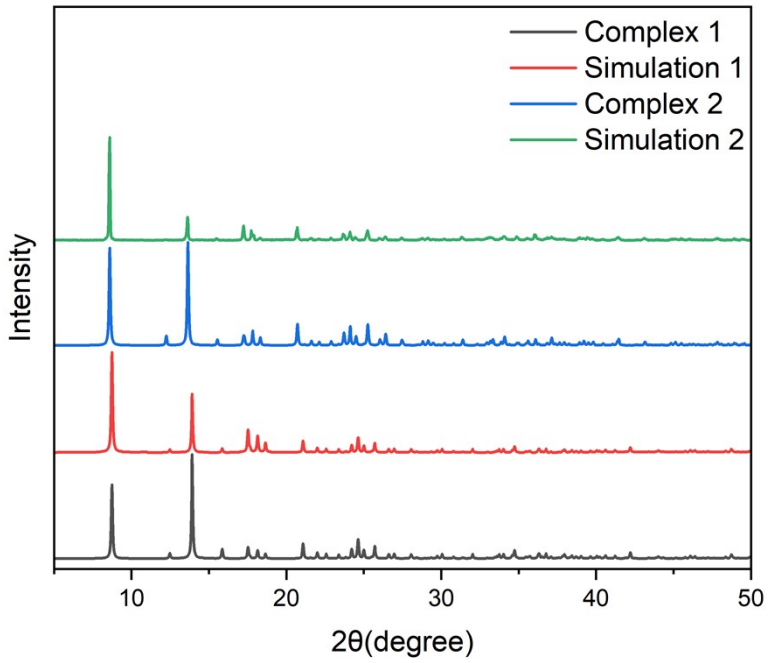

Fig. S5. PXRD spectra of complex **2** and complex **1** together.

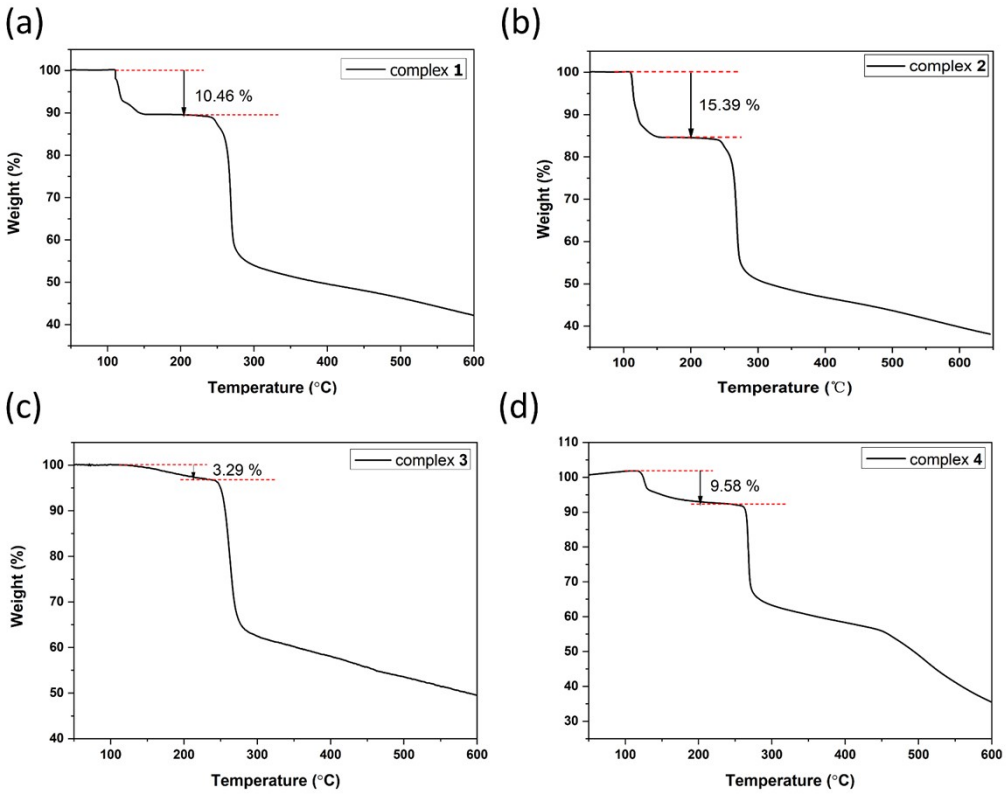

Fig. S6. TG curves of complex **1**, complex **2**, complex **3** and complex **4**. The losses of **1**, **2**, **3** and **4** in the first stage were 10.46 %, 15.39 %, 3.29 % and 9.58 % respectively.

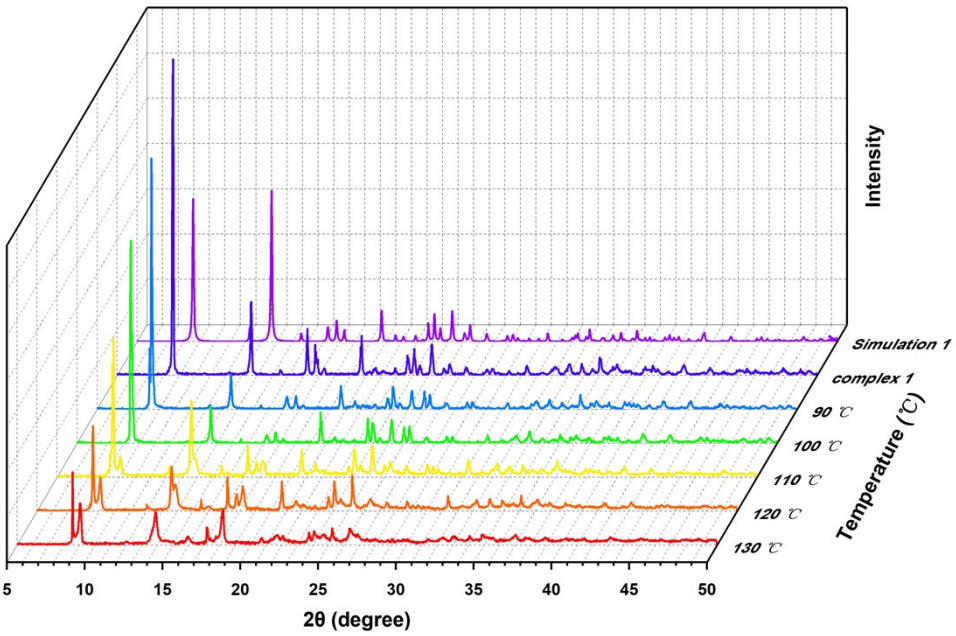

Fig. S7. PXRD curves of **1** changed with temperature.

