Electronic supplementary information (ESI)

A Series of 2D to 3D Metal Organic Frameworks Based on Different Polycarboxylate Anions and Flexible 2,2'-bis(1*H*-imidazolyl)ether Ligand

Lai-Ping Zhang, Jin Yang, Jian-Fang Ma,* Zhi-Fang Jia Yun-Peng Xie and Guo-Hua Wei

Key Lab of Polyoxometalate Science, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

* Correspondence author: Prof. Jian-Fang Ma

E-mail: jianfangma@yahoo.com.cn

Fax: +86-431-85098620

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

Ni(1)-N(1)	**2.0344(18)**	**Ni(1)-O(2)**	**2.0843(18)**
Ni(1)-O(1)	**2.1644(14)**		
N(1)-Ni(1)-N(1)$^{\#2}$	**88.24(10)**	**N(1)-Ni(1)-O(2)**	**95.93(7)**
N(1)-Ni(1)-O(1)	**157.98(6)**	**O(2)-Ni(1)-O(1)**	**62.09(5)**
O(1)-Ni(1)-O(1)$^{\#2}$	**93.72(8)**	**O(2)-Ni(1)-O(2)$^{\#3}$**	**161.07(8)**

Symmetry codes for **1**: $^{\#2}$ -x,y,3/2-z; $^{\#3}$ 1+x,-y,1/2+z

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

Cu(1)-N(1)	**1.965(3)**	**Cu(1)-O(1)**	**1.986(3)**
Cu(2)-O(5)	**1.982(2)**	**Cu(2)-N(4)**	**2.000(3)**
N(1)-Cu(1)-N(1)$^{\#1}$	**180**	**N(1)-Cu(1)-O(1)**	**89.83(12)**
O(1)-Cu(1)-O(1)$^{\#1}$	**180**	**O(5)$^{\#3}$-Cu(2)-O(5)**	**180**
O(5)-Cu(2)-N(4)	**89.46(11)**	**N(4)-Cu(2)-N(4)$^{\#3}$**	**180**

Symmetry codes for **2**: $^{\#1}$ 2-x,2-y,2-z; $^{\#3}$ 1-x,1-y,3-z

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

Cu(1)-O(1)	**1.991(2)**	**Cu(1)-N(4)$^{\#1}$**	**1.991(3)**
Cu(2)-O(4)	**1.978(2)**	**Cu(2)-N(1)$^{\#4}$**	**2.005(3)**
Cu(2)-O(3)	**2.599(2)**		
O(1) -Cu(1)-O(1)$^{\#3}$	**180**	**O(1)-Cu(1)-N(4)$^{\#1}$**	**91.44(10)**
O(1)$^{\#2}$-Cu(1)-N(4)$^{\#1}$	**88.56(10)**	**N(4)$^{\#1}$-Cu(1)-N(4)$^{\#2}$**	**180**
O(4)$^{\#4}$-Cu(2)-O(4)	**180**	**O(4)$^{\#4}$-Cu(2)-N(1)**	**88.91(11)**
O(4)$^{\#4}$-Cu(2)-N(1)$^{\#4}$	**91.09(11)**	**N(1) -Cu(2)-N(1)$^{\#4}$**	**180**

Symmetry codes for **3**: $^{\#1}$ 1/2-x,1/2+y,1/2-z; $^{\#2}$ -1/2+x,1/2-y,-1/2+z; $^{\#3}$ 1-x,-y,1-z; $^{\#4}$ -x,-y,-z

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

Co(1)-N(1)	**2.1281(18)**	**Co(1)-N(4)$^{\#1}$**	**2.1126(16)**
Co(1)-O(1)	**2.1030(14)**	**Co(1)-O(2)$^{\#2}$**	**2.1417(16)**
Co(1)-O(3)	**2.1137(14)**	**Co(1)-O(4)$^{\#3}$**	**2.1471(14)**

