Electronic Supplementary Material (ESI) for Dalton Transactions.

Assessment of the energetic performances of various ZIFs with SOD or RHO topology using high pressure water intrusion-extrusion experiments

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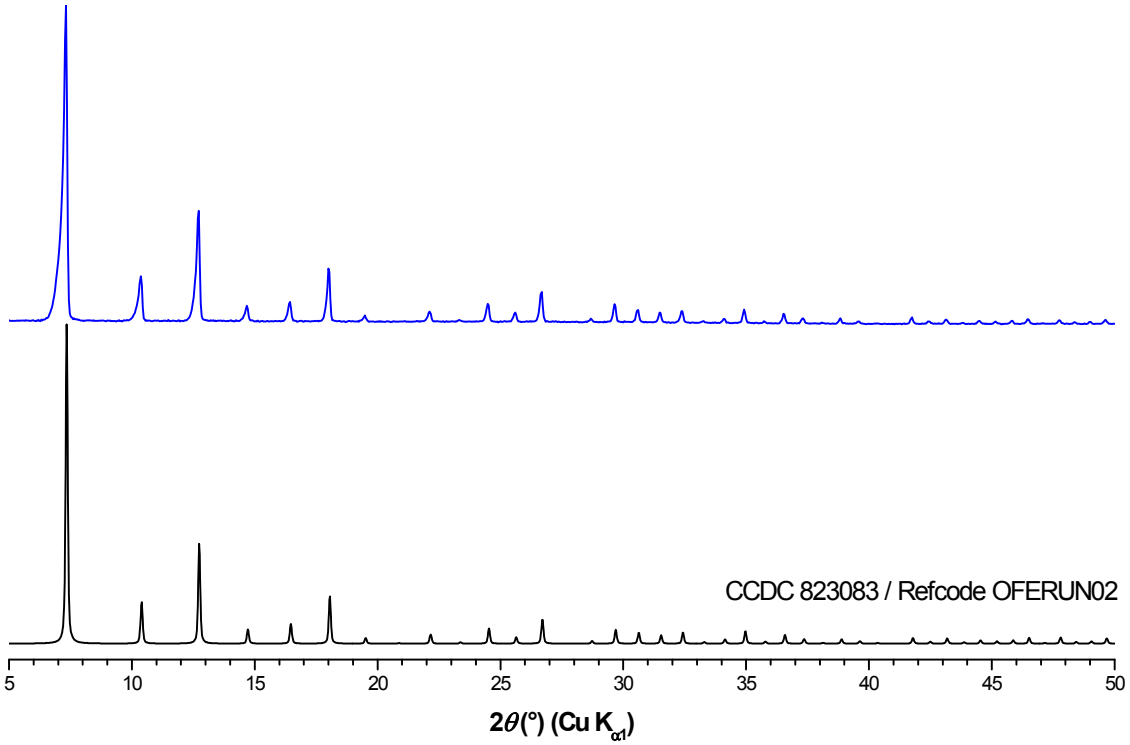
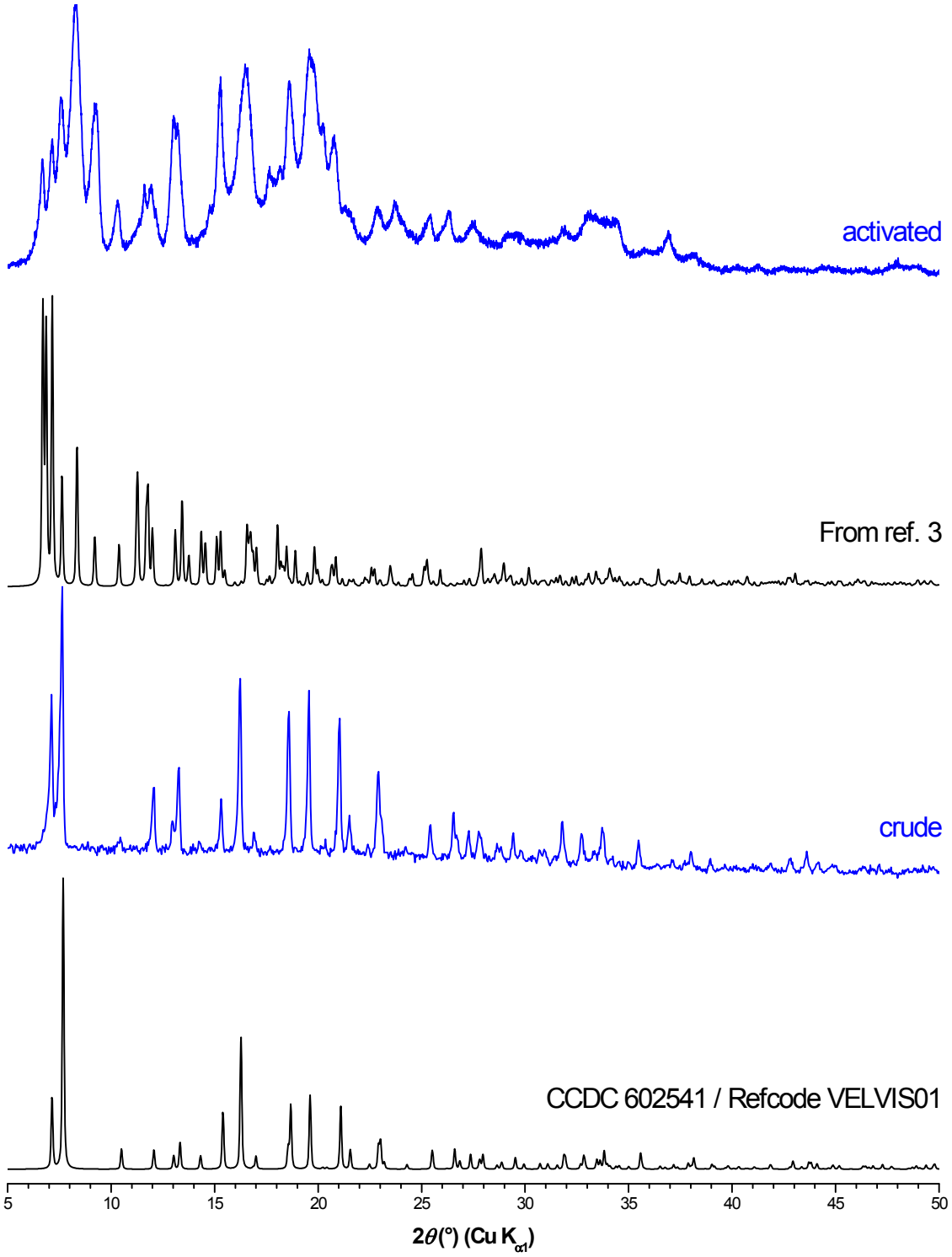
1. Characterisations of materials

