Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Structure-induced catalytic activity of Co-Zn double-metal cyanide complexes for terpolymerization of propylene oxide, cyclohexene oxide and CO_2

Joby Sebastian[†, ‡], Darbha Srinivas[†, ‡, *]

[†] Catalysis Division, CSIR-National Chemical Laboratory, Pune-411 008, India.

[‡] Academy of Scientific and Innovative Research (AcSIR), New Delhi- 110 001, India.

E-mail: d.srinivas@ncl.res.in, Tel: +91 20 2590 2018, Fax: +91 20 2590 2633.

S1. ^{1}H NMR spectrum of PCHC.

S2. ^{1}H NMR spectrum of PPC.

S3. ^{1}H NMR spectra of all polycarbonates.

S4. ^{13}C inverse gated NMR of the copolymers and terpolymer in the CH and CH_2 regions of PPC.

S5. ^{13}C inverse gated NMR of the copolymers and terpolymer in the CH_3 region.

S6. Thermograms of PPC, PCHC and terpolymer.

S7. FTIR of Co-Zn DMC catalysts.

S8. DRIFT spectrum of adsorbed pyridine on DMC-II showing bands due to Lewis acid sites..

S9. NH_3-TPD of DMC-II.

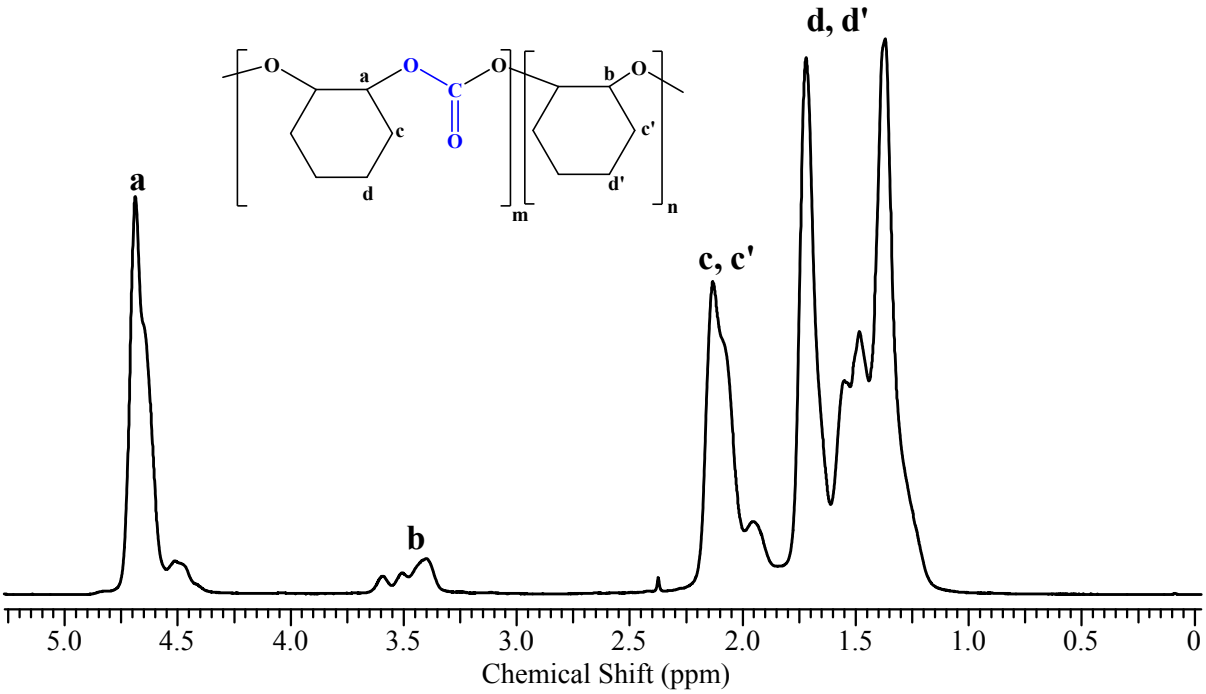
S10 Powder XRD of PCHC and terpolymer produced using DMC-II catalyst.

S11 SEM images of PCHC and terpolymer produced over DMC-II

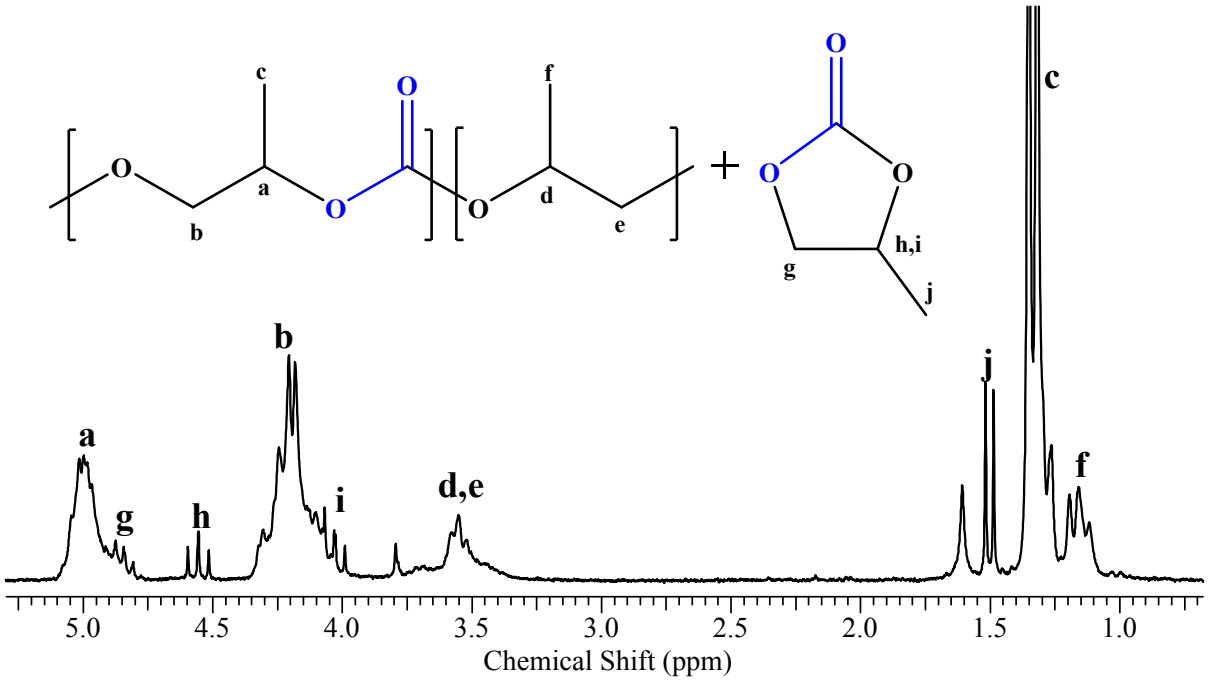
S12. ^{1}H NMR spectrum of crude terpolymer synthesised over DMC-II.

