Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information

A reversible chromogenic covalent organic polymer for gas sensing applications

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1. Experimental

1.1. Materials and Instrumentation

Cyanuric Chloride was purchased from Sigma-Aldrich Pvt. Ltd. and used as received. 2,4,6-tris(*p*-aminophenyl)-1,3,5-triazine was synthesized using *p*-amino benzonitrile with slight modification in reported procedure.[1] THF and Methanol were obtained from commercial suppliers from SpectroChem. Pvt. Ltd. All the chemicals were of A.R. grade. The double deionised water was obtained from USIC, University of Delhi, India. IR experiments were carried out within the range of 400–4000 cm^{-1} using ThermoScientific INCOLET iS50 spectrometer. PXRD patterns were obtained using Shimadzu D8 DISCOVER X-ray diffractometer. XPS experiment was carried out on PHI 5000 Versa Prob III, FEI Inc. with Auger electron spectroscopy module. Morphological characterizations were obtained from TECNAI 200 kV TEM with UHV FEI, Germany (Electron Optics) equipped with digital imaging and 35 mm photography system and ZEISS Gemini SEM-500 FESEM spectroscopy. TGA experiment was performed through Perkin Elmer TG/DTA instrument. N_2 adsorption-desorption isotherm and Pore size distribution was measured by ASI-CT-11 Quantachrome Instruments. Emission studies were carried out on Varian Cary Eclipse Fluorescence spectrometer.

1.2. Synthesis of CC-TAPT-COP

In two different oven-dried R.B. flasks, the cyanuric chloride **1** (104 mg, 0.564 mmol) and 2, 4, 6-*tris* (*p*-aminophenyl)-1, 3, 5-triazine **2** (200 mg, 0.564 mmol) were separately dissolved in THF (10mL). Then after, a solution of DIPEA (0.295mL, 1.692mmol) in THF was added to **2** and the solution **1** was added dropwise to the above reaction mixture over 30 min with constant stirring and heated under reflux for next 24h (Scheme 1). The resulting solid was filtered and washed successively with THF, MeOH and deionised water; dried in oven. Yield: 272 mg.

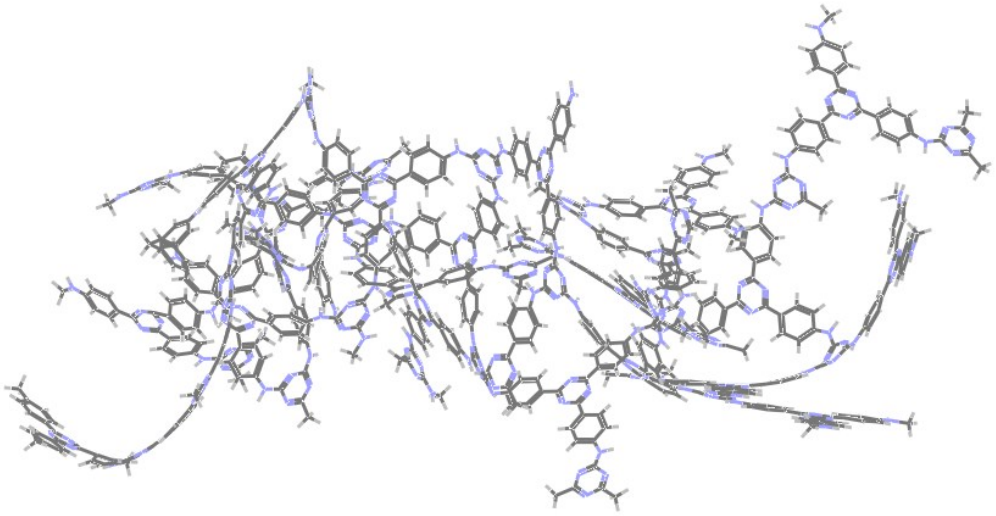

Fig. S1. 3D-Wireframe model of CC-TAPT-COP.

