

Supporting Information

“Solvent Processable and Recyclable Covalent Adaptive Organogels Based on Dynamic Trans-esterification Chemistry: Separation of Toluene from Azeotropic Mixtures”

Suman Debnath, Swaraj Kaushal, Subhankar Mandal, Umaprasana Ojha*

Department of Chemistry, Rajiv Gandhi Institute of Petroleum Technology, Jais, Amethi, UP,
229304, India

E-mail: uojha@rgipt.ac.in

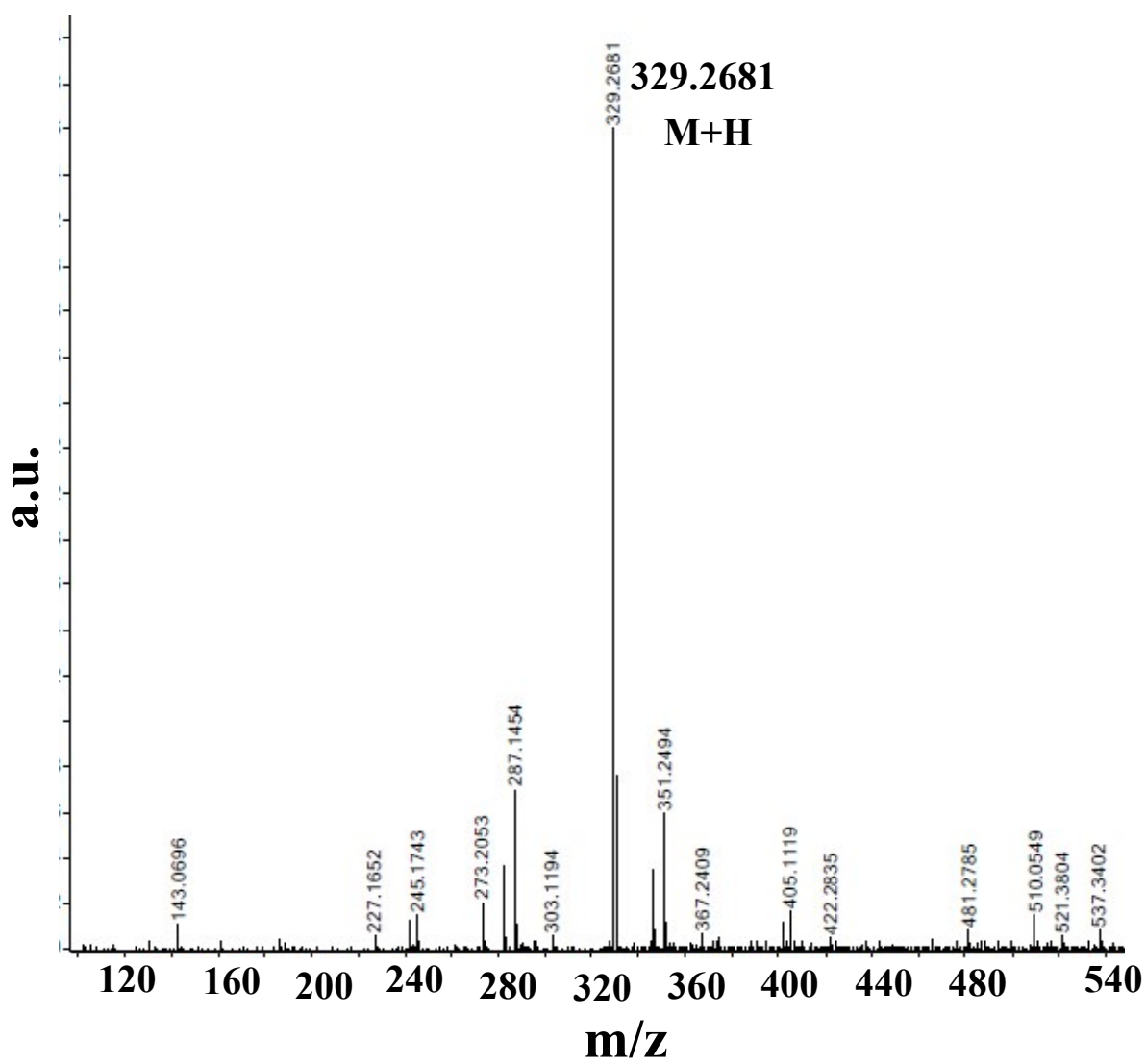


Figure S1: HRMS spectra of the exchange reaction product of BEM with n-hexanol.

