Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Electronic Supporting Information

Copolymerization of Terephthalaldehyde with Pyrrole, Indole and Carbazole Gives Microporous POFs Functionalized with Unpaired Electrons

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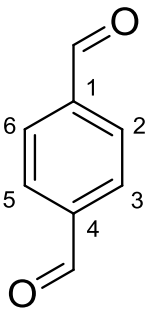
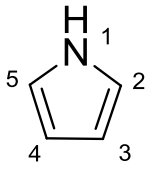
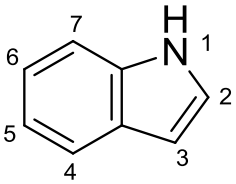
Scheme S1 Starting materials for Pyr-POF, Ind-POF and Car-POF



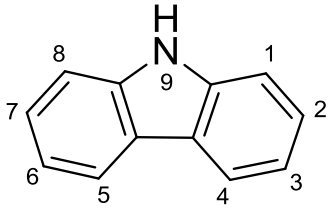
Terephthalaldehyde



Pyrrole



Indole



Carbazole

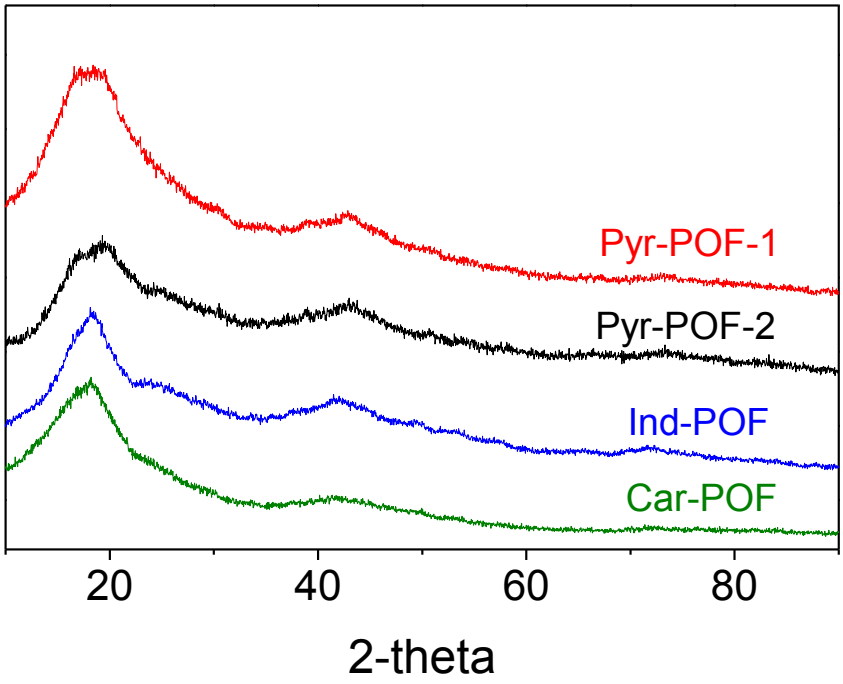


Figure S1 XRD patterns of Pyr-POF-1, Pyr-POF-2, Ind-POF and Car-POF. The broad peaks at 18^{o} and 42^{o} come from the tape that was used on the glass slide.

