CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Synthesis, X-ray Crystal Structures and Gas Sorption Properties of Pillared Square Grid Nets Based on Paddle-wheel Motifs: Implications for Hydrogen Storage in Porous Materials

Hyungphil Chun,[a] Danil N. Dybtsev,[a] Hyunuk Kim,[a] and Kimoon Kim*[a]

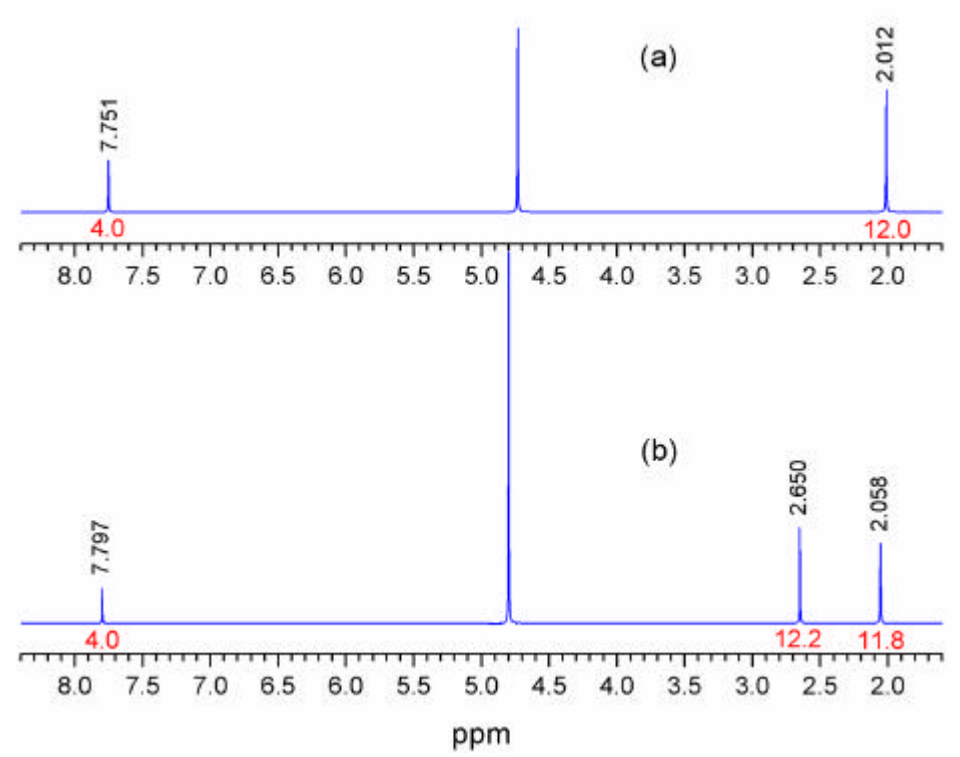

Figure S1. ^{1}H-NMR spectra of (a) 1:1 mixture of H_2bdc and H_2tmbdc in NaOH/D_2O, and (b) [Zn_2(1,4-bdc)(tmbdc)(dabco)] (**2**) digested in NaOH/D_2O. Integral values are shown in red.

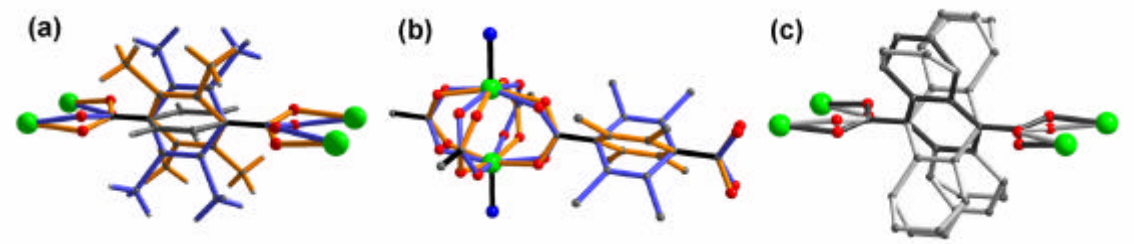

Figure S2. Disordered dicarboxylate linkers in the structure of **2** (a), **3** (b) and **4** (c). Hydrogen atoms are not shown in (b) and (c).