S13. Reaction time verses reactor pressure at different reaction conditions.

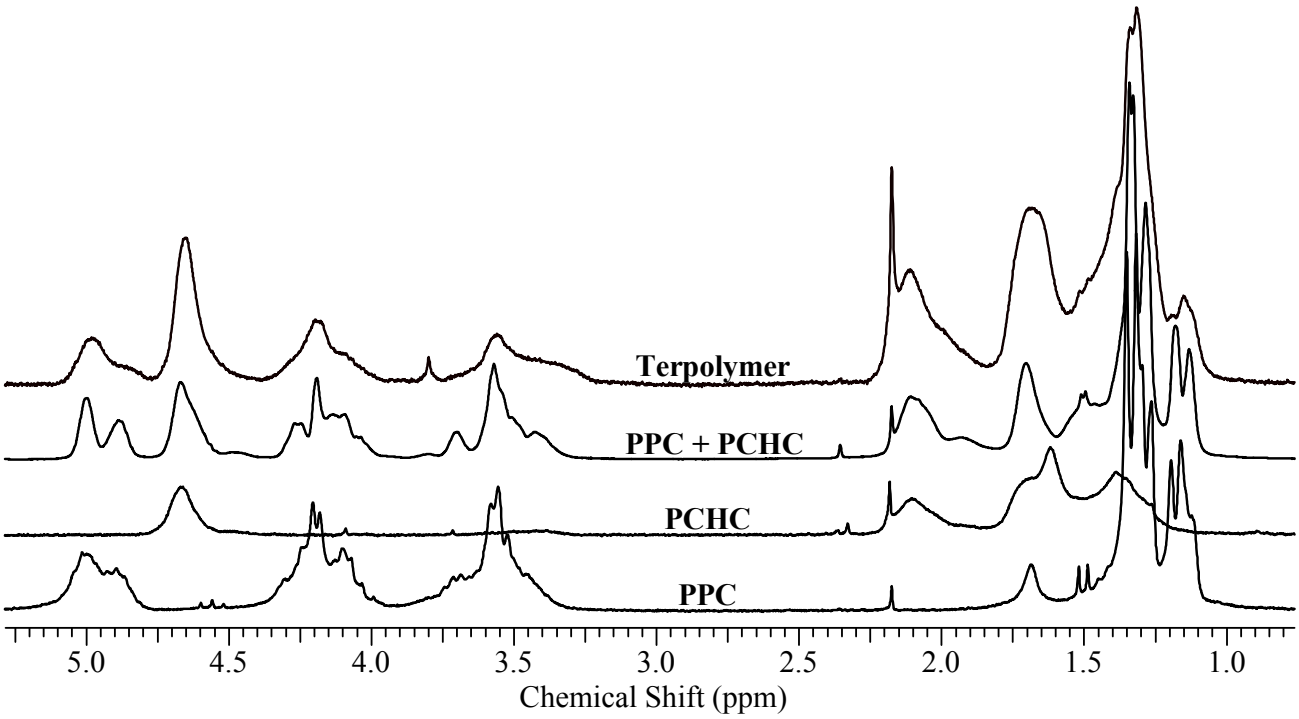
S14. PXRD patterns of fresh and spent DMC-II catalyst.