O(1)-Co(1)-N(4)$^{\#1}$	**97.54(6)**	**O(1)-Co(1)-O(3)**	**169.73(5)**
N(4)$^{\#1}$-Co(1)-O(3)	**89.69(6)**	**O(1)-Co(1)-N(1)**	**90.75(6)**
N(4)$^{\#1}$-Co(1)-N(1)	**94.26(7)**	**O(3)-Co(1)-N(1)**	**96.00(6)**
O(1)-Co(1)-O(2)$^{\#2}$	**78.53(5)**	**N(4)$^{\#1}$-Co(1)-O(2)$^{\#2}$**	**91.64(6)**
O(3)-Co(1)-O(2)$^{\#2}$	**94.04(6)**	**N(1)-Co(1)-O(2)$^{\#2}$**	**168.37(6)**
O(1)-Co(1)-O(4)$^{\#3}$	**94.66(6)**	**N(4)-Co(1)-O(4)$^{\#3}$**	**167.53(6)**
O(3)-Co(1)-O(4)$^{\#3}$	**94.56(6)**	**N(1)-Co(1)-O(4)$^{\#3}$**	**88.62(6)**
O(2)$^{\#2}$-Co(1)-O(4)$^{\#3}$	**87.76(6)**		

Symmetry codes for **4**: $^{\#1}$ 1-x,-y,1-z; $^{\#2}$ 1-x,-y,-z; $^{\#3}$ -x,-y,-z

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

Cu(1)-N(1)	**1.976(5)**	**Cu(1)-O(4)**	**2.006(4)**
Cu(1)-O(5)	**2.614(1)**	**Cu(2)-O(3)**	**2.596(1)**
Cu(2)-N(4)	**1.986(5)**	**Cu(2)-O(2)**	**2.030(4)**
N(1)-Cu(1)-N(1)$^{\#1}$	**180**	**N(1)-Cu(1)-O(4)**	**89.2(2)**
N(1)$^{\#1}$-Cu(1)-O(4)	**90.8(2)**	**O(4)$^{\#1}$-Cu(1)-O(4)**	**180**
N(4)$^{\#3}$-Cu(2)-N(4)	**180**	**N(4)$^{\#3}$-Cu(2)-O(2)**	**91.00(19)**
N(4)-Cu(2)-O(2)	**89.0(2)**	**O(2)-Cu(2)-O(2)$^{\#3}$**	**180**

Symmetry codes for **5**: $^{\#1}$ 1-x,2-y,1-z; $^{\#3}$ -x,2-y,-z

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

Co(1)-O(2)	**1.983(2)**	**Co(1)-O(5)$^{\#3}$**	**1.9980(19)**
Co(1)-N(1)$^{\#4}$	**2.033(2)**	**Co(1)-N(4)**	**2.014(3)**
Co(2)-O(9)$^{\#1}$	**1.980(2)**	**Co(2)-N(5)**	**2.021(3)**
Co(2)-O(6)	**2.018(2)**	**Co(2)-N(8)$^{\#2}$**	**2.022(3)**
O(2)-Co(1)-O(5)$^{\#3}$	**112.09(9)**	**O(2)-Co(1)-N(4)**	**121.33(10)**
O(5)$^{\#3}$-Co(1)-N(4)	**110.26(9)**	**O(2)-Co(1)-N(1)$^{\#4}$**	**104.15(9)**
O(5)$^{\#3}$-Co(1)-N(1)$^{\#4}$	**98.28(9)**	**N(4)-Co(1)-N(1)$^{\#4}$**	**107.86(10)**
O(9)$^{\#1}$-Co(2)-O(6)	**97.76(9)**	**O(9)$^{\#1}$-Co(2)-N(5)**	**105.45(10)**

O(6)-Co(2)-N(5)	**107.52(10)**	**O(9)$^{\#1}$-Co(2)-N(8)$^{\#2}$**	**112.21(10)**
O(6)-Co(2)-N(8)$^{\#2}$	**112.18(10)**	**N(5)-Co(2)-N(8)$^{\#2}$**	**119.36(11)**

