

Supporting Information

Separation of Gas Mixtures Using Co(II)-Carborane-Based Porous Coordination Polymers

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Experimental

Carborane precursor **1** was purchased from KatChem (Czech Republic) and used as received. All other chemicals and solvents were purchased from the Aldrich Chemical Company and used without further purification. Ligand **2** and materials **3** and **4** were made according to previously published methods.¹ Material **3** in this paper is material **2** in reference 1, and Material **4** in this paper is material **3** in reference 1. **3a** and **4a** were obtained by thermal activation of **3** and **4** at 300°C under dynamic vacuum for 12 h. **4b** was obtained by heating **4** at 120°C under dynamic vacuum for 12 h.

Adsorption measurements of CO₂, CH₄, O₂ and N₂ were done volumetrically at 298 K up to 17 bar on samples of 50-70 mg. All gases were 99.9% purity or higher obtained from Airgas, Inc. Equilibrium pressures were measured with an MKS Baratron transducer 627B (accuracy +/- 0.12%). Adsorbate gas was dosed in increments, and equilibrium was assumed when no further change in pressure was observed (within 0.01 kPa).

Magnetization was measured with a commercial Quantum Design MPMS SQUID magnetometer (5 Tesla magnet).

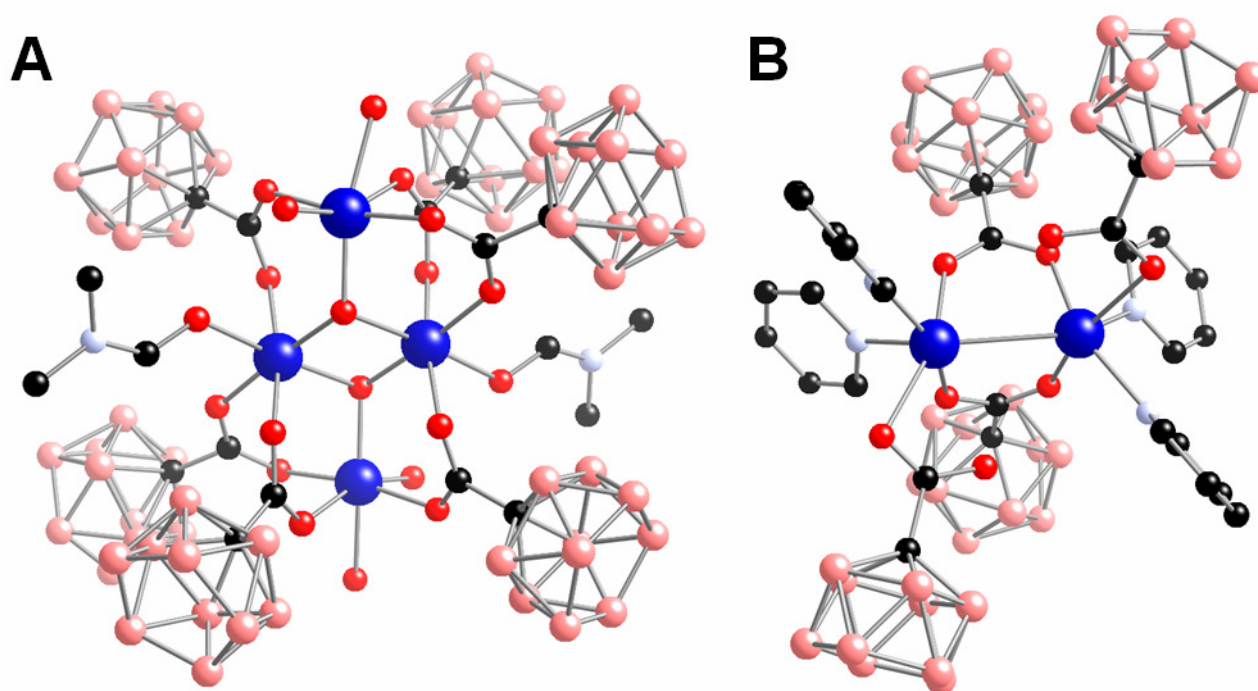


Figure S1. Coordination environments within (a) **3** and (b) **4**, respectively. Cobalt atoms are dark blue, oxygens are red, carbons are black, nitrogens are light blue and borons are beige (made by CrystalMaker 2.2).