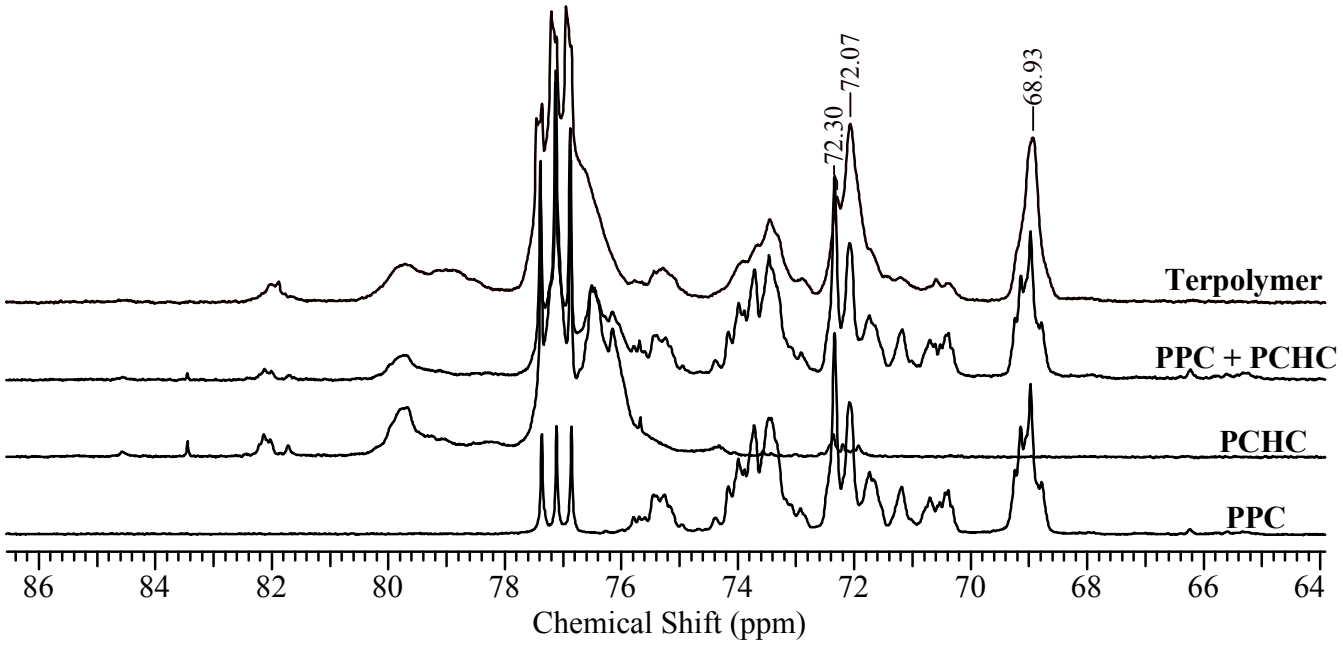
S1. ^{1}H NMR spectrum of purified PCHC.



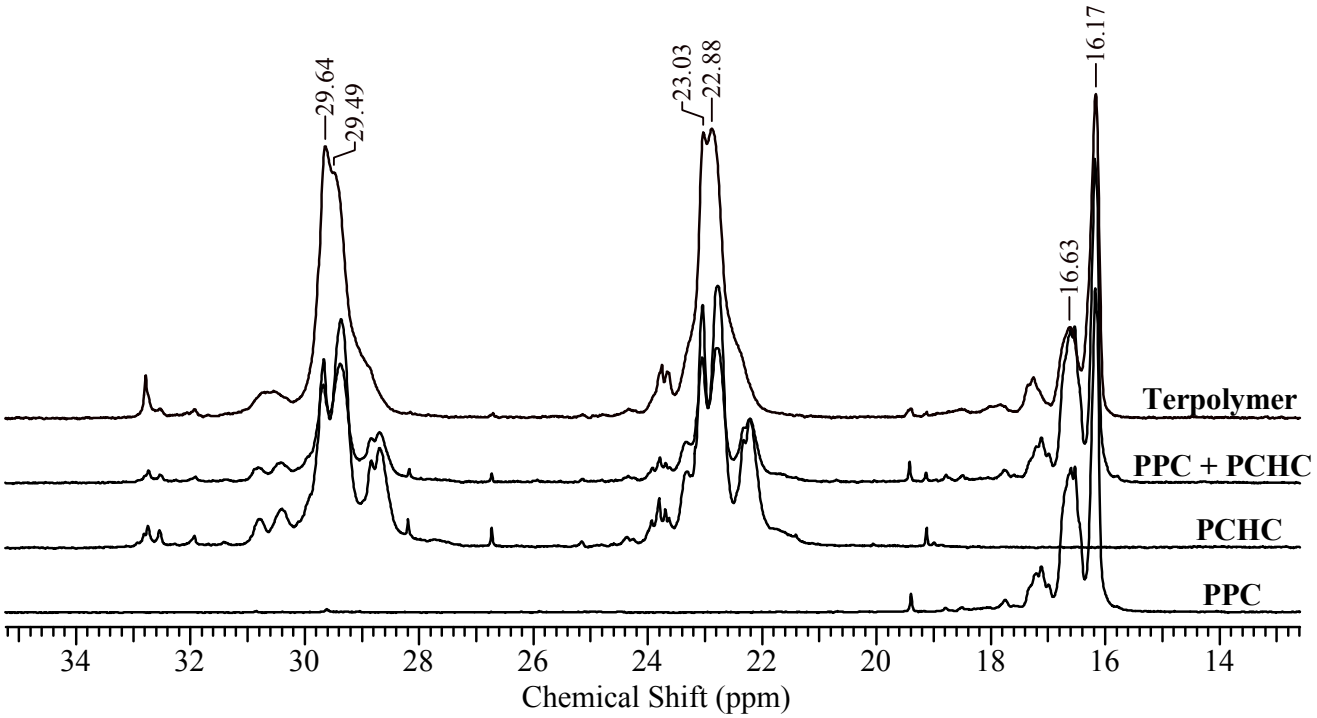
S2. ^{1}H NMR spectrum of purified PPC.