Symmetry codes for **6**: $^{\#1}$ x,3/2-y,-1/2+z; $^{\#2}$ 2-x,1-y,1-z; $^{\#3}$ x,1/2-y,-1/2+z; $^{\#4}$ 1-x,-y,1-z

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

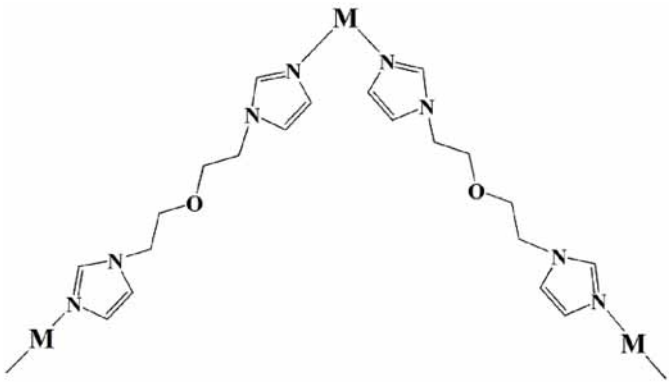
Cu(1)-O(4)	**1.936(2)**	**Cu(1)-O(5)**	**1.967(2)**
Cu(1)-O(6)	**1.973(2)**	**Cu(1)-N(4)**	**1.992(3)**
Cu(1)-O1W$^{\#1}$	**2.541(6)**	**Cu(2)-O3$^{\#2}$**	**2.456(4)**
Cu(2)-O6$^{\#3}$	**2.533(8)**	**Cu(2)-O(1)**	**1.962(2)**
Cu(2)-O(5)$^{\#3}$	**1.9766(19)**	**Cu(2)-O(8)$^{\#4}$**	**1.952(2)**
Cu(2)-N(1)	**1.985(3)**	**Cu(3)-O(2)**	**1.985(2)**
Cu(3)-O(3)$^{\#7}$	**2.257(2)**	**Cu(3)-O(5)$^{\#6}$**	**1.978(2)**
O1W$^{\#1}$···O7	**2.643(5)**		
O(4)-Cu(1)-O(5)	**96.26(9)**	**O(4)-Cu(1)-O(6)**	**174.05(13)**
O(5)-Cu(1)-O(6)	**86.68(8)**	**O(4)-Cu(1)-N(4)**	**87.46(11)**
O(5)-Cu(1)-N(4)	**167.84(11)**	**O(6)-Cu(1)-N(4)**	**88.63(10)**
O(8)$^{\#4}$-Cu(2)-O(1)	**169.68(10)**	**O(8)$^{\#4}$-Cu(2)-O(5)$^{\#7}$**	**93.04(9)**
O(1)-Cu(2)-O(5)$^{\#7}$	**89.49(9)**	**O(8)$^{\#4}$-Cu(2)-N(1)**	**88.16(10)**
O(1)-Cu(2)-N(1)	**90.42(10)**	**O(5)$^{\#7}$-Cu(2)-N(1)**	**173.73(10)**
O(5)$^{\#7}$-Cu(3)-O(5)$^{\#6}$	**180**	**O(5)$^{\#7}$-Cu(3)-O(2)$^{\#5}$**	**88.75(9)**
O(5)$^{\#7}$-Cu(3)-O(2)	**91.25(9)**	**O(5)$^{\#6}$-Cu(3)-O(2)**	**88.75(9)**
O(2)$^{\#5}$-Cu(3)-O(2)	**180**	**O(5)$^{\#7}$-Cu(3)-O(3)$^{\#7}$**	**94.36(8)**
O(5)$^{\#6}$-Cu(3)-O(3)$^{\#7}$	**85.64(8)**	**O(2)$^{\#5}$-Cu(3)-O(3)$^{\#7}$**	**94.72(10)**
O(2)-Cu(3)-O(3)$^{\#7}$	**85.28(10)**	**O(5)$^{\#7}$-Cu(3)-O(3)$^{\#6}$**	**85.64(8)**
O(5)$^{\#6}$-Cu(3)-O(3)$^{\#6}$	**94.36(8)**	**O(2)$^{\#5}$-Cu(3)-O(3)$^{\#6}$**	**85.28(10)**
O(2)-Cu(3)-O(3)$^{\#6}$	**94.72(10)**	**O(3)$^{\#7}$-Cu(3)-O(3)$^{\#6}$**	**180**

