

## SUPPORTING INFORMATION

### **Synthesis and Characterization of Isostructural Cadmium Zeolitic Imidazolate Frameworks *via* Solvent-Assisted Linker Exchange**

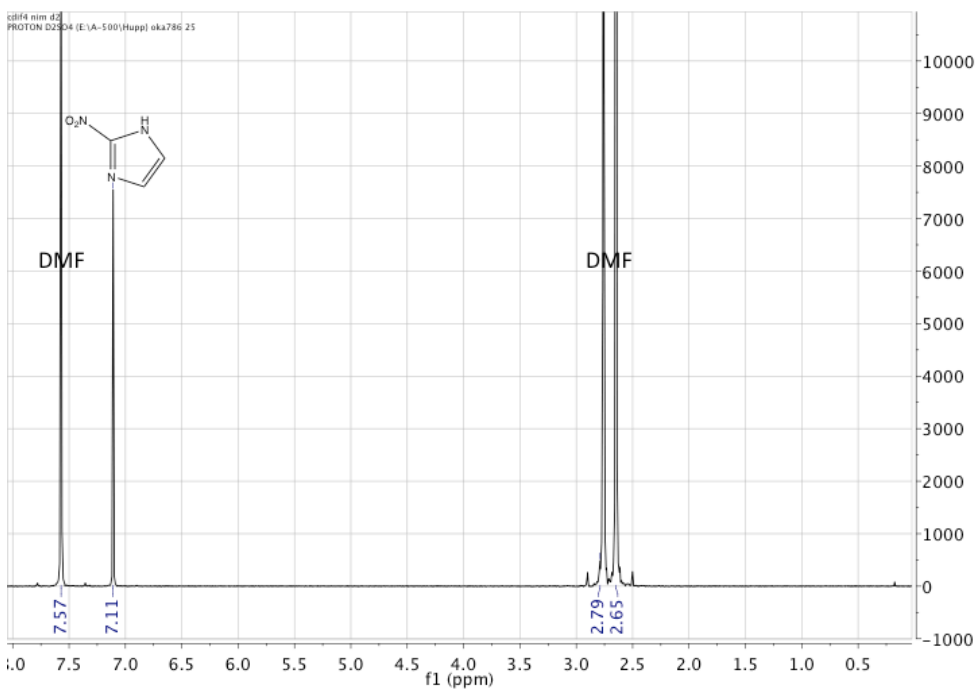
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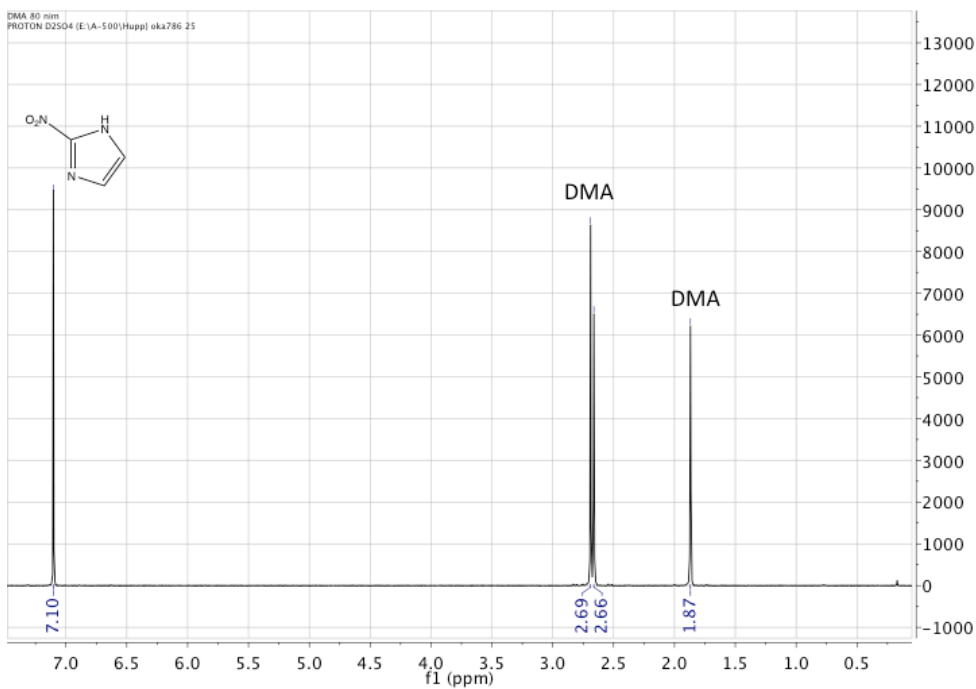
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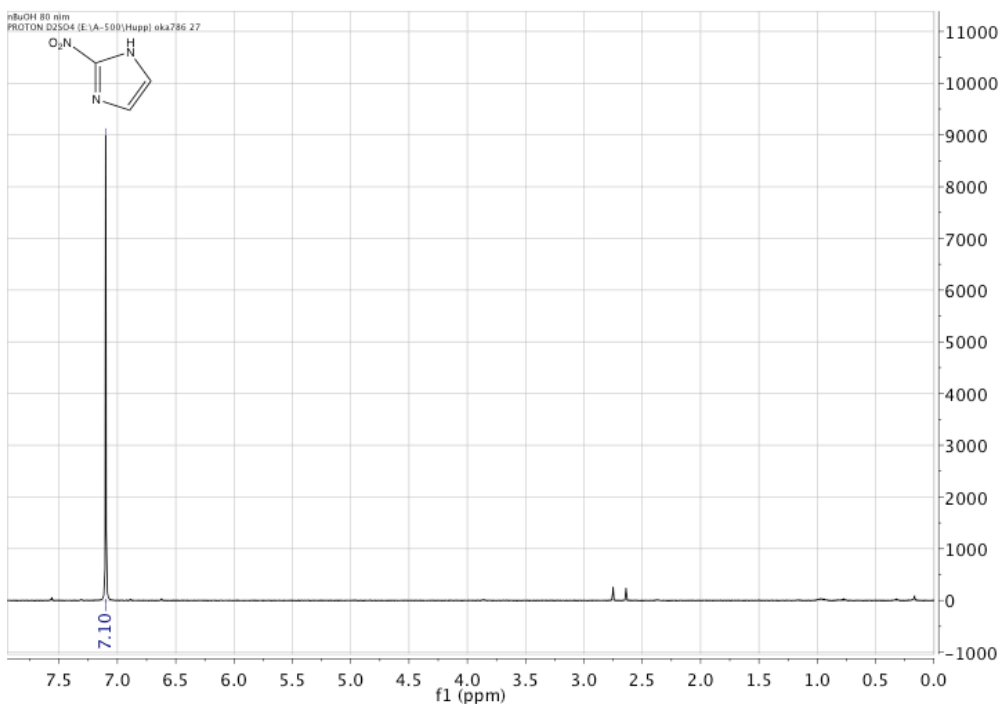
### Section S-1. $^1\text{H}$ NMR measurements.



