## Supporting Information

Organic Cations Templated Synthesis of three

## Zinc-2,5-thiophenedicarboxylate Frameworks for Selective Gas Sorption

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Figure S1. The coordination environment of $\mathrm{Zn}^{2+}$ ions in $\mathbf{1}$ and a view of 3D structure from a and b directions.


B unit

Figure S2. The A unit and B unit in 2.


Figure S3. A view of 3D structure of $\mathbf{2}$ from b and c directions.


Figure S4. The C unit and D unit in 3.


Figure S5. A view of 3D structure of $\mathbf{3}$ from b and c directions.


Figure S6. TGA curve of 1.


Figure S7. PXRD patterns of simulated from the single-crystal data of $\mathbf{1}$ (black); as-synthesized 1 (red); desolvated solid 1-ht (blue).


Figure S8. PXRD patterns of 1 and 1 in different solvents such as DMF, EtOH, $\mathrm{MeCN}, \mathrm{CH}_{2} \mathrm{Cl}_{2}, \mathrm{H}_{2} \mathrm{O}$.


Figure S9. $\mathrm{H}_{2}$ adsorption isotherms for 1-ht fitting by virial method.


Figure S10. The isosteric heat of $\mathrm{H}_{2}$ adsorption for 1-ht estimated by the virial equation.


Figure S11. $\mathrm{CO}_{2}$ adsorption isotherms for 1-ht fitting by virial method.


Figure S12. The isosteric heat of $\mathrm{CO}_{2}$ adsorption for 1-ht estimated by the virial equation.