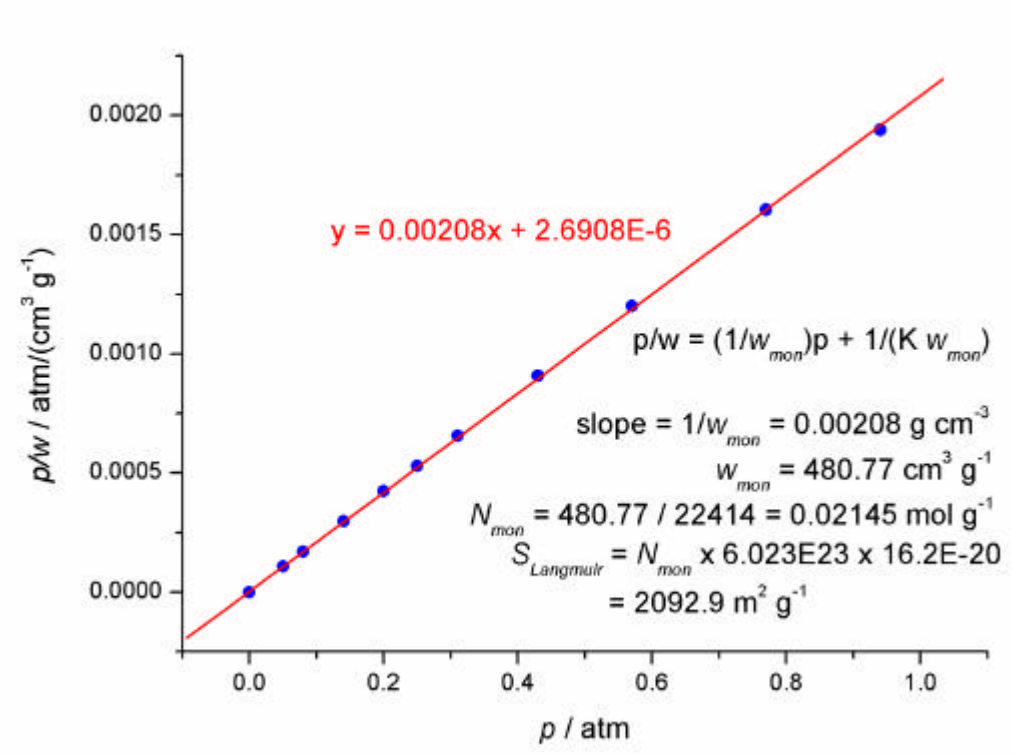

Figure S3. N_2 gas sorption data of $[Zn_2(1,4\text{-bdc})_2(dabco)]$ (**1**) and their fit to a Langmuir equation used to derive Langmuir surface area.

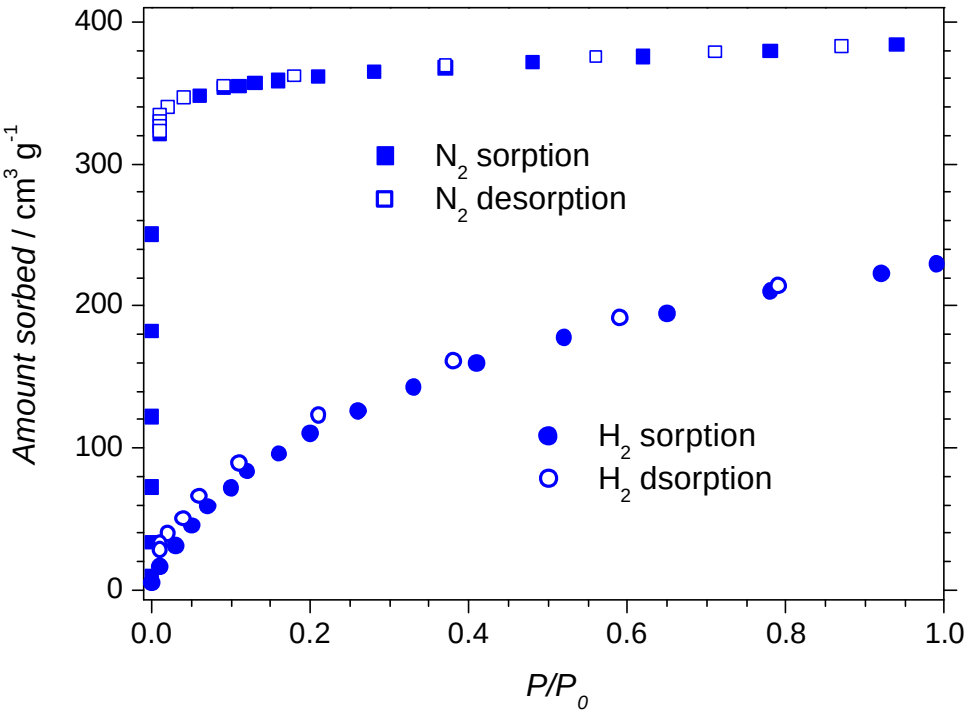

Figure S4. N_2 and H_2 gas sorption isotherms for **2**.

