Electronic Supplementary Information for

## Troger's Base Functionalized Covalent Triazine Frameworks for CO<sub>2</sub> Capture

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Fig. S1. FT-IR spectra of DCTB and the precursor (KBr pellets)



Fig. S2. FT-IR spectra of the CTF-TBs obtained from different ratios of  $ZnCl_2$  to

DCTB (KBr pellets)



Fig. S3. FT-IR spectra of the CTF-TBs obtained from different reaction temperatures

(KBr pellets)



Fig. S4. TGA curve of DCTB and CTF-TB-7 (N<sub>2</sub>, 10 °C /min)



Fig. S5. DSC curves of DCTB and CTF-TB-7 (10 °C/min, N<sub>2</sub>)



Fig. S6. XRD patterns of CTF-TB-3 and CTF-TB-7



Fig. S7. FESEM images of CTF-TB-3 (a), (b) and (c) and CTF-TB-7 (d), (e) and (f)



Fig. S8. TEM images of CTF-TB-3 (a), (b) and (c) and CTF-TB-7 (d), (e) and (f)



Fig. S9. Nitrogen adsorption and desorption isotherms at 77.3 K for CTF-TB-S



Fig. S10. Nitrogen adsorption and desorption isotherms at 77.3 K for all CTF-TBs derived from different ratios of ZnCl<sub>2</sub> to DCTB (Filled symbols for adsorption and Unfilled symbols for desorption. Square: CTF-TB-

1; Circle: CTF-TB-2; Triangle: CTF-TB-3; Diamond: CTF-TB-4; Star: CTF-TB-5)



Fig. S11. Pore size distributions (PSD) calculated by the NLDFT method for all CTF-TBs derived from different ratios of ZnCl<sub>2</sub> to DCTB



Fig. S12. Nitrogen adsorption and desorption isotherms at 77.3 K for all CTF-TBs obtained from different reaction temperatures
(Filled symbols for adsorption and Unfilled symbols for desorption. Square: CTF-TB-6; Circle: CTF-TB-3; Triangle: CTF-TB-7; Diamond: CTF-TB-8; Star: CTF-TB-9)



Fig. S13. Pore size distributions (PSD) calculated by the NLDFT method for all CTF-TBs obtained from different reaction temperatures



Fig. S14. High resolution N1s XPS spectra of (a) DCTB, (b) CTF-TB-6 (350 °C), (c) CTF-TB-3 (400 °C), (d) CTF-TB-7 (450 °C), (e) CTF-TB-8 (500 °C), and (f) CTF-

TB-9 (550 °C)



Fig. S15. Heats of adsorption for the CTF-TBs



Fig. S16. Representative  $CO_2/N_2$  selectivity for CTF-TB-7 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar)



Fig. S17.  $CO_2/N_2$  selectivities for (a) CTF-TB-1, (b) CTF-TB-2, (c) CTF-TB-3, (d) CTF-TB-4, (e) CTF-TB-5, (f) CTF-TB-7, (g) CTF-TB-8, and (h) CTF-TB-9, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar)

Polymer Code	N (%)	C (%)	Н (%)
Calculated	20.58	74.98	4.440
CTF-TB-6 (350 °C)	11.82	75.12	3.735
CTF-TB-3 (400 °C)	11.75	69.50	3.071
CTF-TB-7 (450 °C)	10.53	67.67	2.560
CTF-TB-8 (500 °C)	10.11	66.80	2.995
CTF-TB-9 (550 °C)	8.52	62.67	2.801

Table S1 Elemental Analysis of the CTF-TBs