Supporting Information

Structure-induced catalytic activity of Co-Zn double-metal cyanide complexes for terpolymerization of propylene oxide, cyclohexene oxide and CO₂

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S1. ¹H NMR spectrum of PCHC.
S2. ¹H NMR spectrum of PPC.
S3. ¹H NMR spectra of all polycarbonates.
S4. ¹³C inverse gated NMR of the copolymers and terpolymer in the CH and CH₂ regions of PPC.
S5. ¹³C inverse gated NMR of the copolymers and terpolymer in the CH₃ 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. NH₃-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. ¹H 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.

<table>
<thead>
<tr>
<th>Band position (cm⁻¹)</th>
<th>Band assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>3590</td>
<td>-OH stretch</td>
</tr>
<tr>
<td>2955</td>
<td>-C-H stretch</td>
</tr>
<tr>
<td>2191</td>
<td>-CN stretch</td>
</tr>
<tr>
<td>1614</td>
<td>-OH bending (H₂O)</td>
</tr>
<tr>
<td>1465</td>
<td>-CH scissoring</td>
</tr>
<tr>
<td>1370</td>
<td>-OH bending (tert-butanol)</td>
</tr>
<tr>
<td>1190</td>
<td>3⁰-C-O stretch</td>
</tr>
<tr>
<td>475</td>
<td>Co-CN stretch</td>
</tr>
</tbody>
</table>
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 conditions using 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, $p_{\text{CO}_2}$ = 30 bar, reaction time = 11 h, reaction temperature = 85°C.