Electronic Supplementary Material (ESI) for RSC Advances.

Charged Porous organic frameworks bearing heteroatoms with enhanced isosteric enthalpies of gas adsorption

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Supporting Information

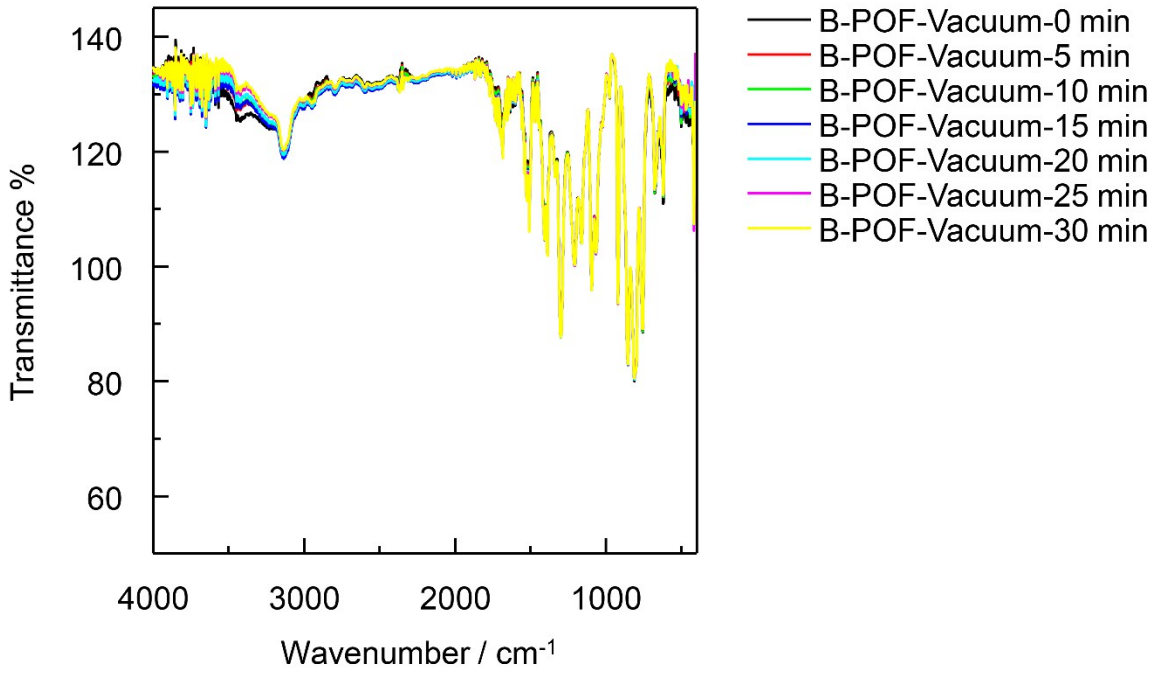

Figure S1. FT-IR spectrum of B-POF under vacuum for different time.

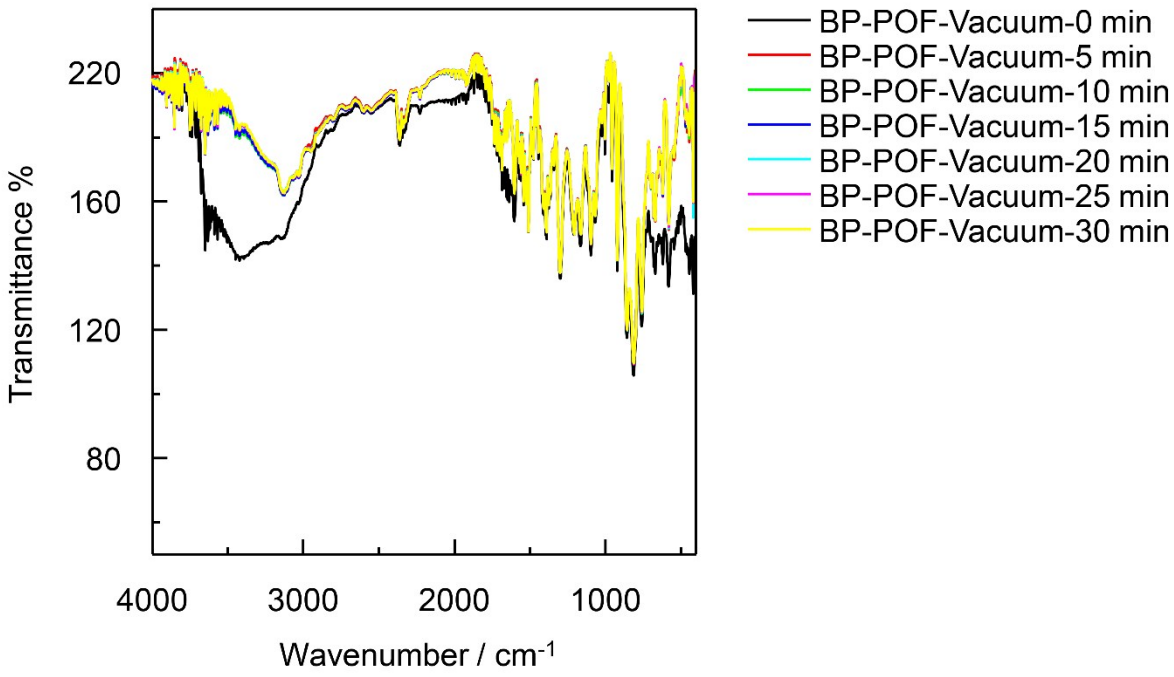

Figure S2. FT-IR spectrum of BP-POF under vacuum for different time.

