**Supporting file**

# Transformation of a Copper-based Metal-Organic Polyhedra into a Mixed Linker MOF for $CO_2$ Capture

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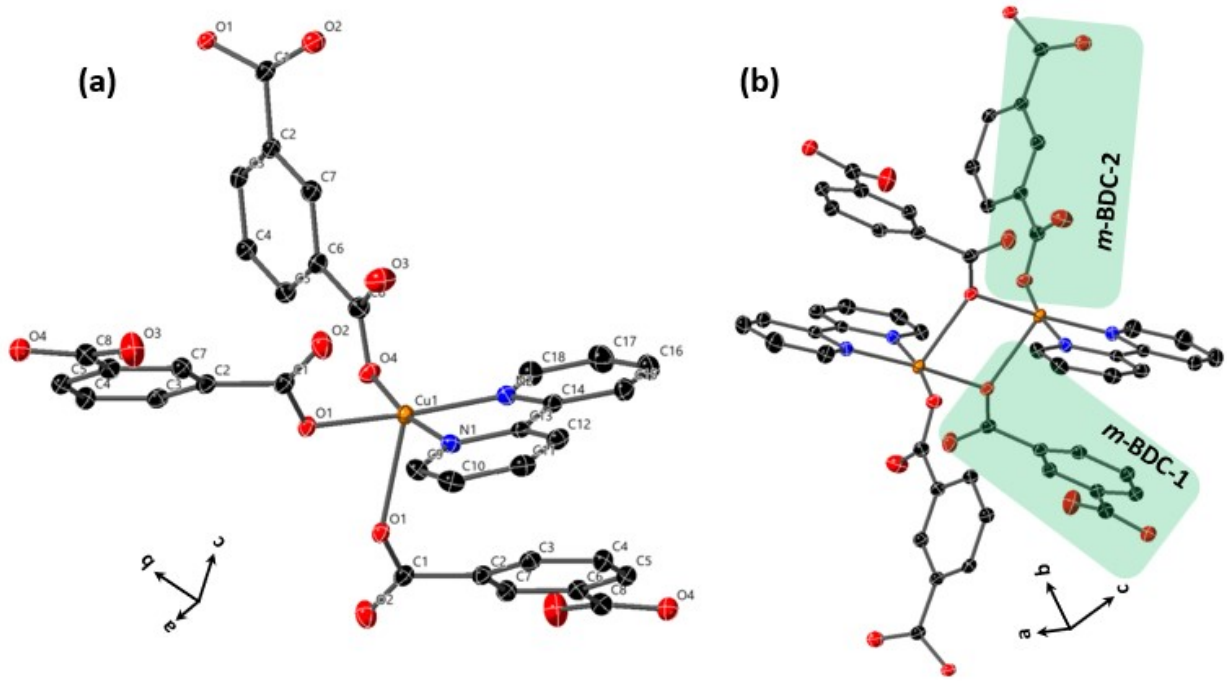


**Figure S1**. **CuMOF-Bipy** crystal structure displaying the (a) asymmetric unit with atom numbering and (b) the binuclear copper node and isophthalic acid linkers, highlighted to show their structural differences.