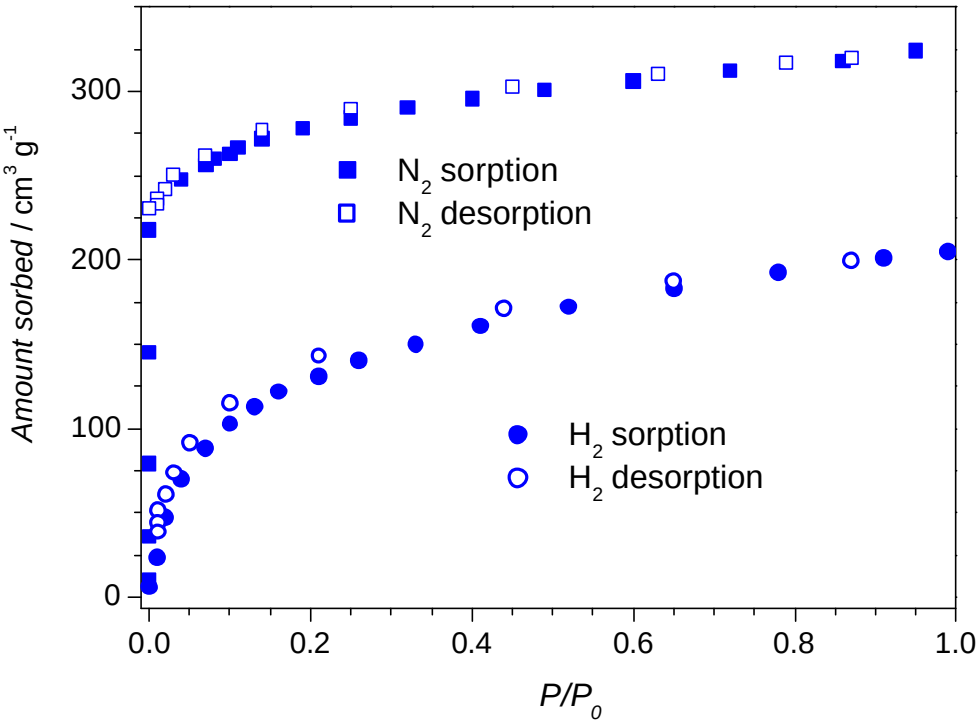

Figure S5. N_2 and H_2 gas sorption isotherms for **3**.

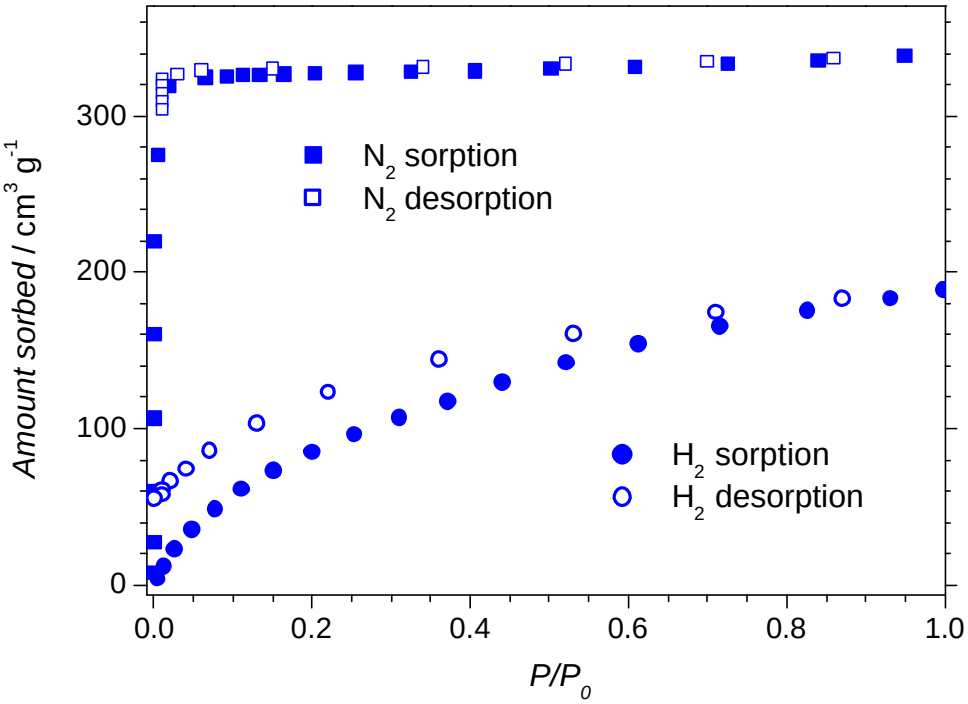

Figure S6. N_2 and H_2 gas sorption isotherms for **4**.

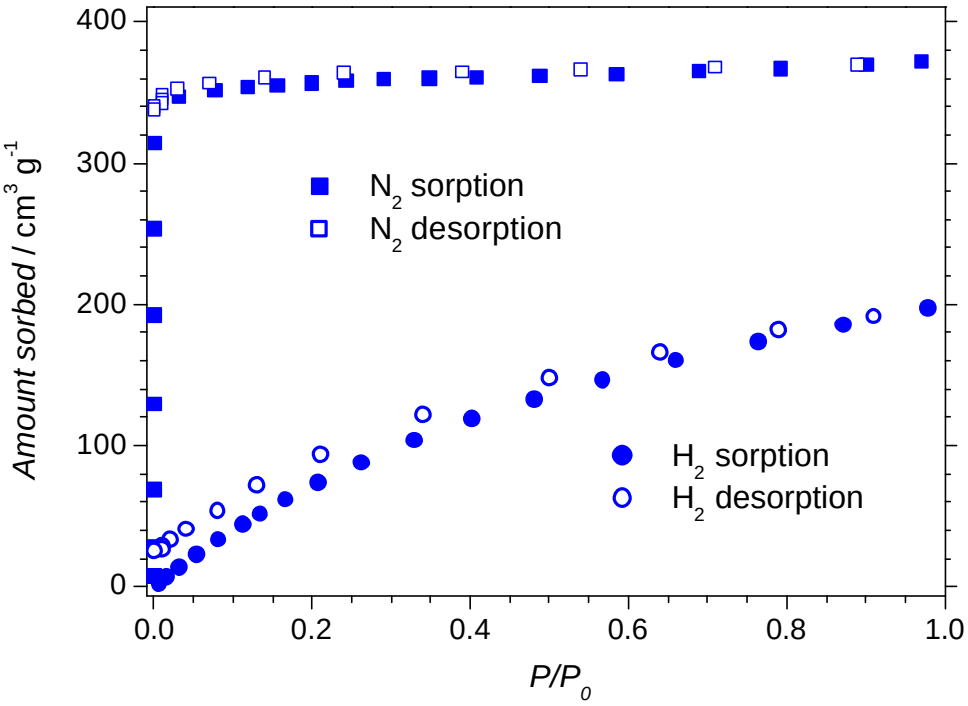

Figure S7. N_2 and H_2 gas sorption isotherms for **5**.