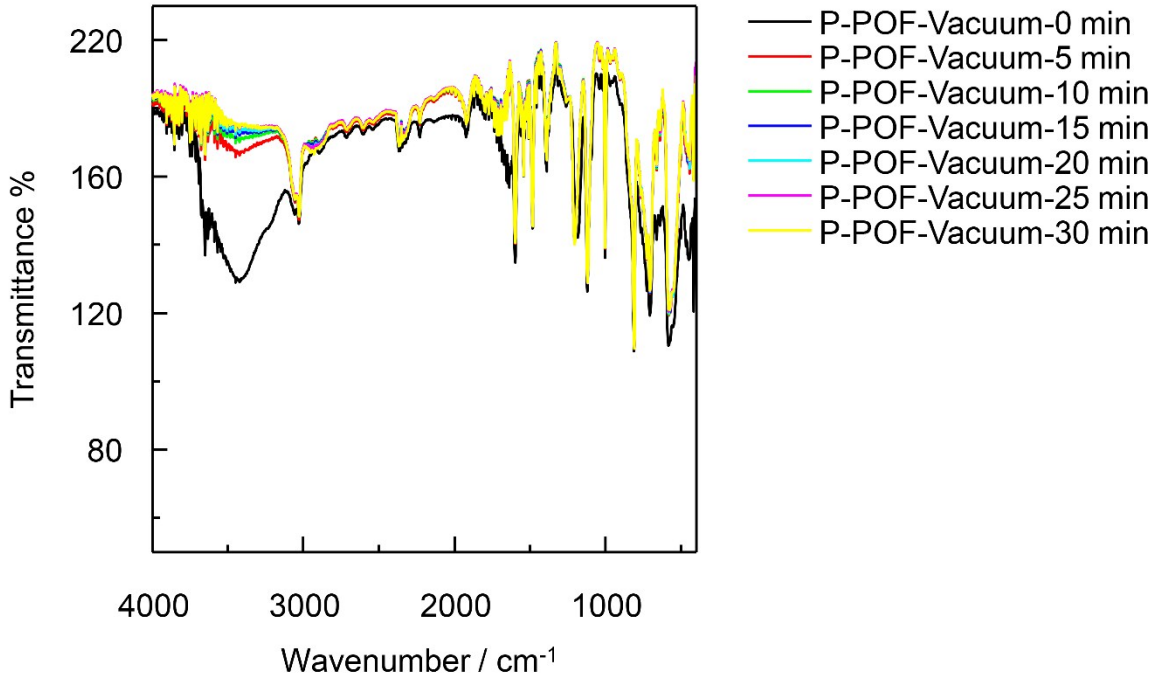

Figure S3. FT-IR spectrum of P-POF under vacuum for different time.

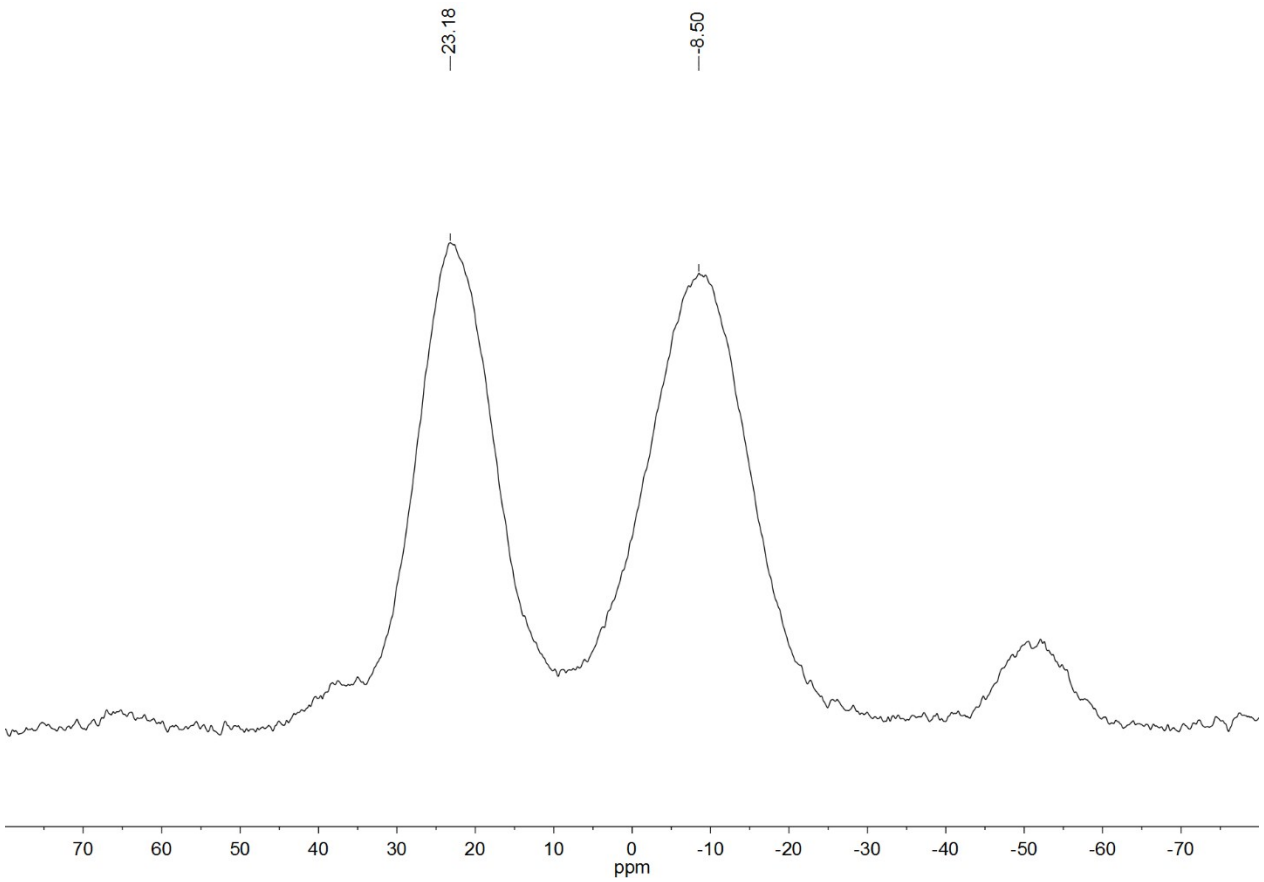

Figure S4. ^{31}P solid state NMR spectra of BP-POF.