1.1. X-Ray Diffraction Patterns

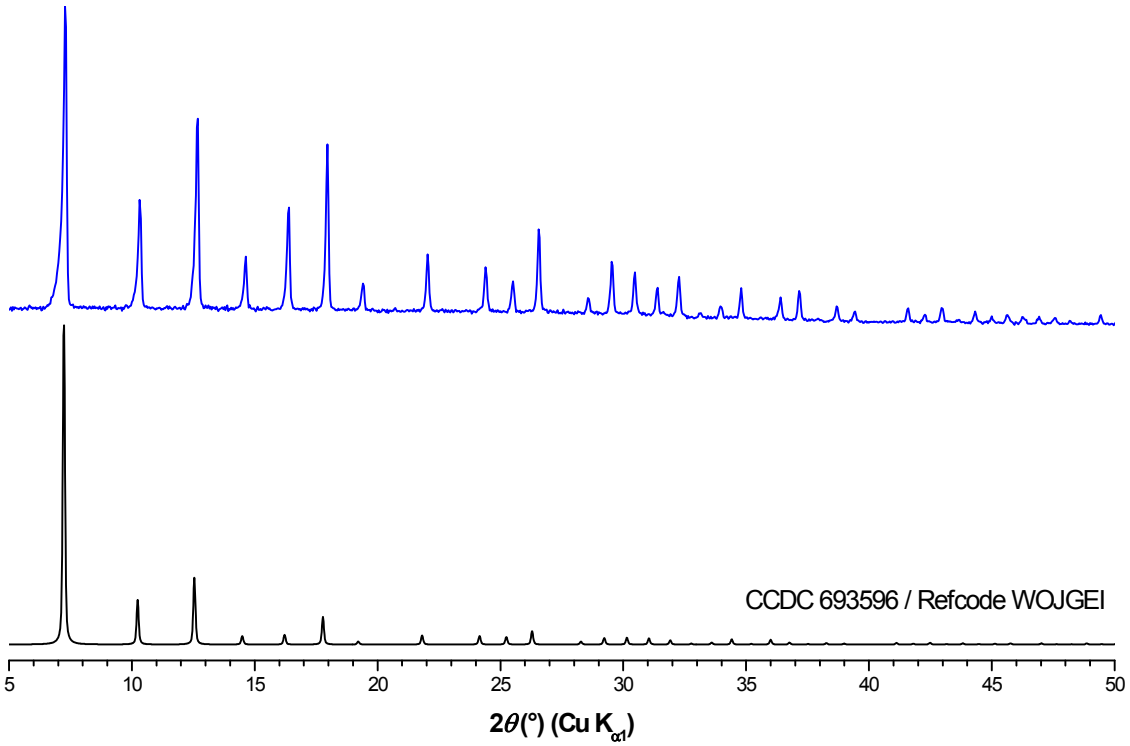
a) **ZIF-8 (SOD)**



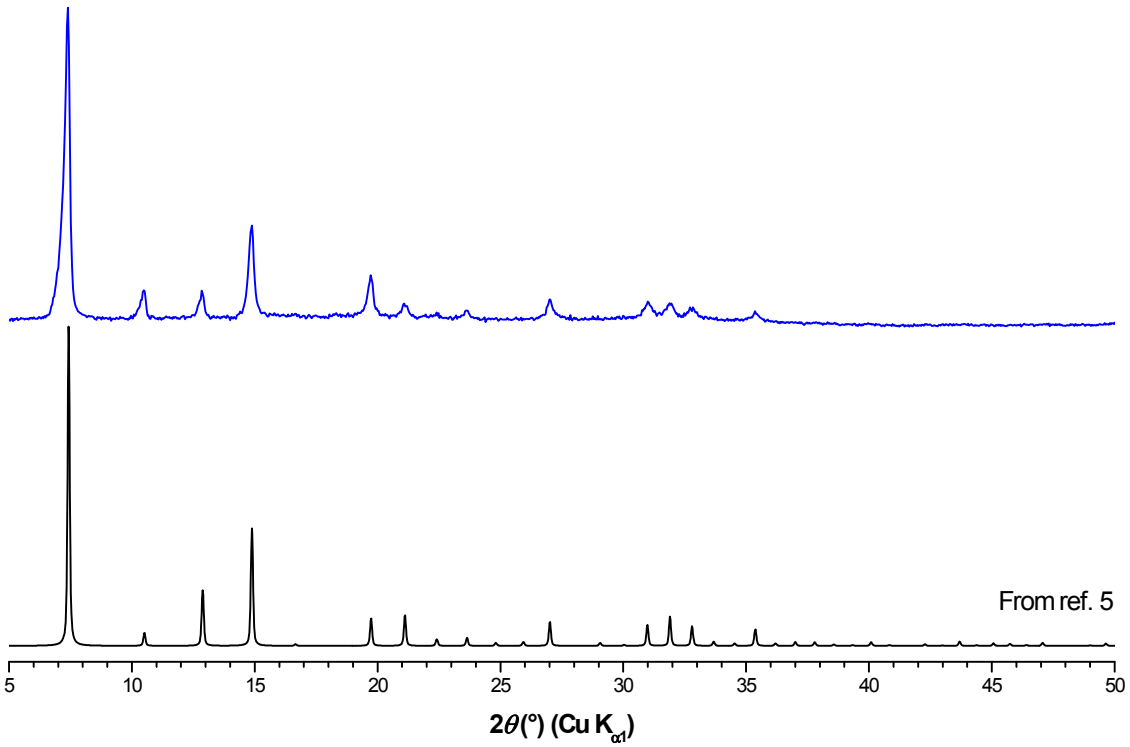
b) **ZIF-7 (SOD)**


activated
From ref. 3
crude
CCDC 602541 / Refcode VELVIS01
5
10
15
20
25
30
35
40
45
50
2θ(°) (Cu Kα1)