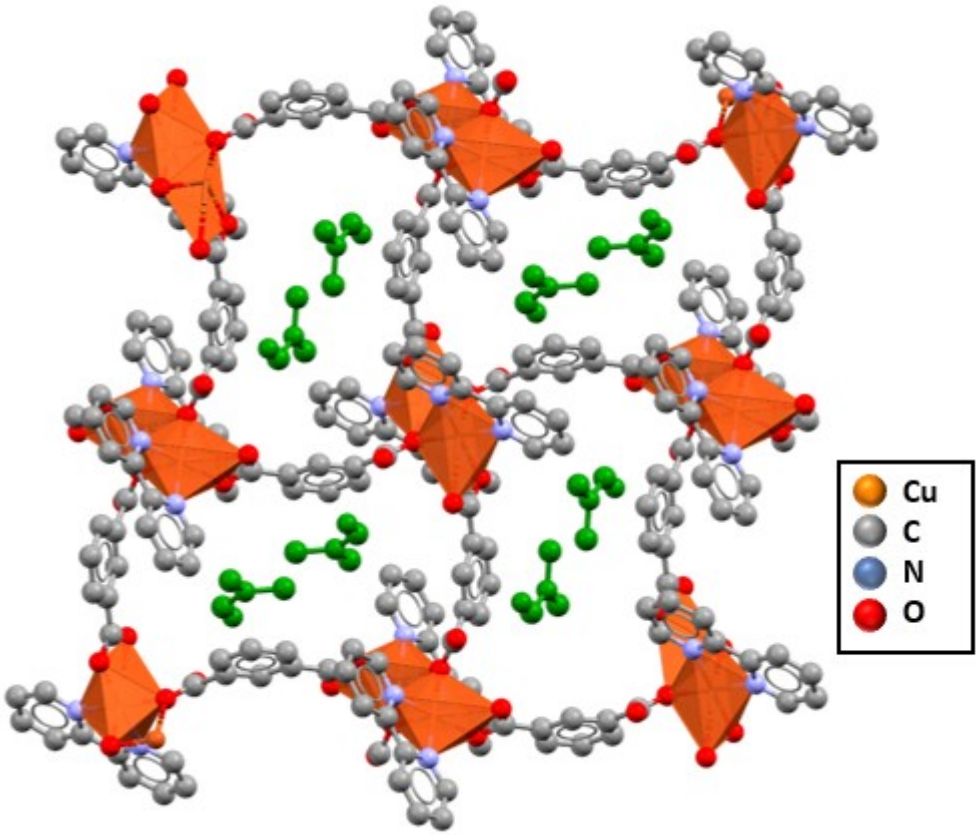


**Figure S2.** The extended structure of **CuMOF-Bipy** along *a*-axis showing uncoordinated DMF molecules (highlighted green) in the pores.

**Table S1.** Crystallographic data and structure refinement results for **CuMOF-Bipy**

| **Compound** | **CuMOF-Bipy** |
|---|---|
| **CCDC number** | 2212850 |
| **Empirical formula** | $C_{42}H_{38}Cu_2N_6O_{10}$ |
| **Formula weight** | 913.86 |
| **Crystal system** | Monoclinic |
| **Space group** | $P2_1/c$ |
| ***a* (Å)** | 9.8053(2) |
| ***b* (Å)** | 15.5940(3) |

| | |
|---|---|
| ***c*** **(Å)** | 13.0691(3) |
| ***β*** **(°)** | 95.514(1) |
| **Volume (Å$^3$)** | 1989.1(7) |
| **Z** | 2 |
| **ρ (calc.)(g/cm$^3$)** | 1.526 |
| **λ** | 0.71073 Å |
| **Temp. (K)** | 110 |
| **F(000)** | 1632.0 |
| **μ (mm$^{-1}$)** | 1.137 |
| **$T_{min}$, $T_{max}$** | 0.7489, 0.6907 |
| **$2\theta_{range}$ (°)** | 4.924 to 90.99 |
| **Reflections collected** | 441443 |
| **Independent reflections** | 16776 [$R_{int}$ = 0.0590, $R_{sigma}$ = 0.0175] |
| **Completeness** | 99.7% |
| **Data/restraints/ parameters** | 16776/18/321 |
| **Final R indexes [I>=2σ (I)]** | $R_1$ = 0.0288, w$R_2$ = 0.0722 |
| **Final R indexes [all data]** | $R_1$ = 0.0412, w$R_2$ = 0.0781 |
| **Goodness-of-fit on $F^2$** | 1.027 |
| **Largest diff. peak and hole (e Å$^{-3}$)** | 0.69/-0.86 |