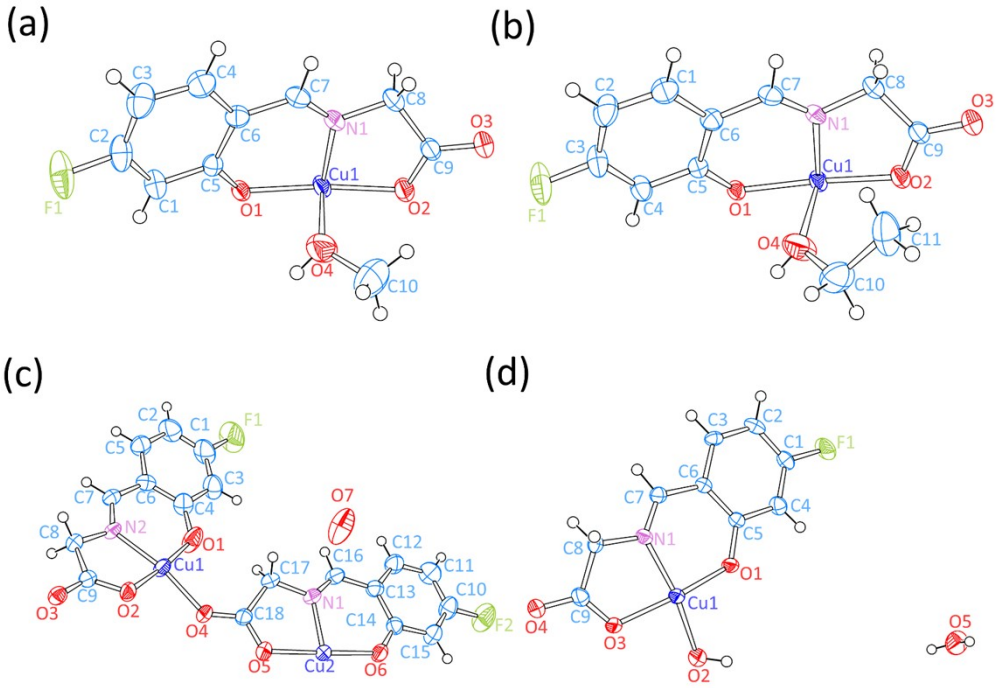

Fig. S8. Oak Ridge thermal ellipsoid plot (ORTEP) views of complexes **1**, **2**, **3**, **4** with 50% thermal ellipsoid probability.

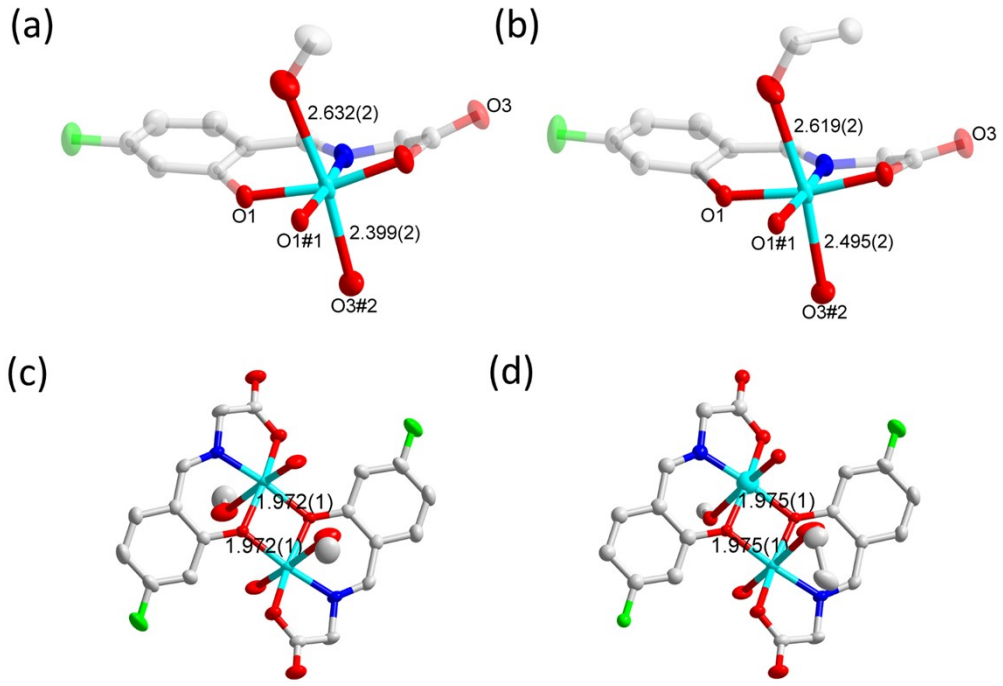

Fig. S9. The axial coordinate bond length in the asymmetric unit of complexes **1** (a) and **2** (b)**.** The binuclear structure and Bond length of bridging coordination bond in complexes **1** (c) and **2** (d). [1]1-X,1-Y,1-Z; [2]-1/2+X,1/2-Y,1-Z.

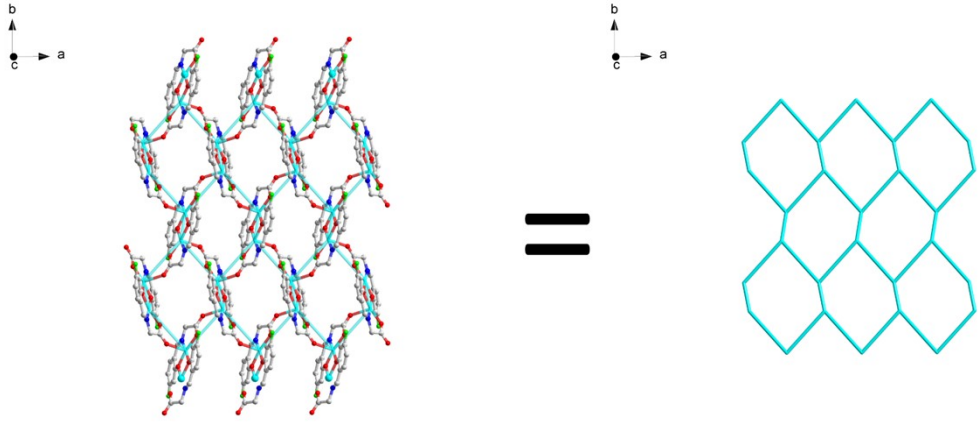

Fig. S10. Simplified honeycomb (hcb) nets of **1** viewed from *c* axis. All atoms except for copper are removed to simplify the structure.