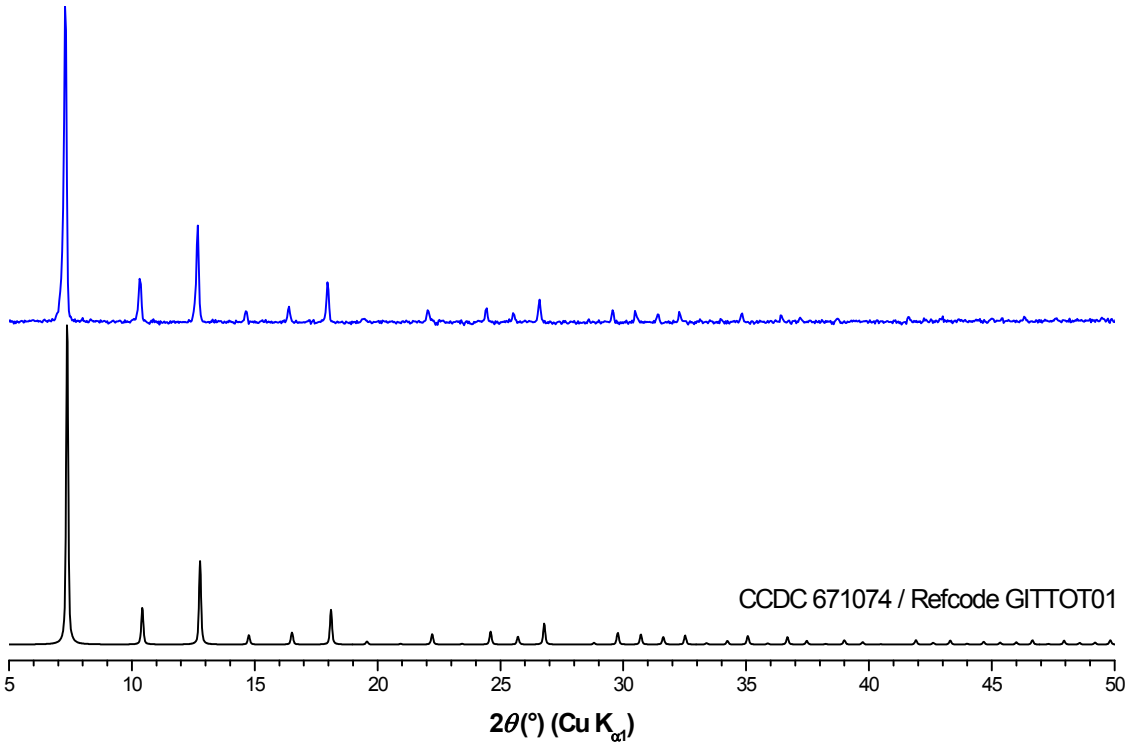
c) **ZIF-90 (SOD)**



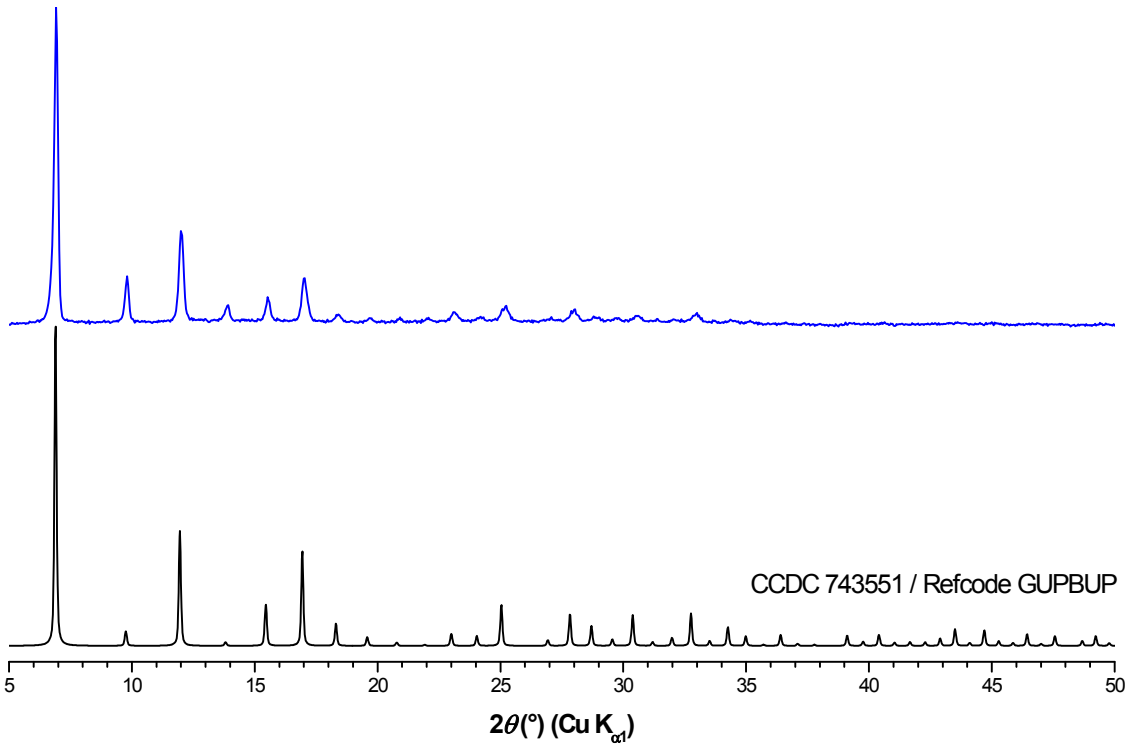
d) **Zn(dcim)$_2$-SALE (SOD)**



e) **ZIF-67 (SOD)**



f) **CdIF-1 (SOD)**



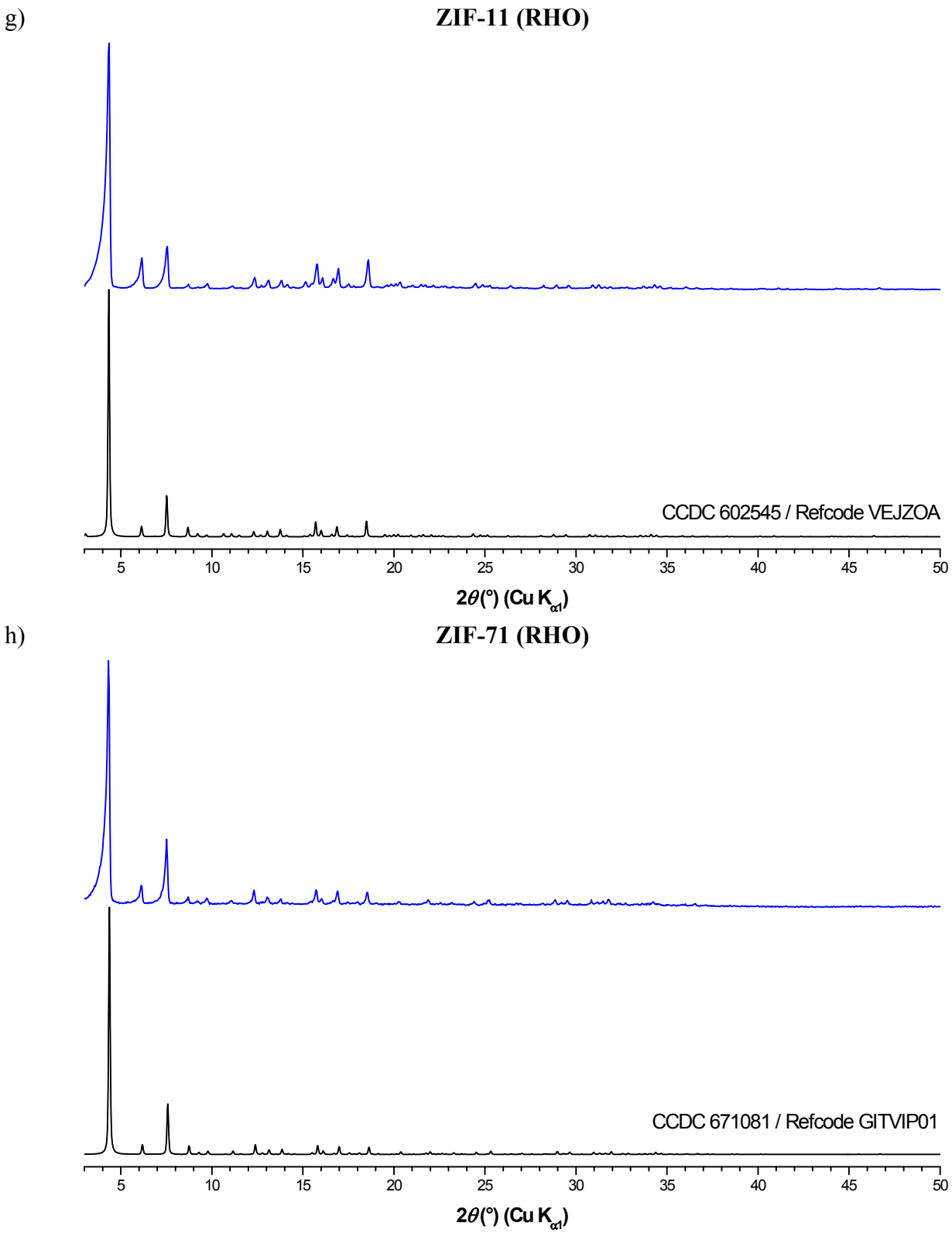


Figure S1. Experimental (blue) and simulated (black) X-ray diffraction patterns of a) ZIF-8, b) crude and activated