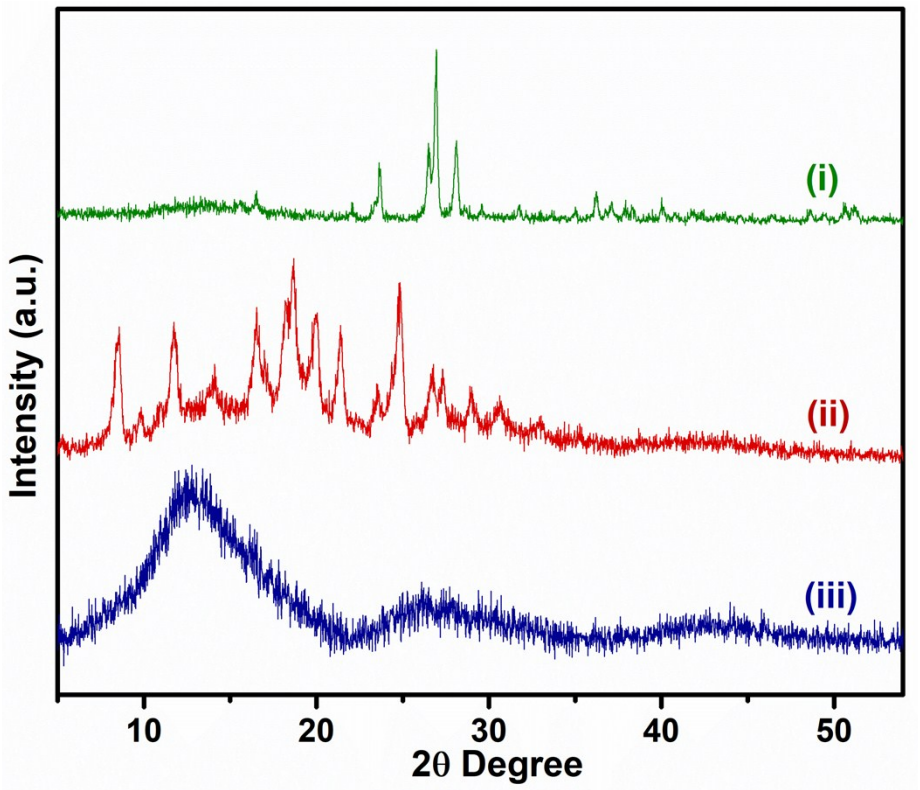

Fig. S2. Powder X-ray Diffraction pattern of (i) (Cyanuric Chloride), (ii) (TAPT) and (iii) (CC-TAPT-COP).

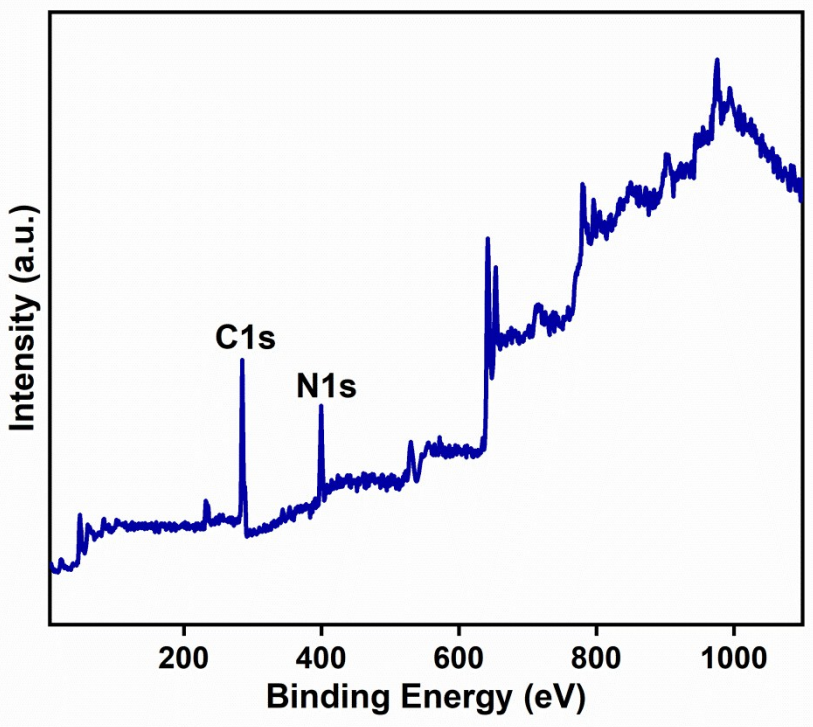

Fig. S3. XPS complete survey spectrum of as-synthesized CC-TAPT-COP.

