Electronic Supplementary Material (ESI) for RSC Advances.

Porous Organic Polymers Derived from Tetrahedral Silicon-Centered Monomers and Stereocontorted Spirobifluorene-Based Precursor: Synthesis, Porosity and Carbon Dioxide Sorption

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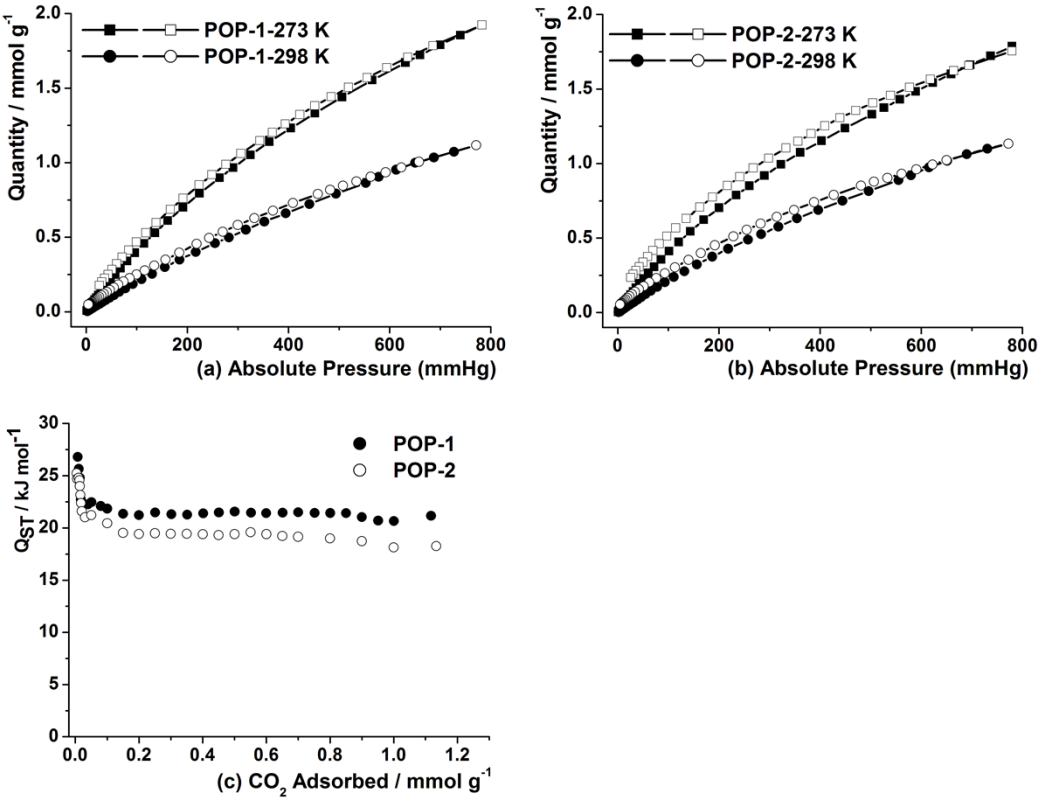

Fig. S1 Carbon dioxide adsorption (closed symbols) and desorption (open symbols) isotherms of POP-1 (a) and POP-2 (b) at 273 K and 298 K; (c) Isosteric heat of carbon dioxide adsorption of POP-1 and POP-2

Henry's Law selectivity of CO_2 over other gases in POP-1 and POP-2 at 298 K

A nice fitting of CO_2 and CH_4 isotherms has been calculated based on Toth isotherm model.[1,2]

$$q = q_{sat}\frac{b^{1/t}P}{(1+b^t)^{1/t}}$$

where q is the uptake in mmol g^{-1}, q_{sat} is the saturation uptake in mmol g^{-1}, P is the pressure in torr, t and b are parameters which are specific for adsorbent pairs.