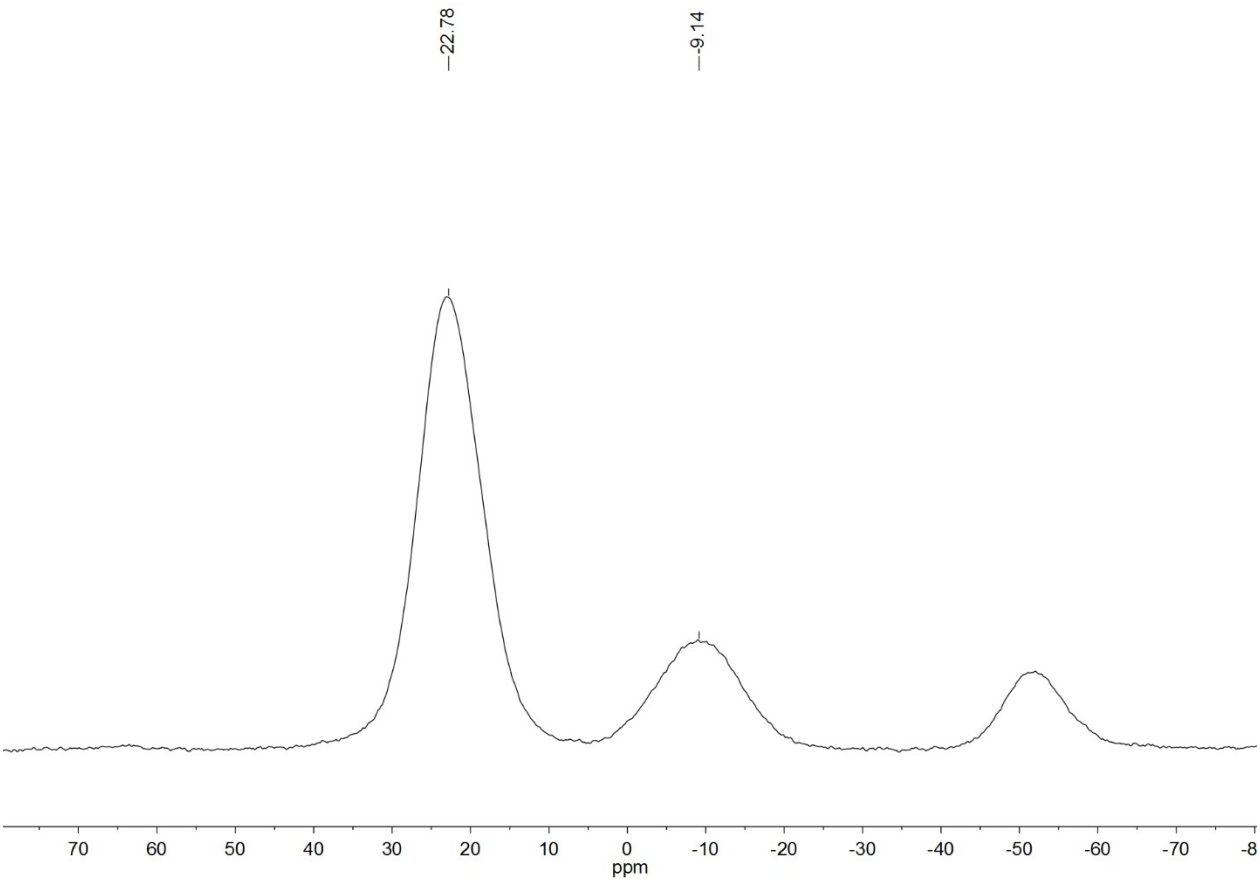

Figure S5. ^{31}P solid state NMR spectra of P-POF.

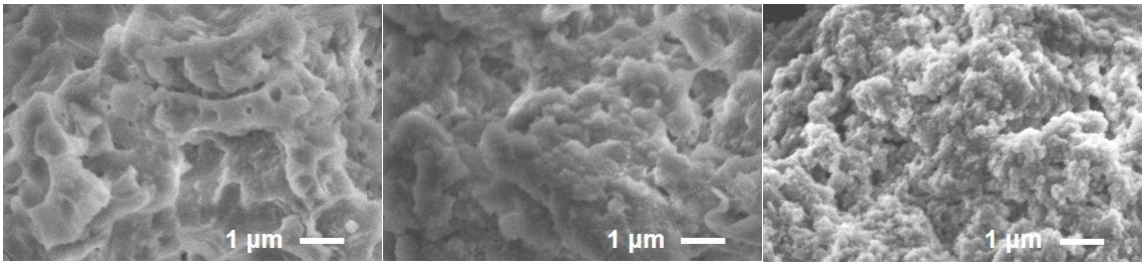

Figure S6. SEM images of (left) B-POF, (middle) BP-POF and (right) P-POF.