Symmetry codes for **7**: $^{\#1}$ -1+x,1/2-y,1-z; $^{\#2}$ -x,-1/2+y,1/2-z; $^{\#3}$ x,1/2-y,-1/2+z; $^{\#4}$ 1/2+x,-1/2+y,1/2-z; $^{\#5}$ -x,-y,-z; $^{\#6}$ -x,-1/2+y,1/2-z; $^{\#7}$ x,1/2-y,-1/2+z

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

Cu(1)-N(4)$^{\#4}$	**1.992(5)**	**Cu(1)-O(1)**	**1.979(3)**
Cu(1)-O(2W)	**2.320(6)**	**Cu(2)-N(1)**	**1.966(5)**
Cu(2)-O(1W)	**1.957(4)**	**Cu(2)-O(4)$^{\#5}$**	**1.963(3)**
Cu(2)-O(5)	**1.948(4)**	**O1W···O6$^{\#2}$**	**2.803(5)**
O2W···O3$^{\#6}$	**2.870(6)**		
O(1)$^{\#3}$-Cu(1)-N(4)$^{\#4}$	**89.62(17)**	**O(1)-Cu(1)-N(4)$^{\#4}$**	**91.04(17)**
O(1)-Cu(1)-N(4)$^{\#1}$	**89.62(17)**	**N(4)$^{\#4}$-Cu(1)-N(4)$^{\#1}$**	**166.9(3)**
O(1)-Cu(1)-O(2W)	**87.10(12)**	**N(4)$^{\#4}$-Cu(1)-O(2W)**	**96.55(14)**
O(5)-Cu(2)-O(1W)	**91.00(17)**	**O(5)-Cu(2)-O(4)$^{\#5}$**	**171.88(16)**
O(1W)-Cu(2)-O(4)$^{\#5}$	**87.76(16)**	**O(5)-Cu(2)-N(1)**	**91.25(18)**
O(1W)-Cu(2)-N(1)	**173.1(2)**	**O(4)$^{\#5}$-Cu(2)-N(1)**	**90.92(18)**

Symmetry codes for **8**: $^{\#1}$ 1-x,1/2+y,3/2-z; $^{\#2}$ 1-x,y,3/2-z; $^{\#3}$ -x,y,3/2-z; $^{\#4}$ 1/2-x,1/2+y,z; $^{\#5}$ 3/2-x,-1/2+y,z; $^{\#6}$ 1/2-x,-1/2+y,z