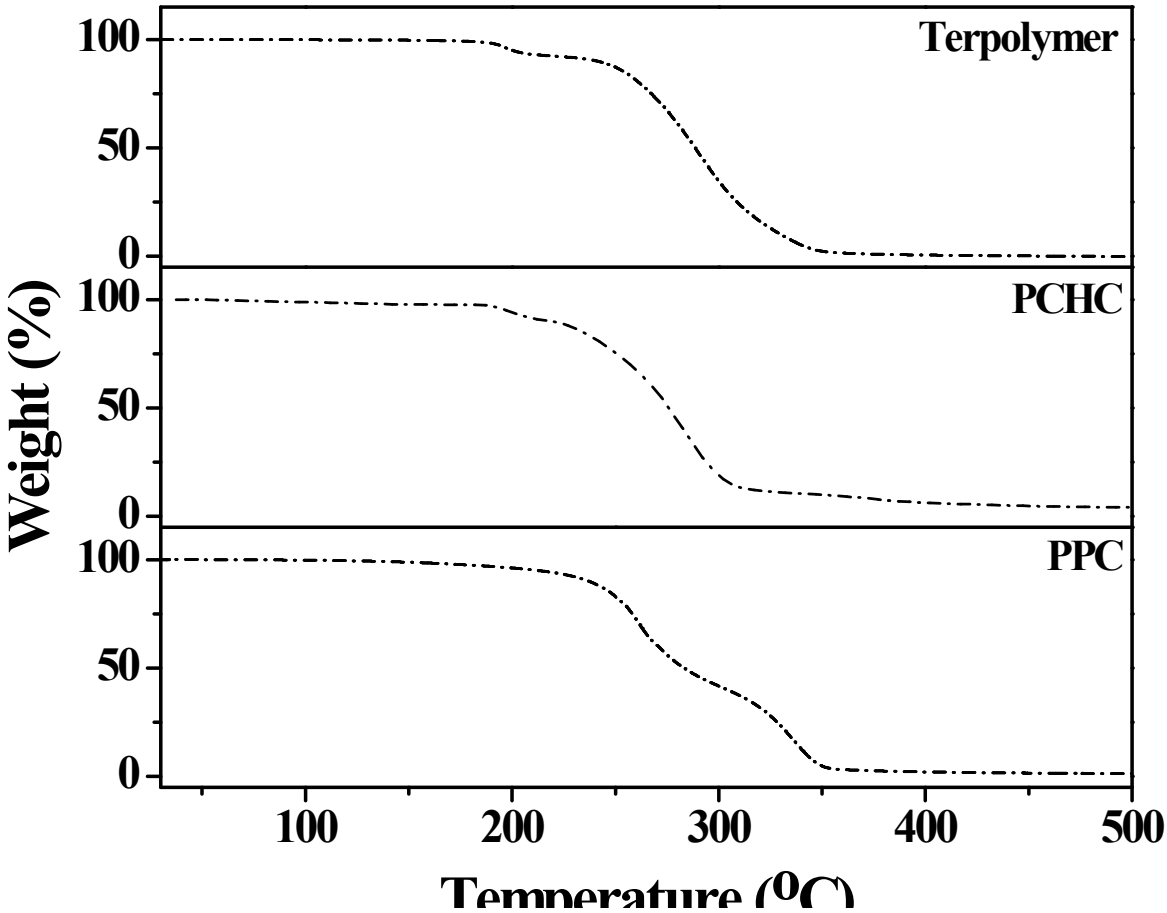
S3. ^{1}H NMR spectra of PPC, PCHC, PPC + PCHC physical blend and PO-CHO-CO_2 terpolymer.



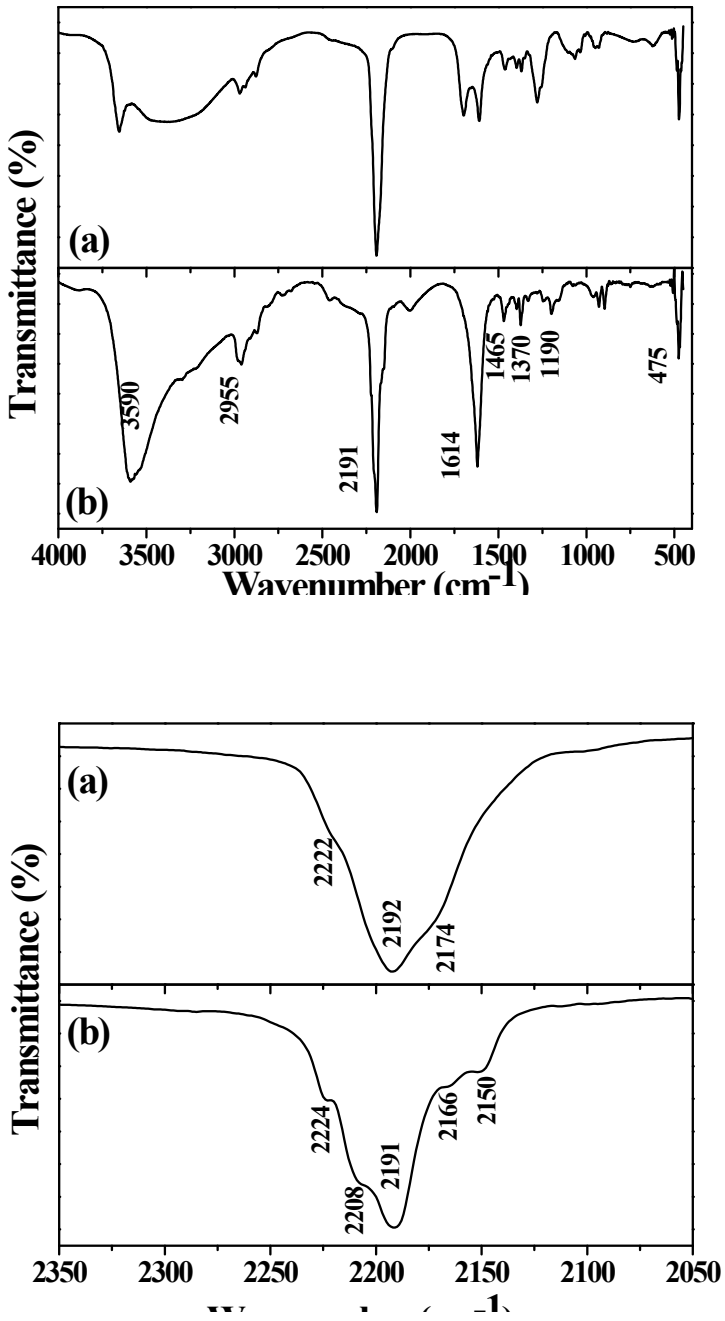
S4. Inverse-gated ^{13}C NMR of the polycarbonates in the CH (72.07 and 72.30 ppm) and CH_2 (68.93 ppm) regions of PPC. The terpolymer spectrum appeared as broad peaks without considerable splits as in the blend and PPC. It also clear that there is a change in tacticity pattern for the terpolymer as compared to PPC (reversal of intensity distribution of 72.30 ppm in terpolymer as compared to PPC).