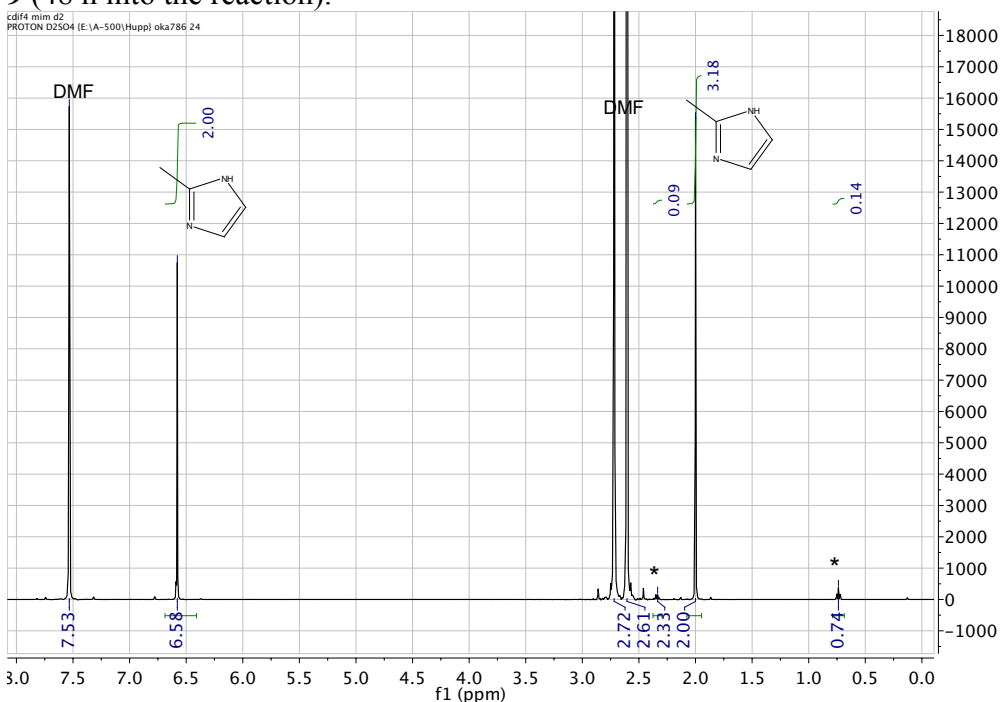
**Figure S1.**  $^1\text{H}$  NMR spectrum of CdIF-4 exchanged to nim in DMF to produce CdIF-9 (48 h into the reaction).



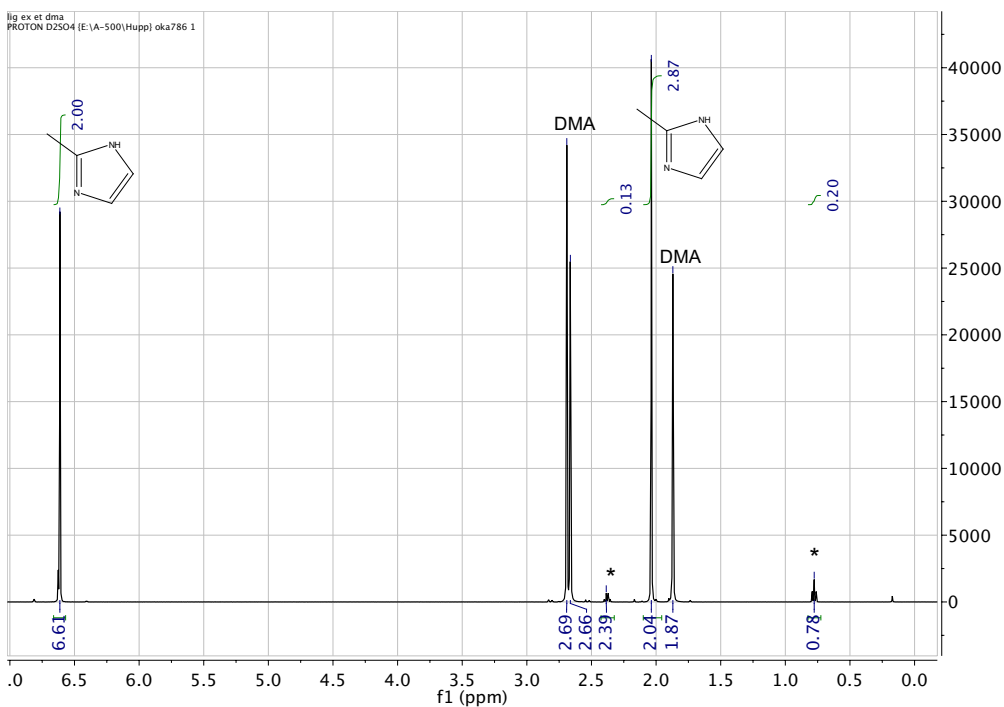
**Figure S2.**  $^1\text{H}$  NMR spectrum of CdIF-4 exchanged to nim in DMA to produce CdIF-9 (48 h into the reaction)



