SUPPORTING INFORMATION

Synthesis and studies on forward and reverse reactions of phenol-blocked polyisocyanates: An insight into blocked isocyanates

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Figure S1. ¹H-NMR spectrum of phenol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S2. ¹H-NMR spectrum of o-cresol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S3. ¹H-NMR spectrum of p-cresol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S4. ¹H-NMR spectrum of o-methoxyphenol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S5. ¹H-NMR spectrum of p-methoxyphenol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S6. ¹H-NMR spectrum of o-chlorophenol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S7. ¹H-NMR spectrum of p-chlorophenol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S8. ¹H-NMR spectrum of p-esterphenol-blocked polyisocyanate (Solvent:CDCl₃).



Figure S9. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with o-cresol; (a) $40 \ ^{\circ}C$ (b) $50 \ ^{\circ}C$ and (c) $60 \ ^{\circ}C$.



Figure S10. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with p-cresol; (a) $40 \ ^{0}C$ (b) $50 \ ^{0}C$ and (c) $60 \ ^{0}C$.



Figure S11. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with o-methoxyphenol; (a) 40 $^{\circ}$ C (b) 50 $^{\circ}$ C and (c) 60 $^{\circ}$ C.



Figure S12. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with p-methoxyphenol; (a) $40 \ ^{\circ}C$ (b) $50 \ ^{\circ}C$ and (c) $60 \ ^{\circ}C$.



Figure S13. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with o-chlorophenol; (a) $40 \ ^{0}C$ (b) $50 \ ^{0}C$ and (c) $60 \ ^{0}C$.



Figure S14. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with p-chlorophenol; (a) $40 \ ^{0}C$ (b) $50 \ ^{0}C$ and (c) $60 \ ^{0}C$.



Figure S15. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with o-esterphenol; (a) $40 \ ^{0}C$ (b) $50 \ ^{0}C$ and (c) $60 \ ^{0}C$.



Figure S16. FT-IR Spectra recorded for different time intervals at different temperatures for the blocking reaction of polyisocyanate with p-esterphenol; (a) 40 0 C (b) 50 0 C and (c) 60 0 C.



Figure S17. Amine-catalysed second-order kinetic plots of blocking reaction of polyisocyanate with o-cresol.

Figure S18.Amine-catalysedsecond-orderkinetic plots ofblockingreactionofpolyisocyanatewithp-cresol.vitalvital





Figure S20. Amine-catalysed second-order kinetic plots of blocking reaction of polyisocyanate with p-methoxyphenol.

Figure S21. Amine-catalysed second-order kinetic plots of blocking reaction of polyisocyanate with o-chlorophenol.

FigureS22.Amine-catalysedsecond-orderkineticplotsofblockingreactionofpolyisocyanatewithp-chlorophenol.



Figure S23.Amine-catalysedsecond-orderkinetic plotsofblockingreactionofpolyisocyanatewitho-esterphenol.

Figure S24.Amine-catalysedsecond-order kinetic plots ofblockingreactionofpolyisocyanate withp-esterphenol.



Figure S25. FT-IR spectra of o-cresol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S26. FT-IR spectra of p-cresol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S27. FT-IR spectra of o-methoxyphenol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S28. FT-IR spectra of p-methoxyphenol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S29. FT-IR spectra of o-chlorophenol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S30. FT-IR spectra of p-chlorophenol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S31. FT-IR spectra of p-esterphenol-blocked polyisocyanate recorded at (a) different temperatures. (b) Zoomed range of isocyanate absorption region.



Figure S32. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of o-cresol-blocked polyisocyanate; (a) 120 ° (b) 130 °C and (c) 140 °C.



Figure S33. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of p-cresol-blocked polyisocyanate; (a) $120 \, {}^{0}\text{C}$ (b) $130 \, {}^{0}\text{C}$ and (c) $140 \, {}^{0}\text{C}$.



Figure S34. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of o-methoxyphenol-blocked polyisocyanate; (a) $120 \ ^{0}C$ (b) $130 \ ^{0}C$ and (c) $140 \ ^{0}C$.



Figure S35. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of p-methoxyphenol-blocked polyisocyanate; (a) $120 \, {}^{0}$ C (b) $130 \, {}^{0}$ C and (c) $140 \, {}^{0}$ C.



Figure S36. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of o-chlorophenol-blocked polyisocyanate; (a) $120 \ ^{\circ}C$ (b) $130 \ ^{\circ}C$ and (c) $140 \ ^{\circ}C$.



Figure S37. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of p-chlorophenol-blocked polyisocyanate; (a) $120 \ ^{\circ}C$ (b) $130 \ ^{\circ}C$ and (c) $140 \ ^{\circ}C$.



Figure S38. FT-IR Spectra recorded for different time intervals at different temperatures for the deblocking reaction of p-esterphenol-blocked polyisocyanate; (a) $120 \ ^{0}C$ (b) $130 \ ^{0}C$ and (c) $140 \ ^{0}C$.



Figure S39. Amine-catalysed first-order kinetic plots of deblocking reaction of o-cresol blocked polyisocyanate.

Figure S40. Amine-catalysedfirst-order kinetic plots ofdeblocking reactionofp-cresolblockedpolyisocyanate.





Figure S42. Amine-catalysed first-order kinetic plots of deblocking reaction of p-methoxyphenol blocked polyisocyanate.

Figure S43. Amine-catalysed first-order kinetic plots of deblocking reaction of o-chlorophenol blocked polyisocyanate.

Figure S44. Amine-catalysed first-order kinetic plots of deblocking reaction of p-chlorophenol blocked polyisocyanate.



Figure S45. Amine-catalysed first-order kinetic plots of deblocking reaction of p-esterphenol blocked polyisocyanate.

Figure S46. Arrhenius plots of forward and reverse reactions of ocresol-blocked polyisocyante showing equilibrium temperature range (ETR) and probable equilibrium temperature.

Figure S47. Arrhenius plots of forward and reverse reactions of p-cresol-blocked polyisocyante showing equilibrium temperature range (ETR) and probable equilibrium temperature.



Figure S48. Arrhenius plots of forward and reverse reactions of o-OMe-phenol-blocked polyisocyante showing equilibrium temperature range (ETR) and probable equilibrium temperature.

Figure S49. Arrhenius plots of forward and reverse reactions of o-Cl-phenol-blocked polyisocyante showing equilibrium temperature range (ETR) and probable equilibrium temperature.

Figure S50. Arrhenius plots of forward and reverse reactions of p-Cl-phenol-blocked polyisocyante showing equilibrium temperature range (ETR) and probable equilibrium temperature.