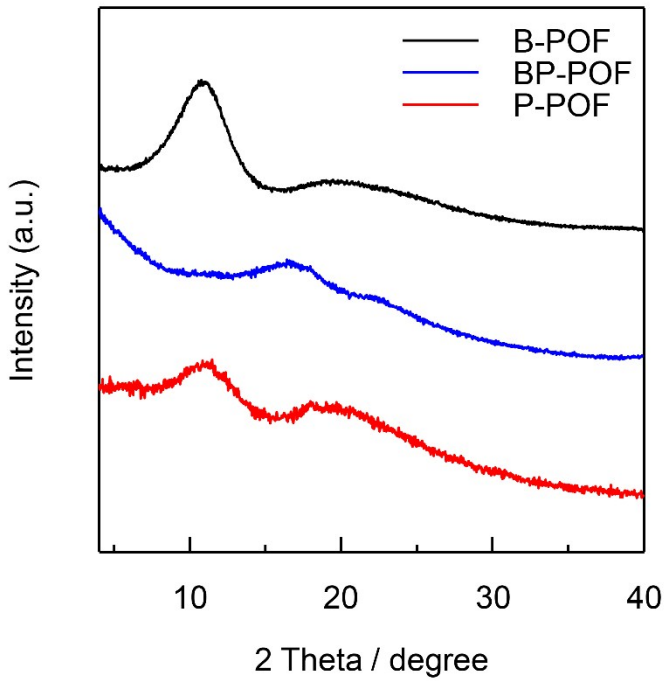

Figure S7. PXRD patterns of B-POF (black), BP-POF(blue) and P-POF(red).

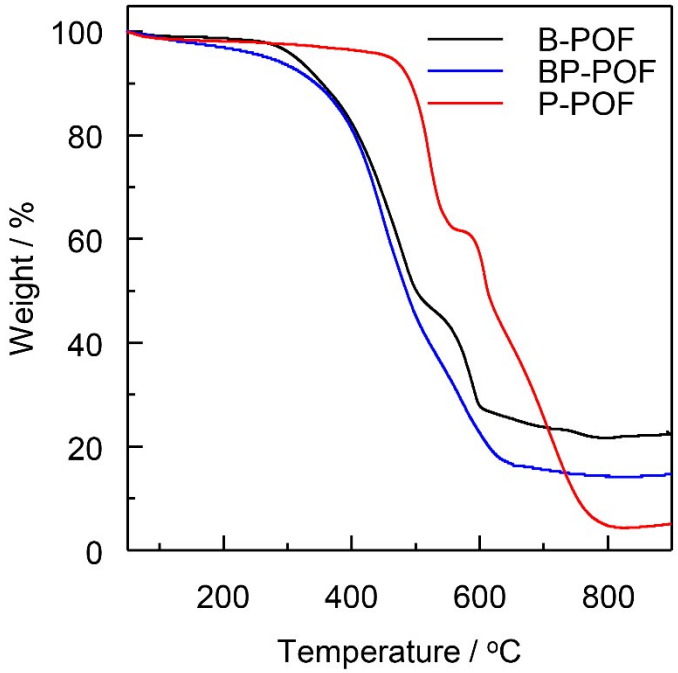

Figure S8. TGA plots of B-POF (black), BP-POF(blue) and P-POF(red).

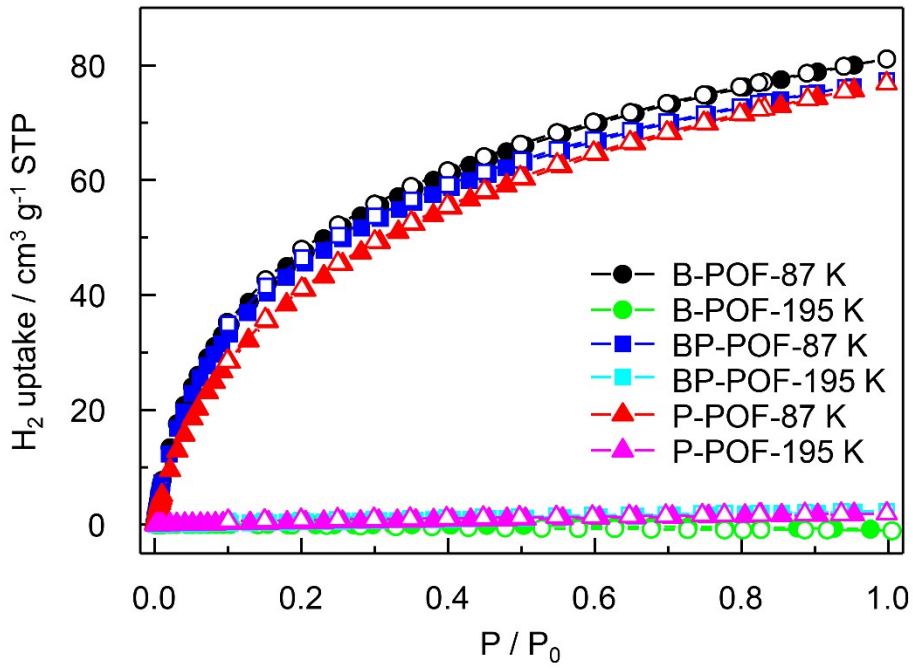

Figure S9. H_2 adsorption isotherms of B-POF (circle), BP-POF (square) and P-POF (triangle) at 87 K (solid symbols, adsorption; open symbols, desorption).