The Henry law constant K, quantifies the extent of the adsorption of a given adsorbate by a solid. The magnitude of K depends on the properties of both adsorbate and solid. For the Toth isotherm, the Henry law constant is defined by the following equation:

$$K = \lim_{P\to 0}(\frac{dq}{dP}) = b^{1/t}q_{sat}$$

Finally, the Henry's Law selectivity $S_{\alpha/\beta}$ of gas α over β is given by the following equation:

$$S_{\alpha/\beta} = \frac{K_\alpha}{K_\beta}$$

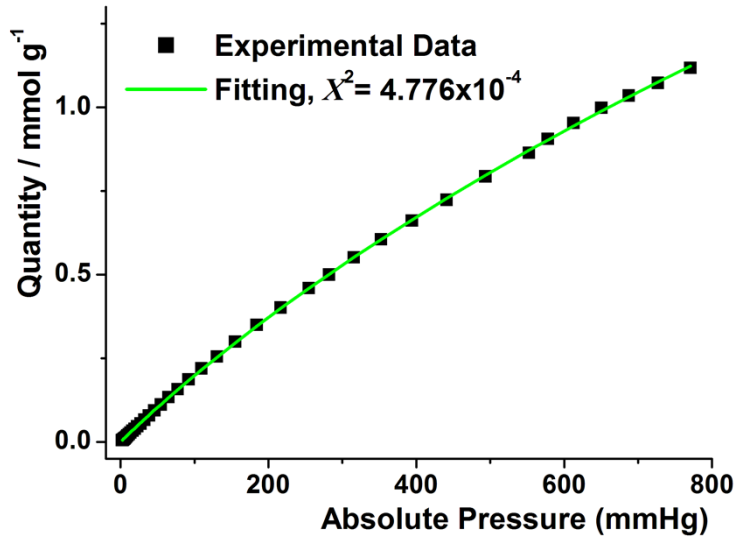

Fig. S2. Toth model fitting of CO_2 adsorption isotherm of POP-1 at 298 K. q_{sat} = 7.24, b = 0.002836, t = 0.724, Henry's law constant, K = 1.68 mmol g^{-1} atm^{-1}

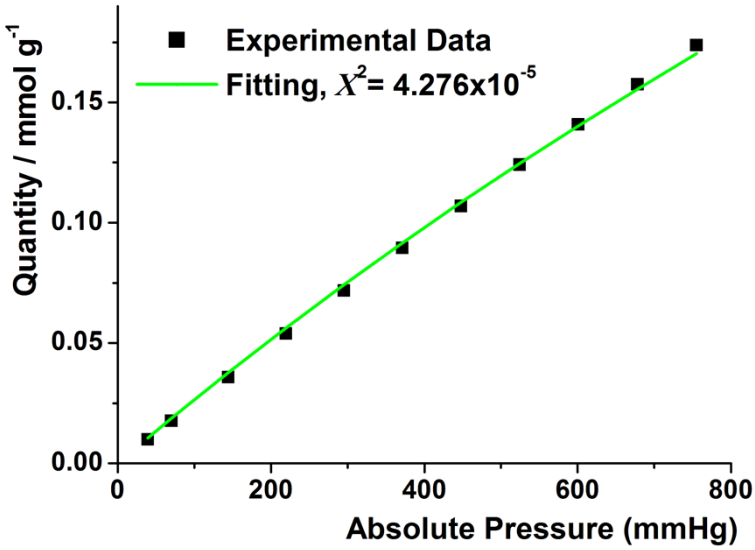

Fig. S3. Toth model fitting of N_2 adsorption isotherm of POP-1 at 298 K. q_{sat} = 0.999, b = 0.000272, t = 0.999, Henry's law constant, K = 0.207 mmol g^{-1} atm^{-1}

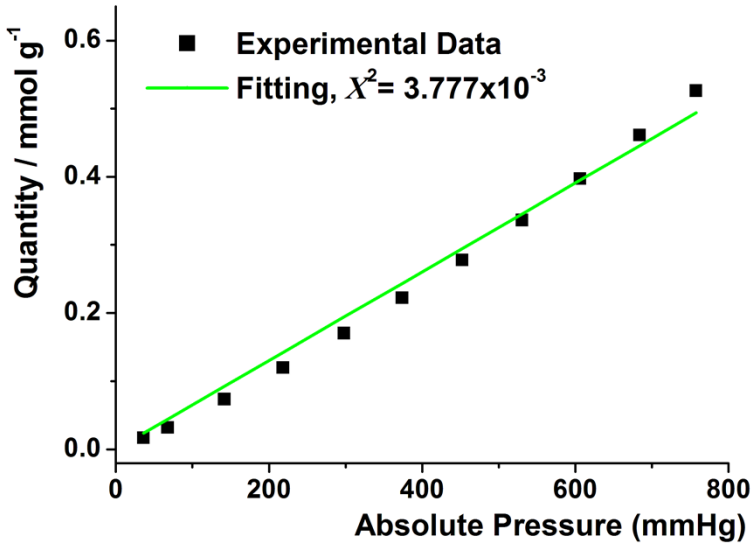

Fig. S4. Toth model fitting of CH_4 adsorption isotherm of POP-1 at 298 K. q_{sat} = 4.99, b = 4.25X10^{-12}, t = 2.927, Henry's law constant, K = 0.496 mmol g^{-1} atm^{-1}