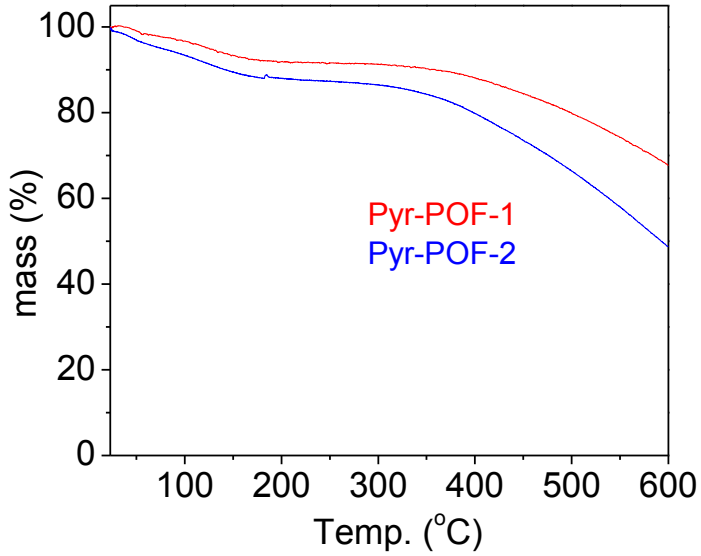


Figure S2 Thermogravimetric analysis of Pyr-POF-1 and Pyr-POF-2 under N_2 flow

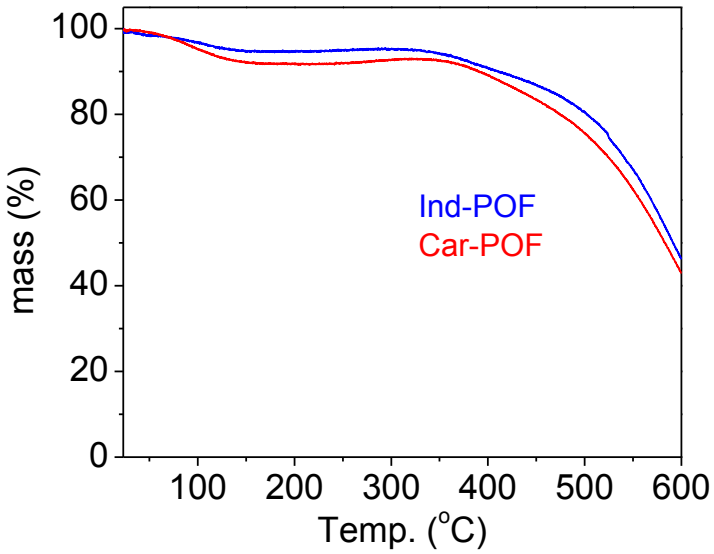


Figure S3 Thermogravimetric analysis of Ind-POF and Car-POF under N_2 flow

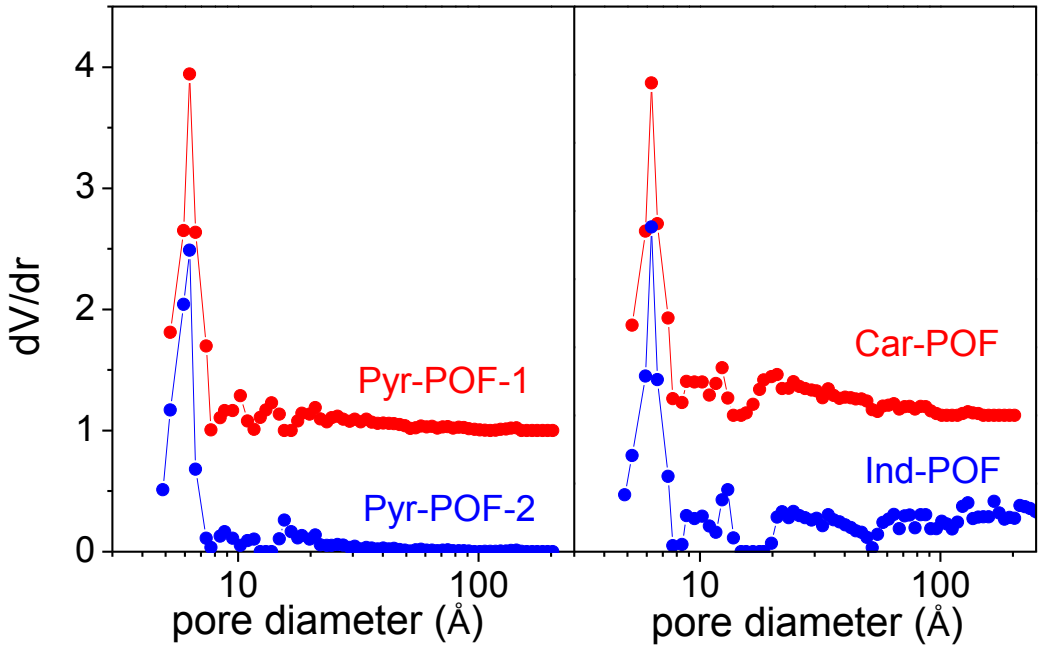


Figure S4 The pore size distribution of Pyr-POF-1, Pyr-POF-2, Ind-POF and Car-POF from N_2 adsorption data analyzed with NLDFT