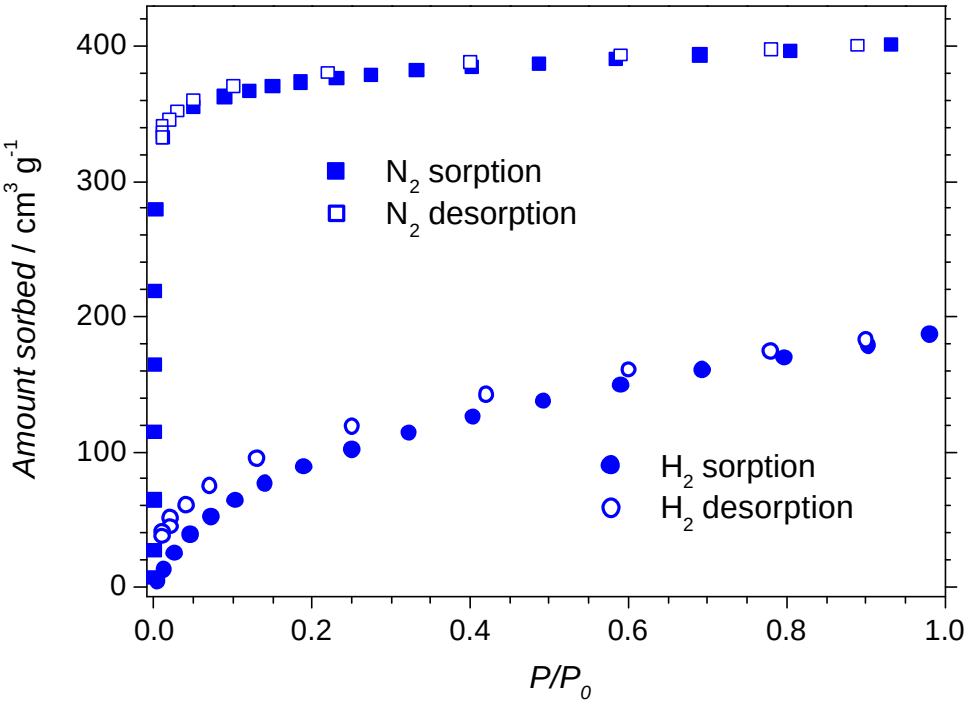

Figure S8. N_2 and H_2 gas sorption isotherms for **8**.