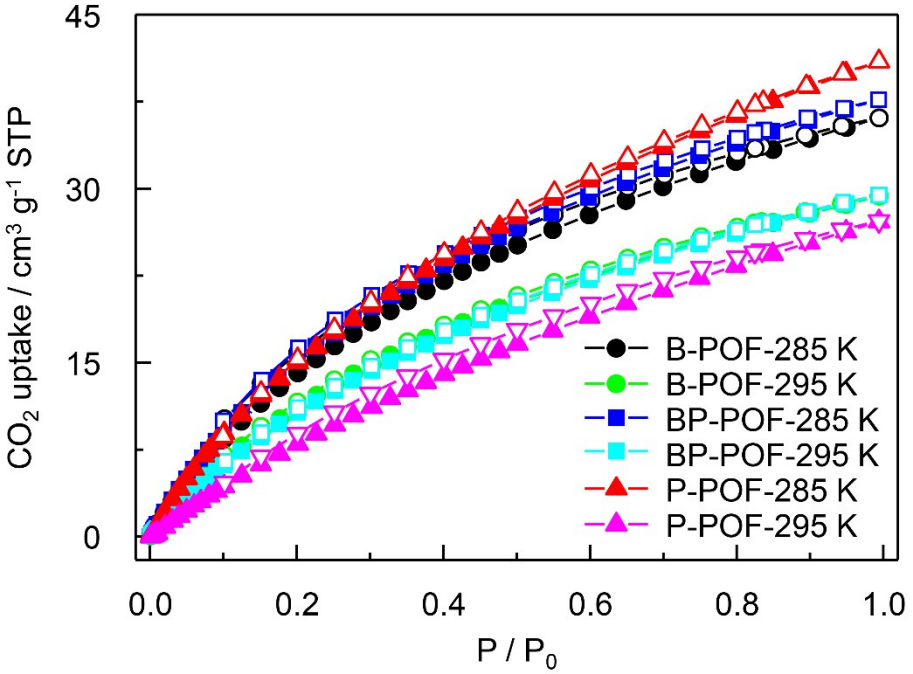

Figure S10. CO_2 adsorption isotherms of B-POF (circle), BP-POF (square) and P-POF (triangle) at 295 K (solid symbols, adsorption; open symbols, desorption).

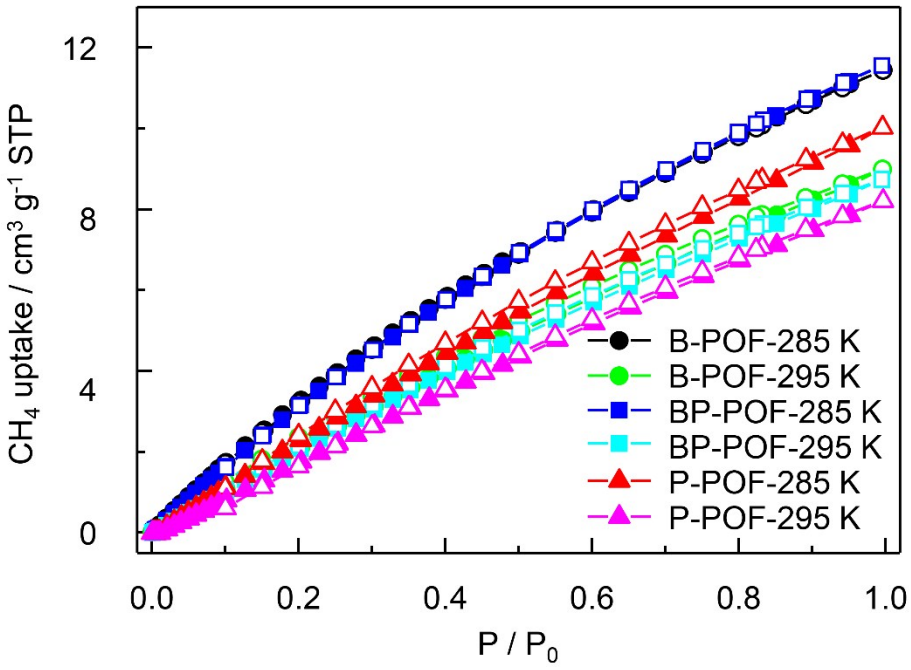

Figure S11. CH_4 adsorption isotherms of B-POF (circle), BP-POF (square) and P-POF (triangle) at 295 K (solid symbols, adsorption; open symbols, desorption).