S5. ^{13}C inverse gated NMR of the polycarbonates in the CH_3 region (16.17 and 16.63 ppm) of PPC and CH_2 region (22.8 and 29.64 ppm) of PCHC. No major difference was observed in the CH_3 region of terpolymer as compared to PPC, but the peaks appeared as merged in case of CH_2 regions of terpolymer as compared to PCHC.

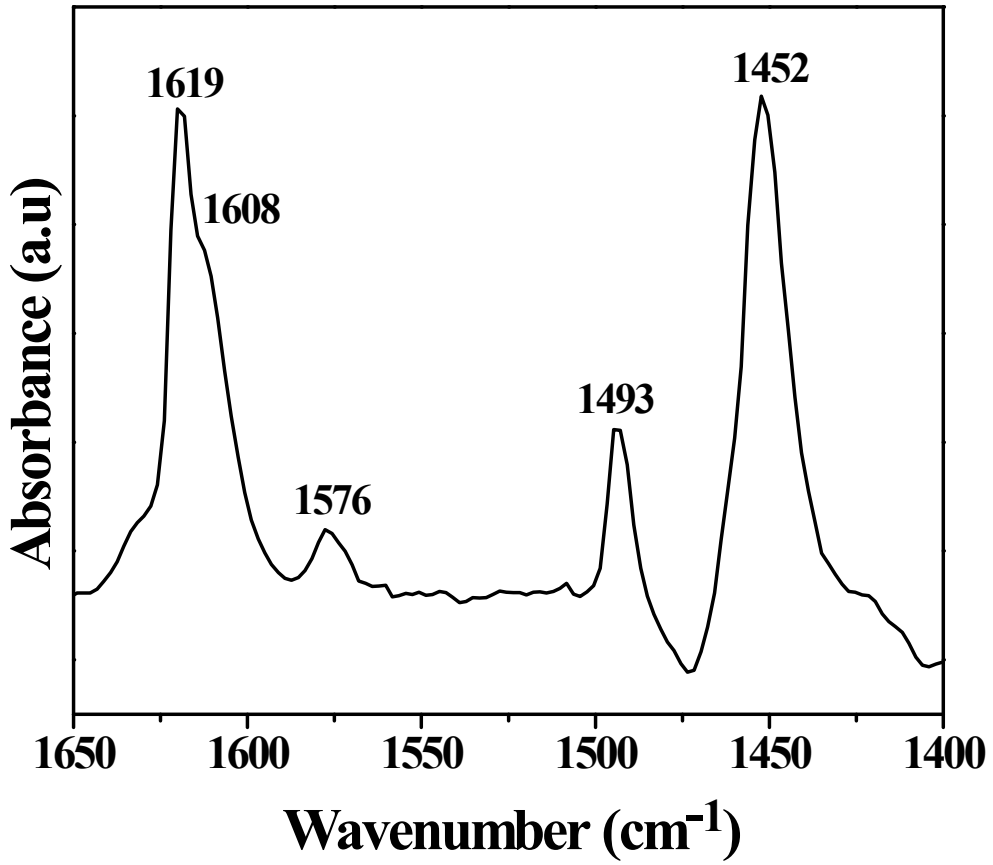


S6. Thermograms of PPC, PCHC and terpolymer synthesized over DMC-II.

