Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Supplementary information

Copper-based MOF, $Cu_3(SDBA)_2(HSDBA)$, as catalyst for efficient reduction of 4-nitrophenol in the presence of sodium borohydride

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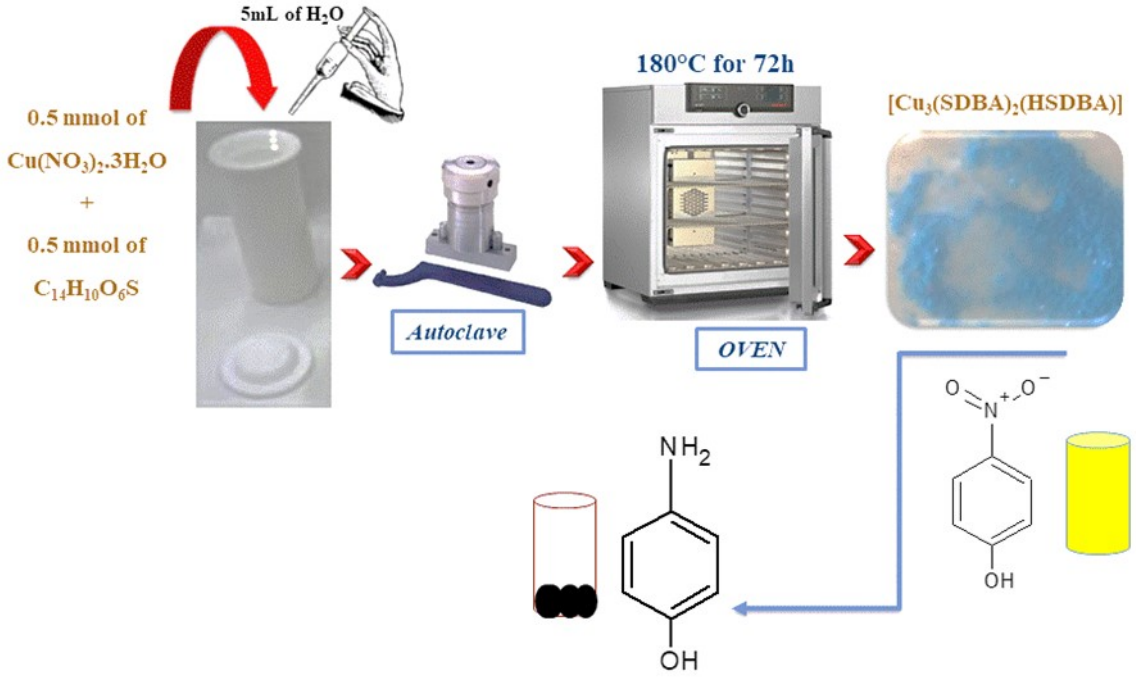

Figure S1. Schematic illustration of the synthesis of blue crystals of $Cu_3(SDBA)_2(HSDBA)$, and their use for the reduction of 4-nitrophenol into 4-aminophenol.