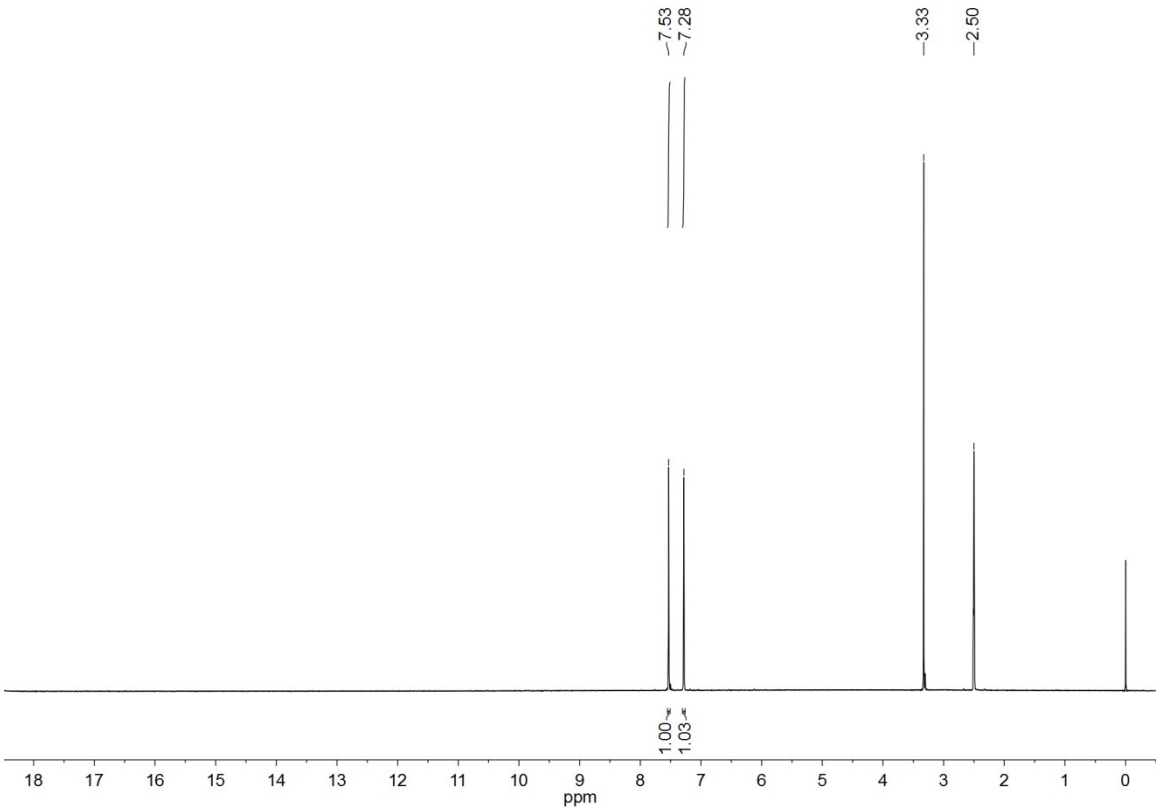

Figure S12. ^{1}H NMR spectra of K[B(4-Brpz)$_4$] in DMSO at room temperature.

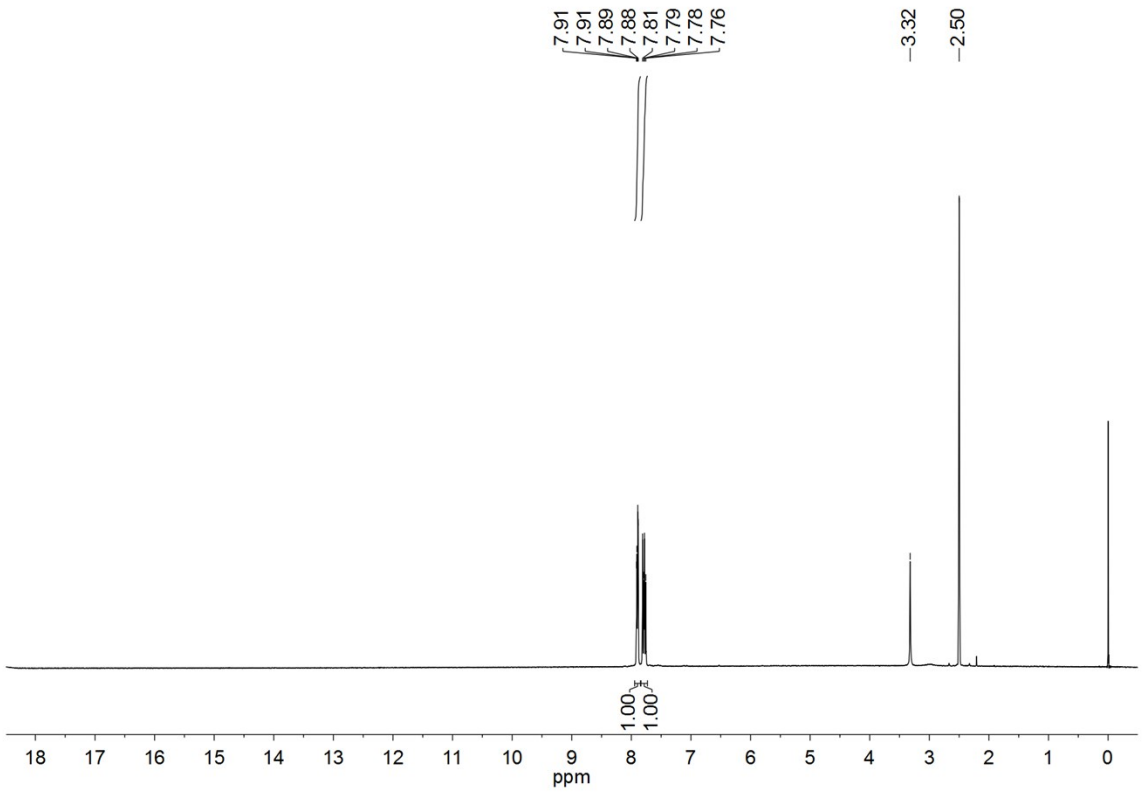

Figure S13. ^{1}H NMR spectra of [P(4-ClPh)$_4$]Br in DMSO at room temperature.