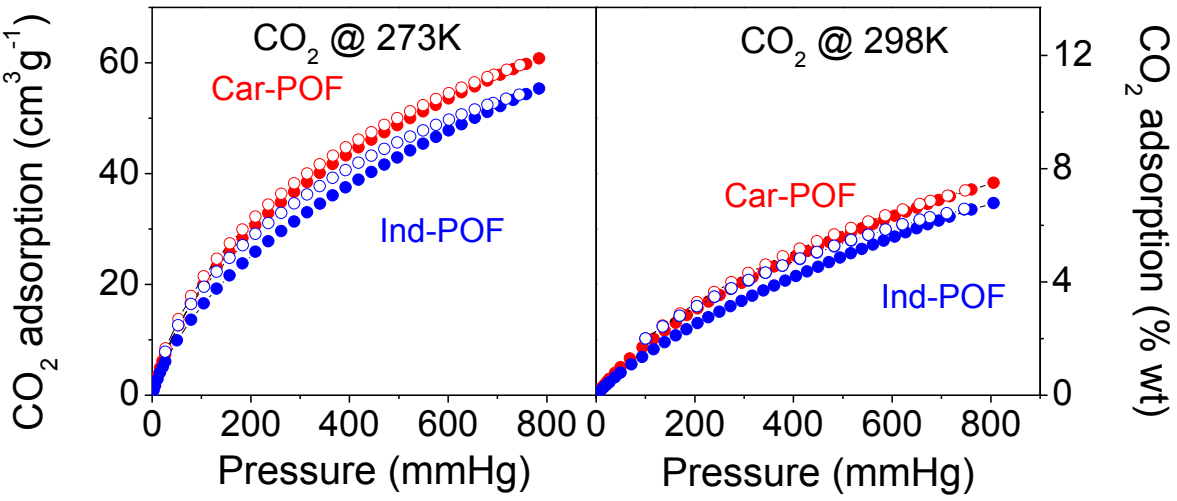


Figure S5 CO_2 adsorption desorption isotherms of Ind-POF and Car-POF at 273 K and 298 K

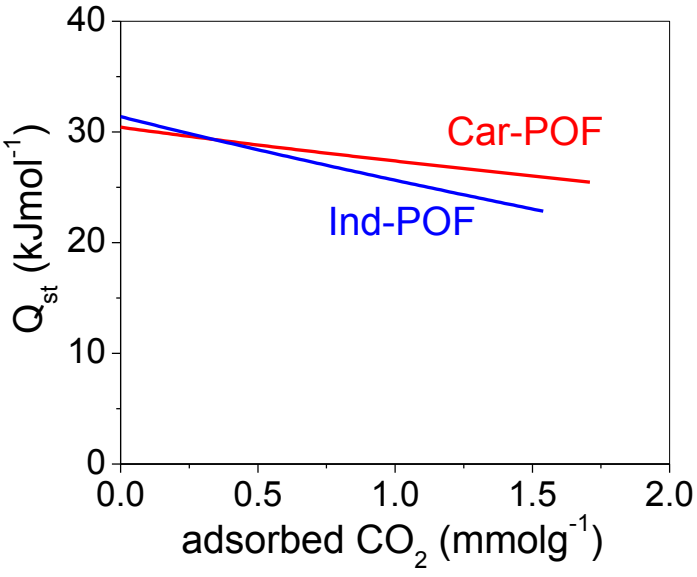


Figure S6 Isosteric heat, Qst, of CO_2 adsorption for Ind-POF and Car-POF calculated from CO_2 adsorption at 273 K and 298 K

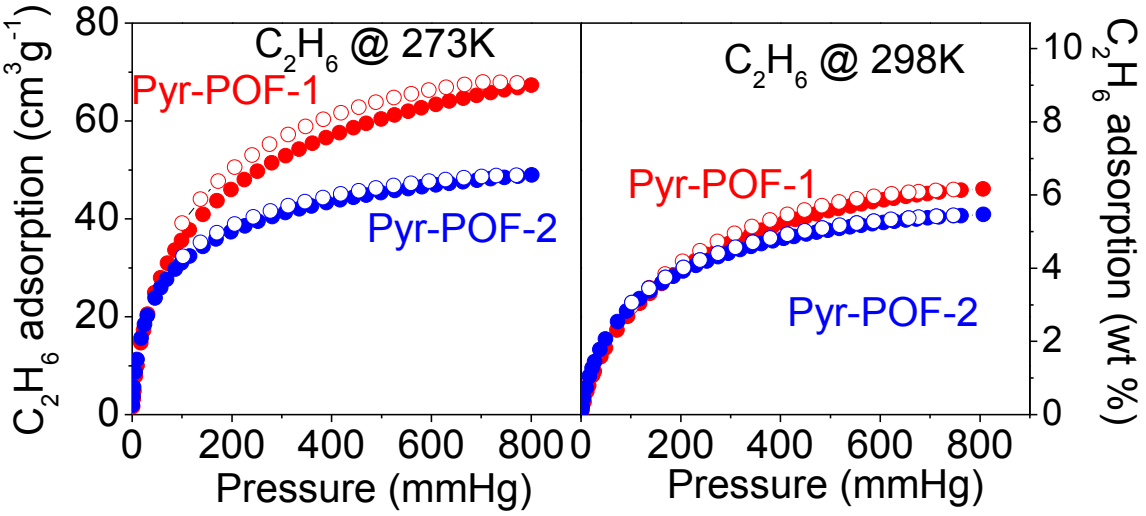


Figure S7 C_2H_6 adsorption desorption isotherms of Pyr-POF-1 and Pyr-POF-2 at 273 K and 298 K