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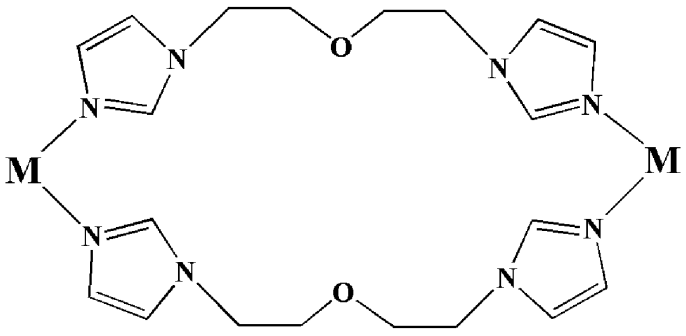
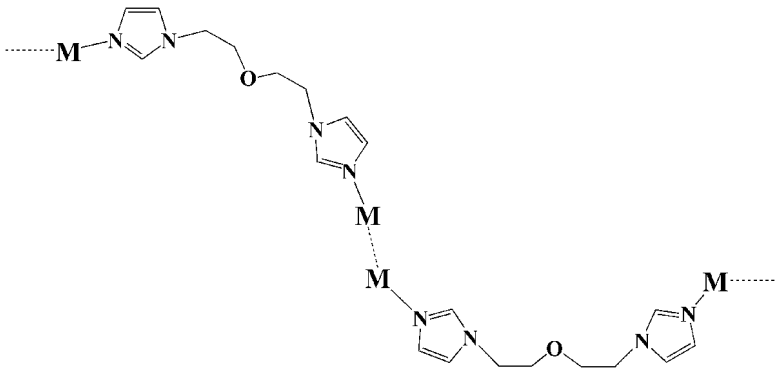
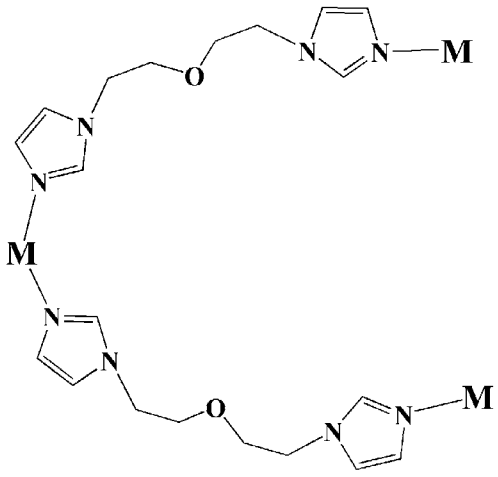


II

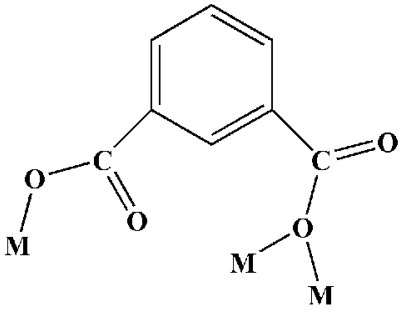


III

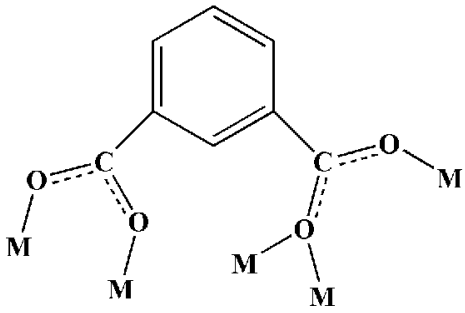


IV

Scheme S1. Four coordination modes of the BIE ligand with the metals in this paper.



I



II

Scheme S2. Coordination modes of L5 anion in compound 7.

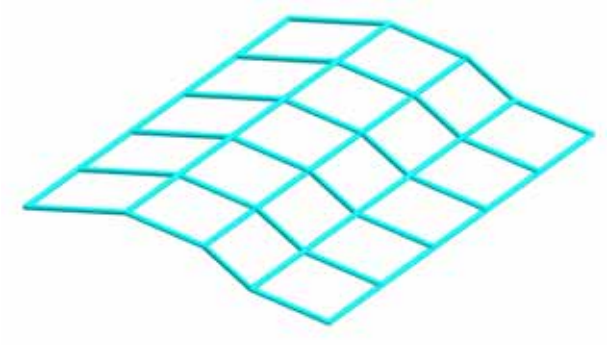


Fig. S1. View of the 2D 4^4-**sql** network of **1**.