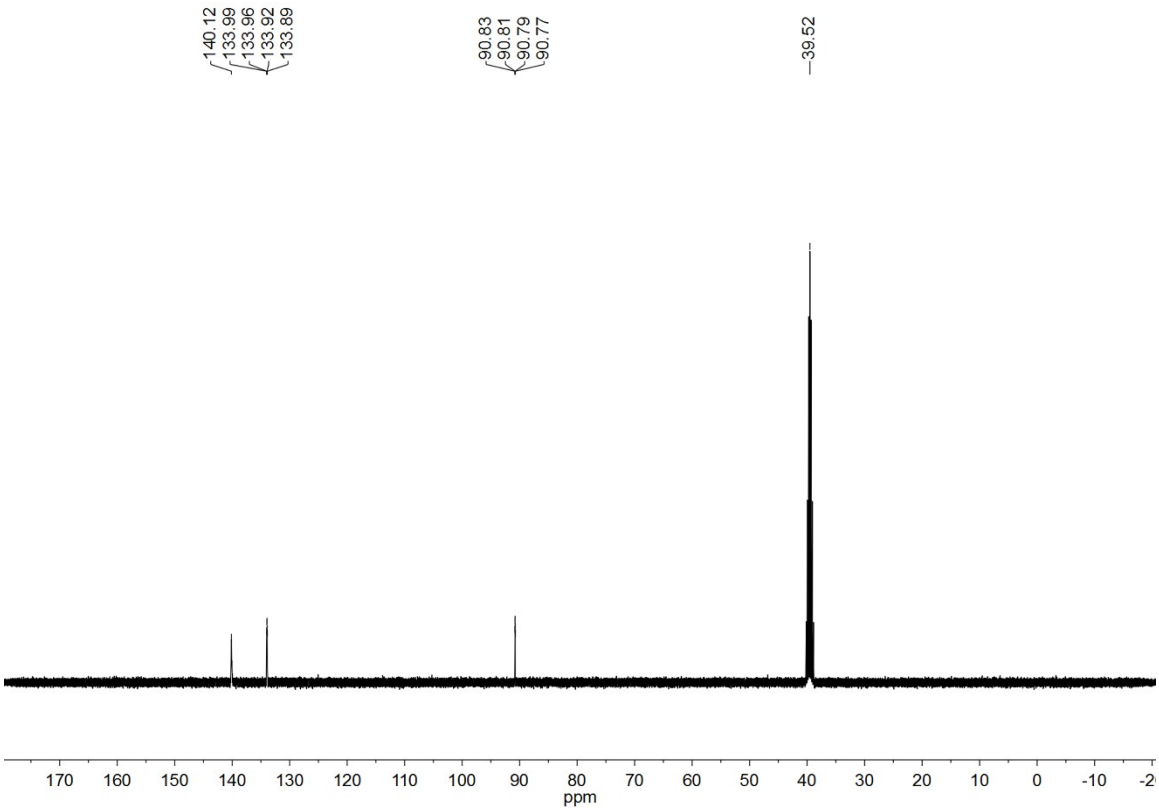

Figure S14. ^{13}C NMR spectra of K[B(4-Brpz)$_4$] in DMSO at room temperature.

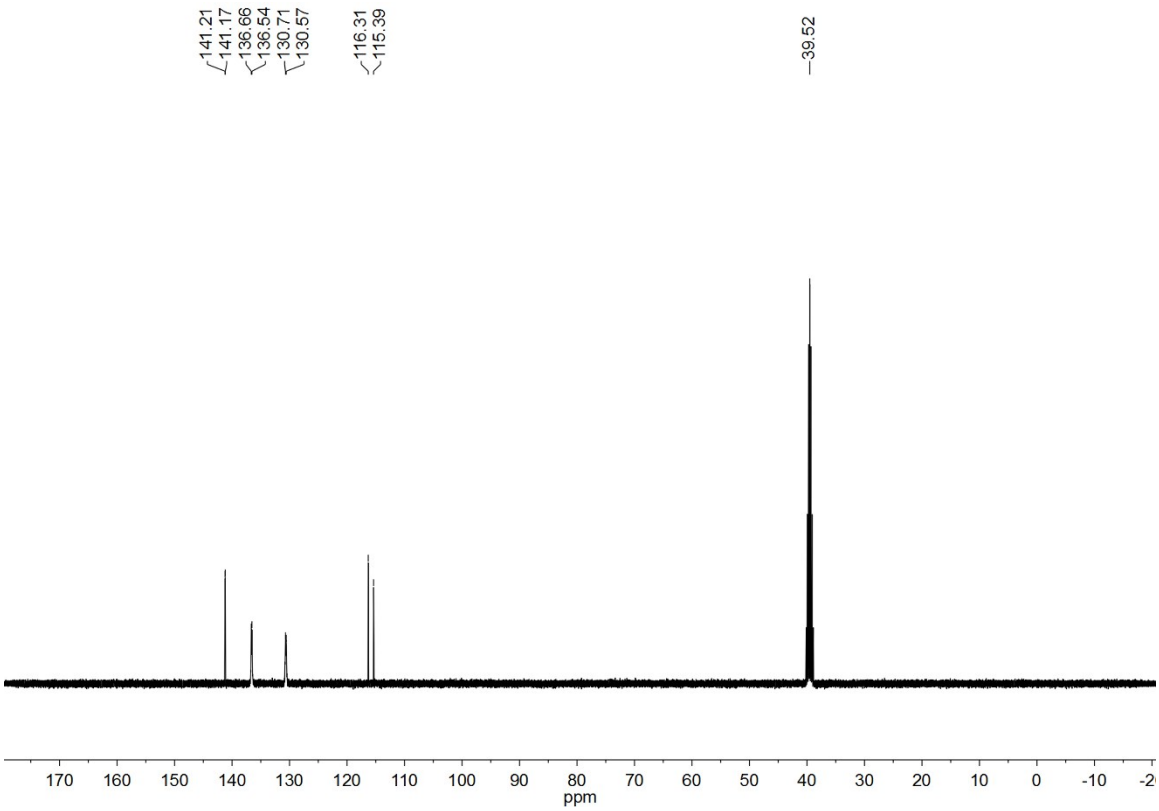

Figure S15. ^{13}C NMR spectra of $[P(4\text{-}ClPh)_4]Br$ in DMSO at room temperature.

Table S1 Comparison of BET surface area, CO_2, CH_4, H_2 sorption capabilities, and isosteric enthalpies for B-POF, BP-POF and P-POF with other porous organic materials.

