Supporting Information

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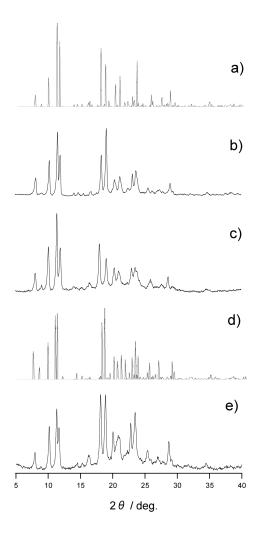


Figure S1. (a) Simulated XRPD pattern from the single crystal model of $3 \supset 4Me_2CO$. (b) Assynthesized $3 \supset 4Me_2CO$. (c) XRPD patterns at room temperature of exposing 3 to acetone for 4 days. (d) Simulated XRPD pattern from the single crystal model of $3 \supset 4THF$. (e) XRPD patterns at room temperature of exposing 3 to THF for 4 days.

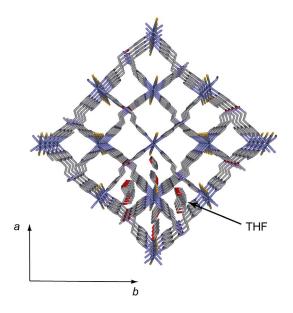


Figure S2. Crystal structure of $3 \supset 4$ THF along the c axis with THF molecules.

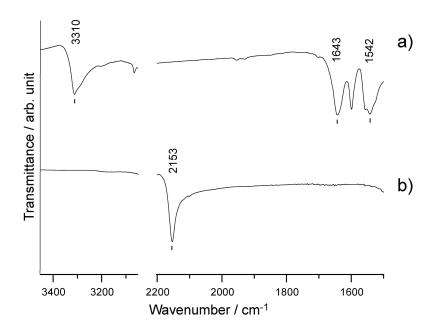


Figure S3. IR spectra in the region of 3450-3050 cm⁻¹ (left) and 2200-1500 cm⁻¹ (right) at room temperature of (a) 4-peia and (b) Co(SCN)₂.

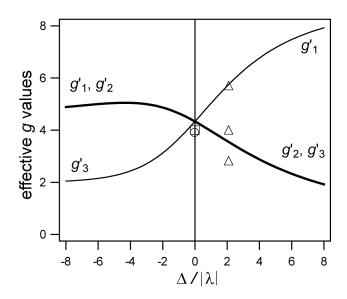


Figure S4. Effective g values calculated from the first-order perturbation equations are plotted versus $\Delta/|\lambda|$. The solid triangles, squares, and circles represent the experimentally-obtained effective g values for $3 \supset 4\text{Me}_2\text{CO}$, $3 \supset \text{Me}_2\text{CO}$, and 3, respectively.

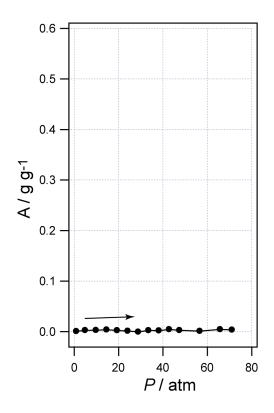


Figure S5. Isotherm for CH_4 adsorption at 298 K of 3 over the pressure range from 0.5 to 70 atom.