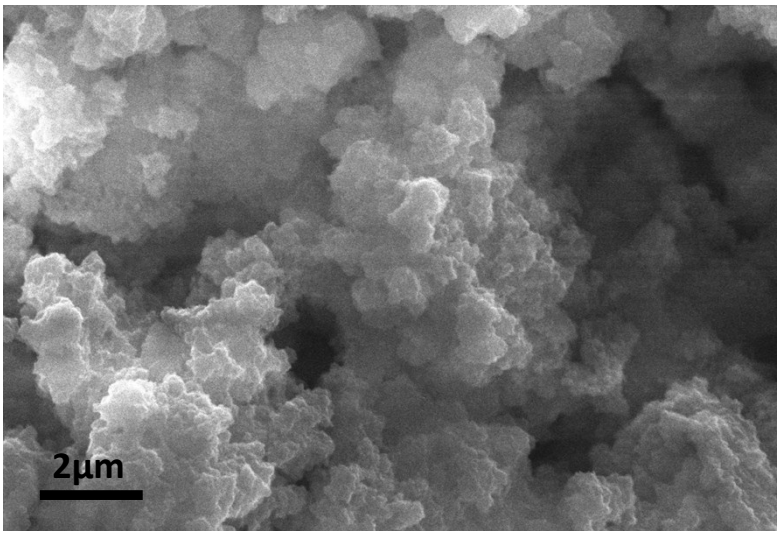

Fig. S4. SEM micrograph of as-synthesized CC-TAPT-COP at 2µm.

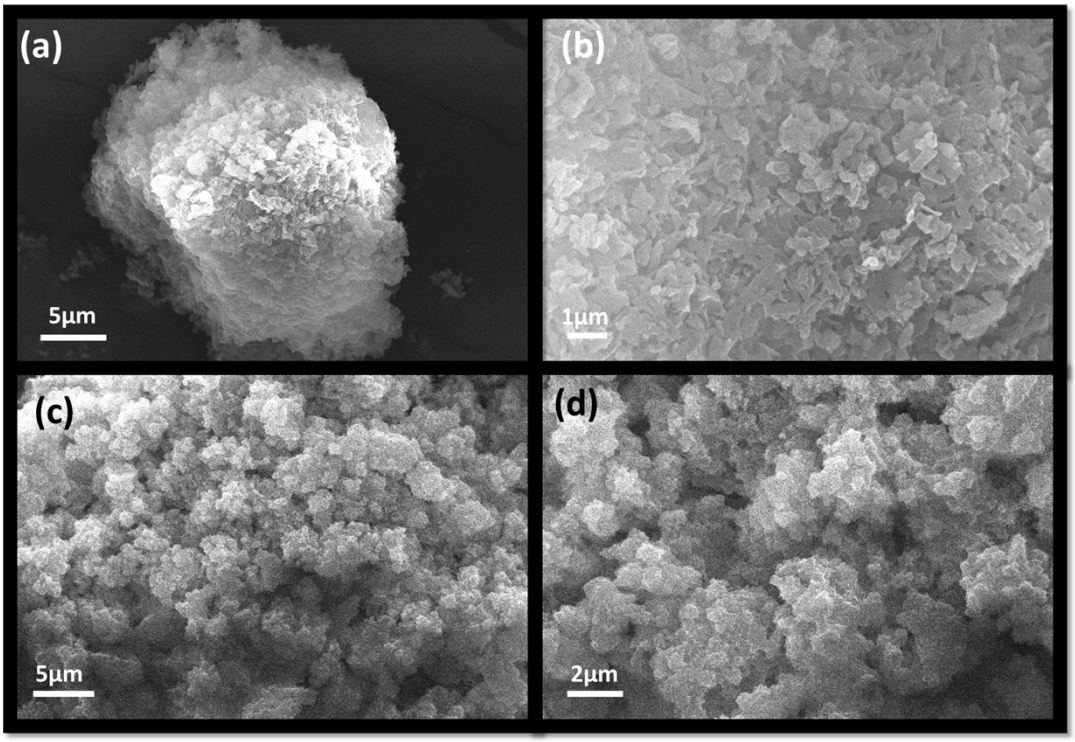

Fig. S5. The SEM micrographs of TAPT (a) 5µm, (b) 1µm and CC-TAPT-COP (c) 5µm (d) 2µm.