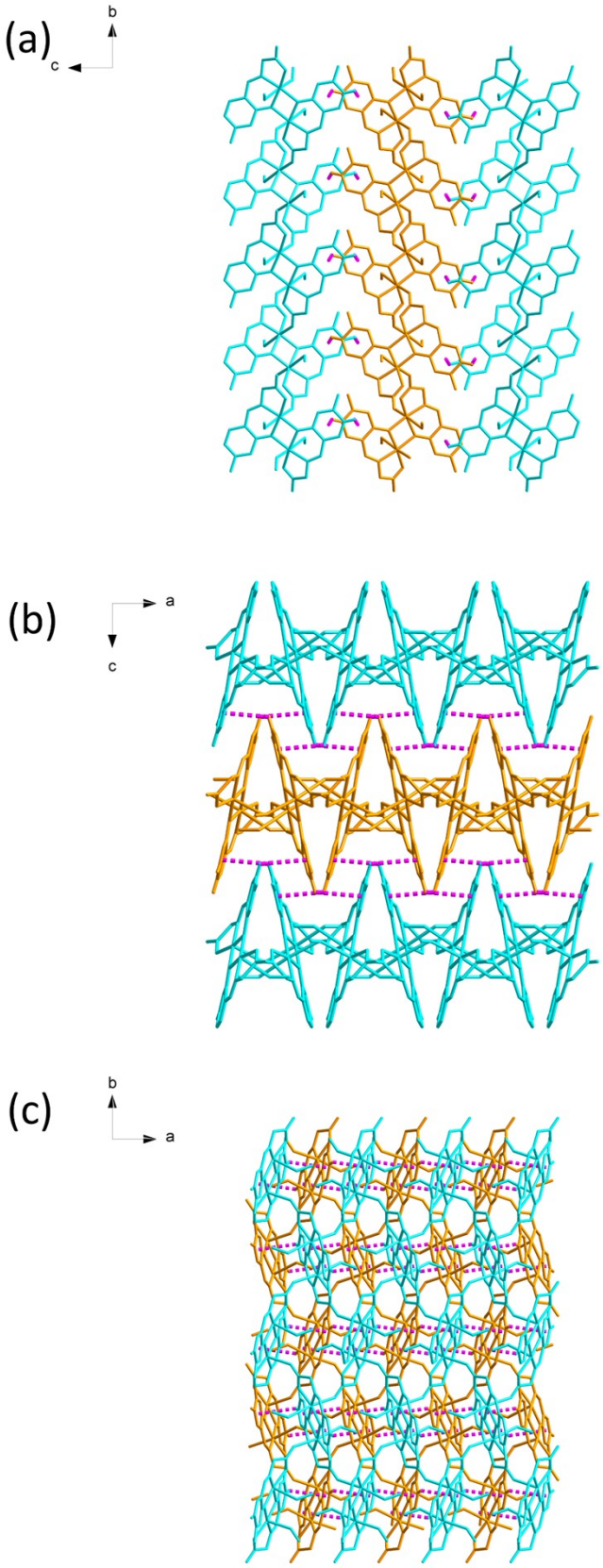

Fig. S11. 3D structure of **1** viewed from *a* axis (a), from *b* axis (b) and from *c* axis (c).(van der Waals C-H…π interactions (3.241(0) Å)

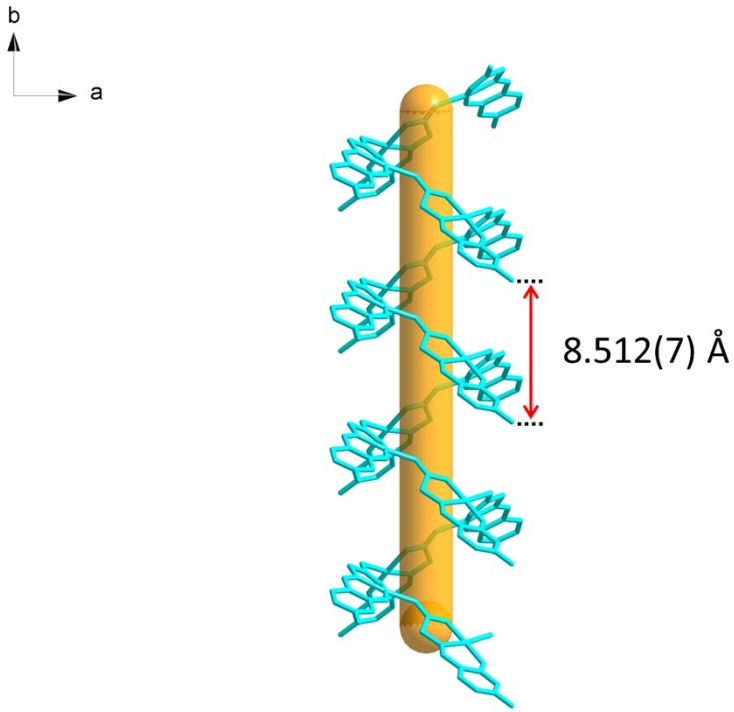

Fig. S12. M-helix structure with a pitch of 5 in complex **3**.

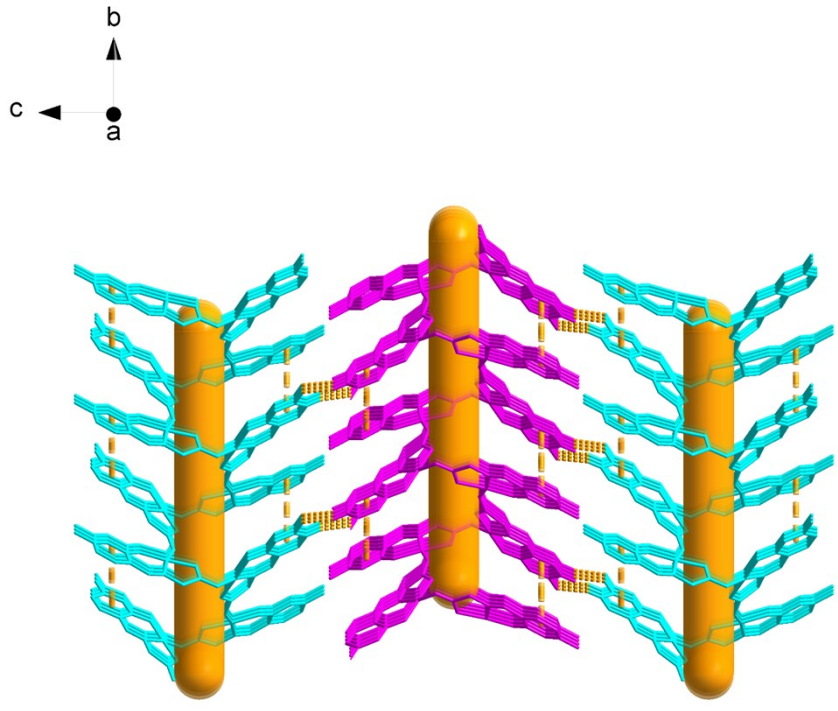

Fig. S13. 3D structures of complex **3** viewed from *a* axis (C11-H11…F2, 0.93 Å, 2.37 Å, 3.208(7) Å, 150.7°).