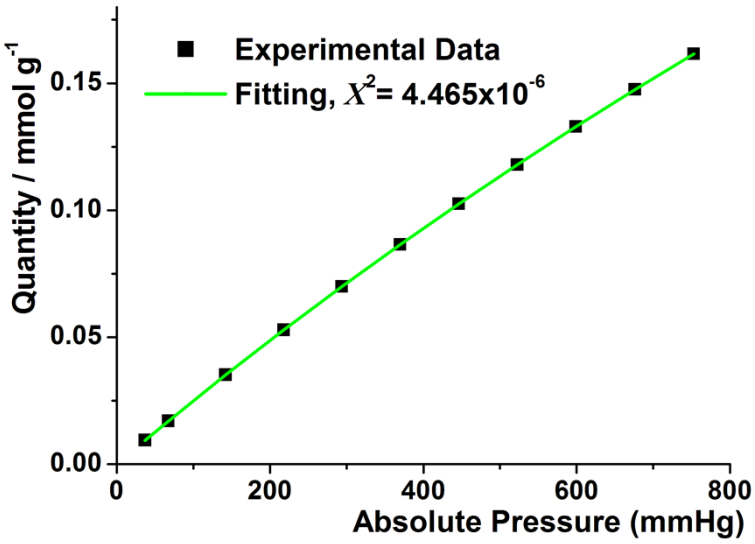

Fig. S5. Toth model fitting of O_2 adsorption isotherm of POP-1 at 298 K. q_{sat} = 1.003, b = 0.000258, t = 0.998, Henry's law constant, K = 0.194 mmol g^{-1} atm^{-1}

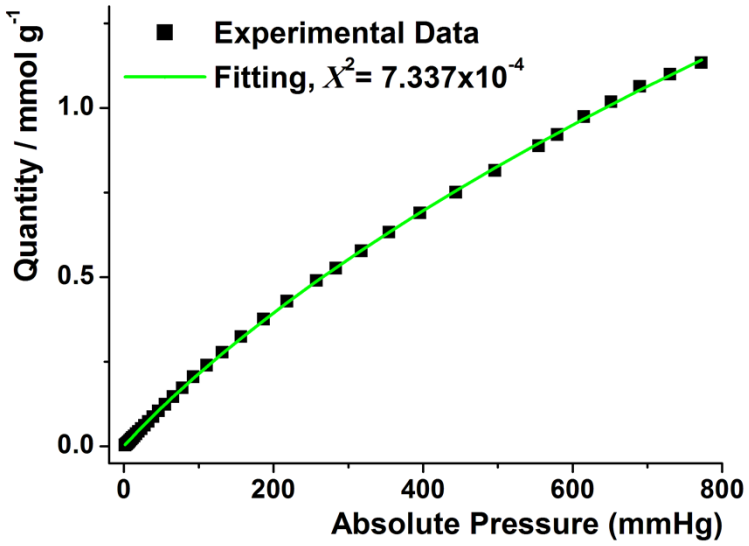

Fig. S6. Toth model fitting of CO_2 adsorption isotherm of POP-2 at 298 K. q_{sat} = 8.30, b = 0.006252, t = 0.6272, Henry's law constant, K = 1.93 mmol g^{-1} atm^{-1}