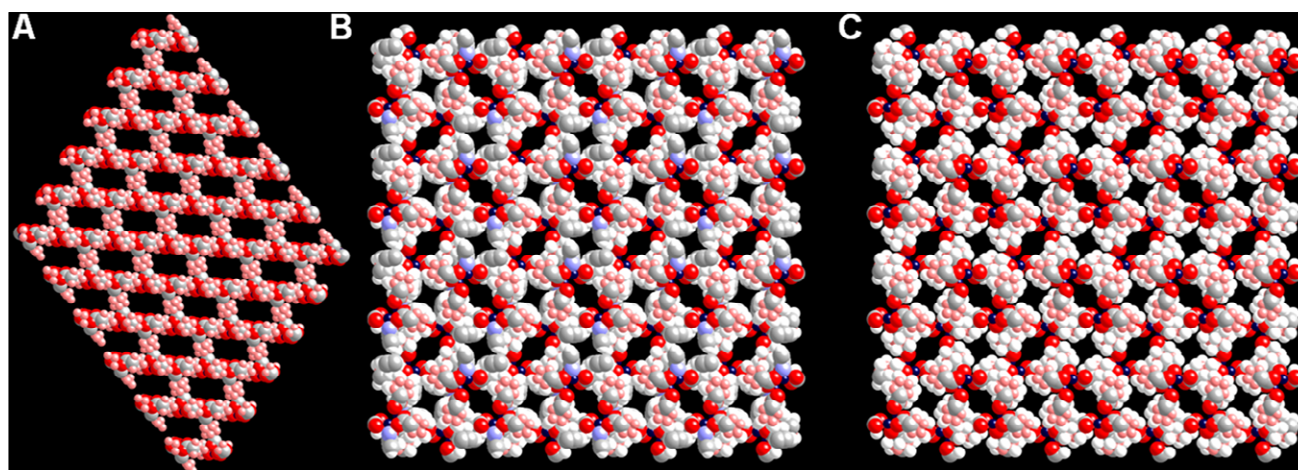


Figure S2. Spaced-filled representations of activated materials. (a) **3a**, (b) **4b**, and (c) **4a**. (made by CrystalMaker 2.2)

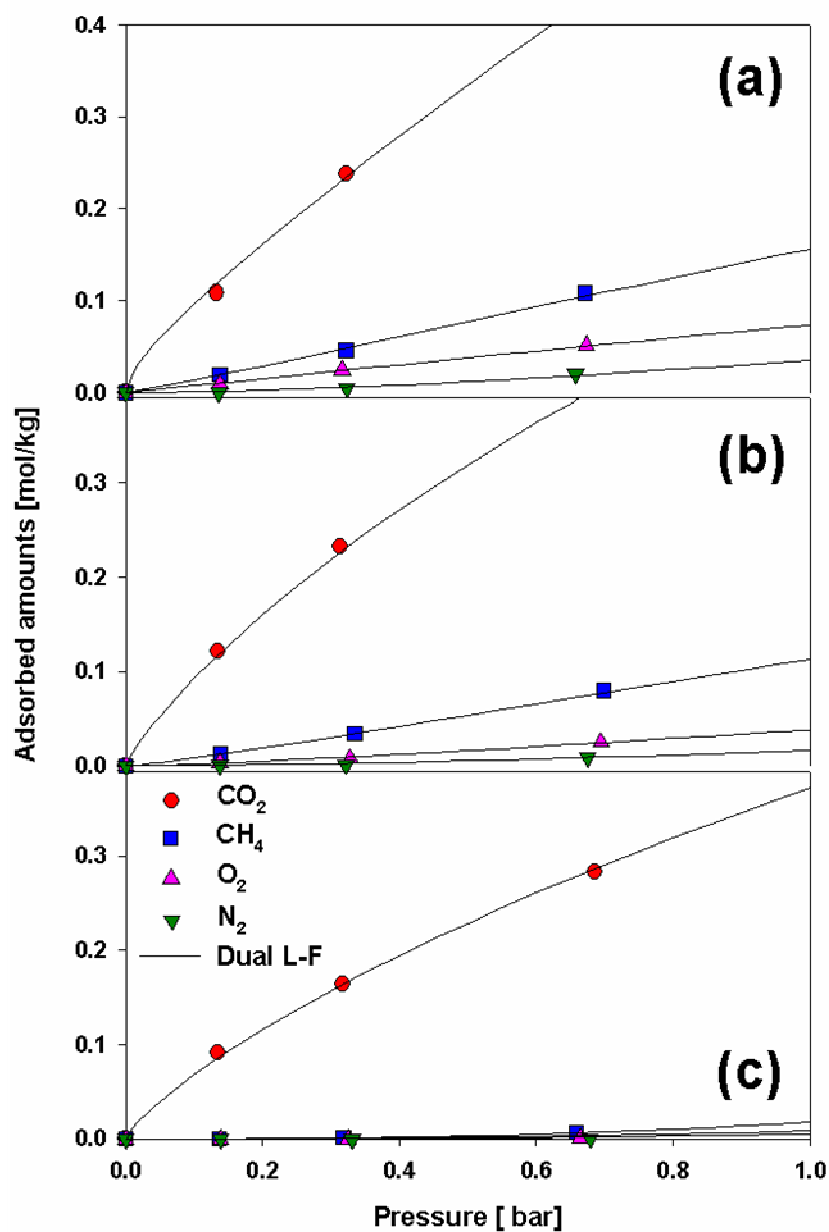


Figure S3. (a)-(c) Low-pressure isotherms of CO₂, CH₄, O₂, and N₂ in **3a**, **4a**, and **4b**, respectively. Solid lines indicate fits from the dual-site Langmuir-Freundlich (Dual L-F) equation.

1. O. K. Farha, A. M. Spokoyny, K. L. Mulfort, S. Galli, J. T. Hupp and C. A. Mirkin, *Small*, 2009, **5**, 1727.