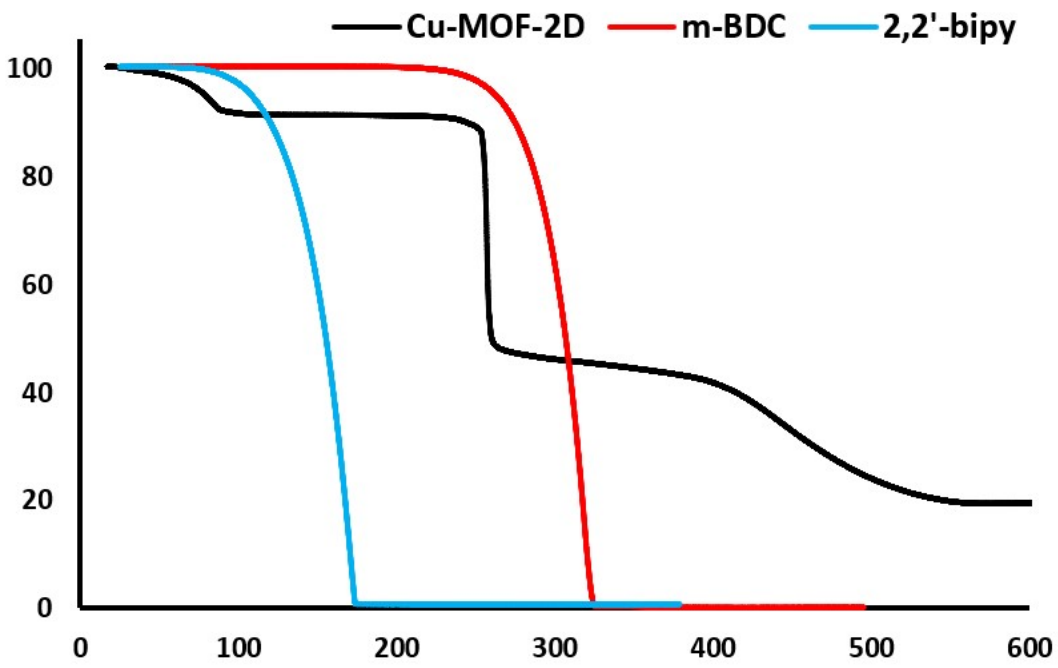


**Figure S3** TGA curves for **CuMOF-Bipy** in comparison to organic linkers used in synthesis

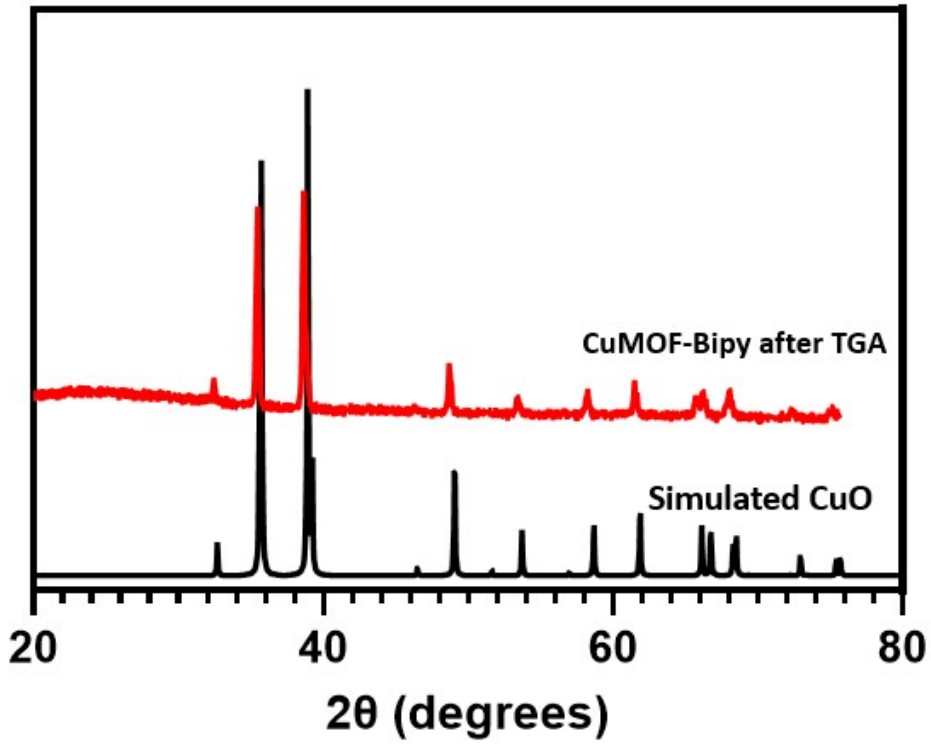


**Figure S4.** PXRD pattern of remaining **CuMOF-Bipy** after TGA under air at 600°C compared to CuO (simulated from ICSD 26715).[1]

