Supporting Information

Synthesis of Zirconium-Based Metal-Organic Frameworks with Iron(II) Clathrochelate Ligands

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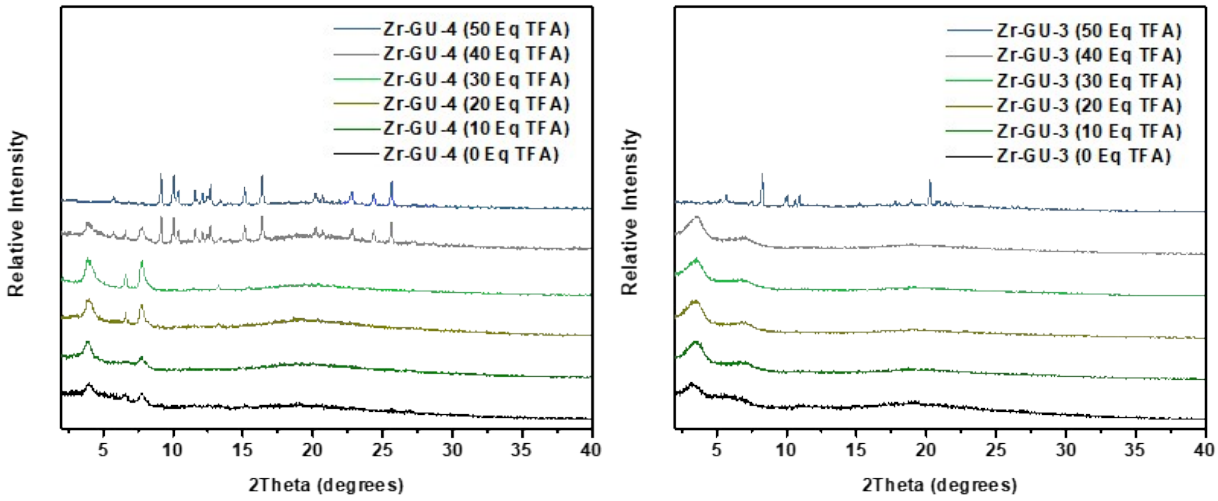