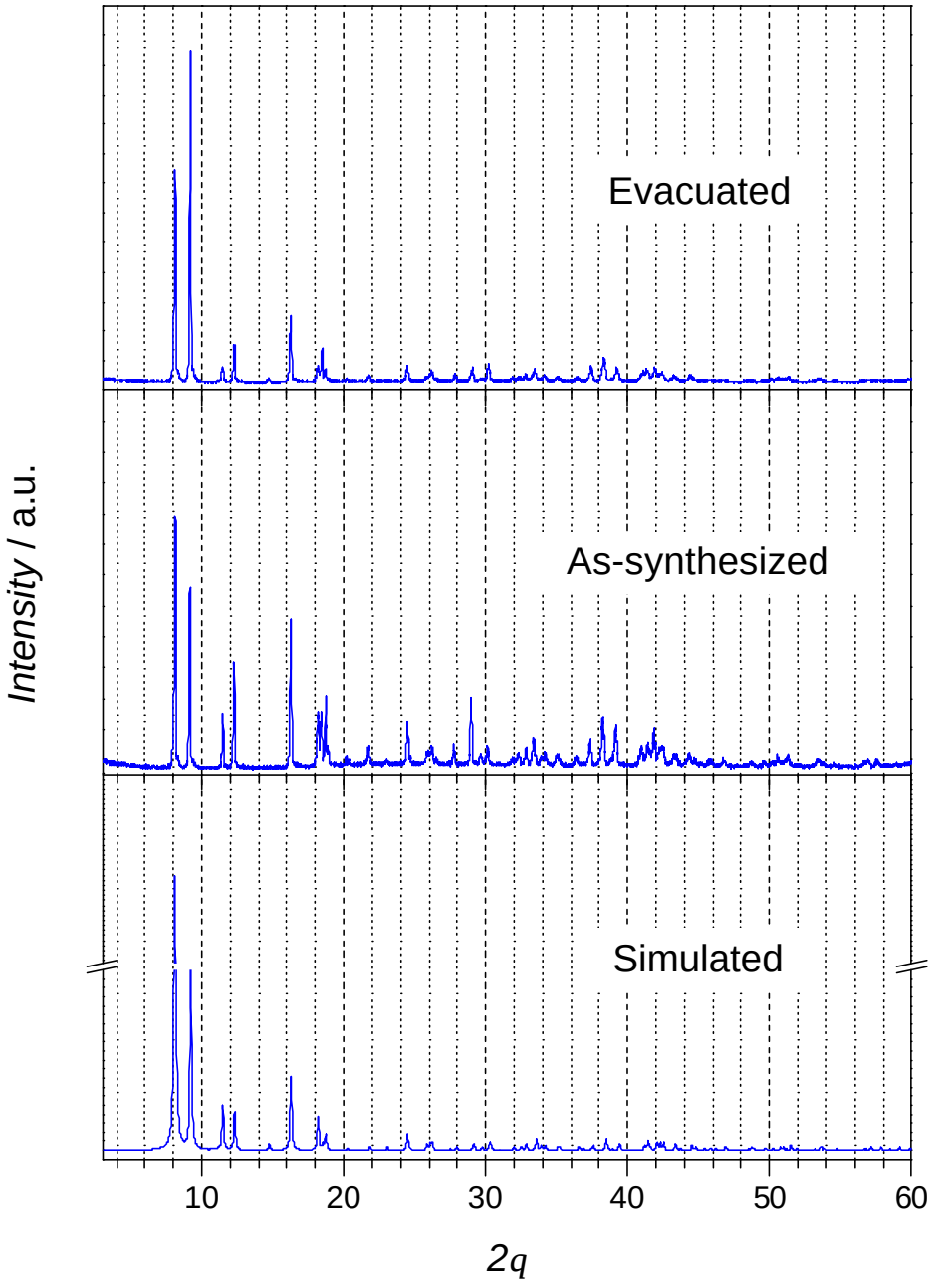

Figure S9. Experimental X-ray powder diffraction patterns of **2** and its simulation based on the single-crystal structure.

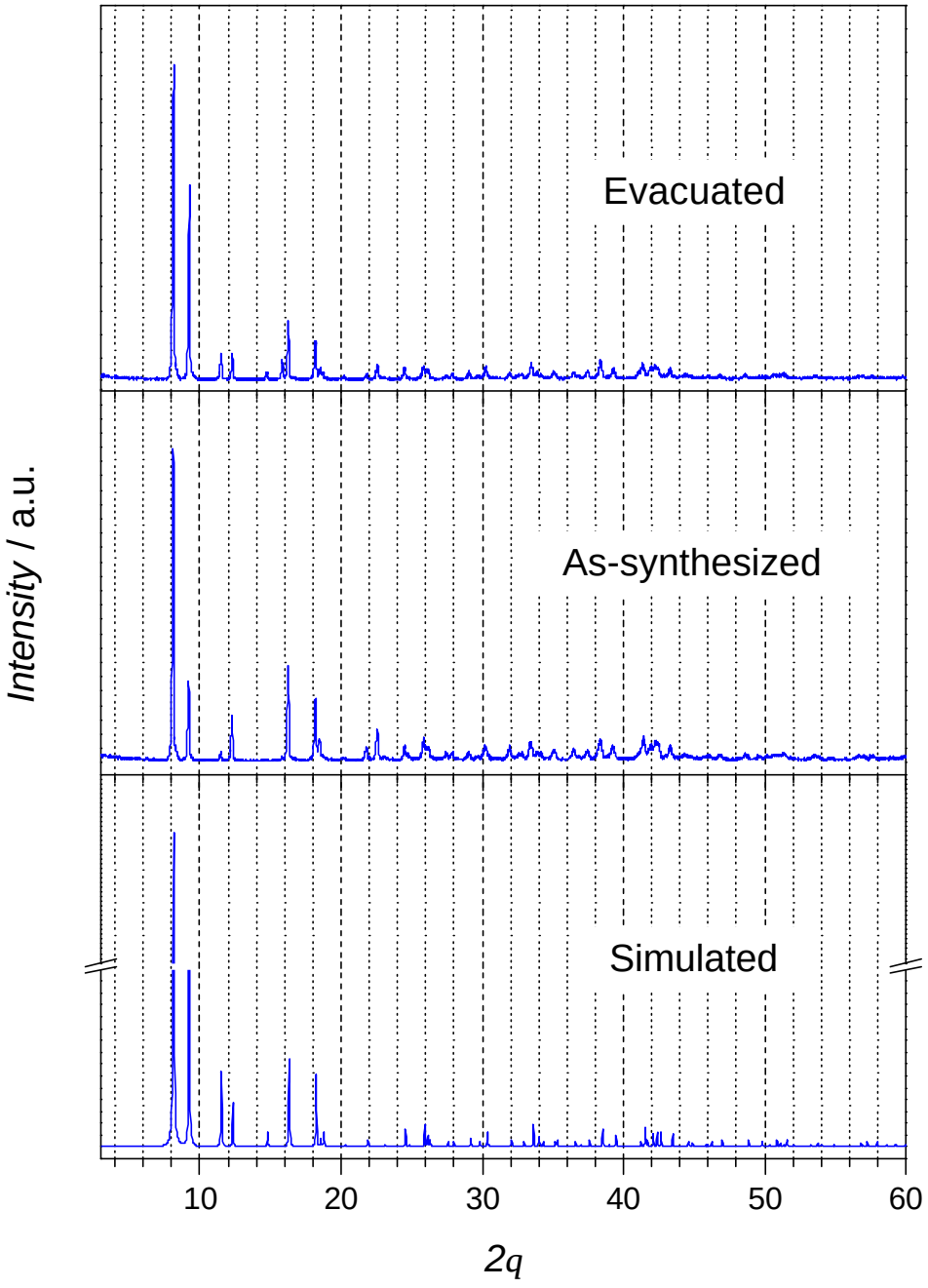

Figure S10. Experimental X-ray powder diffraction patterns of **3** and its simulation based on the single-crystal structure.

