

Supporting Information

Thermally-Crosslinked Hydrogen-Bonded Organic Framework Membranes for Highly Selective Ion Separation

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Table S1. Crystal data and structure refinement for FDU-HOF-1

| Name | FDU-HOF-1 |
|--|--|
| Empirical formula | C ₁₂ H ₁₆ N ₁₀ O ₂ |
| CCDC number | 2238476 |
| Formula weight | 332.35 |
| Temperature/K | 173 |
| Crystal system | orthorhombic |
| Space group | Pnnm |
| a/ Å | 3.6813 (1) |
| b/ Å | 11.5900 (4) |
| c/ Å | 15.8935 (5) |
| α° | 90 |
| β° | 90 |
| γ° | 90 |
| Volume/Å ³ | 678.12 (4) |
| Z | 2 |
| D_c (g·cm ⁻³) | 1.628 |
| μ (mm ⁻¹) | 0.643 |
| $F(000)$ | 348.0 |
| Crystal size (mm) | 0.11 × 0.06 × 0.05 |
| θ range for data collection (°) | 4.107-58.107 |
| Refinement method | Least Squares |

Data/restraints/parameters 760/0/63

Goodness-of-fit on F^2 1.247

Table S2. Different Connolly radius of FDU-HOF-1 of occupied volume, free volume and surface area.

| Connolly radius (Å) | Occupied Volume (Å ³) | Free Volume (Å ³) | Surface area (Å ²) |
|---------------------|-----------------------------------|-------------------------------|--------------------------------|
| 0.6 | 564.07 | 114.05 | 166.78 |
| 0.9 | 593.35 | 84.76 | 123.75 |
| 1.3 | 616.85 | 61.26 | 106.04 |

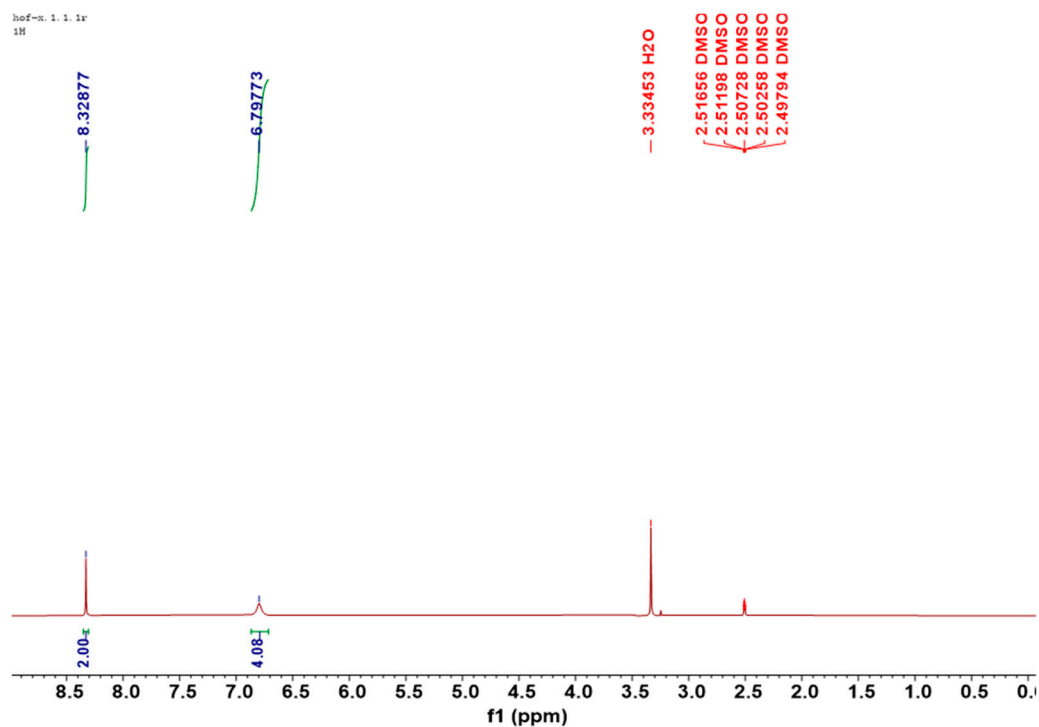


Figure S1. ^1H NMR spectrum of BDQ.