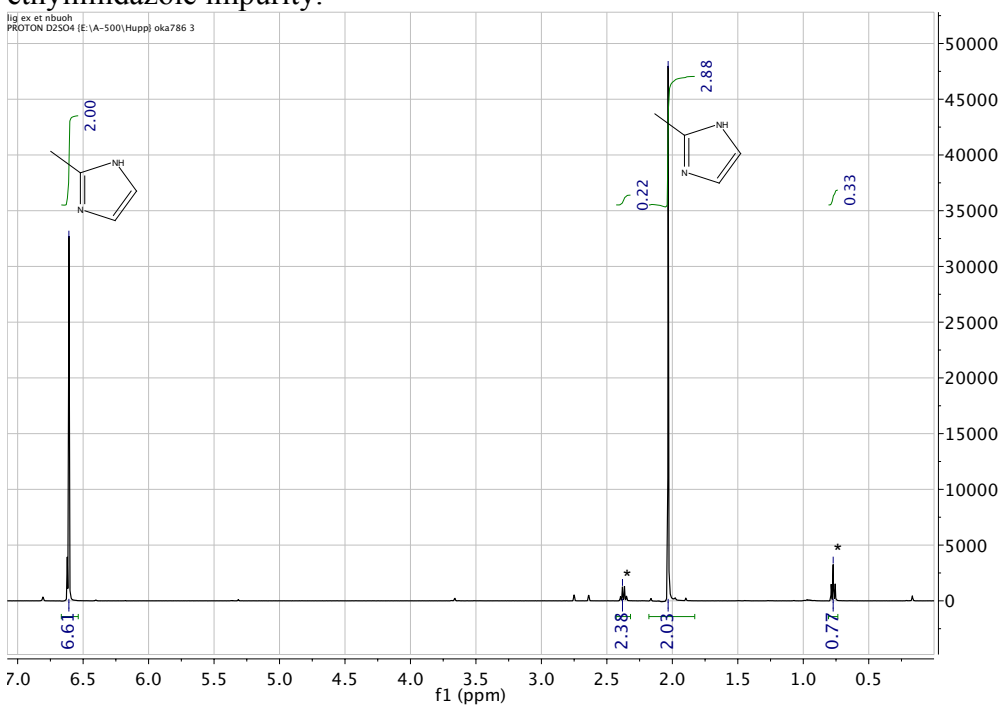
**Figure S3.**  $^1\text{H}$  NMR spectrum of CdIF-4 exchanged to nim in nBuOH to produce CdIF-9 (48 h into the reaction).



**Figure S4.**  $^1\text{H}$  NMR spectrum of CdIF-4 exchanged to mim in DMF to produce SALEM-1 (48 h into the reaction). The asterisks denote the presence of a minor 2-ethylimidazole impurity.

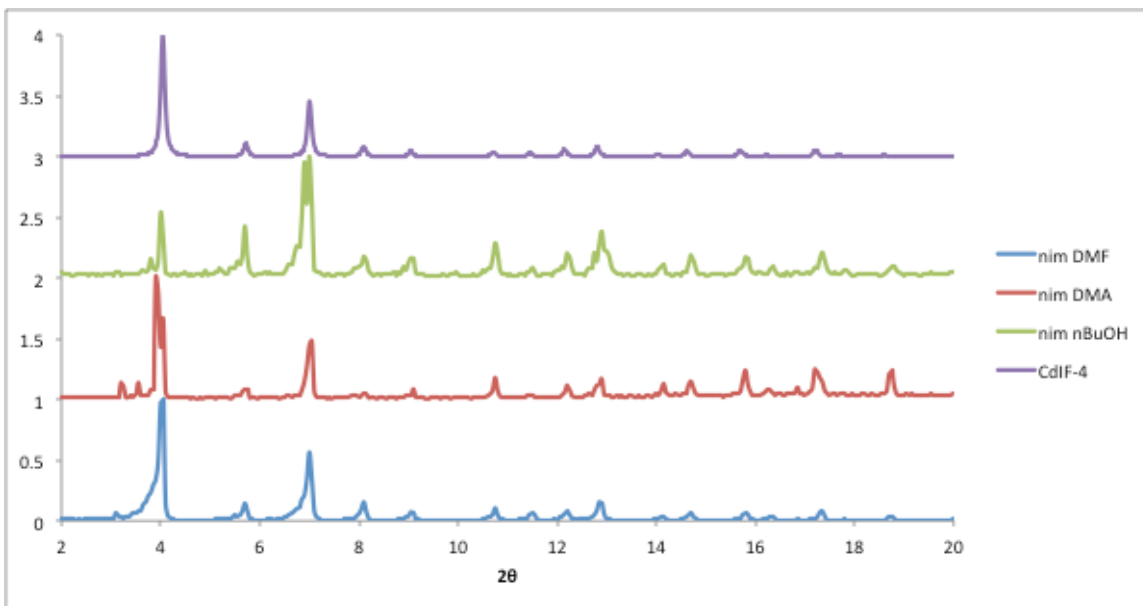


**Figure S5.**  $^1\text{H}$  NMR spectrum of CdIF-4 exchanged to mim in DMA to produce SALEM-1 (48 h into the reaction). The asterisks denote the presence of a minor 2-ethylimidazole impurity.