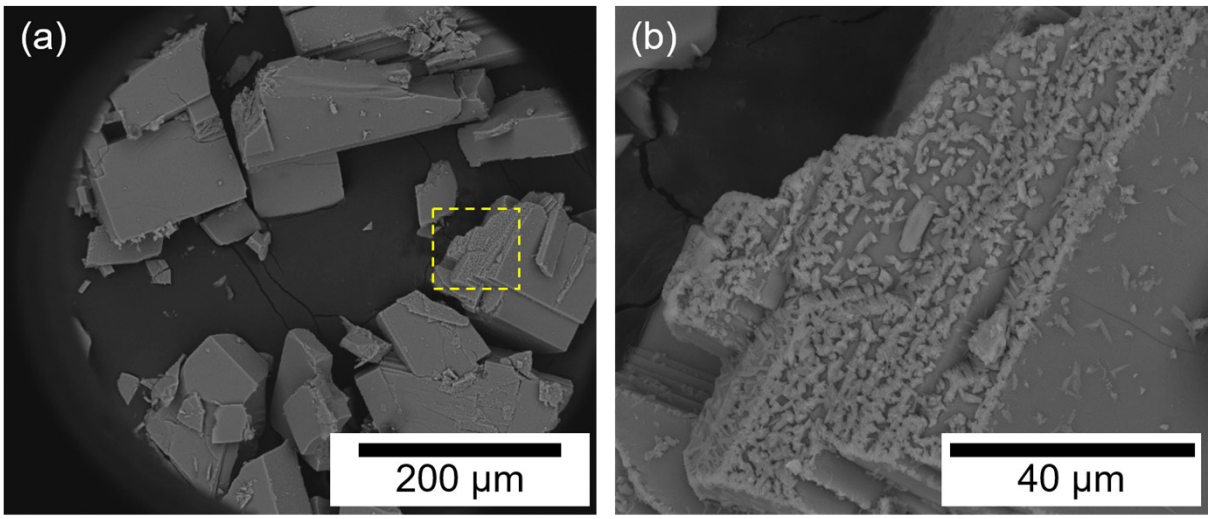

Figure S2. SEM images of $Cu_3(SDBA)_2(HSDBA)$ at two different magnifications. These images are the same as those shown in Figure 1 but at two different magnifications. The image (b) shows a magnification of the area of the image (a) indicated by the yellow box.

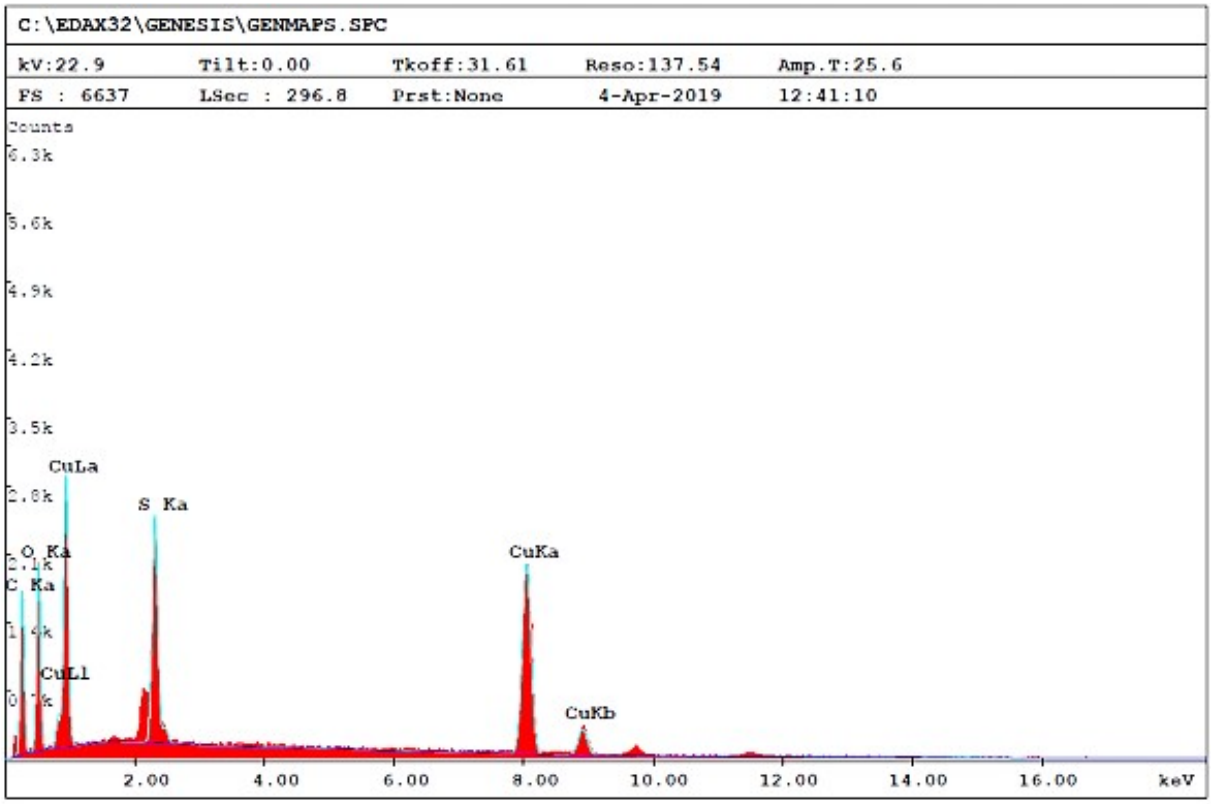

Figure S3. Energy dispersive X-ray spectrum of $Cu_3(SDBA)_2(HSDBA)$.