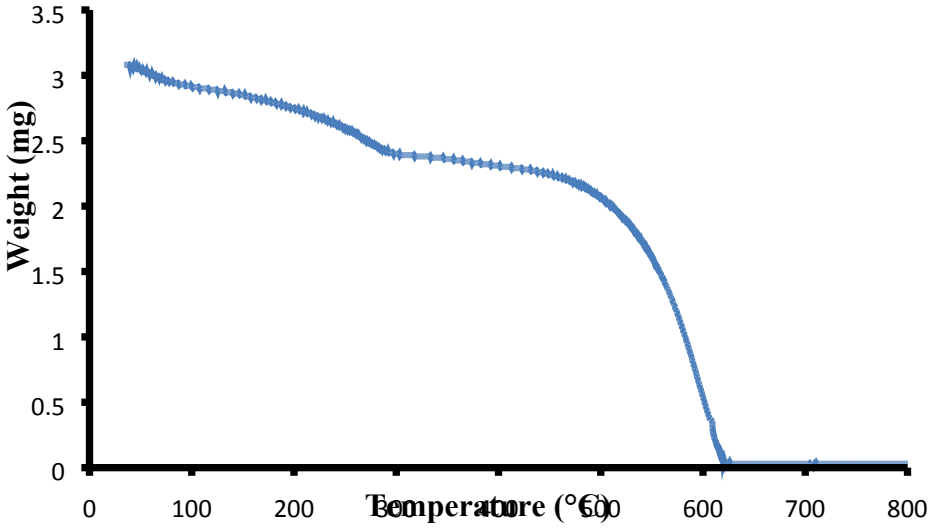

Fig. S6. The TGA thermogram of as-synthesized CC-TAPT-COP.

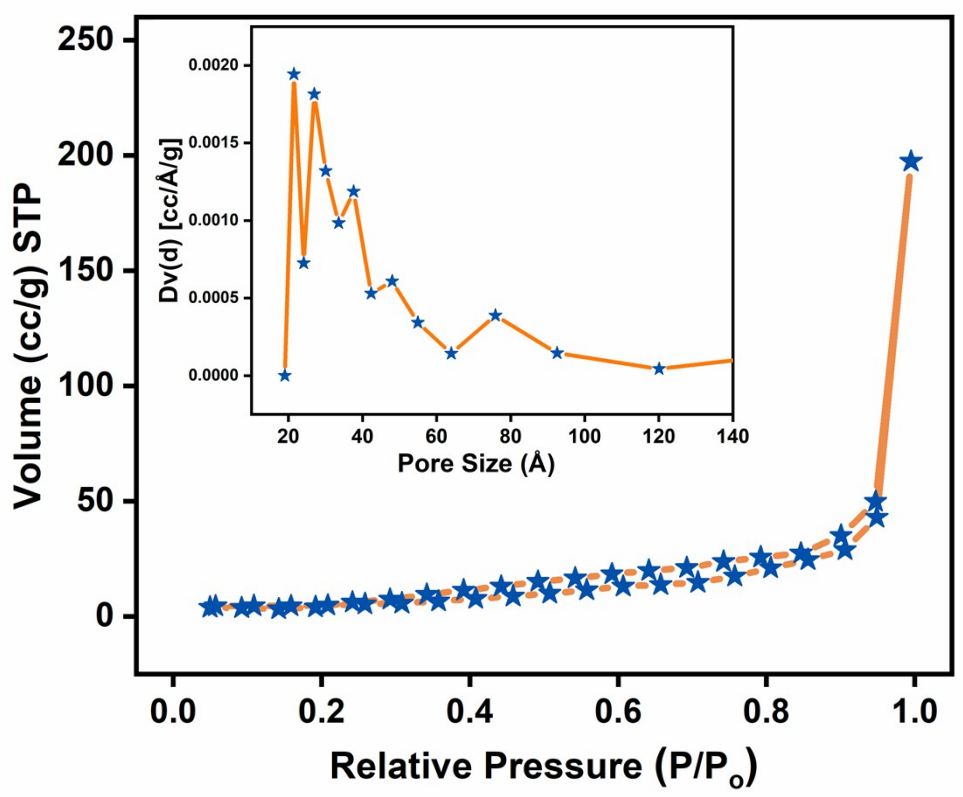

Fig. S7. N_2 adsorption/desorption isotherm of as-synthesized CC-TAPT-COP at 77K. [Inset: The Pore Size distribution of CC-TAPT-COP.]