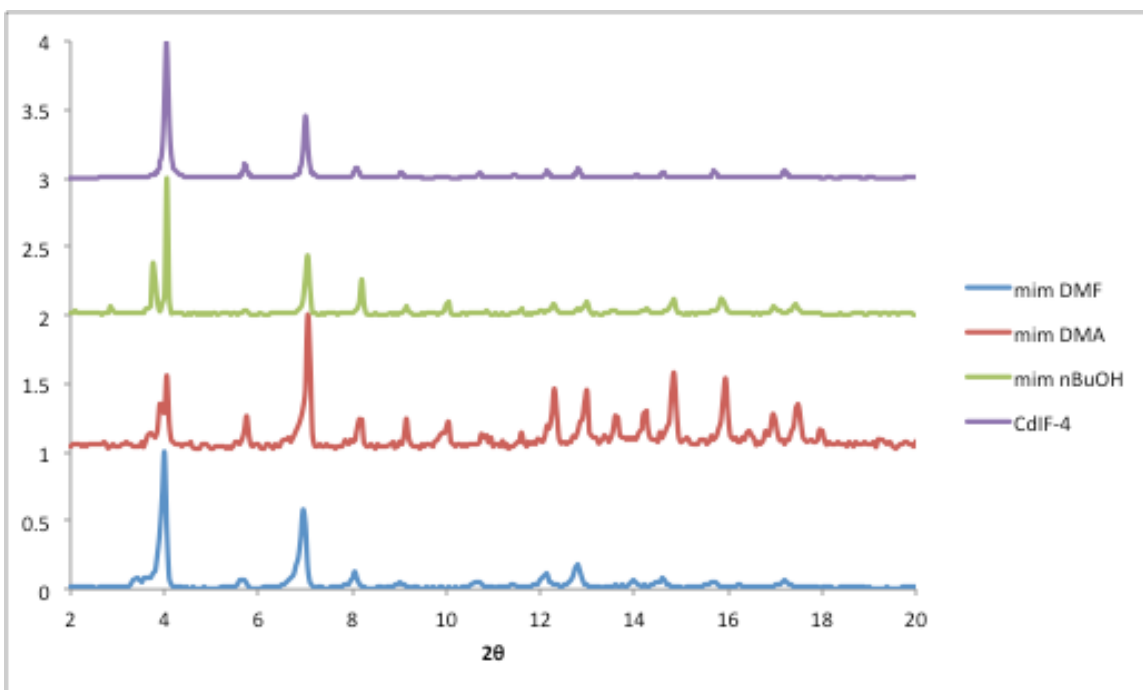


**Figure S6.**  $^1\text{H}$  NMR spectrum of CdIF-4 exchanged to mim in nBuOH to produce SALEM-1 (48 h into the reaction). The asterisks denote the presence of a minor 2-ethylimidazole impurity.

### Section S-3. PXRD measurements



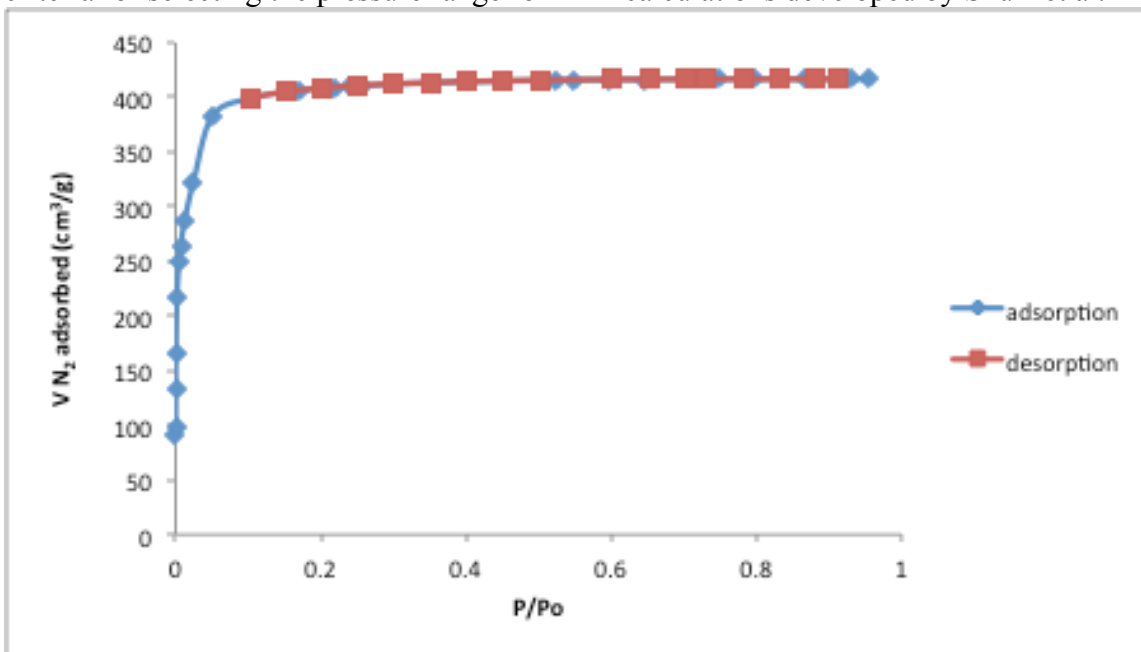
**Figure S7.** PXRD patterns of CdIF-4 exchanged to nim in various solvents.