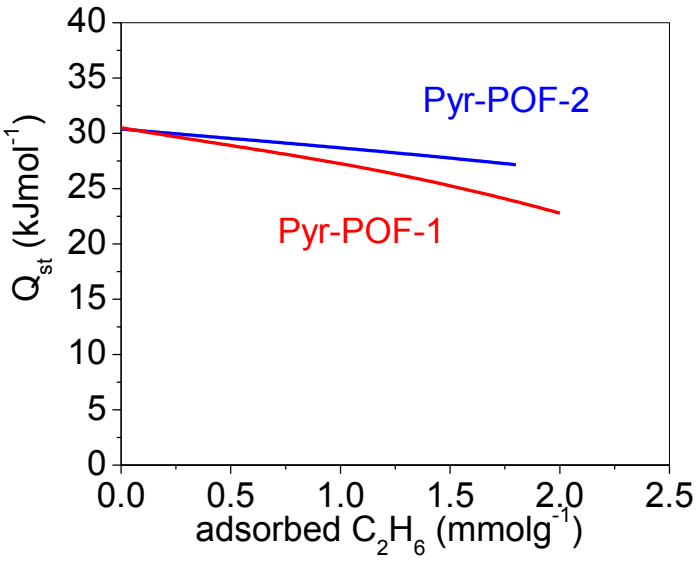


Figure S8 Isosteric heat, Qst, of C_2H_6 adsorption for Pyr-POF-1 and Pyr-POF-2 calculated from C_2H_6 adsorption at 273 K and 298 K

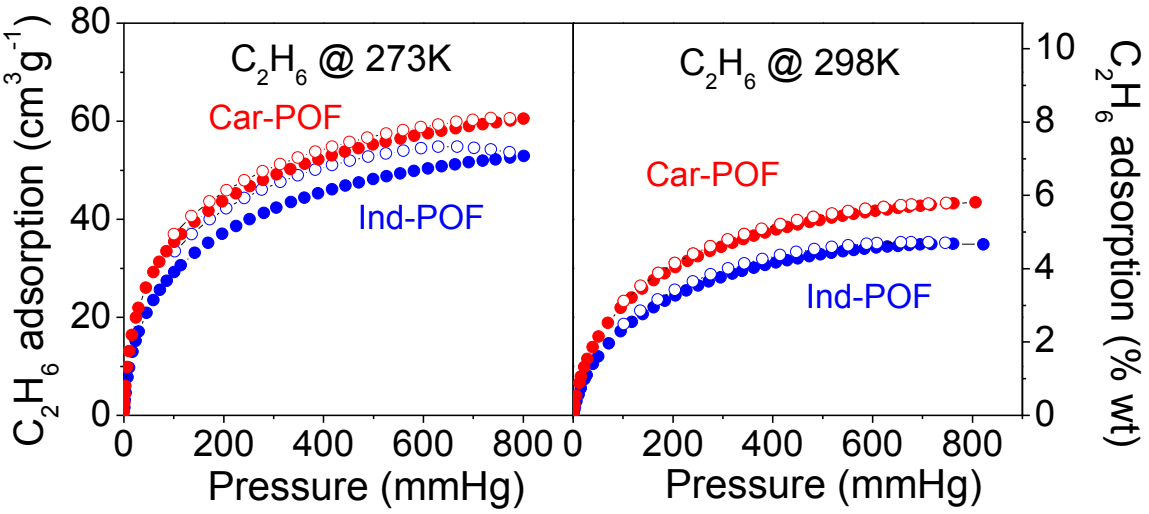


Figure S9 C_2H_6 adsorption desorption isotherms of Ind-POF and Car-POF at 273 K and 298 K