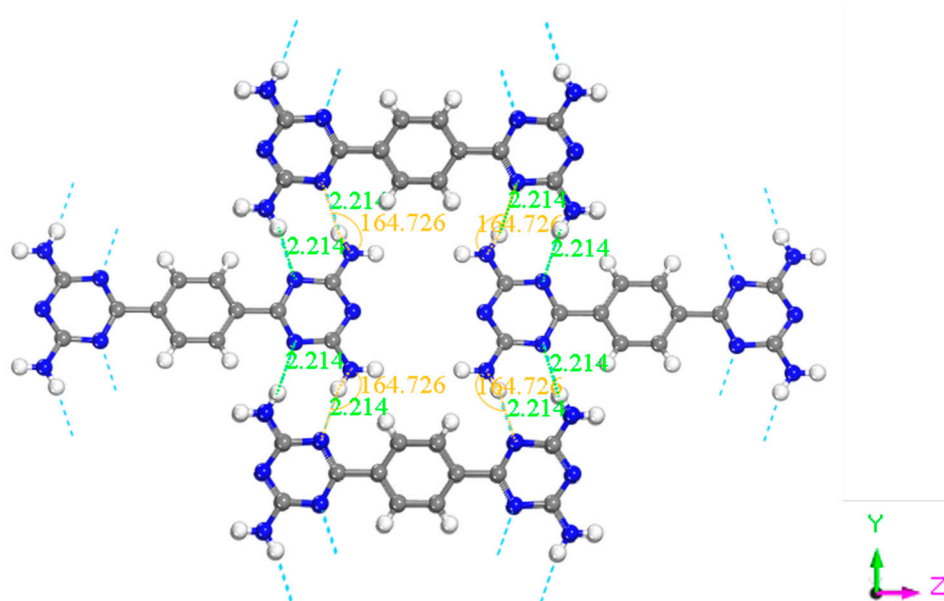


Figure S2. H-bonded distance and angle of BD-T ligand of FDU-HOF-1.

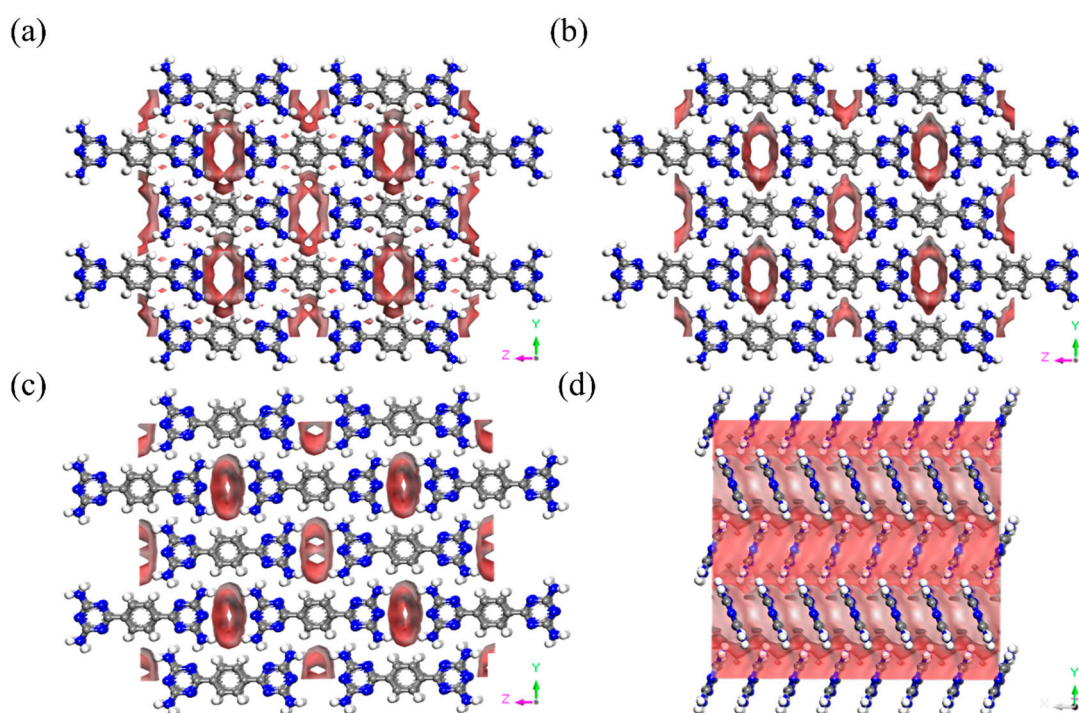


Figure S3. Pore structure at (a) 0.6 Å, (b) 0.9 Å and (c) 1.3 Å probe molecular sizes of FDU-HOF-1 in Materials Studio 2019. (d) Pore structure display along z-axis of FDU-HOF-1.