ZIF-7, c) ZIF-90, d) $Zn(dcim)_2$-SALE, e) ZIF-67, f) CdIF-1, g) ZIF-11 and h) ZIF-71 samples. The crystallographic data referenced as OFERUN02 (823083)[1] for ZIF-8, VELVIS01 (602541)[2] and from ref. [3] for ZIF-7, WOJGEI (693596)[4] for ZIF-90, from ref. [5] for $Zn(dcim)_2$-SALE, GITTOT01 (671074)[6] for ZIF-67, GUPBUP (743551)[7] for CdIF-1, VEJZOA (602545)[2] for ZIF-11 and GITVIP01 (671081)[6] for ZIF-71, were used to plot the simulated patterns.

1.2. Thermogravimetric Analyses

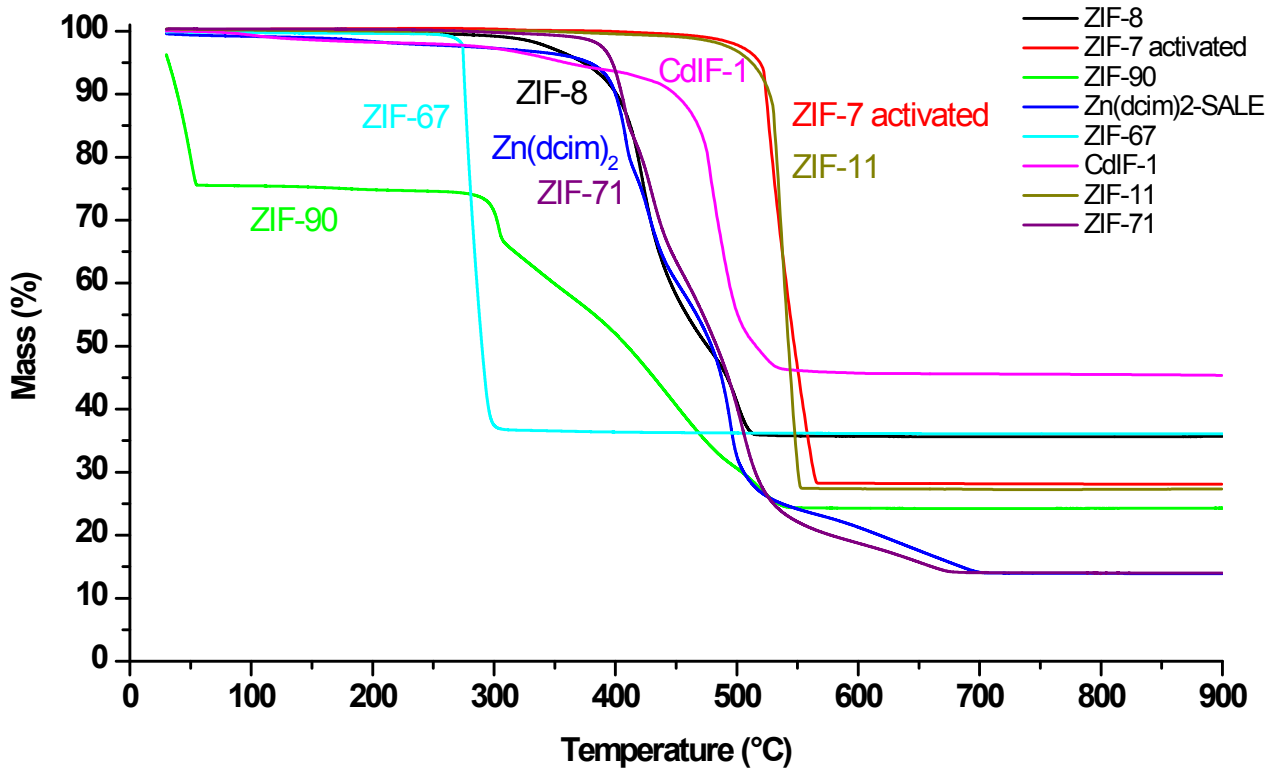


Figure S2. TG curves of ZIF-8 (black), activated ZIF-7 (red), ZIF-90 (green), $Zn(dcim)_2$-SALE (blue), ZIF-67 (cyan), CdIF-1 (magenta), ZIF-11 (dark yellow) and ZIF-71 (purple) samples.

