Heterometal-organic framework with *pcu* net constructed from mixed linear ligands

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Table S1 Selected bond lengths (Å) for compound **1**

Compound **1**			
La(1)-O(1)	2.620(8)	La(2)-O(27)	2.666(5)
La(1)-O(2)	2.547(7)	La(2)-O(28)B	2.634(5)
La(1)-O(21)	2.638(6)	La(2)-O(5)	2.649(8)
La(1)-O(22)	2.478(8)	La(2)-O(6)	2.572(8)
La(1)-O(23)A	2.640(6)	La(2)-O(9)	2.576(7)
La(1)-O(24)A	2.698(5)	Cu(1)-N(3)	2.020(8)
La(1)-O(3)	2.594(7)	Cu(1)-N(6)C	2.011(8)
La(1)-O(4)	2.575(7)	Cu(1)-N(5)D	2.017(7)
La(1)-O(7)	2.615(7)	Cu(1)-O(21)	2.169(6)
La(1)-O(8)	2.613(8)	Cu(1)-O(23)A	2.001(6)
La(2)-O(10)	2.606(7)	Cu(2)-N(1)E	2.015(7)
La(2)-O(11)	2.558(8)	Cu(2)-N(2)F	2.018(8)
La(2)-O(12)	2.625(7)	Cu(2)-N(4)	2.025(8)
La(2)-O(25)	2.677(6)	Cu(2)-O(25)	2.192(5)
La(2)-O(26)B	2.753(4)	Cu(2)-O(28)B	2.014(5)

Symmetry transformations used to generate equivalent atoms A: -*x*+1, *y*-1/2, -*z*+1/2; B: -*x*, *y*-1/2, -*z*+1/2; C: *x*+1, *y*, *z*; D: -*x*+1, -*y*+1, -*z*+1; E: -*x*, -*y*+1, -*z*; F: *x*-1, *y*, *z*.

Table S2 Hydrogen bond lengths (Å) and bond angles (^{o}) for compound **1**

Hydrogen bonds				
D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
O(14)-H(14B)···N(7)^{G}	0.82	1.76	2.582(1)	176.6
O(16)-H(16B)···N(8)^{G}	0.82	1.86	2.66(3)	166.1
O(18)-H(18A)···N(9)^{H}	0.82	1.78	2.601(1)	174.6
O(20)-H(20B)···N(10)^{H}	0.82	1.78	2.591(1)	171.9

Symmetry codes: G *x*, *y*+1, *z*; H *x*, *y*-1, *z*.

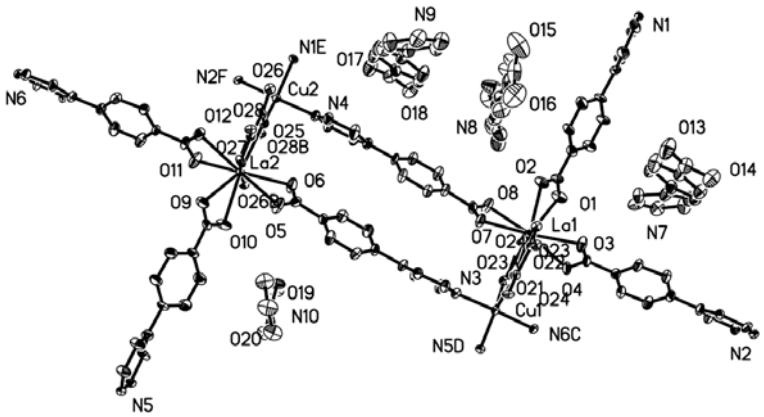

Fig. S1 View of the asymmetric unit of **1**. All hydrogen atoms are omitted for clarity. Atoms having A-F in their labels are symmetry-generated. Symmetry codes A: -*x*+1, *y*-1/2, -*z*+1/2; B: -*x*, *y*-1/2, -*z*+1/2; C: *x*+1, *y*, *z*; D: -*x*+1, -*y*+1, -*z*+1; E: -*x*, -*y*+1, -*z*; F: *x*-1, *y*, *z*.