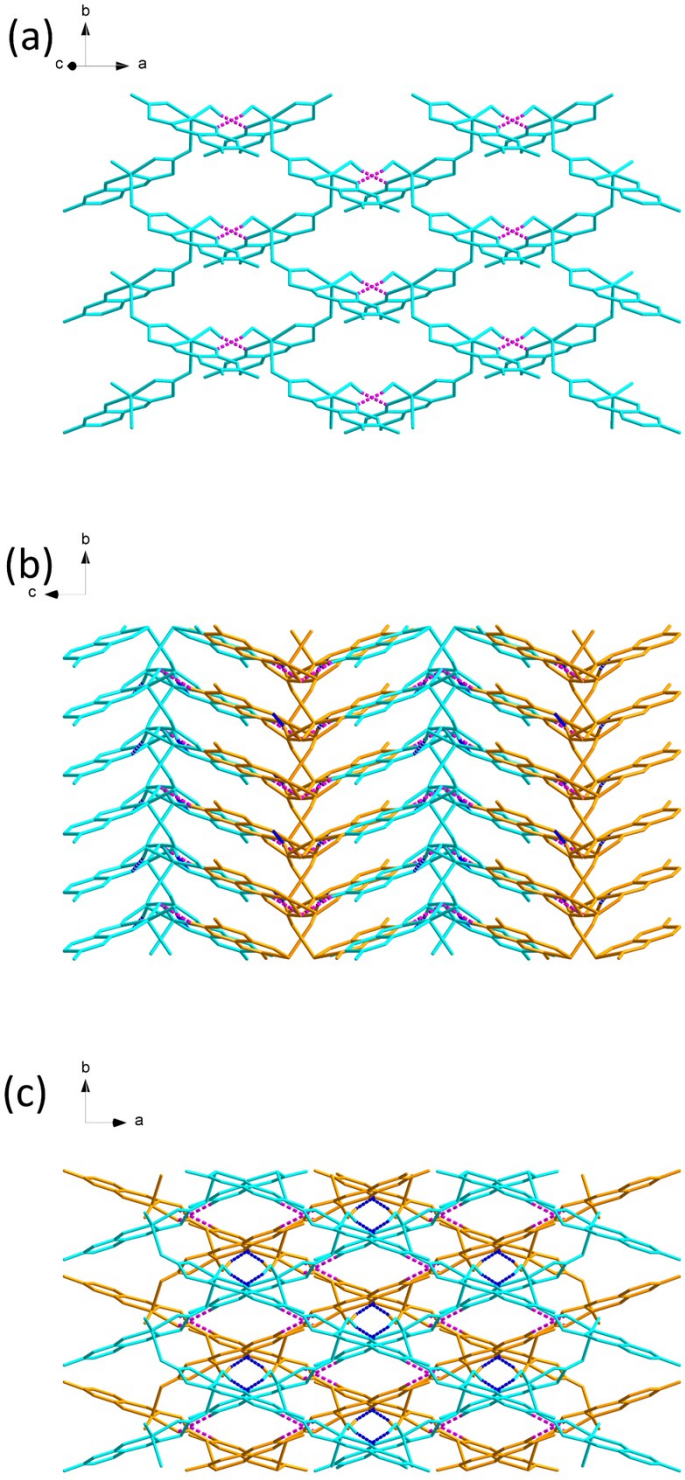

Fig. S14. 2D structure of **4** connected by hydrogen binding(a). 3D structure of **4** viewed from *a* axis (b), from *c* axis (c).

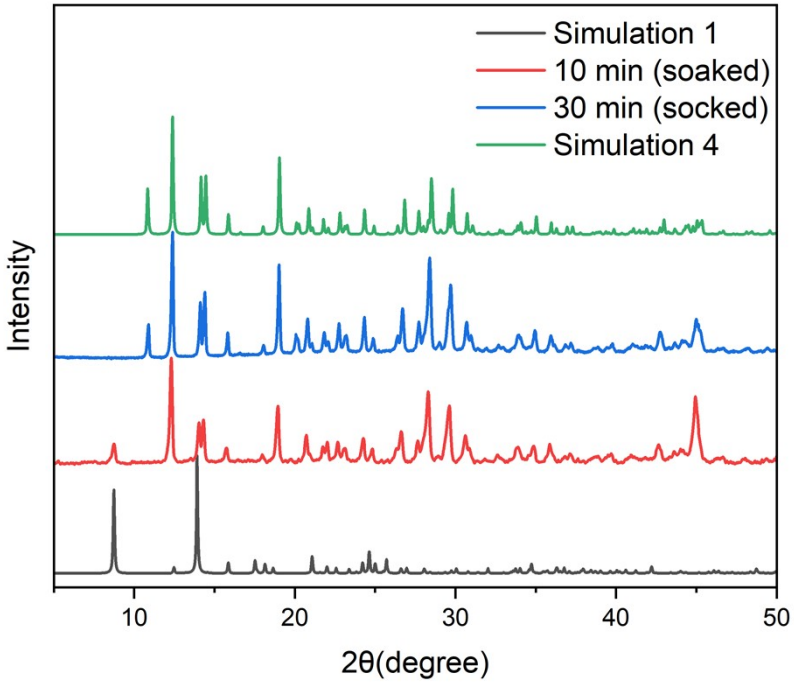

Fig. S15. PXRD patterns of structural transformation induced by water immersion from **1** to **4**.

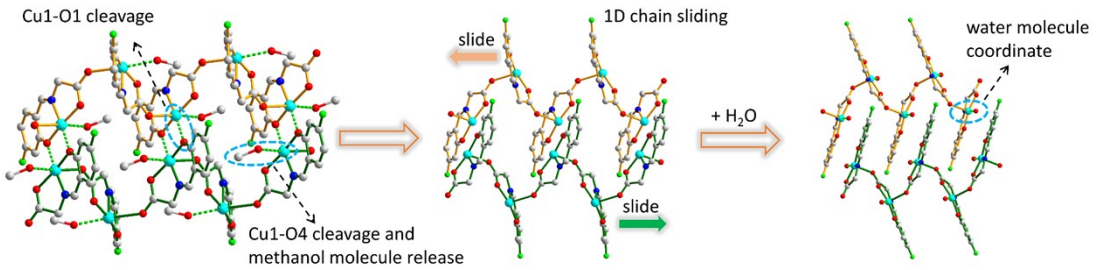

Fig. S16. The mechanism of structural transformation induced by water molecules from **1** to **4**.