Figure S1. Experimental PXRD patterns of **Zr-GU-3,4**

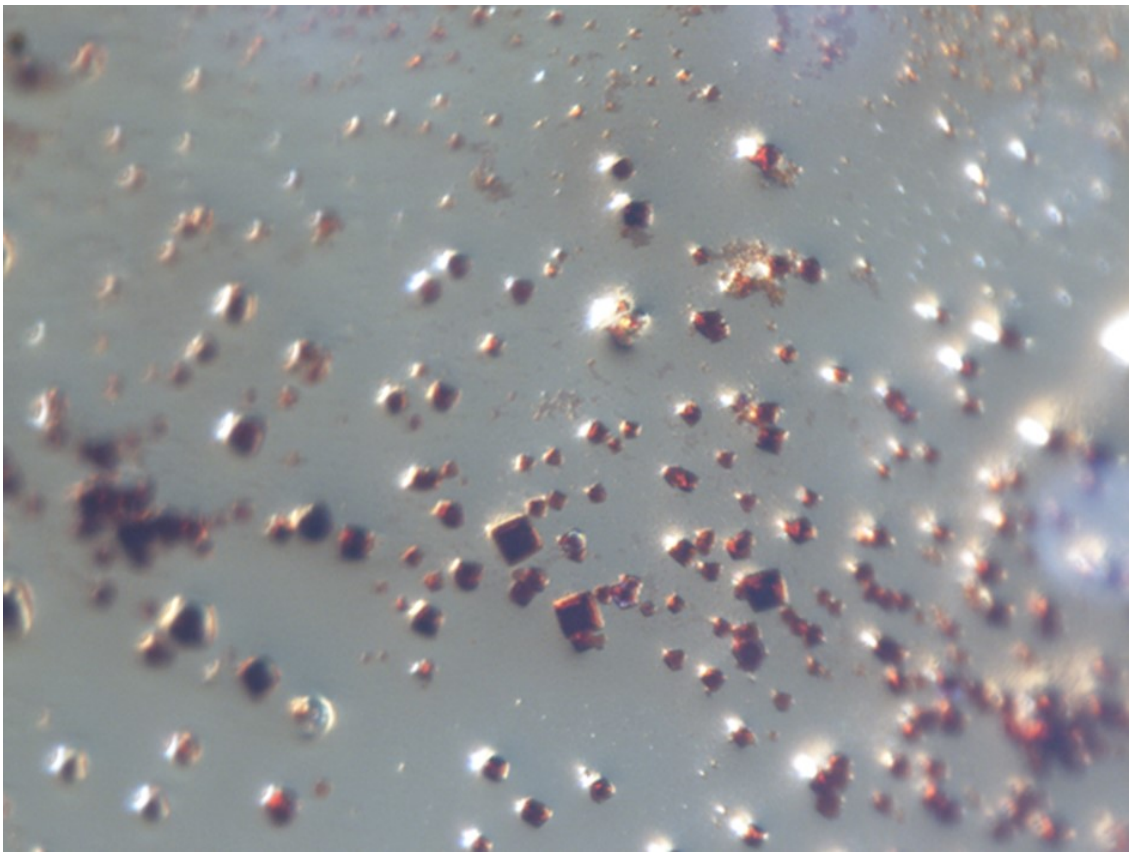

Figure S2. Obtained crystal for **Zr-GU-2** for SCXRD analysis (Crystals were not stable and decomposed during mounting process thus cannot be solved)

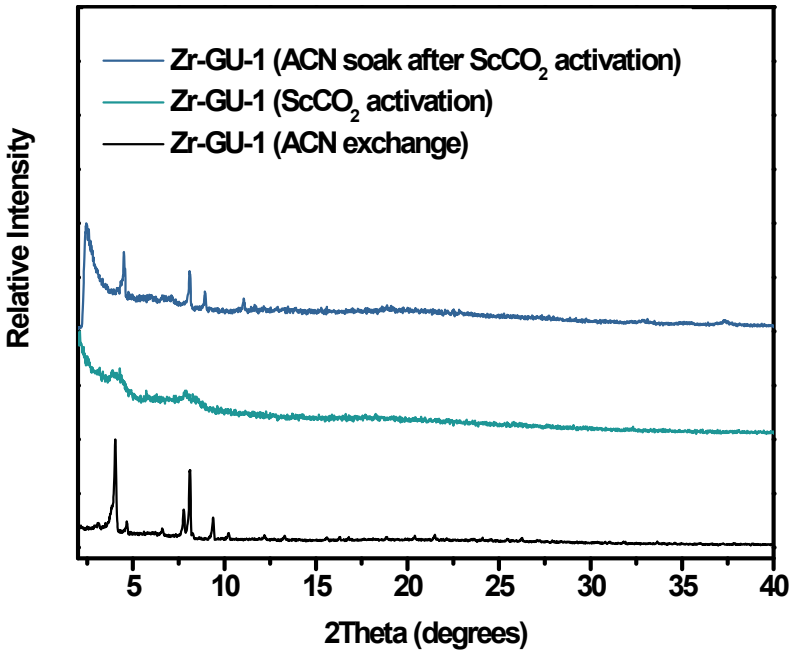

Figure S3. The comparative experimental PXRD patterns of **Zr-GU-1** as-synthesized, after $ScCO_2$ activation and DMF soaked post activation

Table S1. Crystal data and structure refinement for Zr-GU-1

Identification code	Zr-GU-1
Empirical formula	$C_{120}H_{48}B_{12}Fe_6N_{36}O_{68}Zr_6$
Formula weight	4094.08
Temperature/K	200.01(10)
Crystal system	cubic
Space group	*Fm*-3*m*
a/Å	37.5848(3)
b/Å	37.5848(3)
c/Å	37.5848(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	53092.7(14)
Z	4
ρ_{calc}g/cm^3	0.512
μ/mm^{-1}	2.471
F(000)	8080.0
Crystal size/mm^3	0.2 × 0.2 × 0.15
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.802 to 158.742
Index ranges	$-30 \leq h \leq 39$, $-29 \leq k \leq 44$, $-47 \leq l \leq 39$
Reflections collected	26210
Independent reflections	2811 [R_{int} = 0.0909, R_{sigma} = 0.0421]
Data/restraints/parameters	2811/137/106
Goodness-of-fit on F^2	1.058
Final *R* indexes [$I >= 2\sigma(I)$]	R_1 = 0.0793, wR_2 = 0.2163
Final *R* indexes [all data]	R_1 = 0.0879, wR_2 = 0.2257
Largest diff. peak/hole / e Å^{-3}	0.67/-0.94