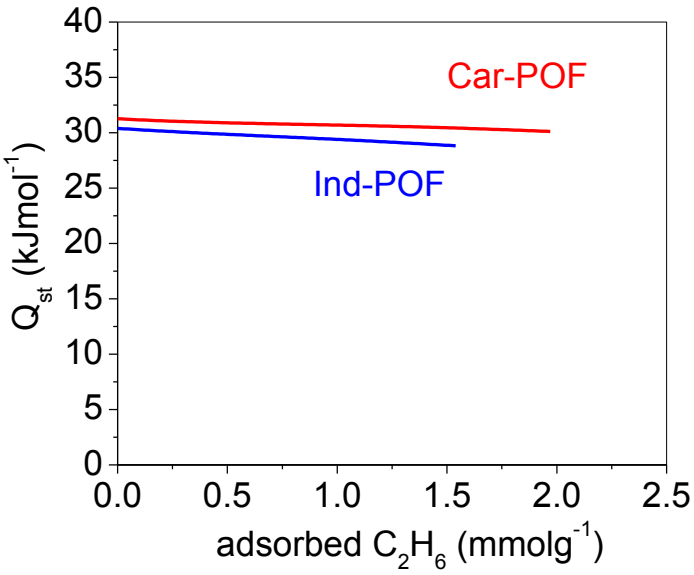


Figure S10 Isosteric heat, Qst, of C_2H_6 adsorption for Ind-POF and Car-POF calculated from C_2H_6 adsorption at 273 K and 298 K

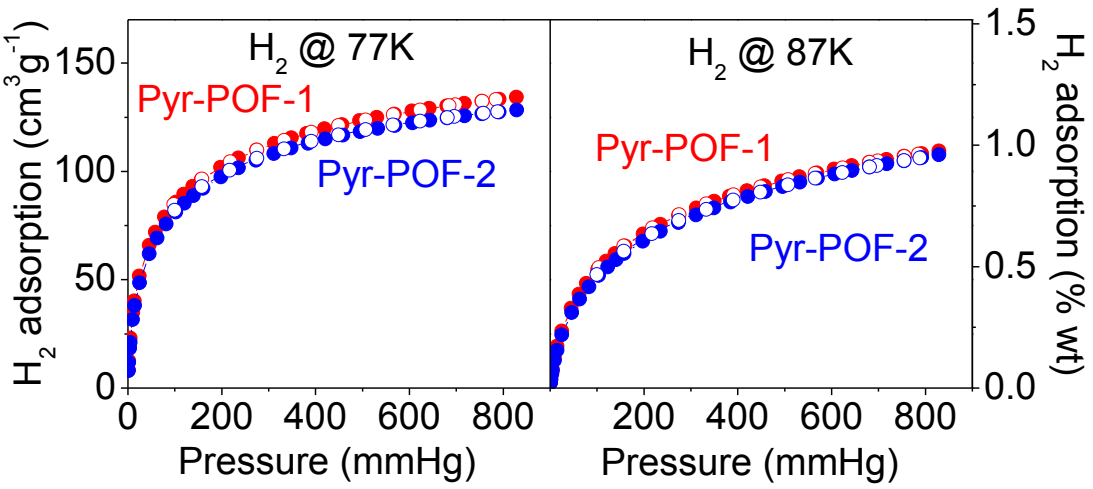


Figure S11 H_2 adsorption desorption isotherms of Pyr-POF-1 and Pyr-POF-2 at 77 K and 87 K

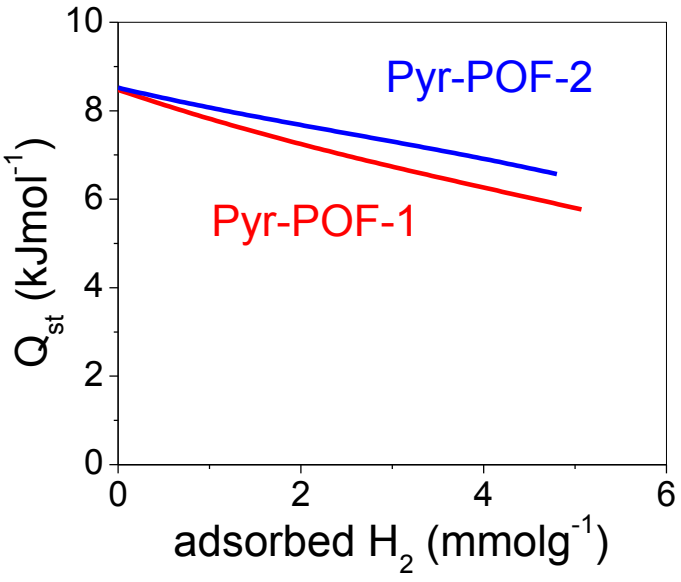


Figure S12 Isosteric heat, Qst, of H_2 adsorption for Pyr-POF-1 and Pyr-POF-2 calculated from H_2 adsorption at 77 K and 87 K