Table S1. Crystal data and refinement table.

Parameters	**$[Cu_3(SDBA)_2(HSDBA)]$**
CCDC deposit No.	1956263
Empirical formula	$C_{42}H_{25}Cu_3O_{19}S_3$
Formula weight g/mol	2175.40
Temperature (K)	296
Wavelength (Å)	1.54178
Crystal system	Triclinic
Space group	*P*-1
a (Å)	12.5482(7)
b (Å)	12.6669(9)
c (Å)	15.7079(8)
α (º)	106.396(4)
β (º)	91.917(3)
γ (º)	119.522 (4)
Volume (Å^3)	2039.2(2)
Z	2
Density (Mg m^{-3})	1.771
Absorption coefficient (mm^{-1})	3.742
F_{000}	1097
Crystal size (mm^3)	0.02 × 0.02 × 0.01
θ range for data collection	3.00º to 65.42º
Index ranges	-14 ≤ h ≤ 14 -14≤ k ≤ 14 -16≤ l ≤18
Reflections collected	16003
Unique reflections	6522 [Rint = 0.0620]
Absorption correction	multi-scan
Refinement method	Full matrix least-squares on F^2
Data/restraints/parameters	6522 / 0 / 601
Goodness-of-fit on F^2	1.070
Final [$I > 2\sigma(I)$]	R_1 = 0.0877, wR_2 = 0.2440
R indices (all data)	R_1 = 0.2440, wR_2 = 0.2647
Largest diff. peak and hole	0.727 and -0.927e Å^{-3}

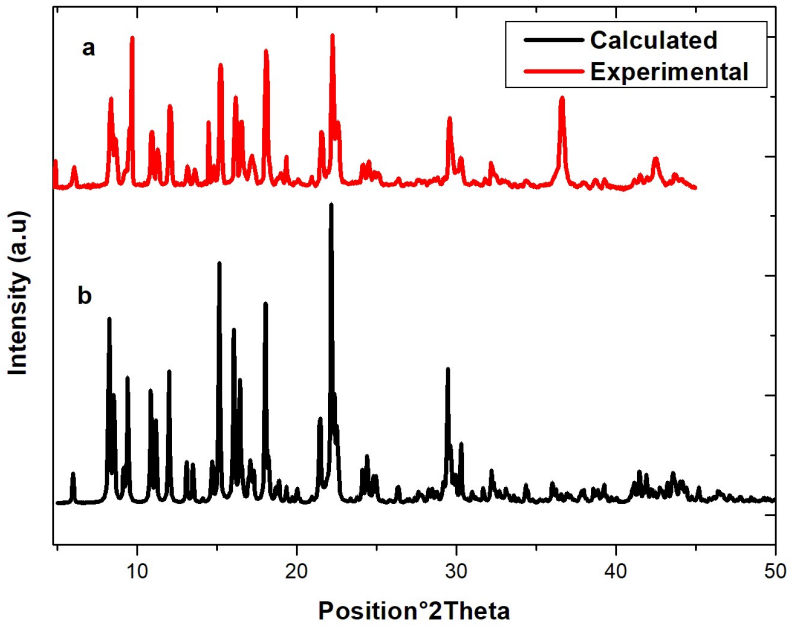

Figure S4. (a) PXRD pattern of bulk $Cu_3(SDBA)_2(HSDBA)$ (blue precipitate) denoted 'experimental'. (b) Calculated XRD pattern, the simulation being from the single XRD data.