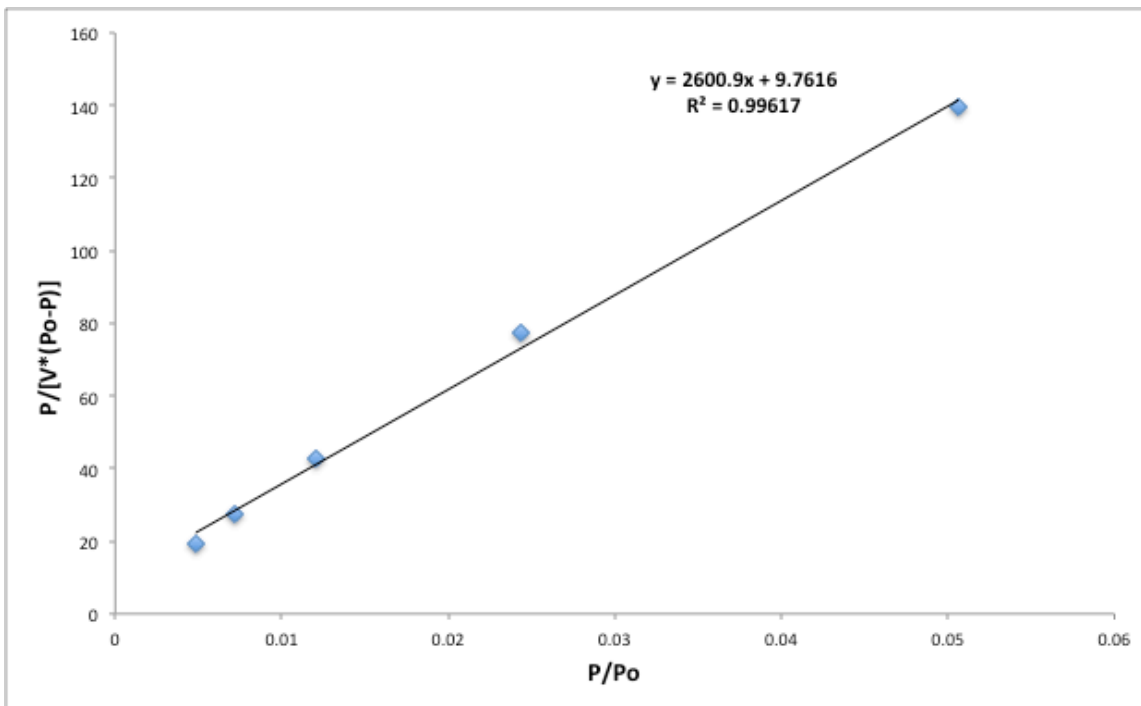
**Figure S8.** PXRD patterns of CdIF-4 exchanged to mim in various solvents.

### Section S-4. BET measurements

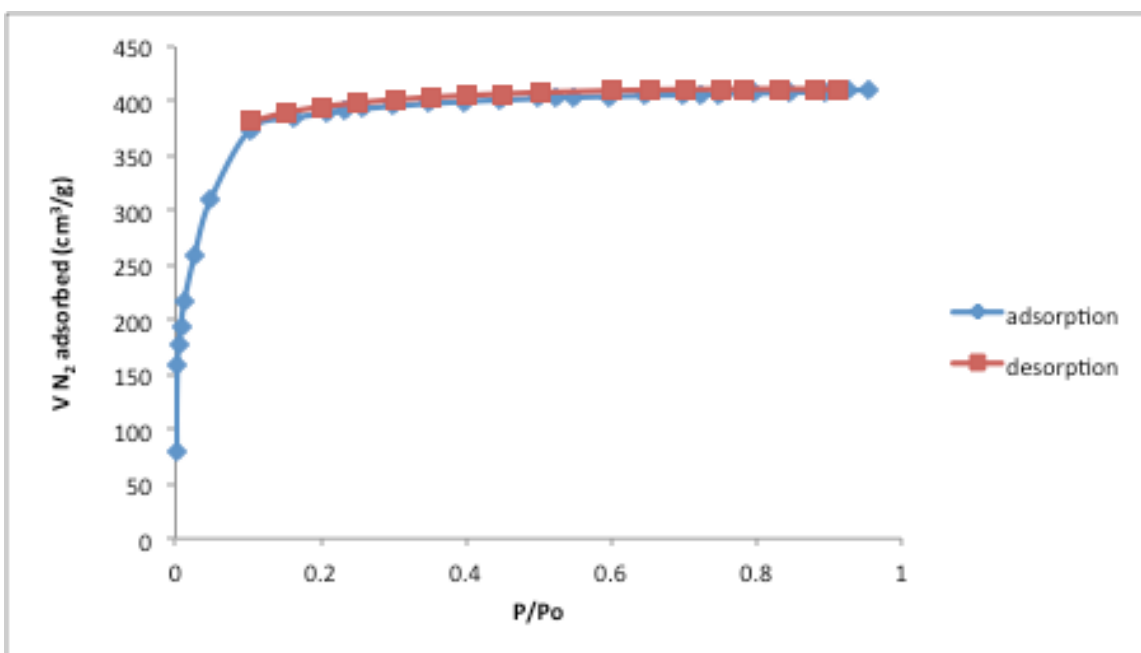
All the BET surface area plots show that the selected data points satisfied the consistency criteria for selecting the pressure range for BET calculations developed by Snurr et al.<sup>1</sup>



