

Supporting Information

A porous β -Cyclodextrin-based terpolymer fluorescence sensor for *in situ* trinitrophenol detection

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Experimental Section:

S1. Synthesis of porous framework polymers (PFP)

β -CD (0.185 g, 0.162 mmol) was purged with N₂ for 5 mins and 5-mL DMA was added. The mixture was equilibrated at -20°C for 30 minutes. DL (0.435 g, 1.645 mmol) pre-dissolved in 5-mL DMA was added dropwise to the reaction mixture over a period of 20 mins with continuous

stirring for 48 h using magnetic stirring. A creamy brown coloured suspension resulted that was washed with distilled water (3×10-mL). Subsequent washing with DMF (3× 10-mL), acetone (3× 10-mL) and finally with distilled water (3×10-mL) to afford light brown solids which were freeze dried for 24 h. The polymers were ground with a mortar and pestle and passed through a size 30 mesh sieve and stored in a desiccator for further use. Figure 2.2 depicts an illustration of the cross-linking reaction for polymer materials containing β -CD and 4, 4'-diisocyanato-3,3'-dimethyl biphenyl (DL), referred to as a porous framework polymer (PFP).

S2. Solid state ^{13}C NMR spectroscopy

Solid-state ^{13}C NMR spectra were obtained with a wide-bore (89 mm) 8.6 T Oxford superconducting magnet system equipped with a 4 mm CP-MAS (cross-polarization with magic angle spinning) solids probe. An Avance DRX360 console and workstation running Top Spin 1.3 (Bruker Bio Spin Corp.; Billerica, MA) was used to control the acquisition parameters using standard pulse programs. The samples were packed in 4-mm-outer-diameter zirconium oxide rotors capped with Teflon MAS rotor caps. Acquisition was carried out with MAS at 8 kHz along with a 2 s recycle delay and 750 μs cross polarization.

Results and Discussion:

S3. Solid-State ^{13}C NMR spectra for PFP and FL-PFP

Solid state ^{13}C NMR spectra give additional structural information to complement the FT-IR results. The broad spectral lines are related to the amorphous nature of the polymers (PFP and FL-PFP) due to the level of cross-linking and the nature in which the reaction occurs within a polymer material as compared with native β -CD. The spectral signatures of β -CD at $\delta=75$ and $\delta=100$ ppm;

whereas the signature at 157 ppm corresponds to the newly formed alkoxy bonds shown in Figure 3.11. The signatures at $\delta = 120-140$ ppm relates to the aromatic carbons of both the TPE and the diisocyanate linker.

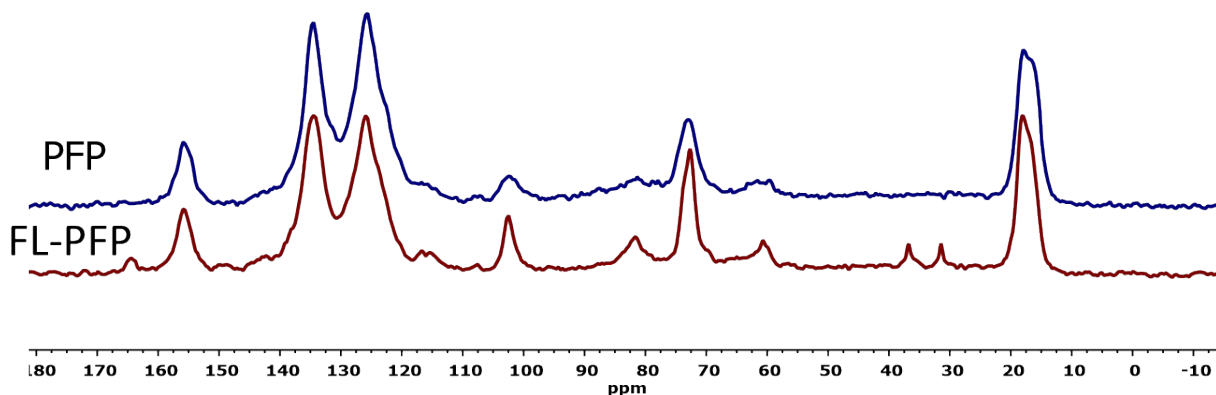


Figure S1. ^{13}C NMR CP-MAS spectra of the PFP and FL-PFP polymer materials. Obtained at a spectrometer frequency of 125 MHz and 8 kHz MAS frequency.

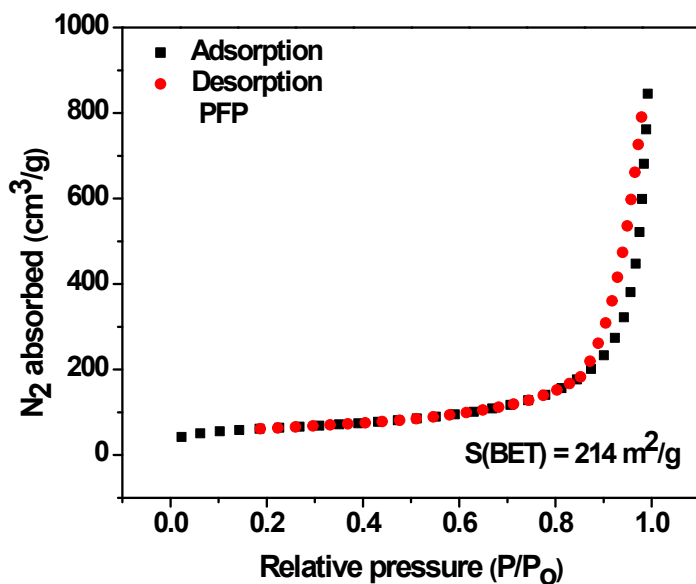


Figure S2. N_2 adsorption-desorption isotherm for PFP at 77 K (CD: linker; 1:10).

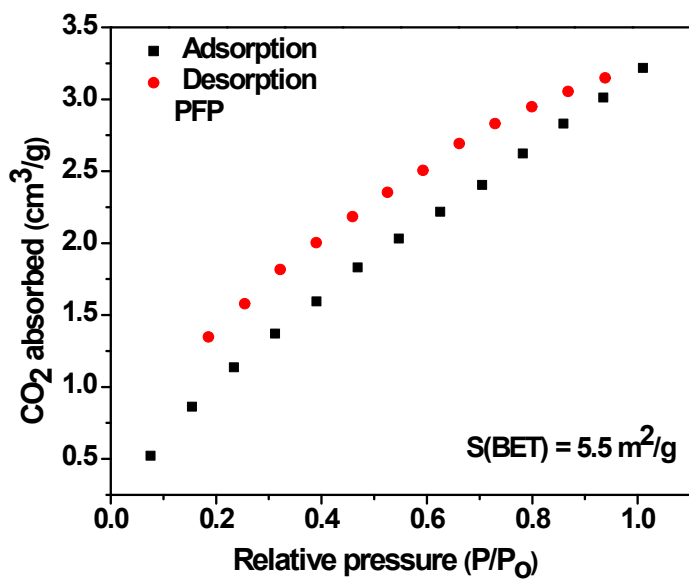


Figure S3. CO₂ adsorption-desorption isotherm for PFP at 273 K (CD: linker; 1:10).