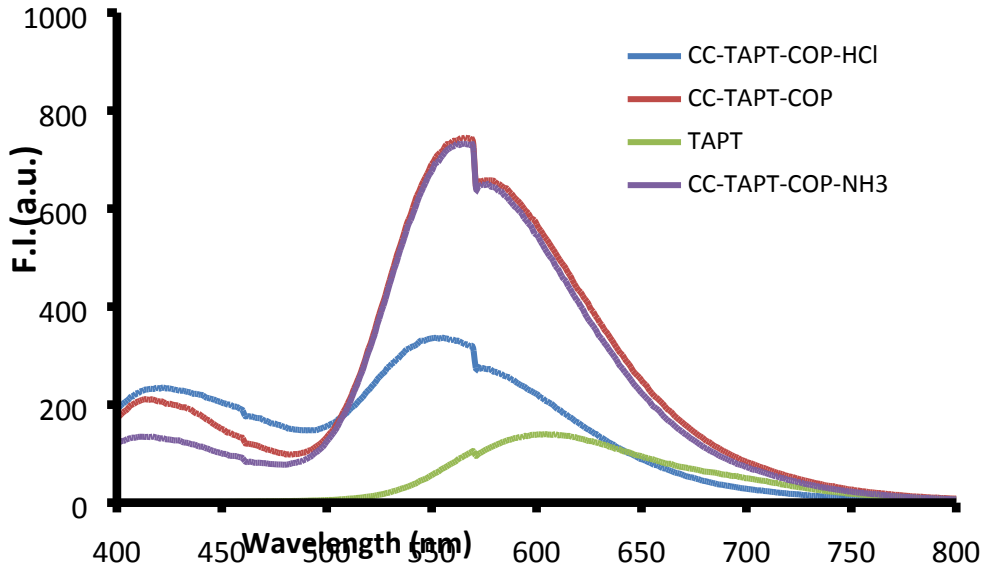

Fig. S8. Fluorescence spectra of TAPT, CC-TAPT-COP, CC-TAPT-COP-HCl and CC-TAPT-COP-NH_3.

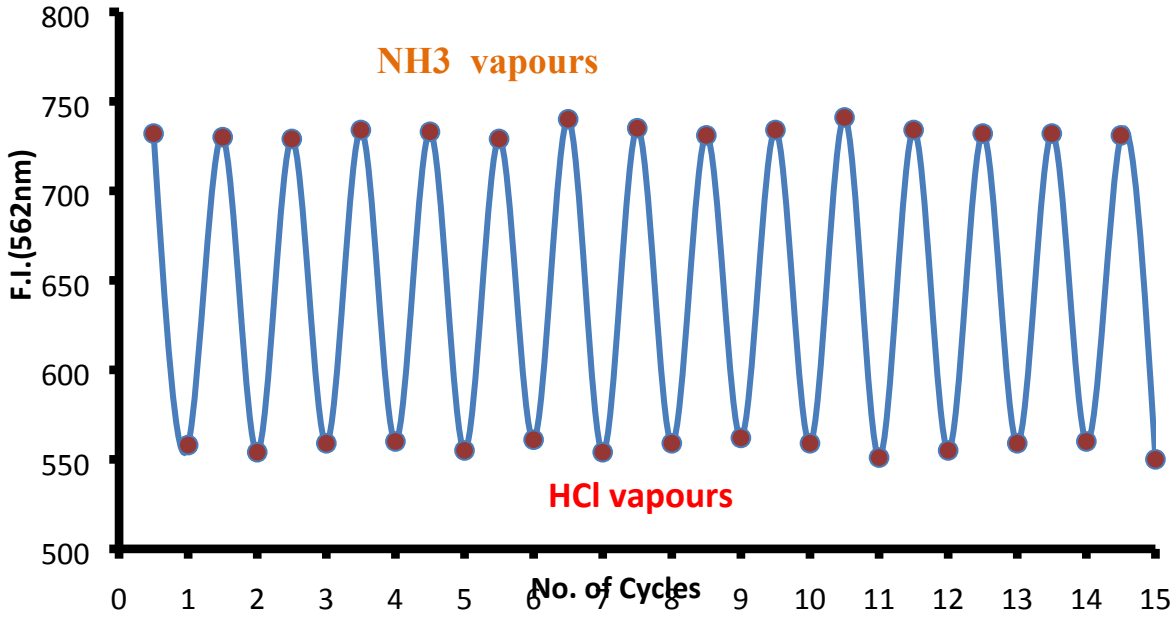

Fig. S9. Reversibility of as-synthesized CC-TAPT-COP upon alternative treatment of HCl and NH_3 vapours.