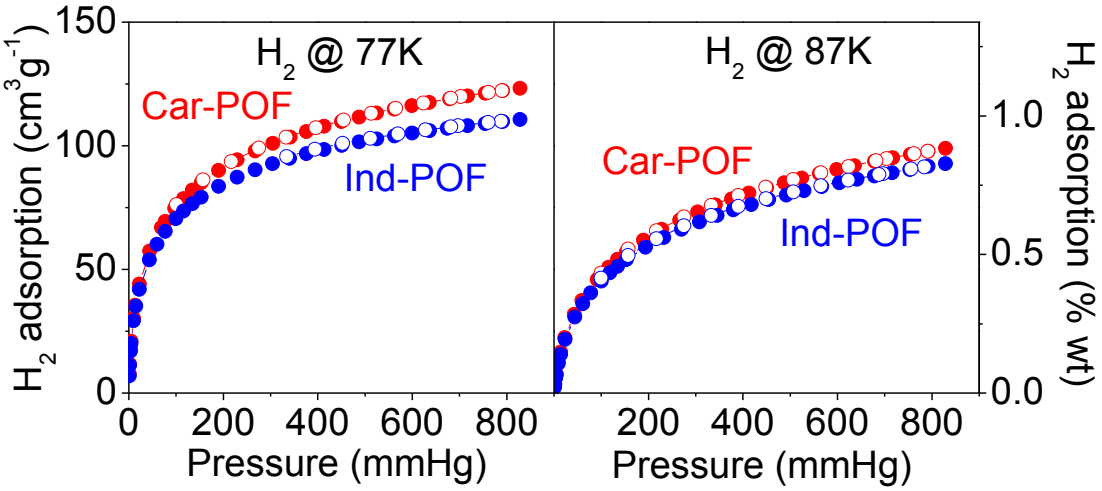


Figure S13 H_2 adsorption desorption isotherms of Ind-POF and Car-POF at 77 K and 87 K

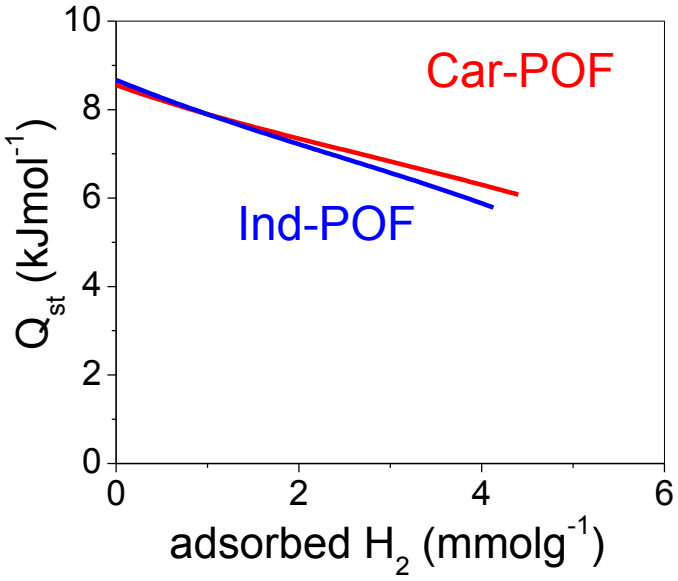


Figure S14 Isosteric heat, Qst, of H_2 adsorption for Ind-POF and Car-POF calculated from H_2 adsorption at 77 K and 87 K

Isosteric heat of adsorption

The isosteric heat of adsorption for CO_2, C_2H_6 and H_2 of each sample was calculated from adsorption isotherms collected at 273 and 298 K, for CO_2 and C_2H_6 and at 77 and 87 K for H_2. The collected data for each sample was fitted to virial equation (1)

$$\ln p = \ln v + \frac{1}{T}\sum_{i=0}^{n1} a_i v^i + \sum_{i=0}^{n2} b_i v^i \qquad (1)$$

where p is the pressure in mmHg, v is the adsorbed amount in $mmolg^{-1}$, T is the temperature in K and a_i and b_i are adjustable parameters.

The isosteric heat of H_2 adsorption, Q_{st}, was calculated according to the equation (2)

$$Q_{st} = -R\sum_{i=0}^{n1} a_i v^i \qquad (2)$$

where R is the gas constant in $Jmol^{-1}K^{-1}$.