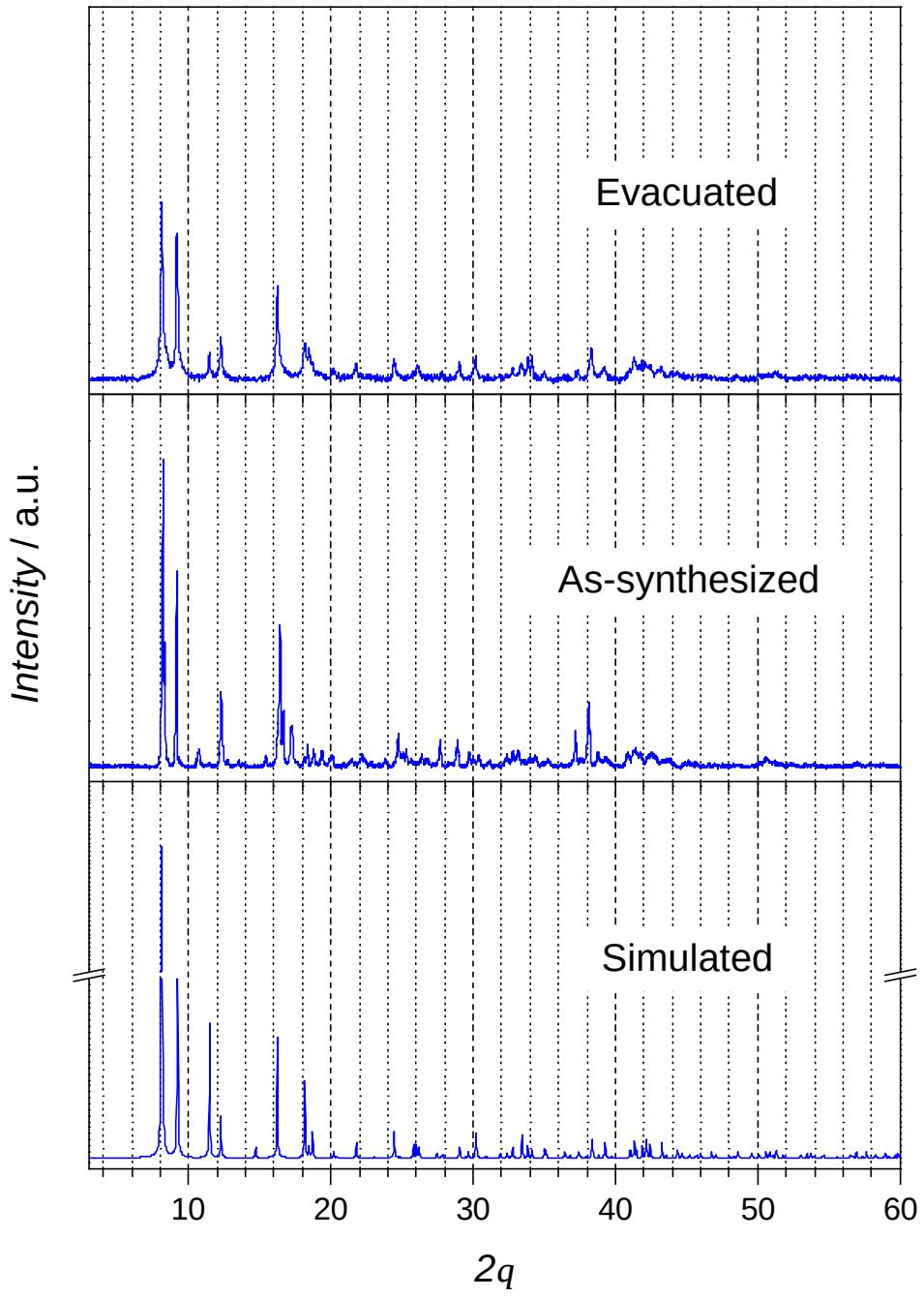

Figure S11. Experimental X-ray powder diffraction patterns of **4** and its simulation based on the single-crystal structure.