Porous organic materials	S_{BET}	H_2 Uptake ($cm^3\ g^{-1}$)	Q_{stH2} (kJ mol^{-1})	CO_2 Uptake ($cm^3\ g^{-1}$)	Q_{stCO2} (kJ mol^{-1})	CH_4 Uptake ($cm^3\ g^{-1}$)	Q_{stCH4} (kJ mol^{-1})	Ref.
B-POF	515	103.3	8.5	46.0	32.3	13.8	22.4	This work
P-POF	629	102.8	7.8	48.4	35.2	13.3	21.4	This work
BP-POF	223	100.0	7.9	43.5	27.7	13.6	21.5	This work
PAF-1	5600	186	4.6	46	15.6	18	14.0	1
COF-102	3620	~136	3.9	~28.5	-	-	-	2
HCP-1	1646	-	-	38 (1 bar 298 K)	~23.5	-	-	3
CTF-1	746	-	-	55.3	~27.5	-	-	4
FCTF-1	662	-	-	104.6	~35			5
BILP-1	1172	~212.8	7.9	~95.7	26.5	~32.2	16.3	5
BILP-3	1306	~235	8.0	~114	28.6	~34	16.6	6
BILP-6	1261	~246	8.2	~108	28.4	~38	13.2	6
PMOP-1	806	-	-	~65.5	18.5	~17.7	~11	7
PMOP-2	559	-	-	~57.8	18.9	~15.2	~11	7
PCTF 1-7	79-2235	~101.7-~212.3	-	41.5-73.0	25-30	14.6-23.6	-	8
CTF-DCBT	500	-	-	37.8 (1 bar 298 K)	44.2	8.9 (1 bar 298 K)	22.8	9
BDPCMP-1-4	482-725	~90.3-~115.4 (77.3 K, 1.13 bar)	-	~37.6-~50.4 (273 K, 1.13 bar)	23-27.3	~10.8-~15.7 (273 K, 1.13 bar)	-	10
N4CMP-1-5	592-1426	-	-	~45.9-~81.1	25.5-35.1	-	-	11
Polycarbazole CPOP-1	2220	~322.6	-	137.0	27	-	-	12
P-THIDT					29			13
P-DTBDT								13
pre-GNF	672	~102.9	6.6	~38.2	29.8	~13.3	22.7	14
GNF-1	679	~116.6	7.7	~48.2	28.7	~16.1	24.1	14
CMP 0-5	512-1018	67-155	~10	-	-	-	-	15
JUC-Z7-10	3305-4889	217-245	5.63-6.88	58-85	15.94-23.17	23-27	15.69-15.96	16
Carbazole-based CMPs	540-917	~108.6-~192.5 (77.3 K, 1.13 bar)	-	~43.9-~65.6	27.1-30.8	~14.6-~22.6	-	17
Isoindigo-based MOPs	654-763	~107.4-~139.5 (77.3 K, 1.13 bar)	-	~55.1-~73.9	27.4-33.5	~16.8-~19.3	-	18
CPN-1-Br		-	-	~55.8	31.0	-	-	19
cCTFs	744-1247	-	-	~50.4-~67.7	43-49	-	-	20

Reference

1. T. Ben, Y. Li, L. Zhu, D, Zhang, D. Cao, Z. Xiang, X. Yao and S. Qiu, *Energy Environ. Sci.*, 2012, **5**, 8370-8376.
2. H. Furukawa and O. M. Yaghi, *J. Am. Chem. Soc.*, 2009, **131**, 8875-8883.
3. C. F. Martin, E. Stöckel, R. Clowes, D. J. Adams, A. I. Cooper, J. J. Pis, F. Rubiera and C. Pevida, *J. Mater. Chem.*, 2011, **21**, 5475−5483.
4. Y. Zhao, K. X. Yao, B. Teng, T. Zhang and Y. A. Han, *Energy Environ. Sci.*, 2013, **6**, 3684−3692.
5. M. G. Rabbani and H. M. El-Kaderi, *Chem. Mater.*, 2011, **23**, 1650−1653.
6. M. G. Rabbani, T. E. Reich, R. M. Kassab, K. T. Jackson and H. M. El-Kaderi, *Chem. Commun.*, 2012, **48**, 1141−1143.
7. J. Liu, Y. Liu, X. Jiang, Y. Luo and Y. Lyu, *Microporous and Mesoporous Materials*, 2017, **250**, 203-209.

8. A. Bhunia, I. Boldog, A. Möller and C. Janiak, *J. Mater. Chem. A*, 2013, **1**, 14990.
9. K. Wang, Y. Tang, Q. Jiang, Y. Lan, H. Huang, D. Liu and C. Zhong, *Journal of Energy Chemistry*, 2017, **26**, 902-908.
10. Y. Xu, D. Chang, S. Feng, C. Zhang and J.-X. Jiang, *New Journal of Chemistry*, 2016, **40**, 9415-9423.
11. G. Li, L. Qin, C. Yao and Y. Xu, *Sci. Rep.*, 2017, **7**, 15394.
12. Q. Chen, M. Luo, P. Hammershoj, D. Zhou, Y. Han, B. W. Laursen, C. G. Yan and B. H. Han, *J. Am. Chem. Soc.*, 2012, **134**, 6084-6087.
13. H. Liu, Q. Li, Q. Li, W. Jin, X. Li, A. Hameed and S. Qiao, *Poly. Chem.*, 2017, **8**, 6733-6740.
14. Y. Byun and A. Coskun, *Chem. Mater.*, 2015, **27**, 2576-2583.
15. J.-X. Jiang, F. Su, A. Trewin, C. D. Wood, H. Niu, J. T. A. Jones, Y. Z. Khimyak, A. I. Cooper, *J. Am. Chem. Soc.*, 2008, **130**, 7710-7720.
16. C. Pei, T. Ben, Y. Li and S. Qiu, *Chem. Commun.*, 2014, **50**, 6134-6136.
17. X. Wang, Y. Zhao, L. Wei, C. Zhang, X. Yang, M. Yu and J.-X. Jiang, *Macromolecular Chemistry and Physics*, 2015, **216**, 504-510.
18. Y. Zhao, X. Wang, C. Zhang, F. Xie, R. Kong and J.-X. Jiang, *RSC Adv.*, 2015, **5**, 100322-100329.
19. S. Fischer, A. Schimanowitz, R. Dawson, I. Senkovska, S. Kaskel and A. Thomas, J. Mater. Chem. A, 2014, 2, 11825-11829.
20. O. Buyukcakir, S. H. Je, S. N. Talapaneni, D. Kim and A. Coskun, *ACS Appl. Mater. Interfaces*, 2017, **9**, 7209-7216.