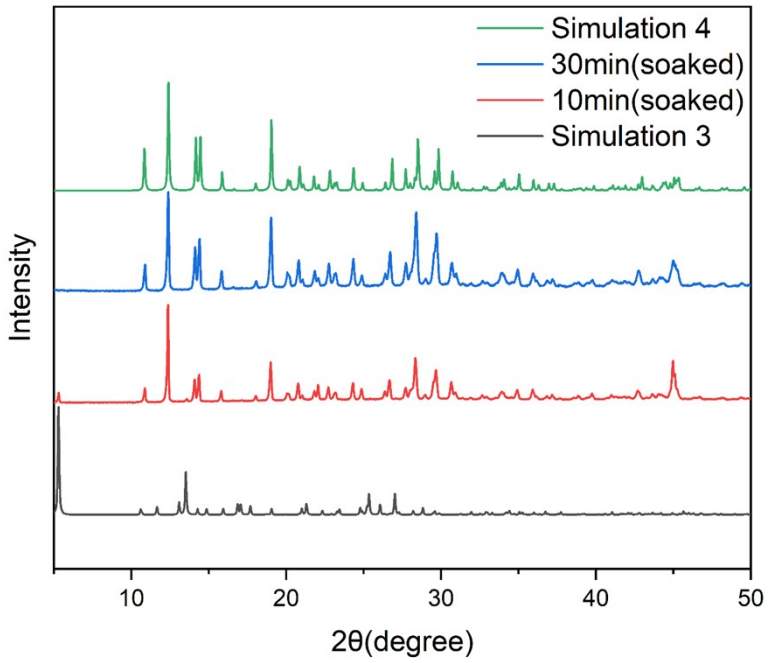

Fig. S17. PXRD patterns of structural transformation induced by water immersion from **3** to **4**.

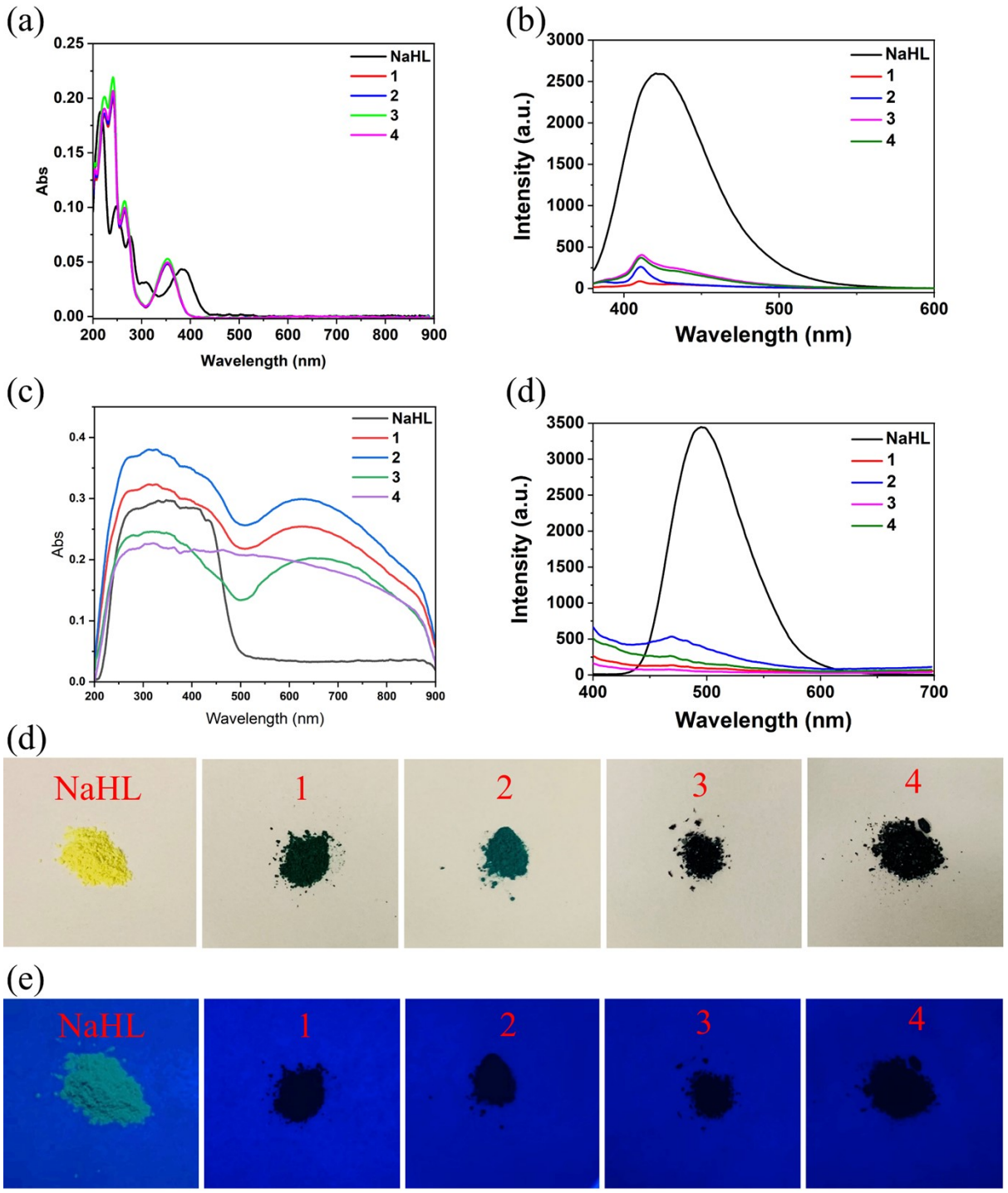

Fig. S18. UV-vis absorption spectra (a) and photoluminescence emission spectra (b) of NaHL, **1**, **2**, **3** and **4** in MeOH solution with a concentration of 1.0×10^{-5} M. Solid state UV-vis absorption spectra (c) and photoluminescence emission spectra (d) of NaHL, **1**, **2**, **3** and **4**. The color of NaHL, **1**, **2**, **3** and **4** under sunlight (d) and ultraviolet light (e). The excited wavelength of **1**, **2**, **3**, and **4** is 352nm in both liquid and solid stated, And the excited wavelength for NaHL is 384nm in both solid and liquid state.