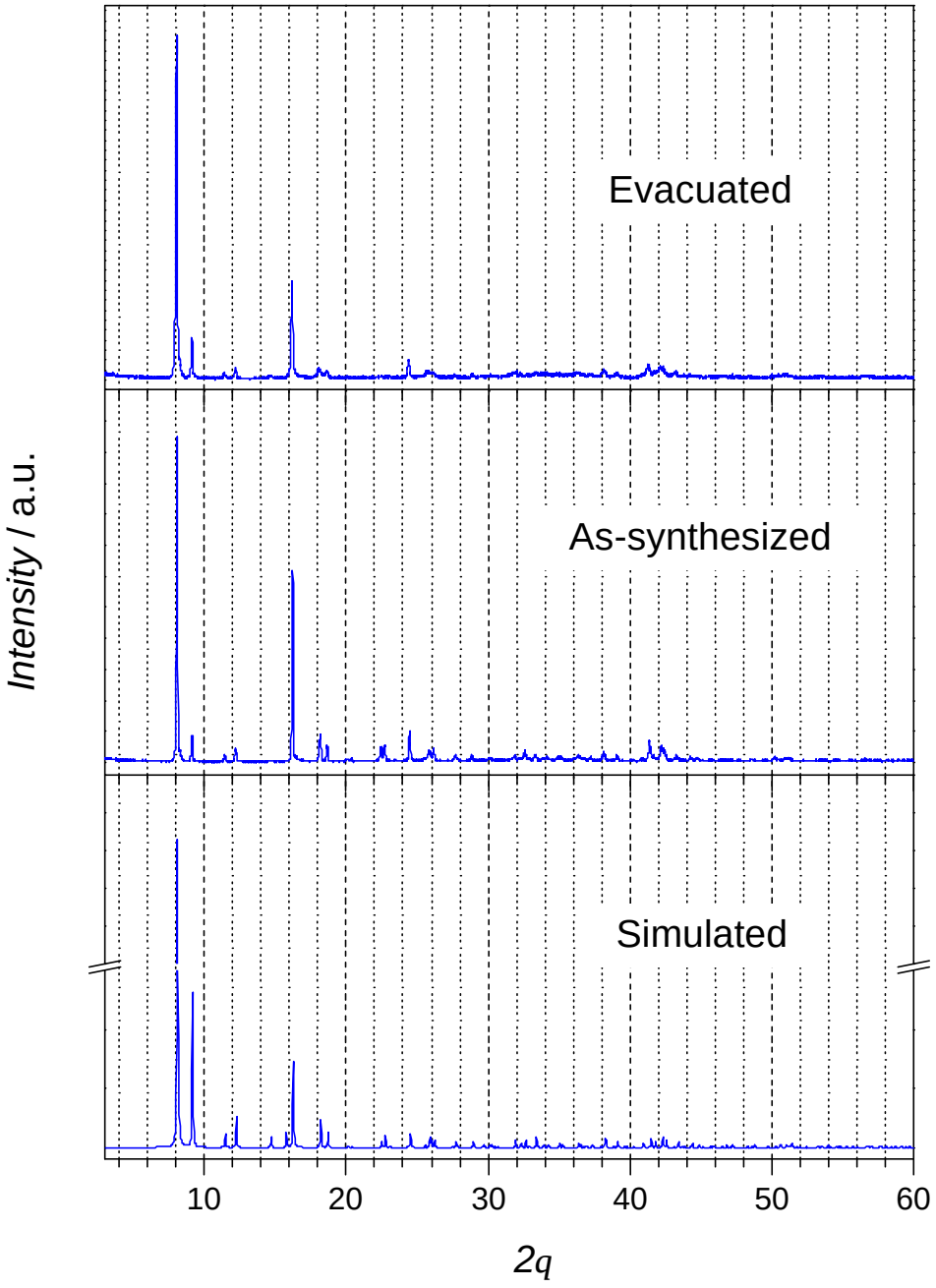

Figure S12. Experimental X-ray powder diffraction patterns of **5** and its simulation based on the single-crystal structure.