Table S1. Experimental and theoretical mass losses corresponding to the formation of ZnO, Co_3O_4, and CdO after thermal analysis of Zn-, Co- and Cd-based ZIFs.

Samples	Topology	Cation	Linker	Mass loss (%) in the 200-800°C temperature range	
				Experimental	Theoretical
ZIF-8	SOD	Zn^{2+}	mim	64.3	64.2
ZIF-7		Zn^{2+}	bim	72.0	72.8
ZIF-90		Zn^{2+}	ica	67.8	68.2
$Zn(dcim)_2$-SALE		Zn^{2+}	dcim	85.8	75.9
ZIF-67		Co^{2+}	mim	63.8	63.7
CdIF-1		Cd^{2+}	mim	53.6	53.2
ZIF-11	RHO	Zn^{2+}	bim	72.7	72.8
ZIF-71		Zn^{2+}	dcim	86.0	75.9

1.3. Scanning Electron Microscopy

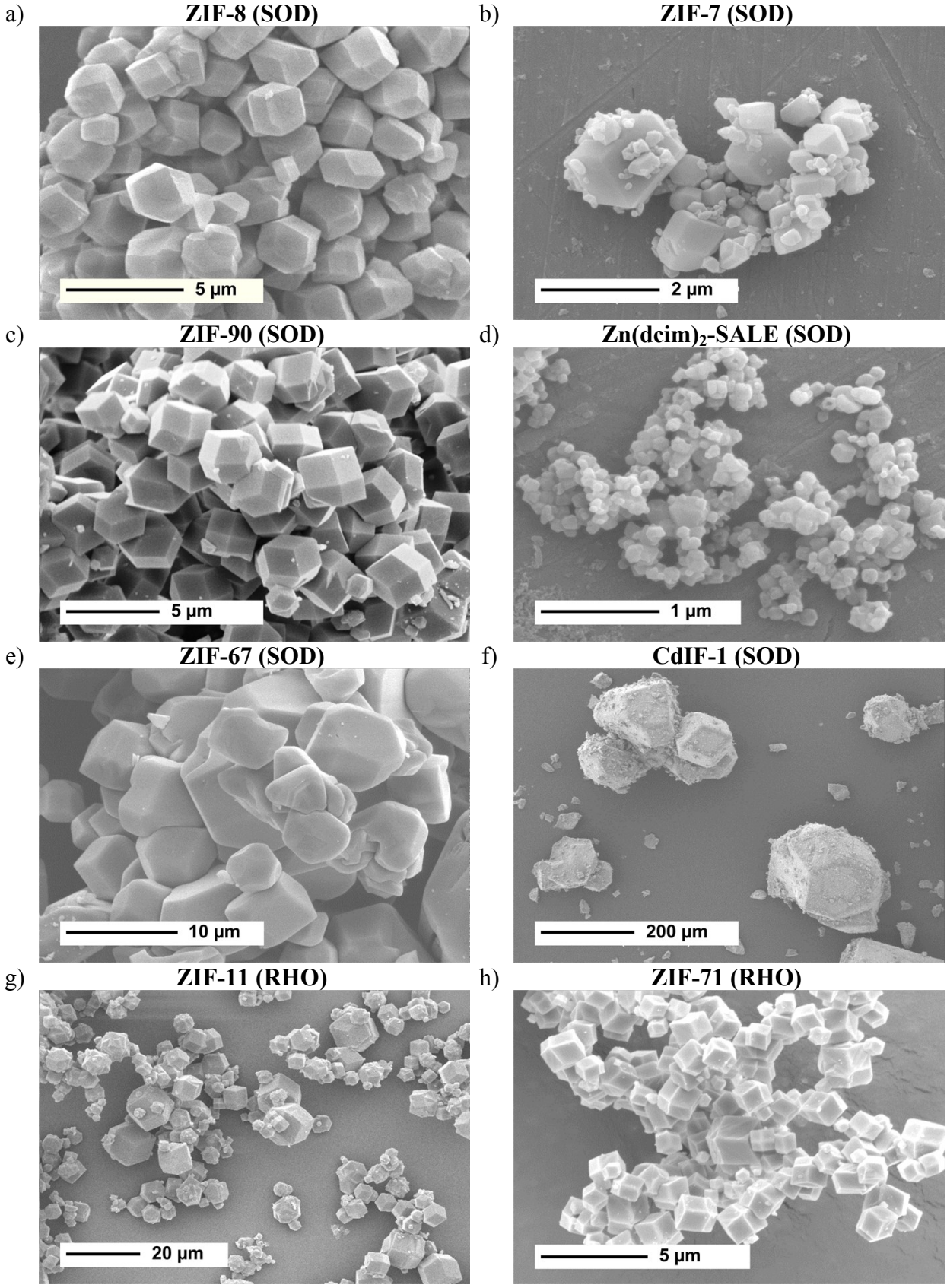