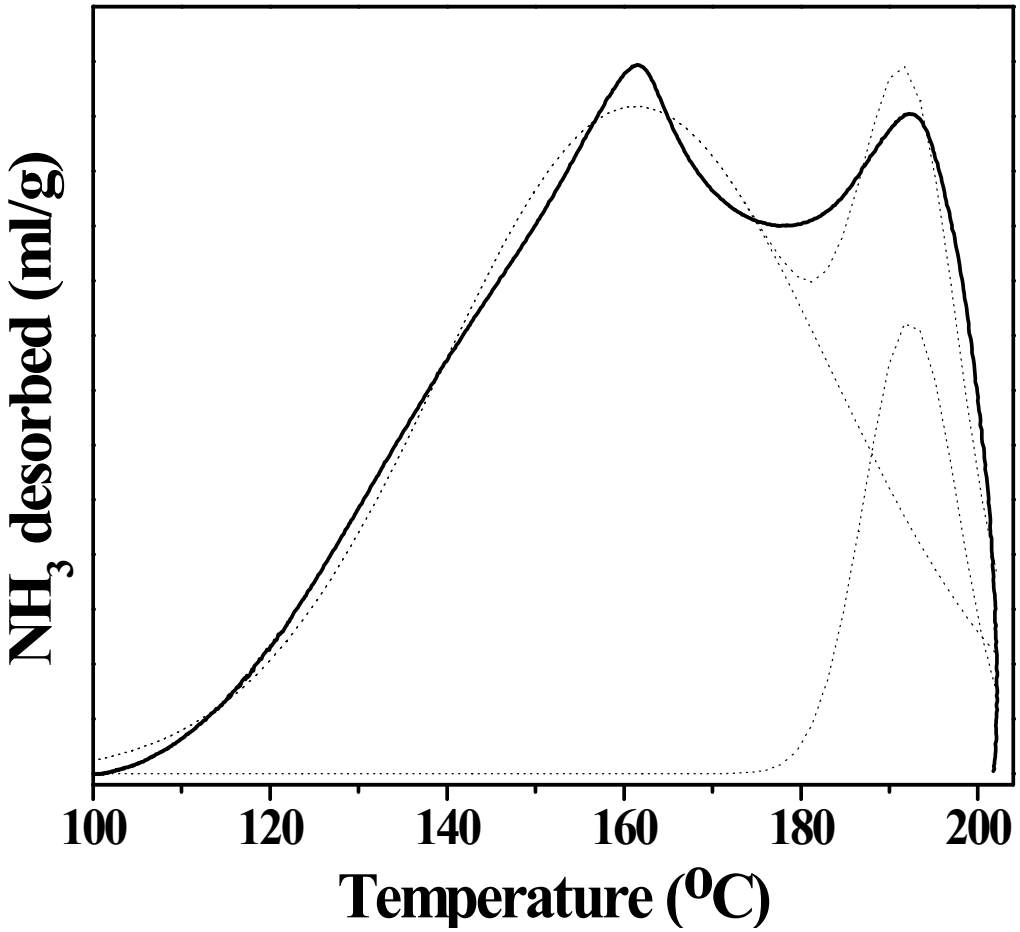


S7. FTIR of (a) DMC-I and (b) DMC-II catalysts. Band assignments are given below.

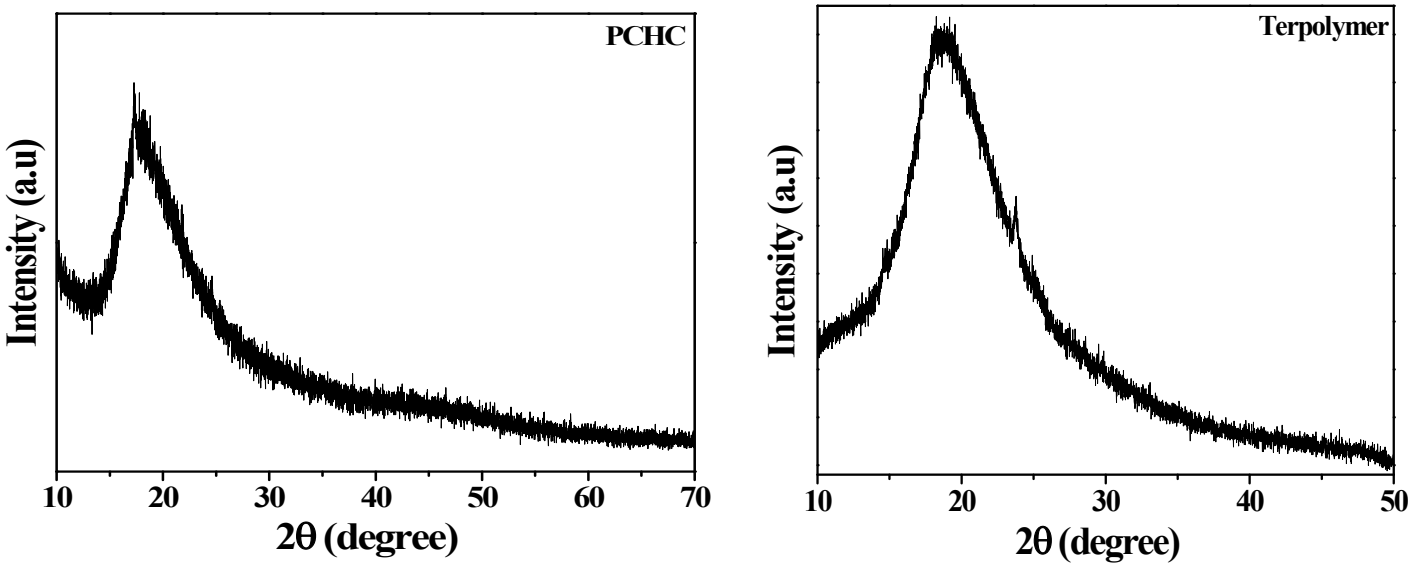
Band position (cm^{-1})	Band assignment
3590	-OH stretch
2955	-C-H stretch
2191	-CN stretch
1614	-OH bending (H_2O)
1465	-CH scissoring
1370	-OH bending (tert-butanol)
1190	3°-C-O stretch
475	Co-CN stretch