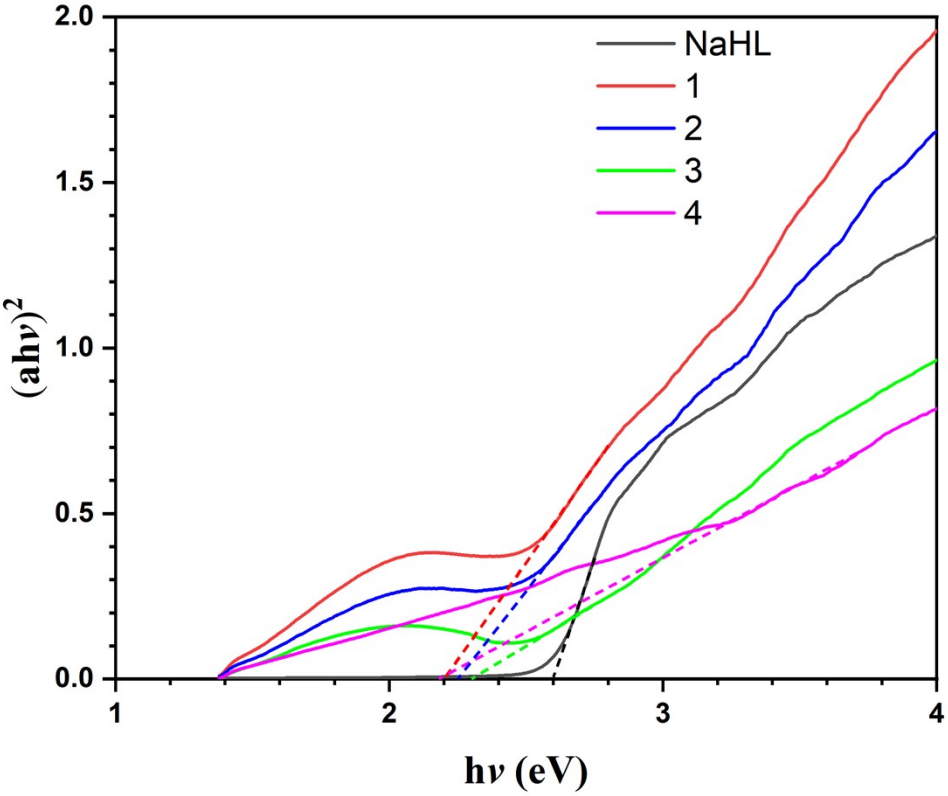

Fig. S19 Bandgap calculated using Kubelka-Munk's function. The bandgap of NaHL, **1**, **2**, **3**, and 4 are 2.60 eV, 2.20 eV, 2.25 eV, 2.31 eV, and 2.18 eV, respectively.

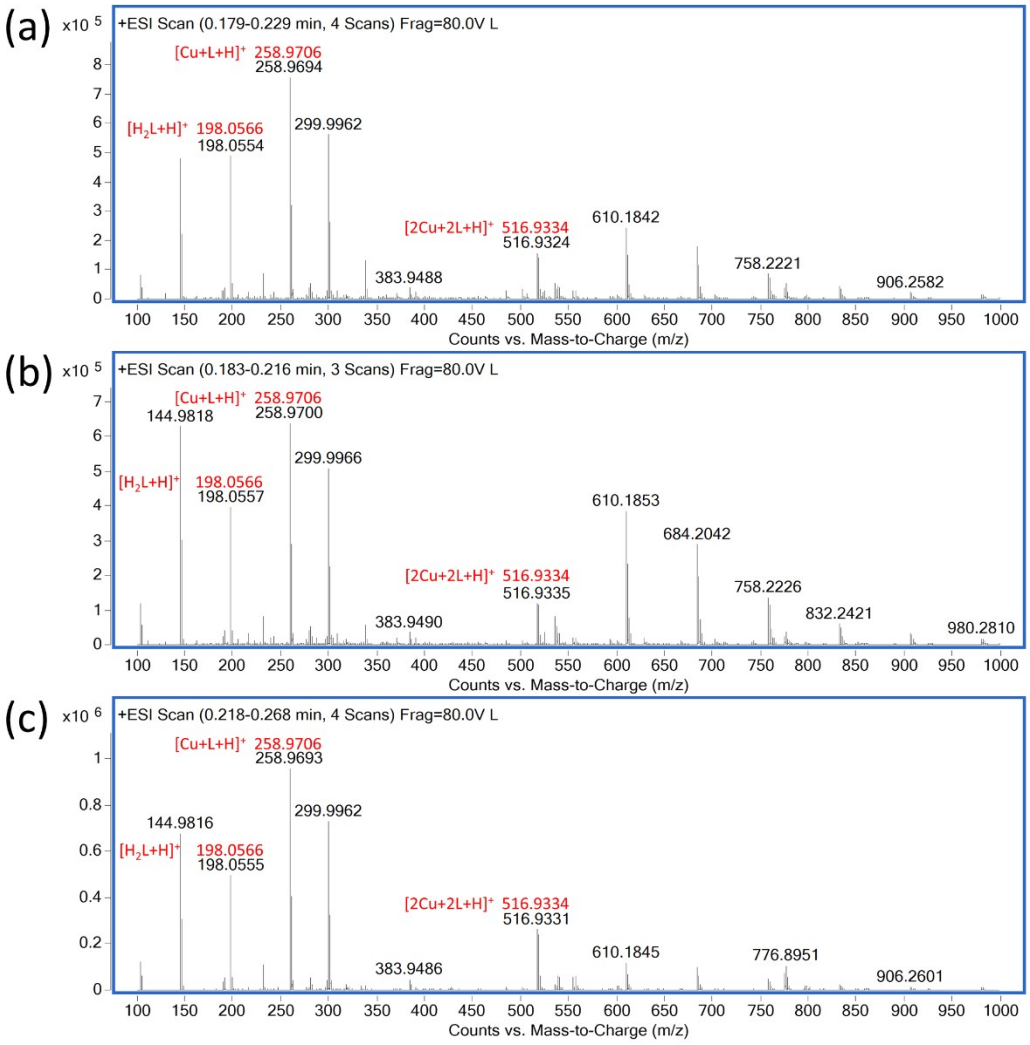

Fig. S20 ESI-MS spectra of complex **1** (a), complex **3** (b) and complex **4** (c)in methanol solution.