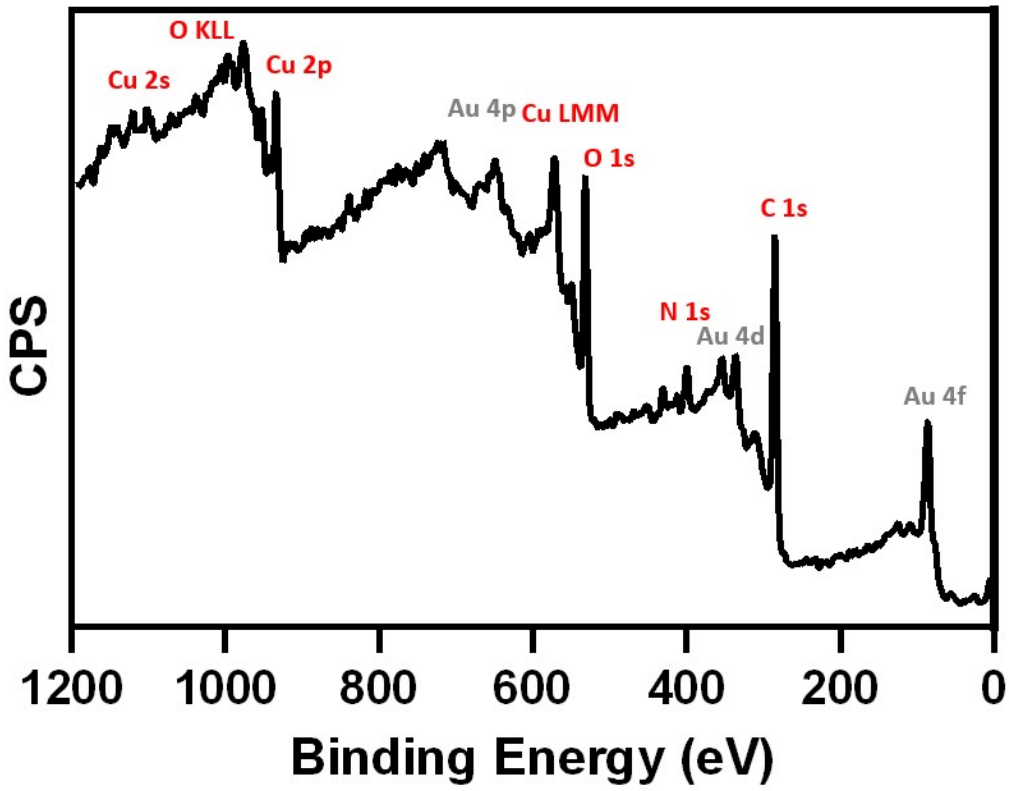


**Figure S5.** The survey XPS spectrum of **CuMOF-Bipy,** Au (4f, 4d, 4p, and 4s) peaks come from the reference used for charge correction

**Table S2.** Atomic concentrations calculated from XPS spectra

| **CuMOF-Bipy** | C (%) | N (%) | O (%) | Cu (%) |
|---|---|---|---|---|
| **Theoretical calculated** | 70 | 10 | 16.6 | 3.33 |
| **Actual** | 71.21 | 8.10 | 17.33 | 3.37 |