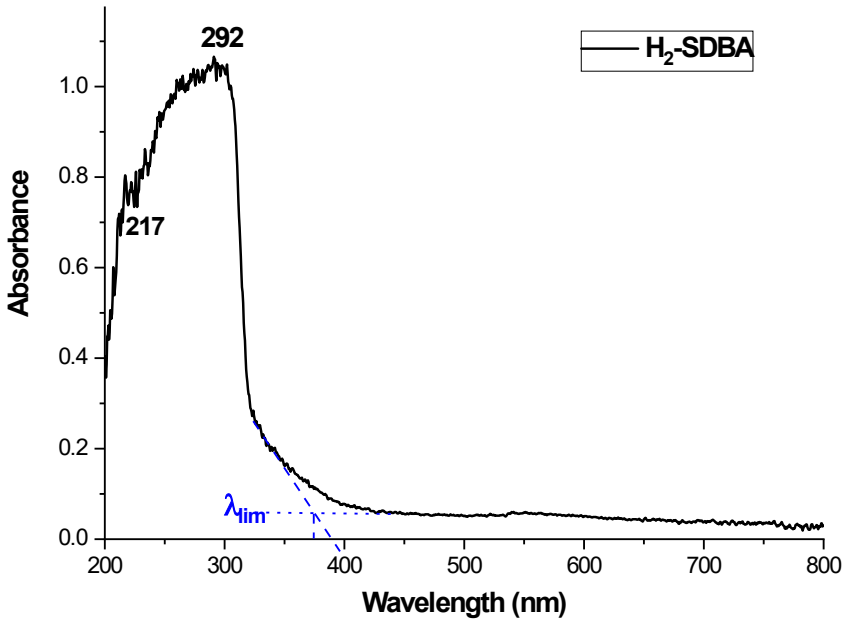

Figure S5. UV-vis absorption spectrum of the H_2-SDBA ligand. The λ_{max} of the two absorption bands and the λ_{lim} are indicated.

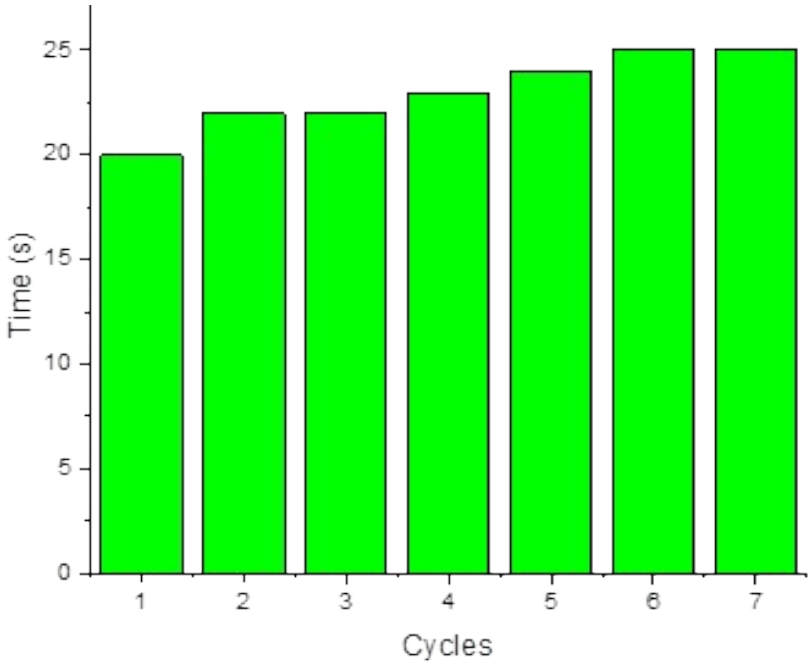

Figure S6. Time for the conversion of 4-NP catalyzed by re-used $Cu_3(SDBA)_2(HSDBA)$ in the presence of aqueous $NaBH_4$, for 7 cycles. Conditions: 5 mL; [4-NP] = 7.1×10^{-4} mol L^{-1}; [$NaBH_4$] = 2.1×10^{-2} mol L^{-1}; 2 mg $Cu_3(SDBA)_2(HSDBA)$; 25 °C.