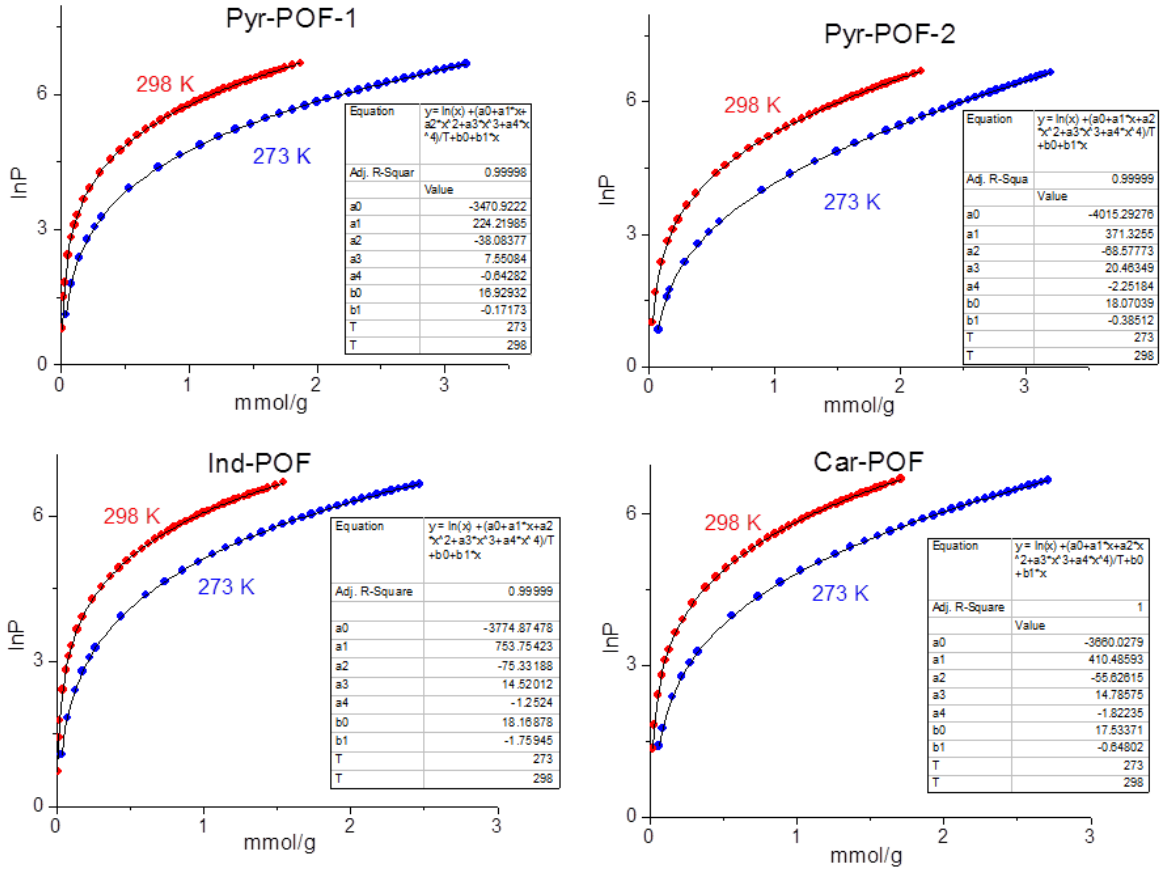


Figure S15 Virial fitting of CO_2 adsorption data points for Pyr-POF-1, Pyr-POF-2, Ind-POF and Car-POF