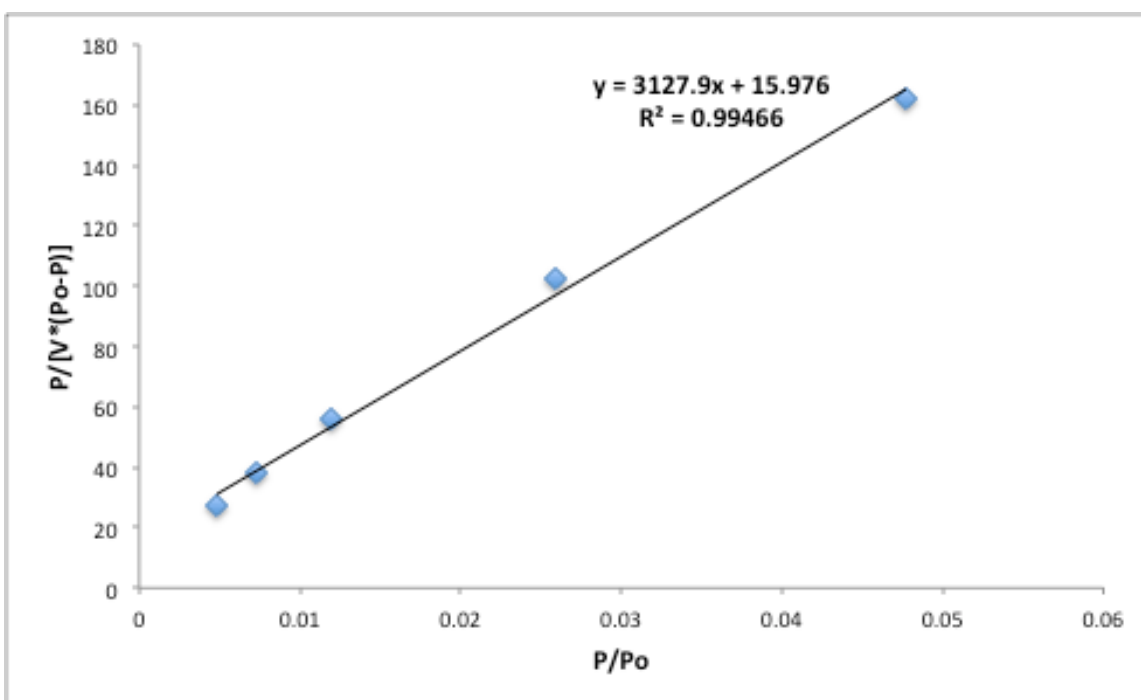
**Figure S9.** Nitrogen gas sorption isotherm at 77 K for CdIF-9.



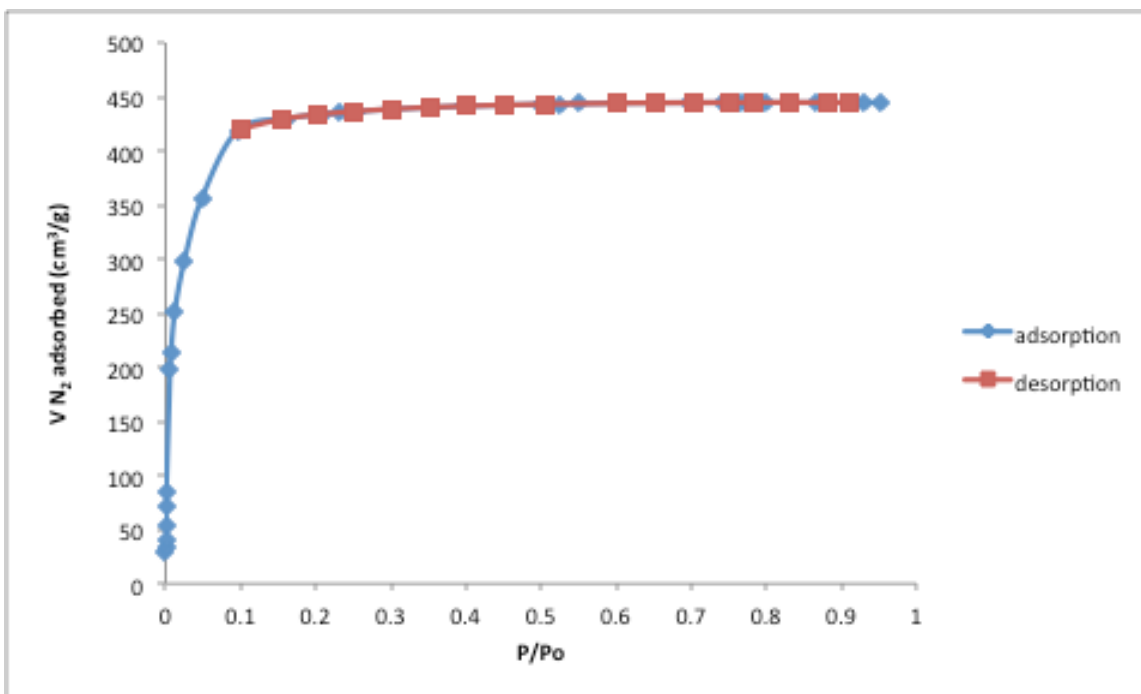
**Figure S10.** BET surface area plot for CdIF-9 for P/Po 0.005-0.05. The BET surface area calculated from this P/Po is 1668 m<sup>2</sup>/g