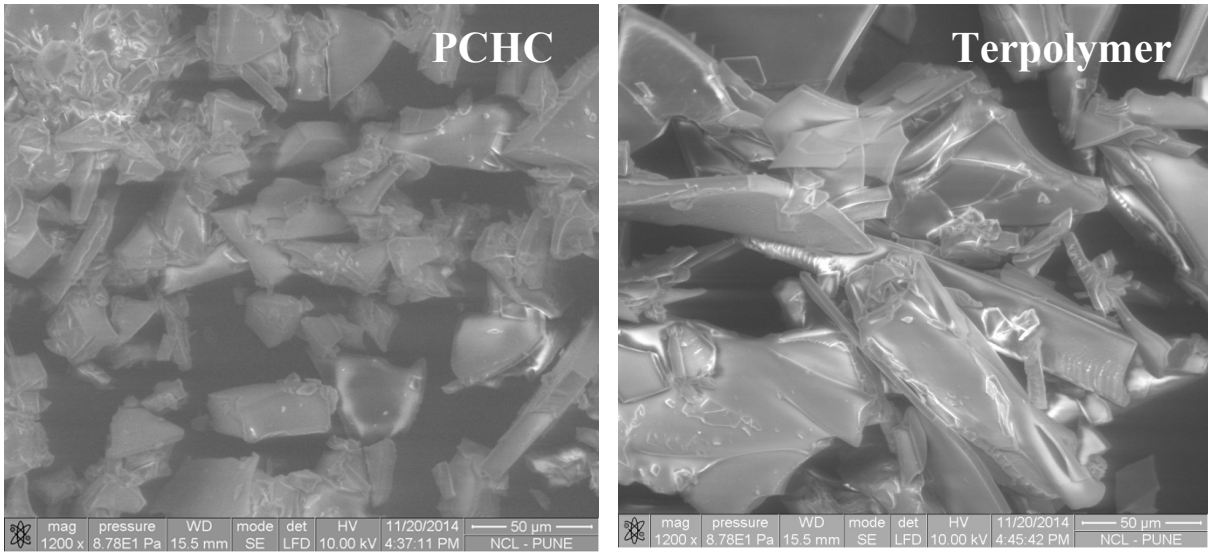
S8. DRIFT spectra of adsorbed pyridine on DMC-II showing bands due to Lewis acid sites.



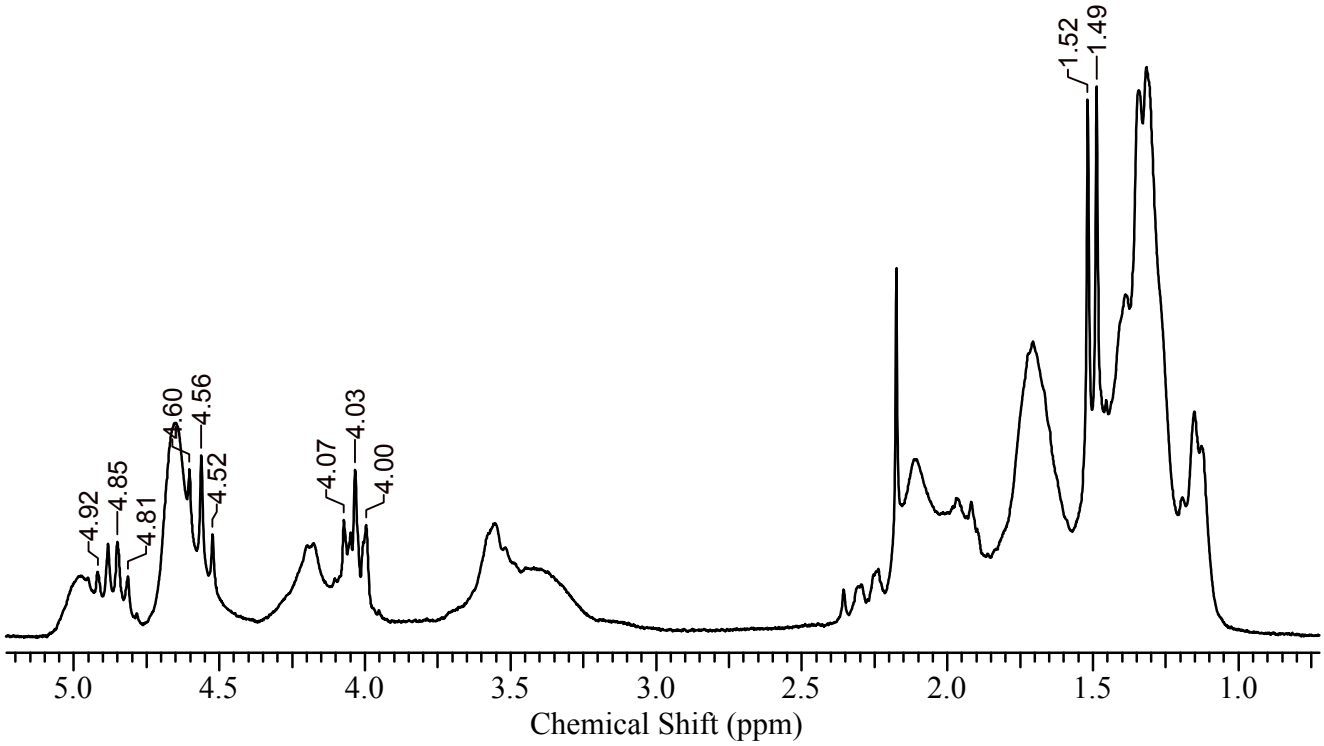
S9. NH_3-TPD of DMC-II.