Figure S3. SEM micrographs of a) ZIF-8, b) ZIF-7, c) ZIF-90, d) $Zn(dcim)_2$-SALE, e) ZIF-67, f) CdIF-1, g) ZIF-11 and h) ZIF-71 samples.

2. Water intrusion-extrusion experiments under high pressure

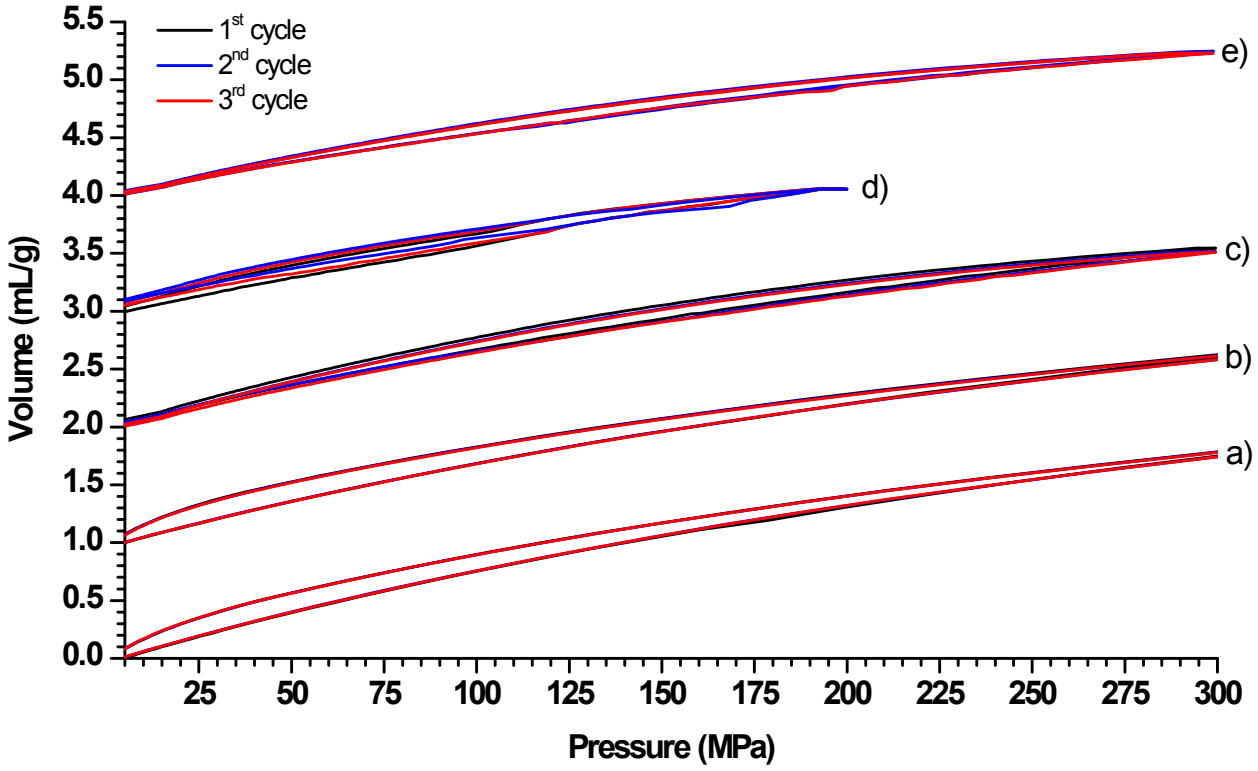


Figure S4. Pressure-volume diagrams of the a) "ZIF-7 crude−water", b) "ZIF-7 activated−water", c) "ZIF-90−water", d) "$Zn(dcim)_2$-SALE−water" and e) "ZIF-11−water" systems. For clarity the diagrams for each system are shifted by 1.0 mL/g along the *y* axis.

3. References

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