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Structural assistants of hydroxyl- and chloro-bridges to construct two new 3D Keggin-based frameworks

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Fig. S1. The btb ligand donates four N atoms to coordinate with four Cu^{I} ions in compound **1**.

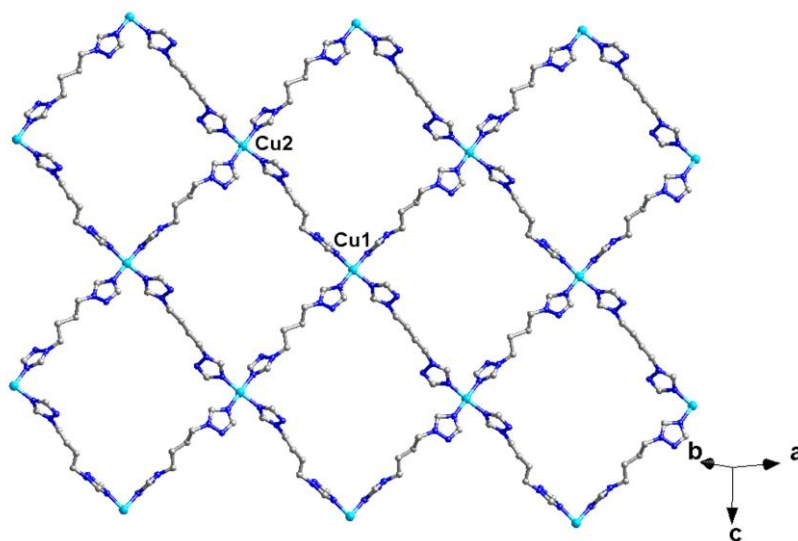


Fig. S2. The 2D metal-organic layer in compound **2** containing quadrangle tetra-nuclear Cu^{II} cycles.

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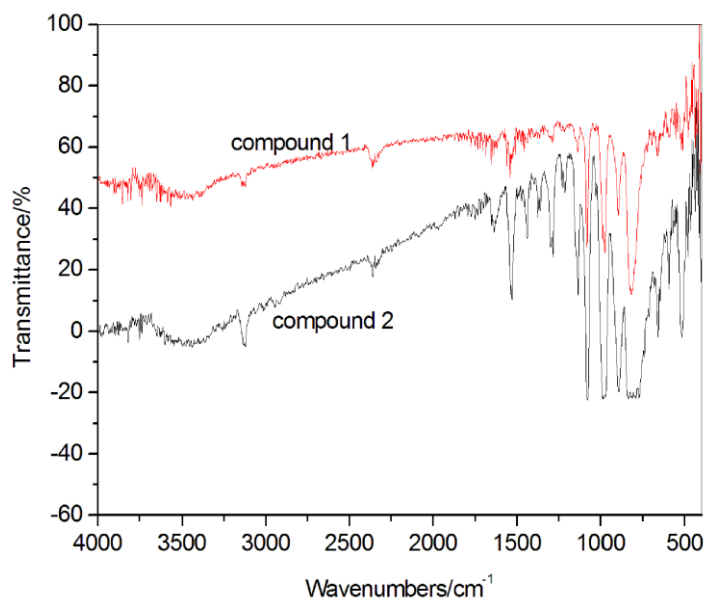


Fig. S3. IR spectra of compounds **1** and **2**.

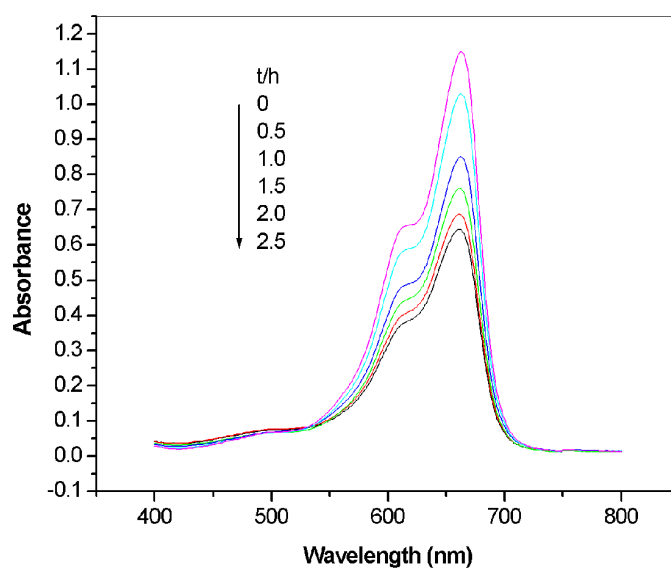


Fig. S4 Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of parent Keggin PW₁₂.

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Table S1. Selected bond lengths (Å) and bond angles (°) for compounds **1** and **2**.

| Compound 1 | | | |
|---|-----------|-----------------------|-----------|
| Cu(1)-N(1)#1 | 1.878(11) | Cu(2)-N(2)#2 | 1.975(13) |
| Cu(2)-O(13) | 1.734(8) | N(1)-Cu(1)-N(1)#1 | 168.7(8) |
| N(2)-Cu(2)-O(13) | 112.2(4) | N(2)-Cu(2)-N(2)#2 | 135.6(9) |
| Cu(2)#3-O(13)-Cu(2) | 180 | | |
| Symmetry codes for 1 : #1 -x,y,-z #2 -x,y,-z+1 #3 -x,-y+1,-z+1 | | | |
| Compound 2 | | | |
| Cu(1)-N(4) | 2.010(17) | Cu(1)-N(10) | 1.956(12) |
| Cu(1)-N(16) | 1.929(14) | Cu(1)-N(22)#4 | 1.999(18) |
| Cu(1)-O(26) | 2.647(17) | Cu(1)-Cl(1) | 2.605(7) |
| Cu(2)-N(1) | 2.032(19) | Cu(2)#1-N(9) | 1.983(19) |
| Cu(2)#2-N(15) | 2.06(2) | Cu(2)#3-N(21) | 2.02(2) |
| Cu(2)-O(44)#5 | 2.589(17) | Cu(2)-Cl(1) | 2.603(7) |
| Cu(2)-Cl-Cu(1) | 177.7(3) | N(10)-Cu(1)-N(16) | 88.5(10) |
| N(22)#4-Cu(1)-N(16) | 93.1(9) | N(10)-Cu(1)-N(22)#4 | 175.9(9) |
| N(4)-Cu(1)-N(16) | 172.1(10) | N(10)-Cu(1)-N(4) | 88.2(9) |
| N(22)#4-Cu(1)-N(4) | 89.7(7) | N(16)-Cu(1)-Cl(1) | 93.6(9) |
| N(10)-Cu(1)-Cl(1) | 92.2(7) | N(22)#4-Cu(1)-Cl(1) | 91.4(6) |
| N(9)#1-Cu(2)-N(21)#3 | 173.4(8) | N(9)#1-Cu(2)-N(1) | 89.0(7) |
| N(9)#1-Cu(2)-O(44)#5 | 88.4(6) | N(9)#1-Cu(2)-Cl(1) | 93.6(5) |
| O(44)#5-Cu(2)-Cl(1) | 175.5(4) | N(1)-Cu(2)-Cl(1) | 92.4(6) |
| N(9)#1-Cu(2)-N(15)#2 | 90.8(7) | N(21)#3-Cu(2)-N(15)#2 | 89.9(7) |
| Symmetry codes for 2 : #1 -x+1,-y,-z+1 #2 -x+1,-y,-z #3 -x,-y+1,-z #4 -x,-y+1,-z+1 #5 x-1,y-1,z | | | |