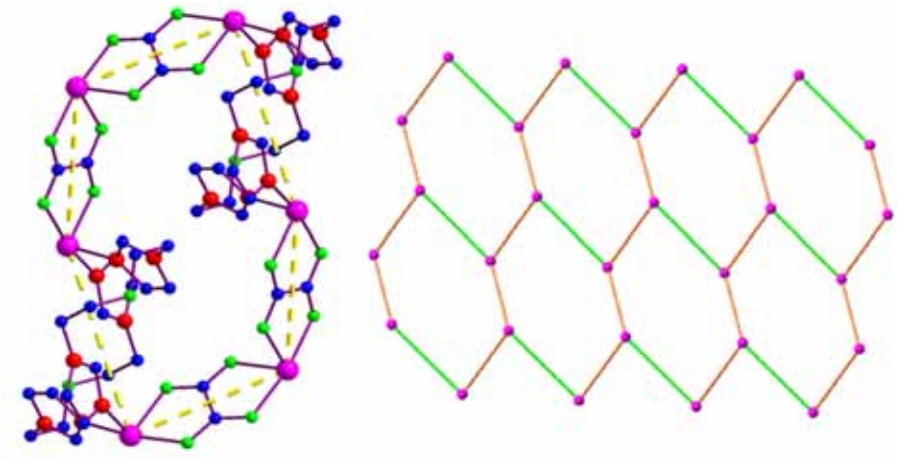


Fig. S2. One 6-membered ring is shown for each net shortest closed circuits, and the **hcb** net of compound **4**.

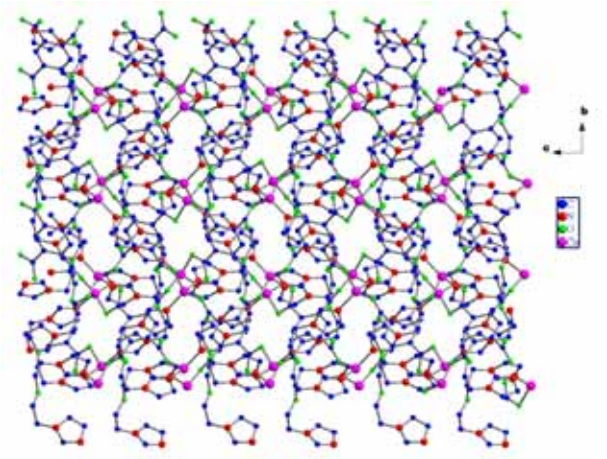


Fig. S3. The 3D complicated framework of compound **6**.

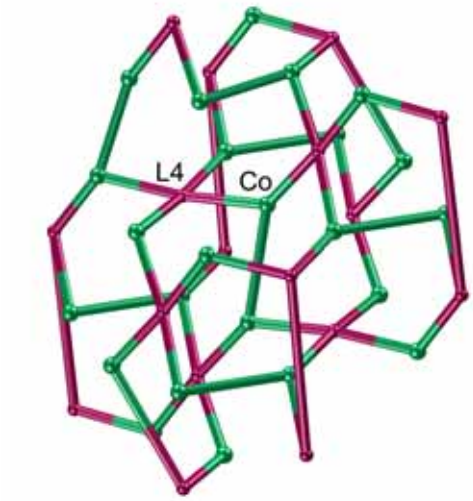


Fig. S4. Schematic diagram (OLEX) showing the $(8^3)_2(8^5{\cdot}10)$ network of **6**.

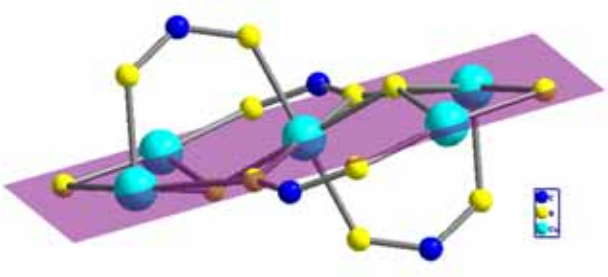


Fig. S5. View of the five coplanar Cu(II) atoms of compound **7**.