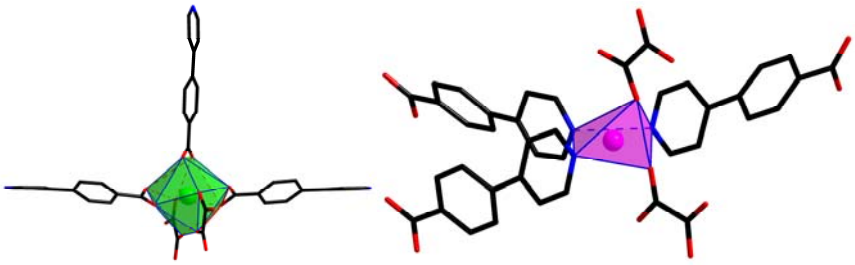

Fig. S2 The coordinate environment of La (left) and Cu atoms in **1** (right).

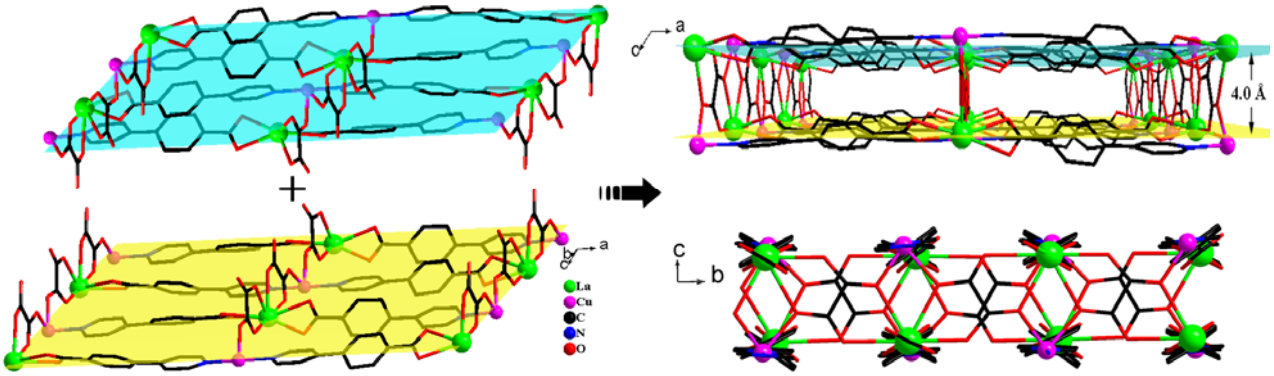

Fig. S3 The scheme representation of the bilayer and the side views along the *b* and *a* axis.

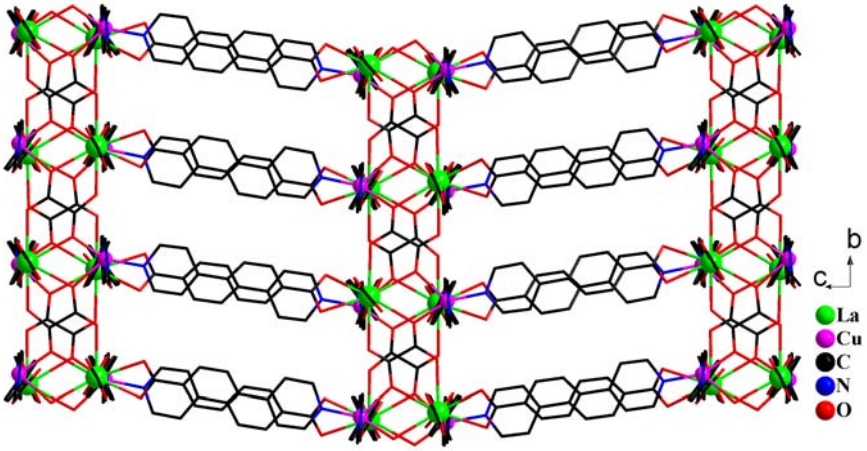

Fig. S4 The side view of the 3D framework of compound **1**.