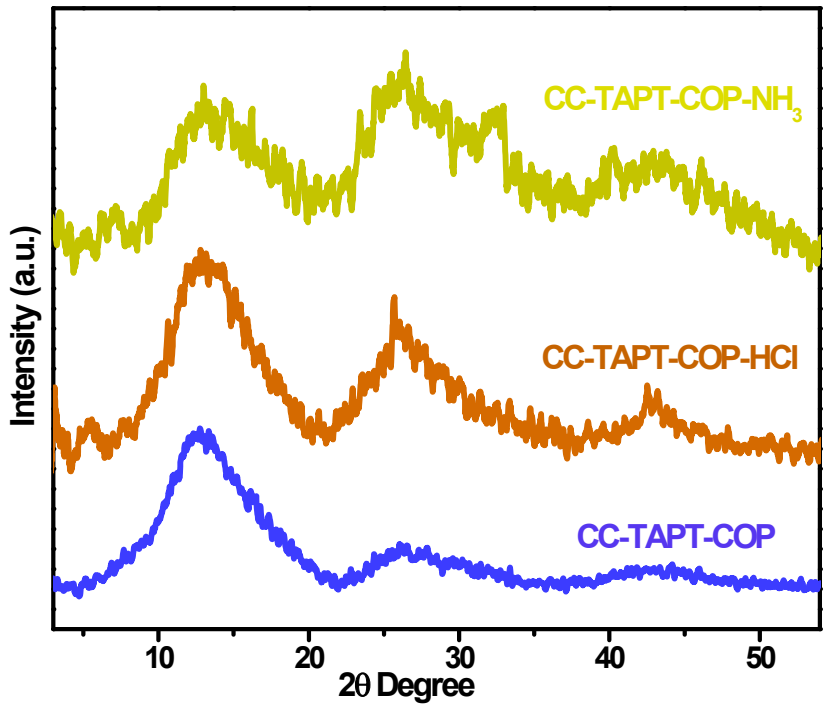

Fig. S10. Stacked view of Powder XRD of CC-TAPT-COP, CC-TAPT-COP-HCl and CC-TAPT-COP-NH_3.

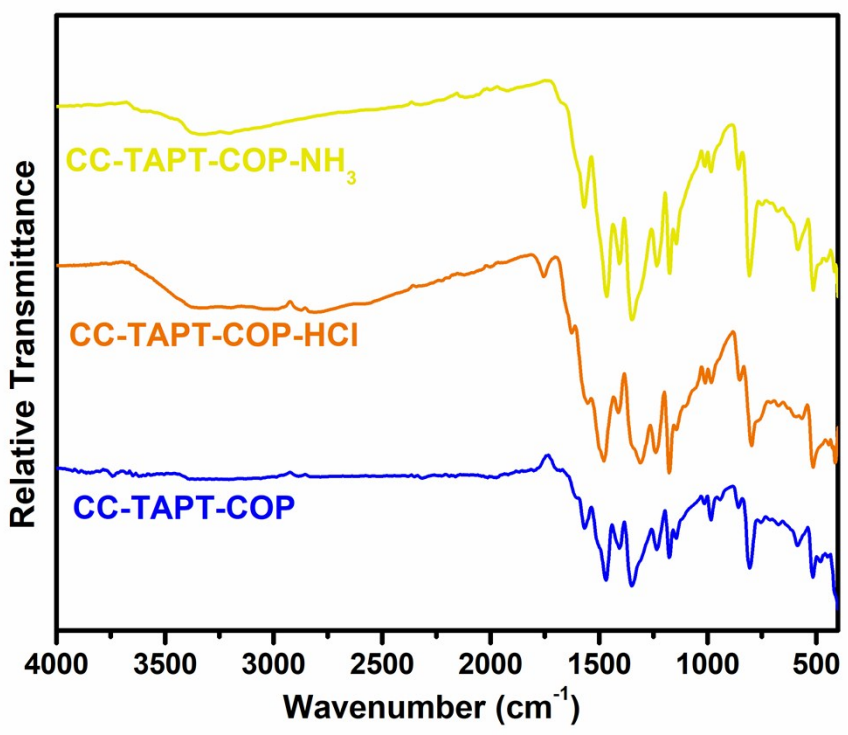

Fig. S11. Stacked view of FT-IR spectra of CC-TAPT-COP, CC-TAPT-COP-HCl and CC-TAPT-COP-NH_3.

References:

1. P. Bhanja, K. Bhunia, S. K. Das, D. Pradhan, R. Kimura, Y. Hijikata, S. Irle and A. Bhaumik, *ChemSusChem*, 2017, **10**, 921-929.