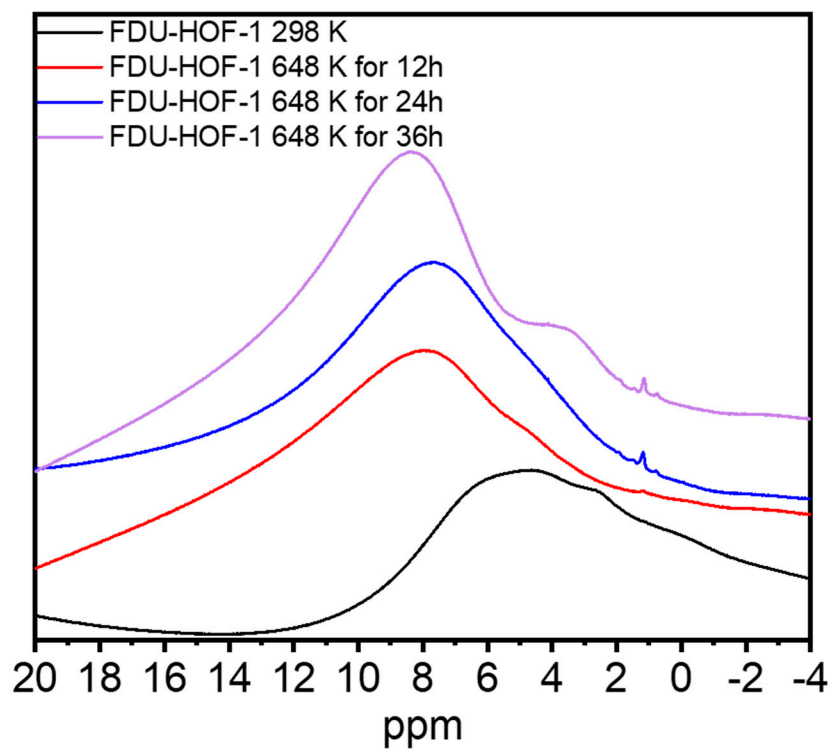


Figure S4. Solid-state ^1H NMR spectrums of FDU-HOF-1.

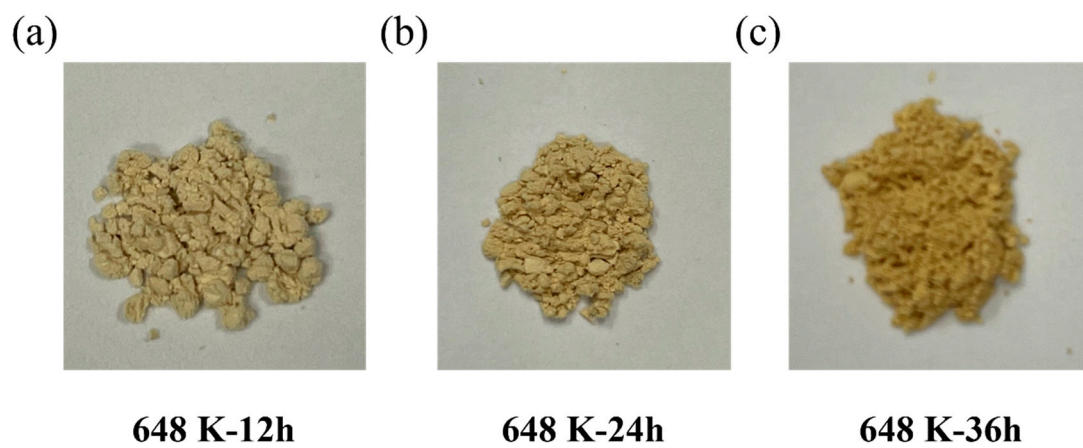


Figure S5. Photographs of FDU-HOF-1 powder after being treated under 648 K of (a) 12 h, (b) 24 h and (c) 36 h.