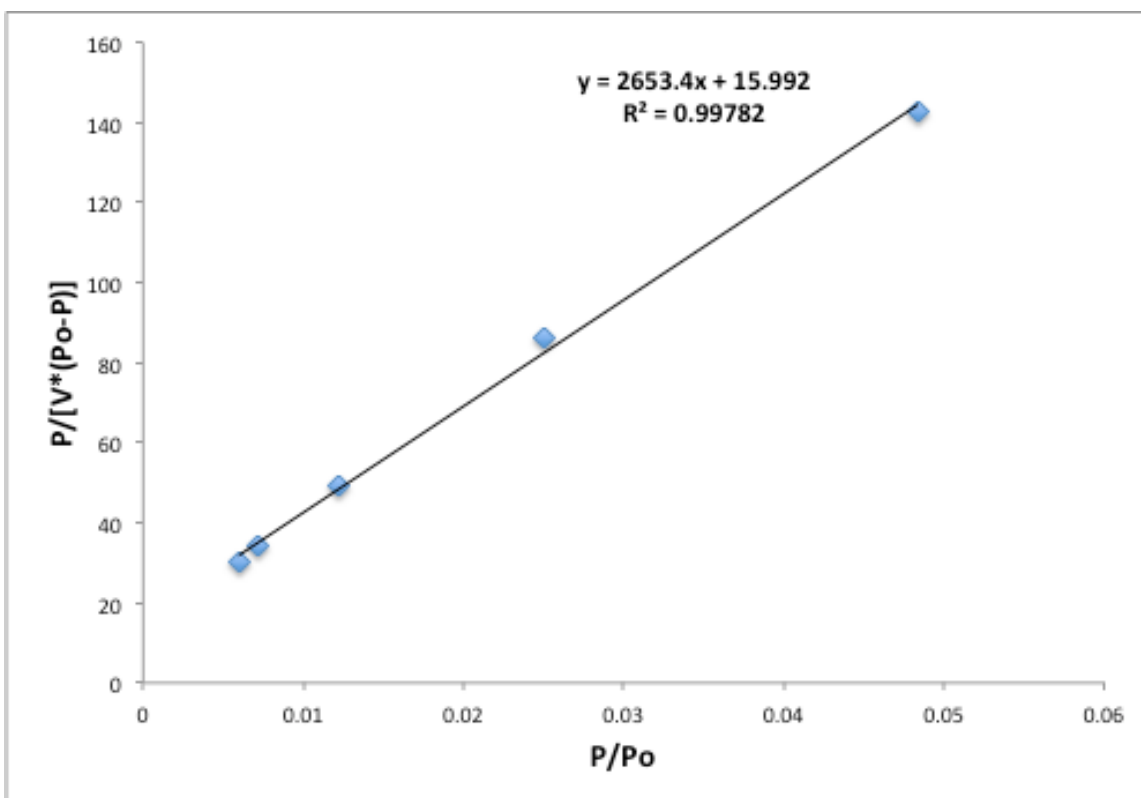
**Figure S11.** Nitrogen gas sorption isotherm at 77 K for SALEM-1.



**Figure S12.** BET surface area plot for SALEM-1 for P/Po 0.005-0.05. The BET surface area calculated from this P/Po is 1385 m<sup>2</sup>/g



**Figure S13.** Nitrogen gas sorption isotherm at 77 K for CdIF-4 obtained through reverse SALE (eim→mim→eim).



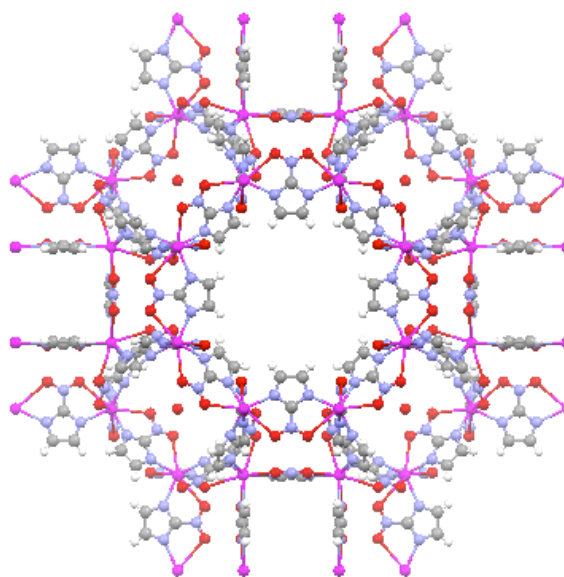
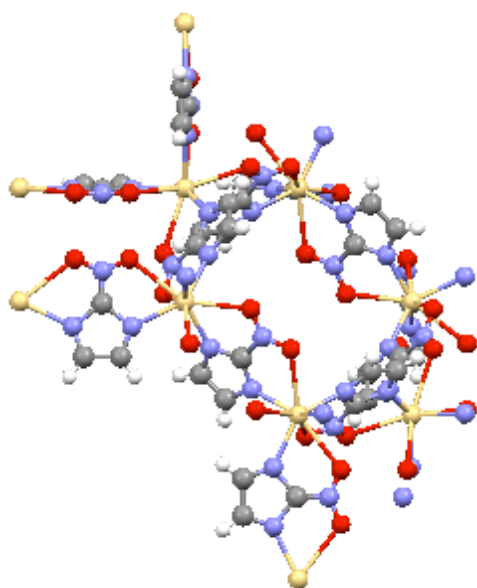
**Figure S14.** BET surface area plot for CdIF-4 for P/Po 0.005-0.05. The BET surface area calculated from this P/Po is 1632 m<sup>2</sup>/g.