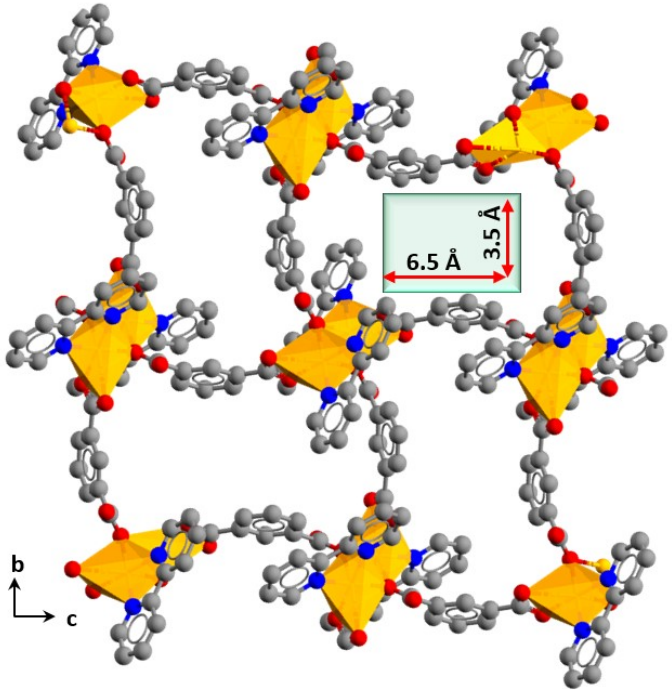


**Figure S6.** Calculated pore-openings in **CuMOF-Bipy** crystal structure viewed along *a*-axis

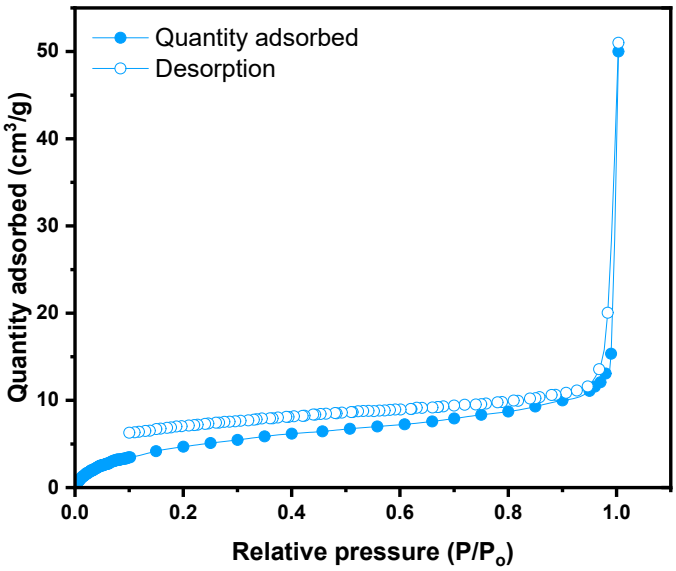


**Figure S7.** Nitrogen adsorption isotherm for **CuMOF-Bipy** at 77 K

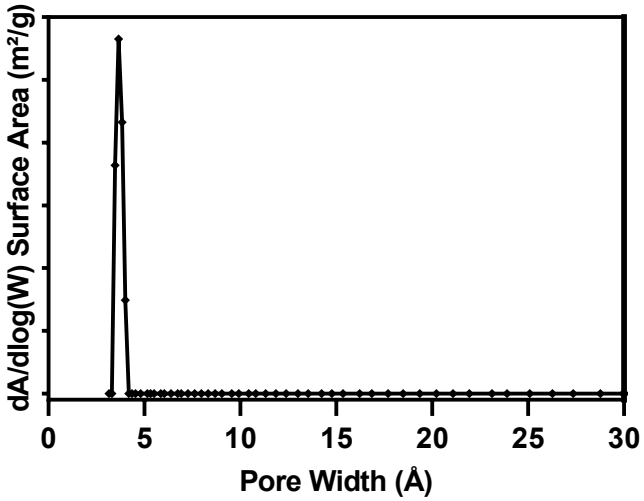


**Figure S8.** Pore size distribution in **CuMOF-Bipy**

## References

1. Tunell, G, Posnjak, E, Ksanda, C J, *Z.Kristallogr.Mineral.Petrogr.Abt .A* (1935), **90**, 120