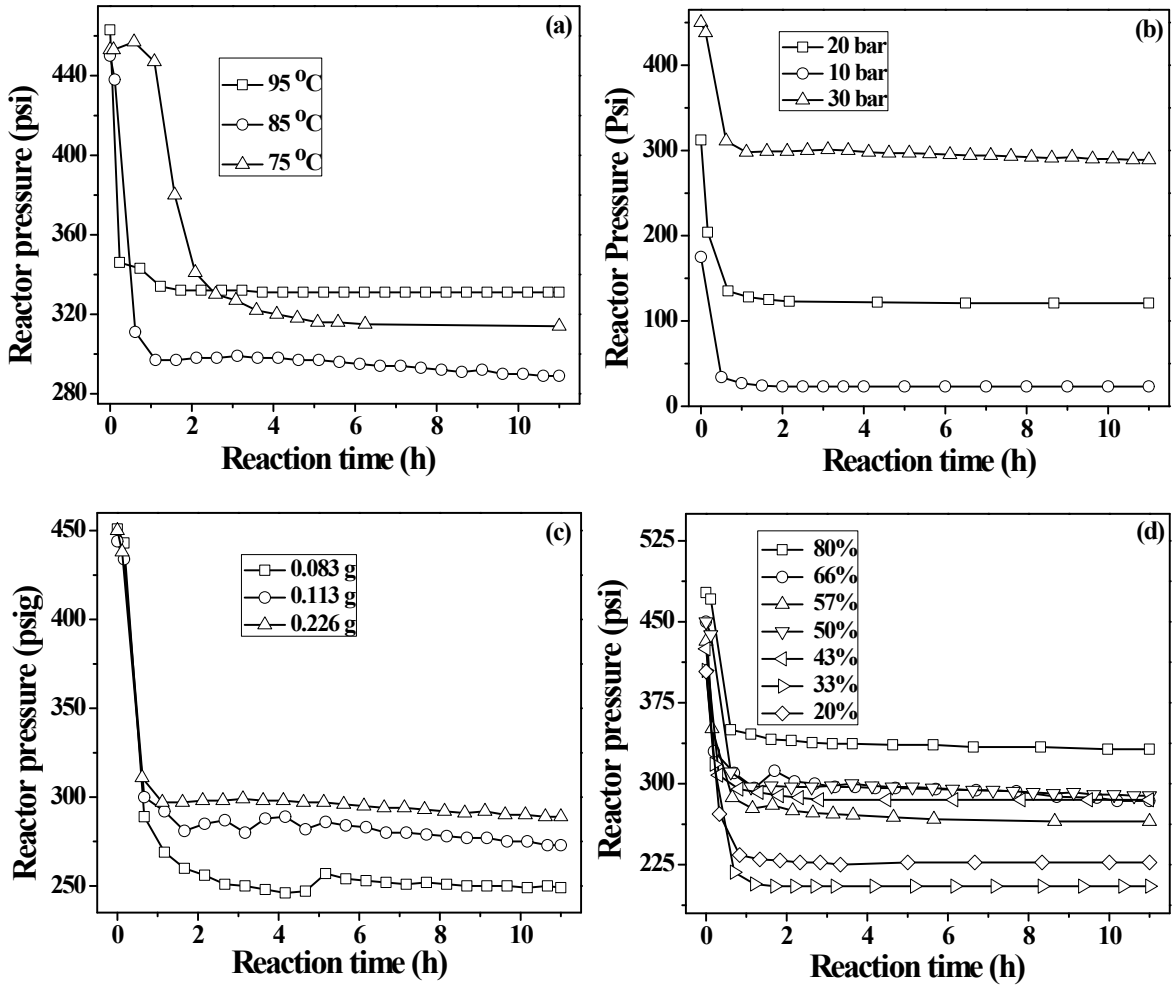
S10. PXRD of PCHC and terpolymer produced using DMC-II catalyst.



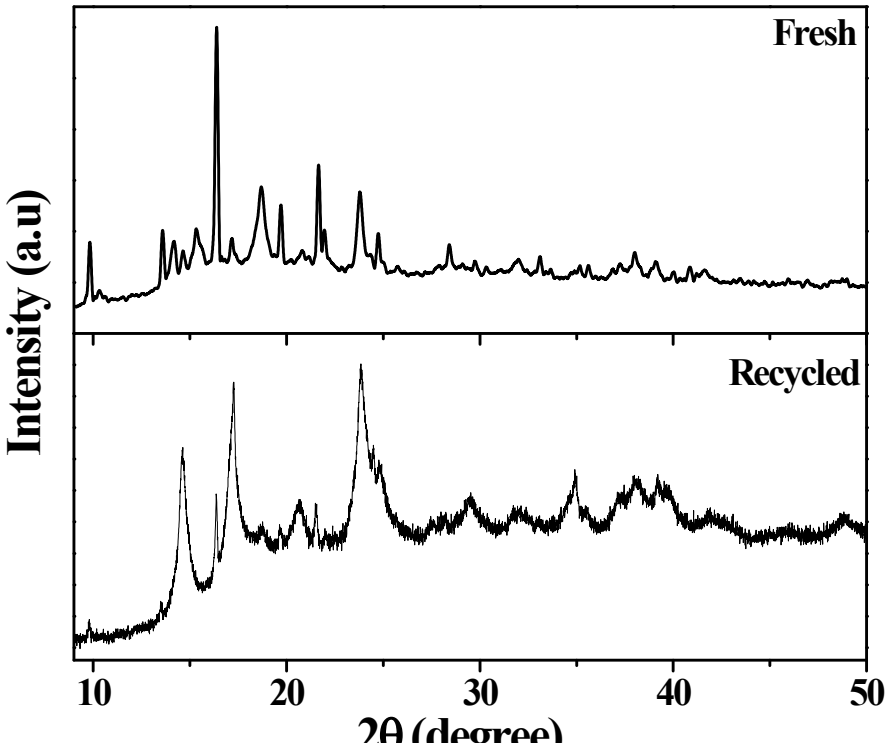
S11. SEM images of PCHC and PO-CHO-CO_2 terpolymer produced over DMC-II.



S12. ^{1}H NMR spectrum of crude terpolymer synthesised over DMC-II. The assigned peaks correspond to cyclic propylene carbonate (PC).



S13. Reaction time verses reactor pressure at different reaction conditionsusing DMC-II as catalyst. (a) effect of temperature, (b) effect of CO_2 pressure, (c) effect of catalyst quantity and (d) effect of % PO in reactant epoxide mixture.



S14. PXRD patterns of fresh and spent DMC-II catalyst. Reaction conditions: CHO = 5.6 g, PO = 3.5 g, CHO : PO molar ratio = 1:1, catalyst = 0.226 g, toluene = 8.7 g, p_{CO2} = 30 bar, reaction time = 11 h, reaction temperature = 85°C.