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

Atom-Atom	Bond length	Atom-Atom	Bond length
Cu1-Cu1[1]	3.022(0)	N1-C7	1.273(2)
Cu1-O1[1]	1.972(1)	N1-C8	1.450(2)
Cu1-O1	1.975(1)	O4-C10	1.382(3)
Cu1-O2	1.973(1)	C6-C7	1.439(3)
Cu1-O3[2]	2.399(2)	C6-C5	1.417(2)
Cu1-O4	2.632(2)	C6-C4	1.411(2)
Cu1-N1	1.920(2)	C5-C1	1.404(2)
O1-C5	1.335(2)	C9-C8	1.519(3)
O2-C9	1.270(2)	C1-C2	1.375(3)
O3-C9	1.235(2)	C4-C3	1.366(3)
F1-C2	1.364(2)	C2-C3	1.374(3)

[1]1-X,1-Y,1-Z; [2]-1/2+X,1/2-Y,1-Z

Atom-Atom-Atom	Bond Angles	Atom-Atom-Atom	Bond Angles
O1[1]-Cu1-Cu1[1]	40.06(3)	C7-N1-Cu1	126.26(13)
O1-Cu1-Cu1[1]	40.00(3)	C7-N1-C8	121.26(15)
O1[1]-Cu1-O1	80.06(5)	C8-N1-Cu1	112.06(12)
O1[1]-Cu1-O2	102.66(5)	C5-C6-C7	124.55(15)
O1-Cu1-O3[2]	94.41(5)	C4-C6-C7	116.00(16)
O11-Cu1-O3[2]	86.14(5)	C4-C6-C5	119.36(16)
O2-Cu1-Cu1[1]	141.18(4)	N1-C7-C6	126.16(16)
O2-Cu1-O1	166.81(6)	O1-C5-C6	122.25(14)
O2-Cu1-O3[2]	98.63(6)	O1-C5-C1	119.94(15)
O3[2]-Cu1-Cu1[1]	90.36(3)	C1-C5-C6	117.81(15)
N1-Cu1-Cu1[1]	133.25(5)	O2-C9-C8	116.51(15)
N1-Cu1-O1[1]	173.31(6)	O3-C9-O2	125.36(17)
N1-Cu1-O1	93.26(6)	O3-C9-C8	118.09(17)
N1-Cu1-O2	83.81(6)	C2-C1-C5	119.13(18)
N1-Cu1-O3[2]	94.64(6)	C3-C4-C6	122.36(19)
Cu1[1]-O1-Cu1	99.94(5)	F1-C2-C1	117.31(19)
C5-O1-Cu1	124.98(10)	F1-C2-C3	118.18(18)
C5-O1-Cu1[1]	132.13(10)	C3-C2-C1	124.51(18)
C9-O2-Cu1	114.49(11)	C4-C3-C2	116.56(17)
C9-O3-Cu1[3]	136.60(13)	N1-C8-C9	108.90(14)

[1]1-X,1-Y,1-Z; [2]-1/2+X,1/2-Y,1-Z; [3]1/2+X,1/2-Y,1-Z

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

Atom-Atom	Bond length	Atom-Atom	Bond length
Cu1-Cu1[1]	3.030(1)	N1-C8	1.463(2)
Cu1-O1	1.971(1)	C7-C6	1.447(3)
Cu1-O1[1]	1.975(1)	C6-C5	1.418(3)
Cu1-O2	1.964(1)	C6-C1	1.405(3)
Cu1-O3[2]	2.495(2)	C5-C4	1.405(3)
Cu1-O4	2.619(2)	C9-C8	1.516(3)
Cu1-N1	1.920(2)	C4-C3	1.373(3)
O1-C5	1.334(2)	C1-C2	1.367(3)
O2-C9	1.275(2)	C3-C2	1.377(3)
F1-C3	1.364(2)	C10-C11	1.479(4)
O3-C9	1.241(2)	C10-O4	1.396(3)
N1-C7	1.271(3)		

[1]1-X,1-Y,1-Z; [2]-1/2+X,1/2-Y,1-Z

Atom-Atom-Atom	Bond Angles	Atom-Atom-Atom	Bond Angles
O1[1]-Cu1-Cu1[1]	39.78(4)	C5-C6-C7	124.56(17)
O1-Cu1-Cu1[1]	39.88(4)	C1-C6-C7	116.12(18)
O1-Cu1-O1[1]	79.66(6)	C1-C6-C5	119.33(18)
O2-Cu1-Cu1[1]	142.30(4)	O1-C5-C6	122.41(17)
O2-Cu1-O1[1]	103.36(6)	O1-C5-C4	120.03(16)
O2-Cu1-O1	170.00(6)	C4-C5-C6	117.56(17)
N1-Cu1-Cu1[1]	133.16(5)	O2-C9-C8	116.62(17)
N1-Cu1-O1	93.33(6)	O3-C9-O2	124.98(19)
N1-Cu1-O1[1]	172.59(6)	O3-C9-C8	118.37(17)
N1-Cu1-O2	83.95(6)	C3-C4-C5	119.49(19)
Cu1-O1-Cu1[1]	100.33(6)	C2-C1-C6	122.7(2)
C5-O1-Cu1[1]	132.41(12)	F1-C3-C4	117.9(2)
C5-O1-Cu1	125.12(11)	F1-C3-C2	117.9(2)
C9-O2-Cu1	114.91(13)	C4-C3-C2	124.2(2)
C7-N1-Cu1	126.28(14)	N1-C8-C9	108.91(15)
C7-N1-C8	121.40(17)	C1-C2-C3	116.4(2)
C8-N1-Cu1	112.00(13)	O4-C10-C11	110.2(2)
N1-C7-C6	125.85(18)		

[1]1-X,1-Y,1-Z

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

Atom-Atom	Bond length	Atom-Atom	Bond length
Cu1-O1	1.889(3)	N2-C7	1.272(5)
Cu1-O2	1.963(3)	N2-C8	1.463(5)
Cu1-O4	1.960(3)	C1-C2	1.366(9)
Cu1-N2	1.937(3)	C1-C3	1.352(8)
Cu2-O3[1]	1.957(3)	C2-C6	1.371(7)
Cu2-O5	1.948(3)	C3-C4	1.429(7)
Cu2-O6	1.885(3)	C4-C5	1.412(7)
Cu2-N1	1.910(3)	C5-C6	1.397(6)
F1-C1	1.367(6)	C5-C7	1.440(6)
F2-C10	1.360(6)	C8-C9	1.503(6)
O1-C4	1.307(6)	C10-C11	1.376(7)
O2-C9	1.263(5)	C10-C13	1.358(6)
O3-C9	1.244(5)	C11-C12	1.355(8)
O4-C18	1.236(5)	C12-C15	1.418(6)
O5-C18	1.268(5)	C13-C14	1.399(6)
O6-C14	1.307(5)	C14-C15	1.422(6)
N1-C16	1.275(5)	C15-C16	1.435(6)
N1-C17	1.458(6)	C17-C18	1.525(6)