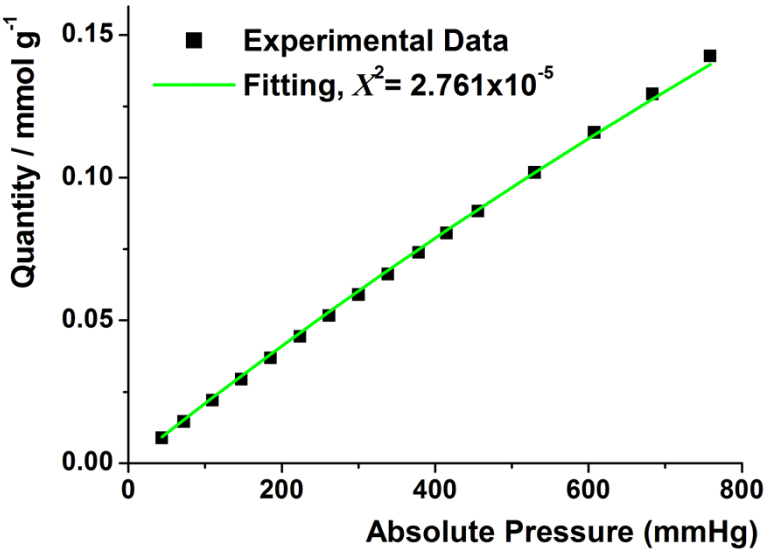

Fig. S7. Toth model fitting of N_2 adsorption isotherm of POP-2 at 298 K. q_{sat} = 0.999, b = 0.000214, t = 0.999, Henry's law constant, K = 0.163 mmol g^{-1} atm^{-1}

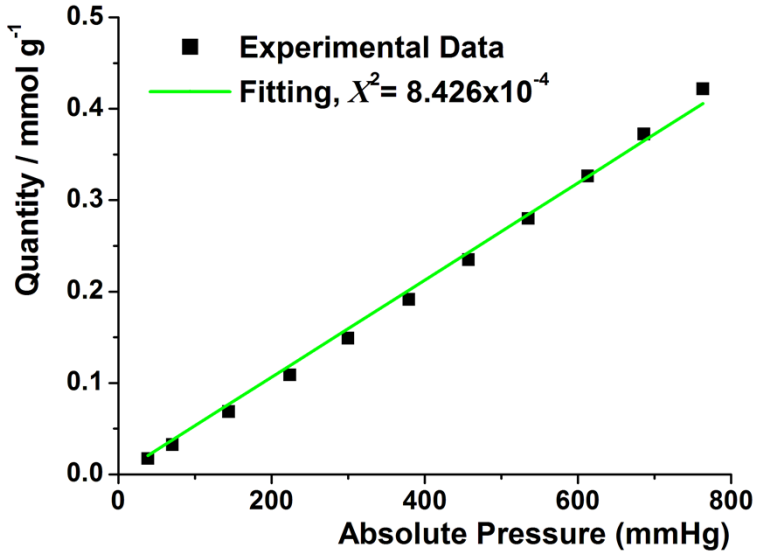

Fig. S8. Toth model fitting of CH_4 adsorption isotherm of POP-2 at 298 K. q_{sat} = 4.999, b = 5.82X10^{-14}, t = 3.331, Henry's law constant, K = 0.404 mmol g^{-1} atm^{-1}

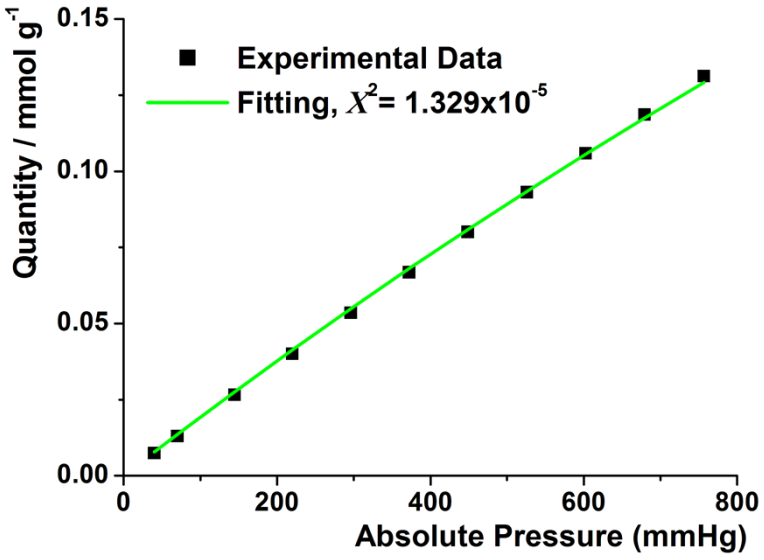

Fig. S9. Toth model fitting of O_2 adsorption isotherm of POP-2 at 298 K. q_{sat} = 0.999, b = 0.000196, t = 0.999, Henry's law constant, K = 0.149 mmol g^{-1} atm^{-1}

References

[1] E. Neofotistou, C. D. Malliakas, P. N. Trikalitis, *Chem. Eur. J.*, 2009, **15**, 4523–4527.

[2] B. Wang, A. P. Côté, H. Furukawa, M. O'Keeffe, O. M. Yaghi, *Nature*, 2008, **453**, 207– 211.