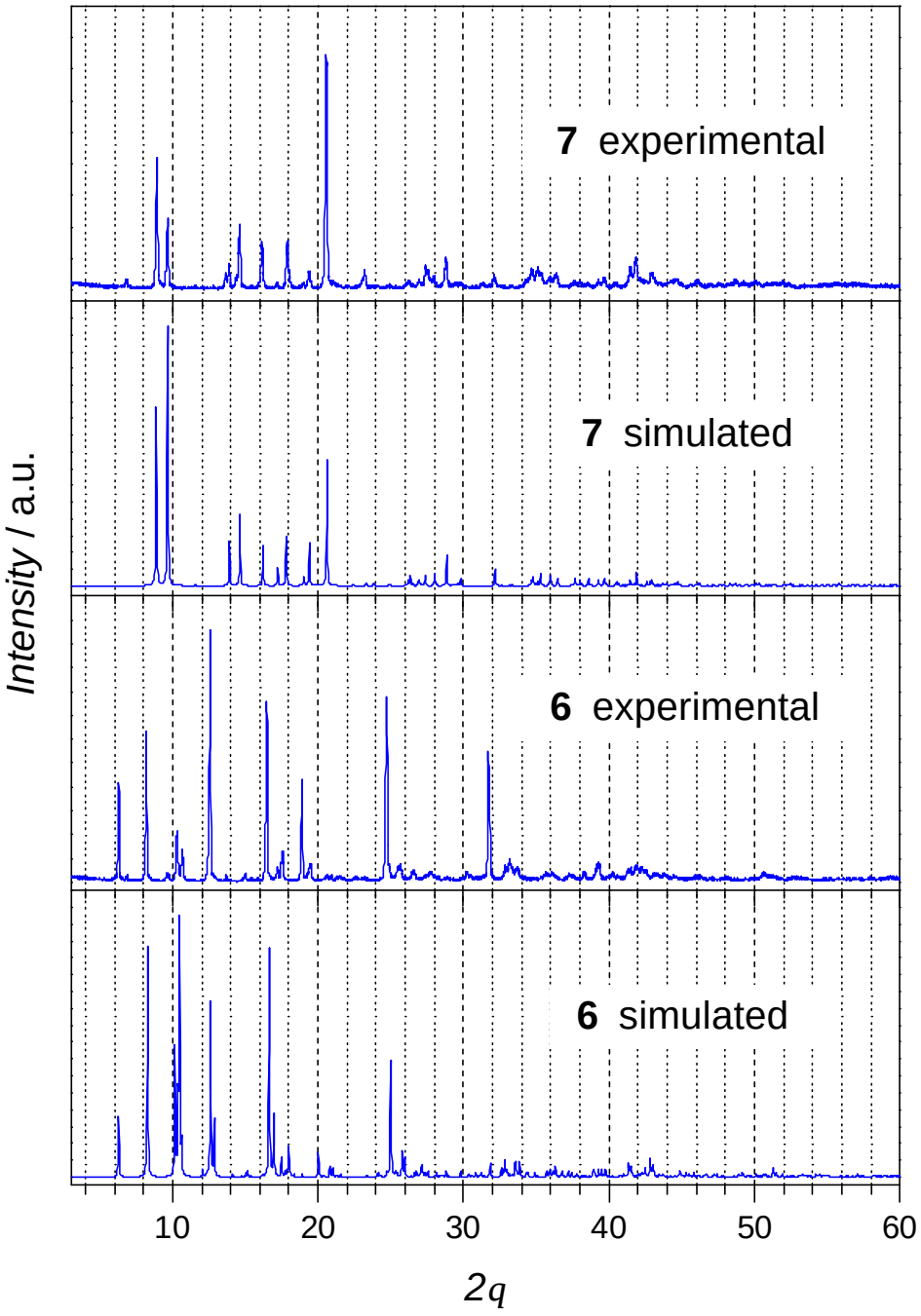

Figure S13. Experimental and X-ray powder diffraction patterns of **6** and **7** and their simulations based on the single-crystal structure.

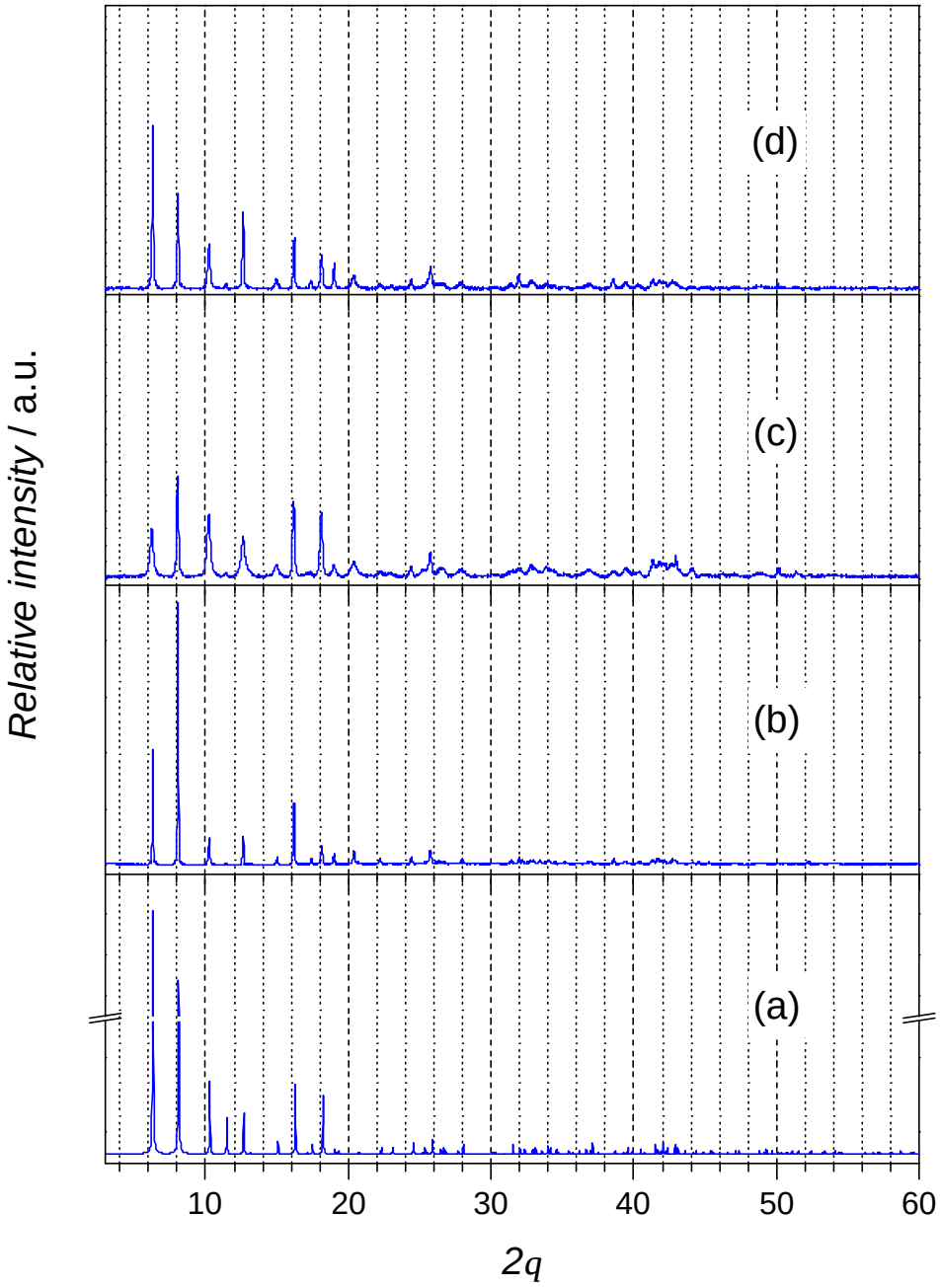

Figure S14. X-ray powder diffraction patterns of **8**. (a) Simulation based on the single-crystal structure, (b) as-synthesized, (c) evacuated under vacuum at 120 °C overnight, (d) dried after soaking the evacuated sample in DMF.