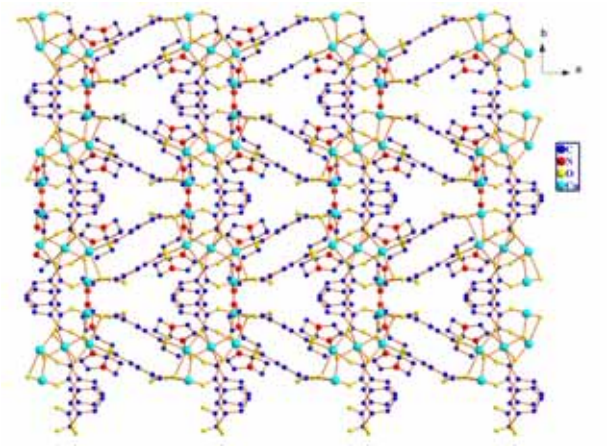


Fig. S6. View of the 3D complicated framework of **7**.

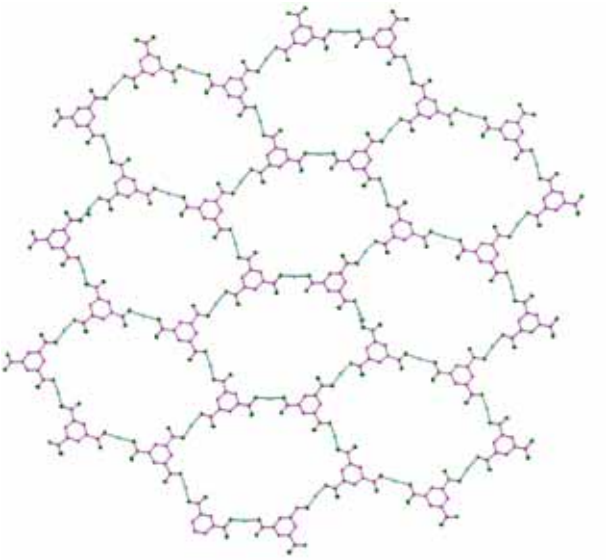


Fig. S7. View of a single layer composed of L6 anions and Cu(II) ions with 6^3 network within compound **8**.

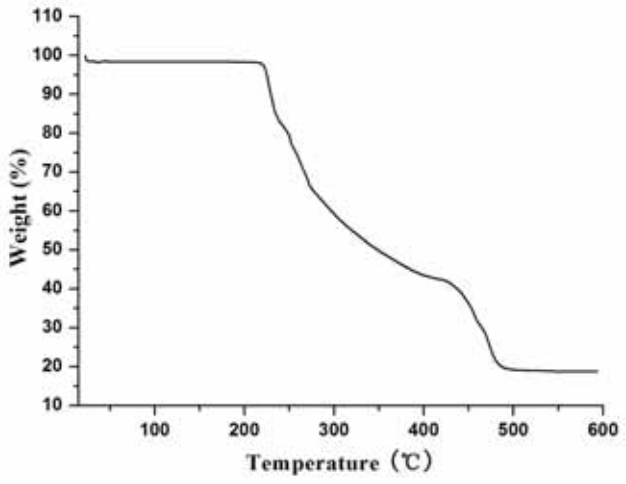


Fig. S8. TGA curve of **3**.

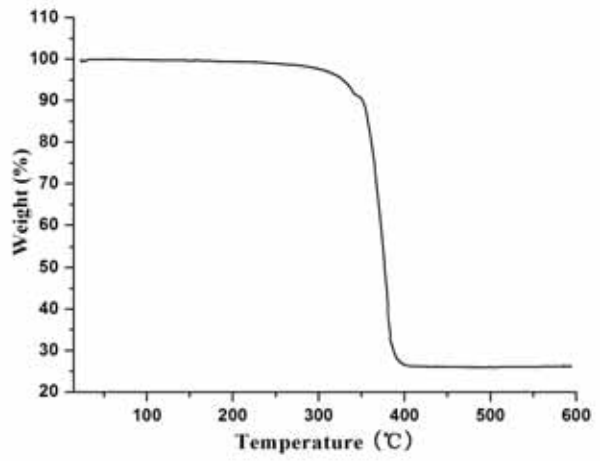


Fig. S9. TGA curve of **4**.