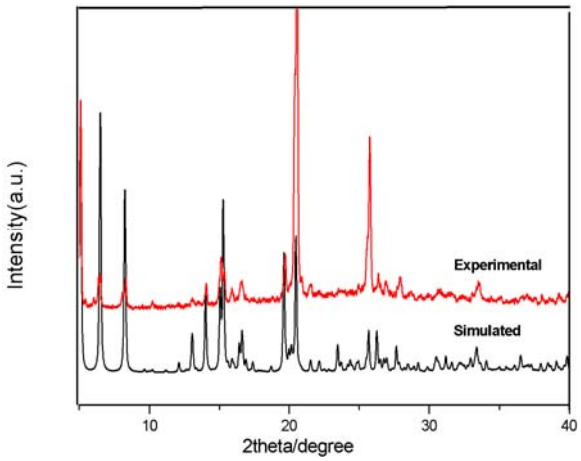

Fig. S5 Simulated and experimental PXRD patterns of **1**.

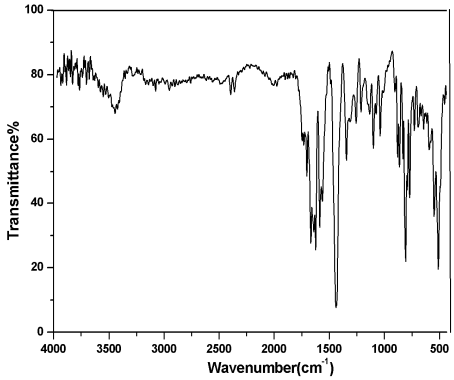

Fig. S6 The IR spectrum of compound **1**.

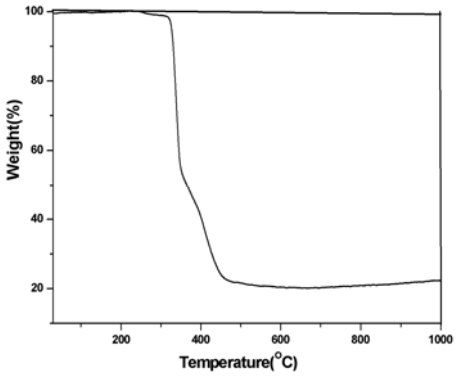

Fig. S7 TGA curve of compound **1**.

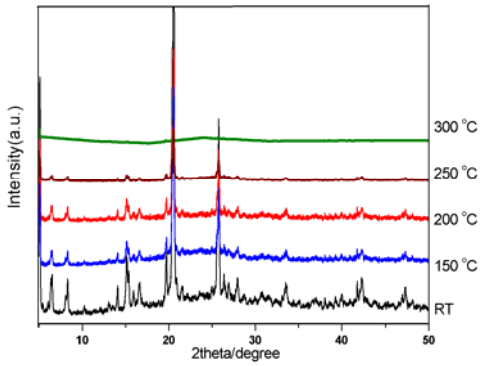

Fig. S8 The experimental PXRD of **1** from room temperature to 300 °C.

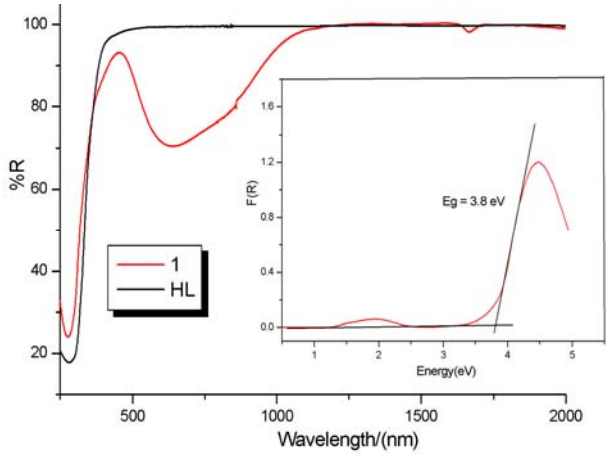

Fig. S9 UV-vis-IR optical diffuse reflectance spectrum for **1**.