[1]1-X,-1/2+Y,3/2-Z

Atom-Atom-Atom	Bond Angles	Atom-Atom-Atom	Bond Angles
O1-Cu1-O2	172.67(17)	O1-C4-C3	117.8(5)
O1-Cu1-O4	95.64(15)	O1-C4-C5	125.2(4)
O1-Cu1-N2	93.22(15)	C5-C4-C3	117.0(5)
O4-Cu1-O2	88.24(12)	C4-C5-C7	122.1(4)
N2-Cu1-O2	83.63(13)	C6-C5-C4	119.8(4)
N2-Cu1-O4	169.29(14)	C6-C5-C7	118.0(4)
O5-Cu2-O3[1]	91.15(13)	C2-C6-C5	122.4(5)
O6-Cu2-O3[1]	89.96(13)	N2-C7-C5	125.1(4)
O6-Cu2-O5	178.27(15)	N2-C8-C9	109.1(3)
O6-Cu2-N1	94.62(14)	O2-C9-C8	118.6(4)
N1-Cu2-O3[1]	170.24(14)	O3-C9-O2	122.8(4)
N1-Cu2-O5	84.48(14)	O3-C9-C8	118.7(4)
C4-O1-Cu1	126.2(3)	F2-C10-C11	117.7(4)
C9-O2-Cu1	114.5(2)	C13-C10-F2	118.3(5)
C9-O3-Cu2[2]	109.3(3)	C13-C10-C11	124.0(5)
C18-O4-Cu1	136.4(3)	C12-C11-C10	117.0(5)
C18-O5-Cu2	115.2(3)	C11-C12-C15	122.4(5)
C14-O6-Cu2	125.7(3)	C10-C13-C14	120.2(5)
C16-N1-Cu2	125.4(3)	O6-C14-C13	118.1(4)
C16-N1-C17	120.7(4)	O6-C14-C15	124.3(4)
C17-N1-Cu2	113.4(3)	C13-C14-C15	117.6(4)
C7-N2-Cu1	126.4(3)	C12-C15-C14	118.8(4)
C7-N2-C8	120.5(4)	C12-C15-C16	118.3(4)
C8-N2-Cu1	112.8(2)	C14-C15-C16	122.9(4)
C2-C1-F1	117.2(6)	N1-C16-C15	125.3(4)
C3-C1-F1	118.0(6)	N1-C17-C18	108.8(3)
C3-C1-C2	124.8(5)	O4-C18-O5	121.8(4)
C1-C2-C6	116.7(5)	O4-C18-C17	121.4(4)
C1-C3-C4	119.3(5)	O5-C18-C17	116.8(4)

[1]1-X, -1/2+Y, 3/2-Z; [2]1-X, 1/2+Y, 3/2-Z

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

Atom-Atom	Bond length	Atom-Atom	Bond length
Cu1-O1	1.911(3)	N1-C8	1.459(5)
Cu1-O3	1.948(3)	C6-C3	1.408(5)
Cu1-O4[1]	2.335(4)	C6-C7	1.448(5)
Cu1-N1	1.923(4)	C6-C5	1.410(6)
Cu1-O2	1.998(4)	C3-C2	1.372(6)
F1-C1	1.352(5)	C9-C8	1.531(6)
O1-C5	1.324(5)	C1-C4	1.372(6)
O3-C9	1.263(6)	C1-C2	1.369(7)
O4-C9	1.239(5)	C5-C4	1.401(5)
N1-C7	1.283(5)		

[1]1/2-X, -1/2+Y, 1/2-Z

Atom-Atom-Atom	Bond Angles	Atom-Atom-Atom	Bond Angles
O1-Cu1-O3	166.14(14)	C3-C6-C5	119.4(4)
O1-Cu1-O4[1]	94.63(13)	C5-C6-C7	123.0(4)
O1-Cu1-N1	93.58(14)	C2-C3-C6	122.4(4)
O1-Cu1-O2	91.29(14)	N1-C7-C6	124.9(4)
O3-Cu1-O4[1]	99.10(14)	O3-C9-C8	116.8(4)
O3-Cu1-O2	87.84(14)	O4-C9-O3	125.3(4)
N1-Cu1-O3	84.45(14)	O4-C9-C8	117.9(4)
N1-Cu1-O4[1]	106.29(14)	F1-C1-C4	118.2(4)
N1-Cu1-O2	166.59(15)	F1-C1-C2	118.2(4)
O2-Cu1-O4[1]	85.73(16)	C2-C1-C4	123.6(4)
C5-O1-Cu1	126.8(2)	O1-C5-C6	124.4(3)
C9-O3-Cu1	115.4(3)	O1-C5-C4	118.1(4)
C9-O4-Cu1[2]	122.8(3)	C4-C5-C6	117.5(4)
C7-N1-Cu1	126.8(3)	N1-C8-C9	108.9(3)
C7-N1-C8	120.6(4)	C1-C4-C5	120.3(4)
C8-N1-Cu1	112.1(3)	C1-C2-C3	116.8(4)
C3-C6-C7	117.6(4)		

[1]1/2-X,-1/2+Y,1/2-Z; [2]1/2-X,1/2+Y,1/2-Z

Table S5. Selected Hydrogen bond for complex **1**.

	D-H	H…A	D…A	<(DHA)
O4-H4-O3[1]	0.82	1.98	2.788(2)	168.1
C7-H7-F1[2]	0.93	2.45	3.127(2)	129.3
C1-H1-O2[3]	0.93	2.35	3.099(2)	137.1
C8-H8B-O2[4]	0.97	2.53	3.275(2)	133.8

[1]3/2-X, 1/2+Y, +Z; [2]1/2-X, -1/2+Y, +Z; [3]1-X, 1-Y, 1-Z; [4]-1/2+X, 1/2-Y, 1-Z

Table S6. Selected Hydrogen bond for complex **2**.

	D-H	H…A	D…A	<(DHA)
C7-H7-F1[1]	0.93	2.53	3.180(3)	126.8
C4-H4-O2[2]	0.93	2.3	3.067(3)	140
O4-H4A-O3[3]	0.82	1.96	2.777(2)	170.9

[1]3/2-X,-1/2+Y,+Z; [2]1-X,1-Y,1-Z; [3]1/2-X,1/2+Y,+Z

Table S7. Selected Hydrogen bond for complex **3**.

	D-H	H…A	D…A	<(DHA)
C11-H11-F2[1]	0.93	2.37	3.208(7)	150.7

[1]1/2+X,3/2-Y,-Z;

Table S8. Selected Hydrogen bond for complex **4**.

	D-H	H…A	D…A	<(DHA)
C4-H4-O4[3]	0.93	2.57	3.444(6)	156.4
C2-H2-O3[4]	0.93	2.64	3.471(5)	148.6
O2-H2B-O1[1]	0.85	1.82	2.650(5)	165.1

[1]3/2-X, 1/2+Y, +Z; [2]1/2-X, -1/2+Y, +Z; [3]1-X, 1-Y, 1-Z; [4]-1/2+X, 1/2-Y, 1-Z