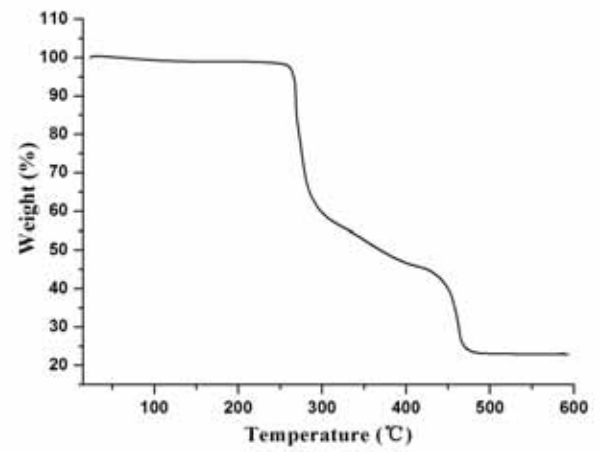


Fig. S10. TGA curve of **5**.

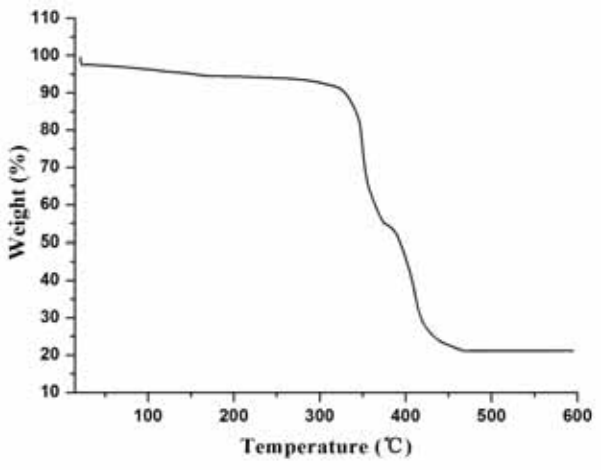


Fig. S11. TGA curve of **6**.

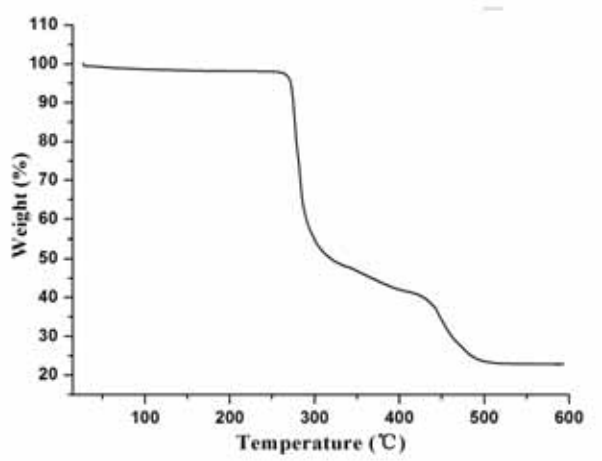


Fig. S12. TGA curve of **7**.

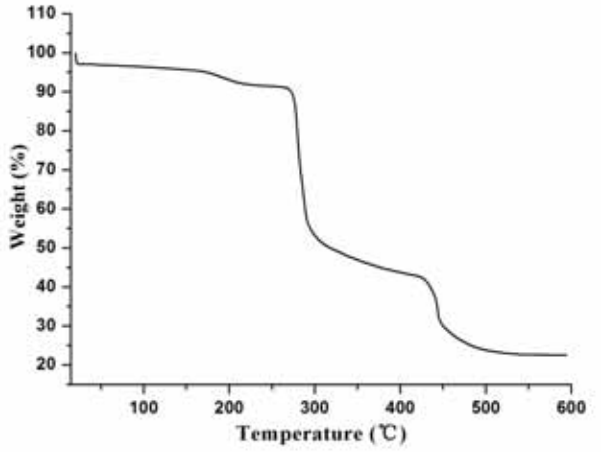


Fig. S13. TGA curve of **8**.