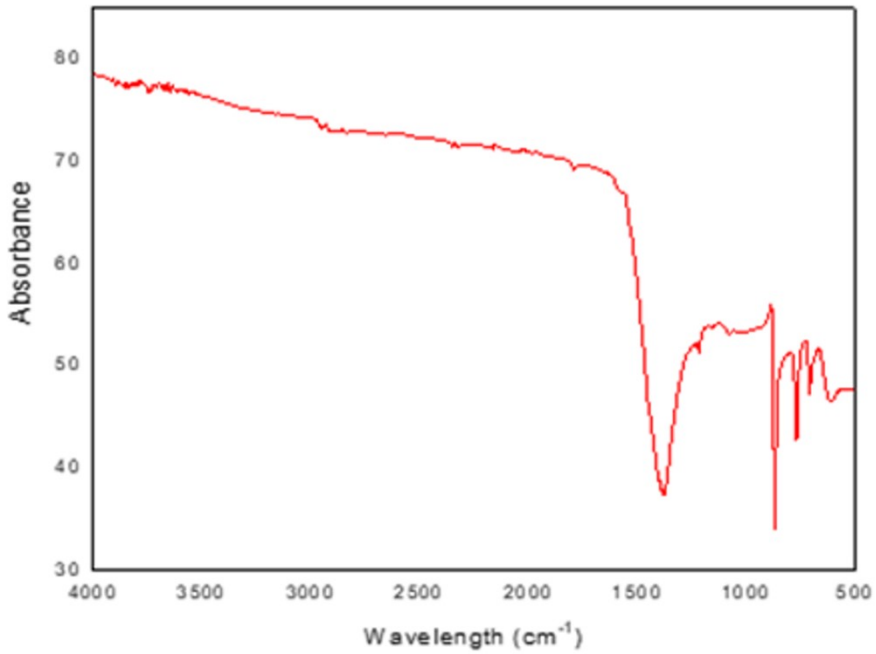

Figure S7. FTIR spectrum of used $Cu_3(SDBA)_2(HSDBA)$, that is, $Cu_3(SDBA)_2(HSDBA)$ recovered after 7 cycles.

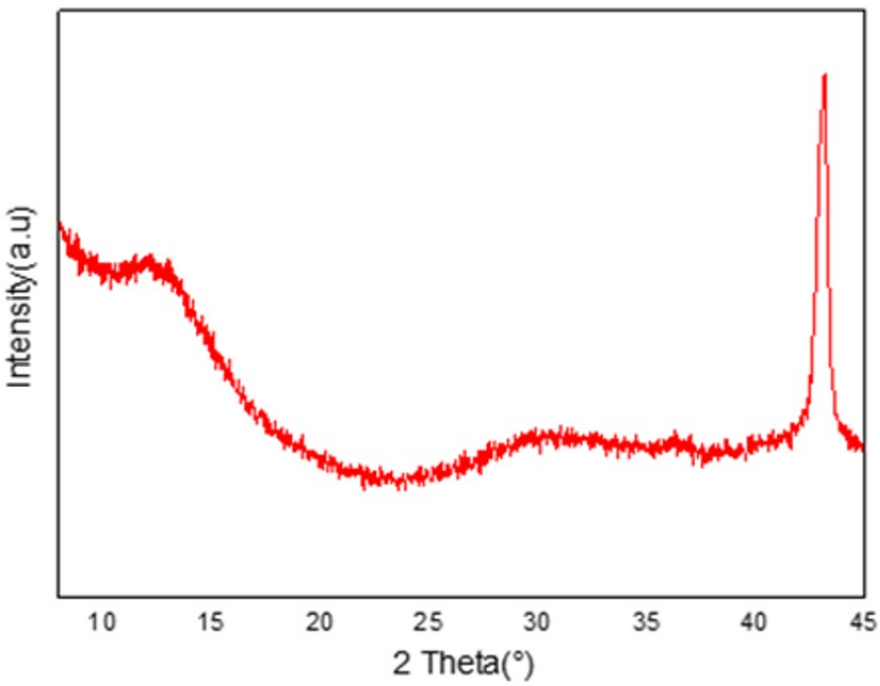

Figure S8. PXRD pattern of used $Cu_3(SDBA)2(HSDBA)$, that is, $Cu_3(SDBA)_2(HSDBA)$ recovered after 7 cycles. The peak at around 43.5° belongs to metallic Cu (the plane (111)).