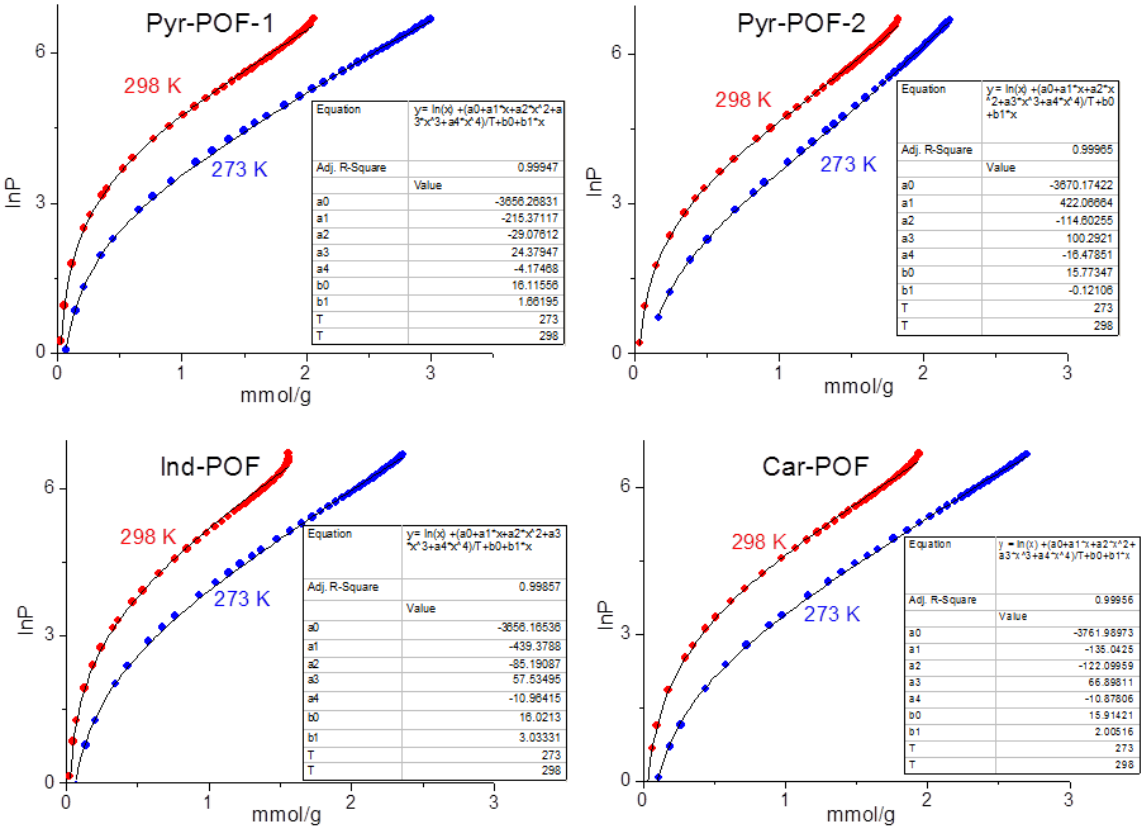


Figure S16 Virial fitting of C_2H_6 adsorption data points for Pyr-POF-1, Pyr-POF-2, Ind-POF and Car-POF

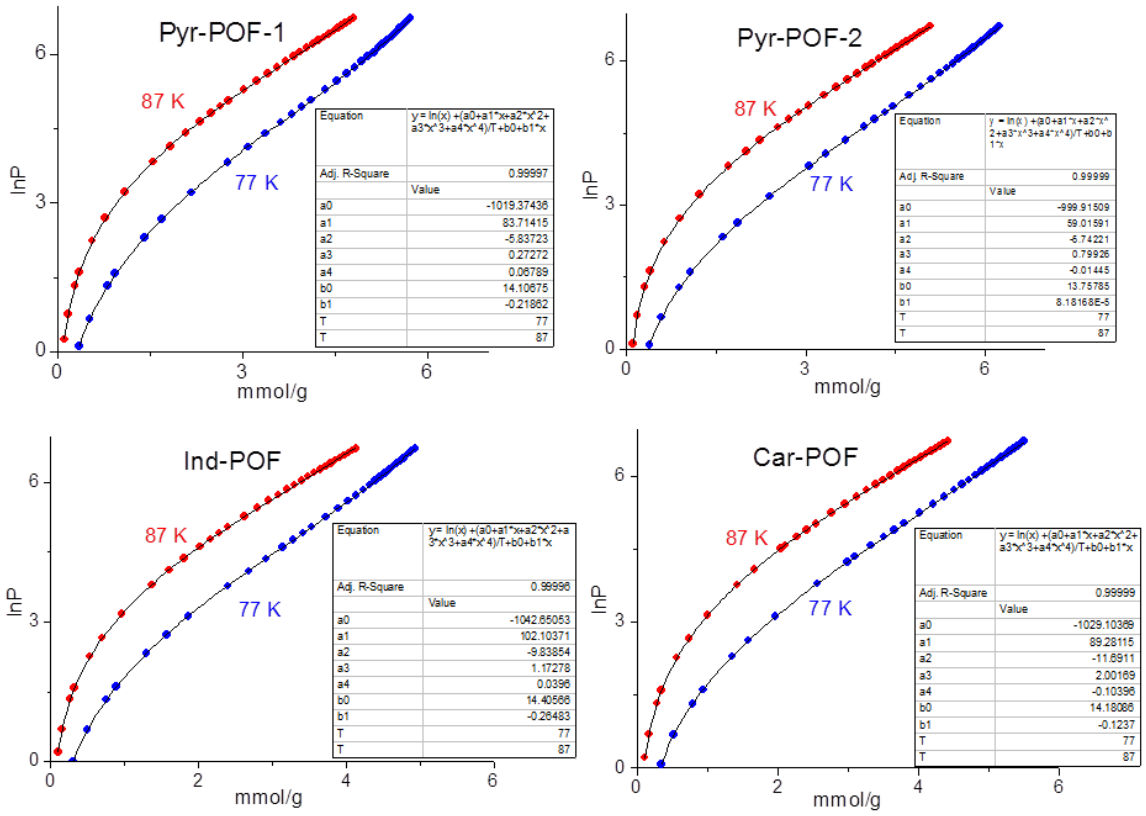


Figure S17 Virial fitting of H_2 adsorption data points for Pyr-POF-1, Pyr-POF-2, Ind-POF and Car-POF