## Section S-5. Single crystal data.

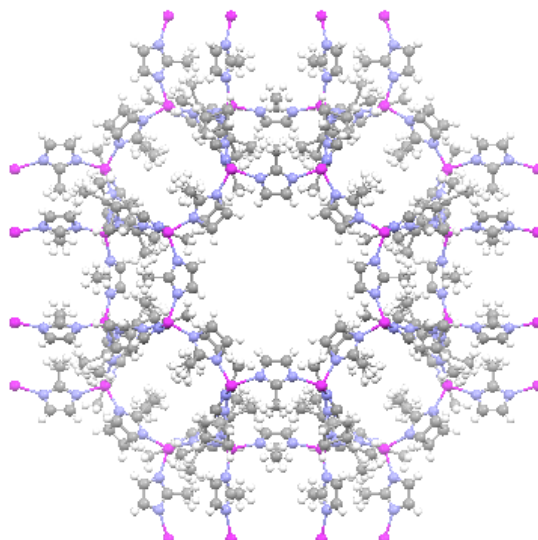
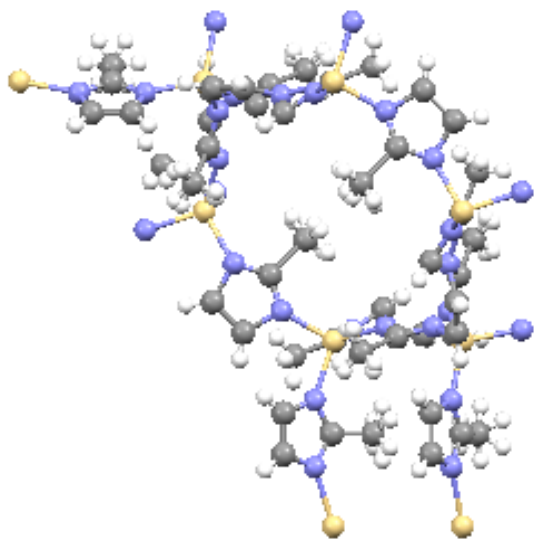
**Table S1** Crystal data and structure refinement for **CdIF-9**

Empirical formula	C <sub>6</sub> H <sub>4</sub> Cd N <sub>6</sub> O <sub>4</sub>
Formula weight	336.55
Temperature	100 K
Wavelength	1.54184 Å
Crystal system	Cubic
Space group	<i>Im</i> 3 <i>m</i>
Unit cell dimensions	$a = b = c = 30.2375 (4) \text{ \AA}$ $\alpha = \beta = \gamma = 90^\circ$
Volume	27646.3 (6) Å <sup>3</sup>
Z	48
Density (calculated)	0.970 Mg m <sup>-3</sup>
Absorption coefficient	7.69 mm <sup>-1</sup>
F(000)	7776
Crystal size	0.05 x 0.05 x 0.05 mm
Theta range for data collection	3.6° - 53.0°
Index ranges	-25 ≤ h ≤ 30 -30 ≤ k ≤ 29 -30 ≤ l ≤ 29
Reflections collected	44426
Independent reflections	1437 [R <sub>int</sub> = 0.090]
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Reflections/restraints/parameters	1437/21/118
Goodness of fit on F <sup>2</sup>	1.05
Final R indices	R[F <sup>2</sup> > 2σ(F <sup>2</sup> )] = 0.047, wR(F <sup>2</sup> ) = 0.162
Largest diff. peak and hole	0.45, -0.31



**Table S2** Crystal data and structure refinement for **SALEM-1**

Empirical formula	C <sub>8</sub> H <sub>10</sub> Cd N <sub>4</sub>
Formula weight	274.60
Temperature	100 K
Wavelength	1.54184 Å
Crystal system	Cubic
Space group	<i>Im3m</i>
Unit cell dimensions	$a = b = c = 30.5539 (5) \text{ \AA}$ $\alpha = \beta = \gamma = 90^\circ$
Volume	28523.3 (5) Å <sup>3</sup>
Z	48
Density (calculated)	0.767 Mg m <sup>-3</sup>
Absorption coefficient	7.22 mm <sup>-1</sup>
F(000)	6432
Crystal size	0.06 x 0.06 x 0.06 mm
Theta range for data collection	4.1° - 46.3°
Index ranges	-28 ≤ h ≤ 24 -23 ≤ k ≤ 29 -22 ≤ l ≤ 32
Reflections collected	16673
Independent reflections	1694 [R <sub>int</sub> = 0.071]
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Reflections/restraints/parameters	1694/2/72
Goodness of fit on F <sup>2</sup>	1.02
Final R indices	R[F <sup>2</sup> > 2σ(F <sup>2</sup> )] = 0.067, wR(F <sup>2</sup> ) = 0.235
Largest diff. peak and hole	0.54, -0.60



**Section S-6. Author Contributions.** J. T. H. conceived the idea behind the experiment. O. K. and W. B. chose the system on which to perform the experiment and performed all the experiments and measurements. O. K. F. and J. T. H. supervised the project and provided guidance with the experiments. A. A. S. and C. S. solved the crystal structures reported in the paper. O. K. wrote the initial drafts of the manuscript. O. K., W. B., O. K. F. and J. T. H. finalized the manuscript.

**Section S-7. References.**

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<sup>1</sup> K. S. Walton, and R. Q. Snurr. *J. Am. Chem. Soc.*, 2007, **129**, 8552-8556.