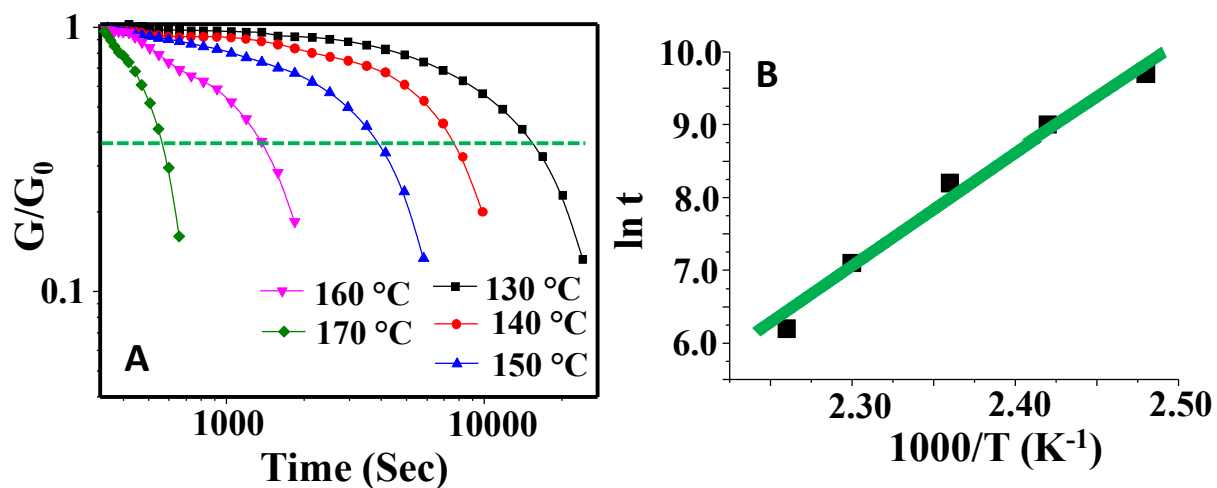


Figure S2: (A) The Stress relaxation plot and (B) Arrhenius plot for TEOC-PTMO-PTE.

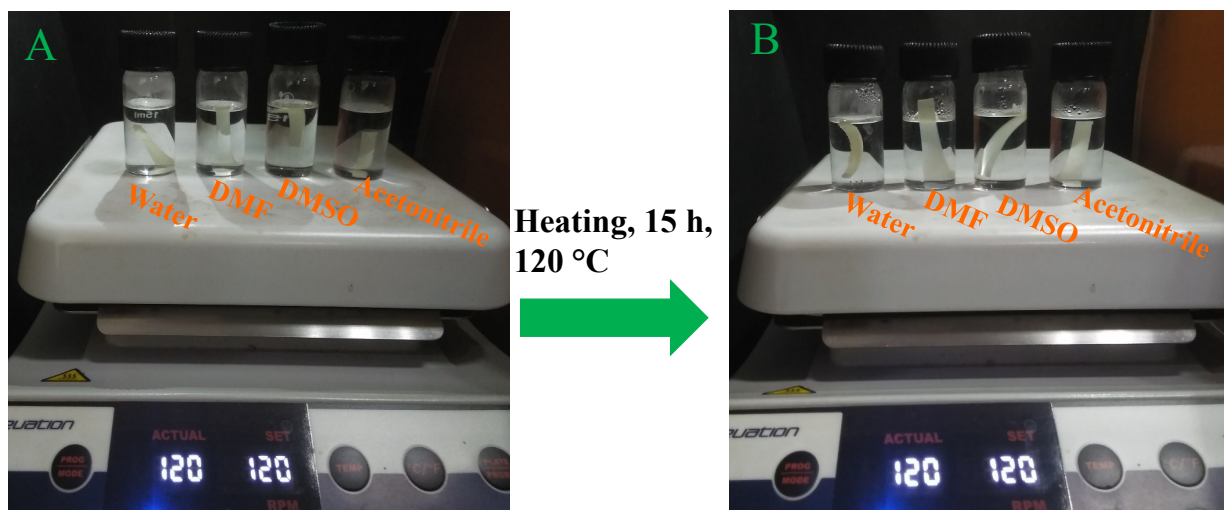


Figure S3: TEOC-PTMO-PTE CAN samples kept in non-alcoholic solvent for heating at 120 °C for 15 h.

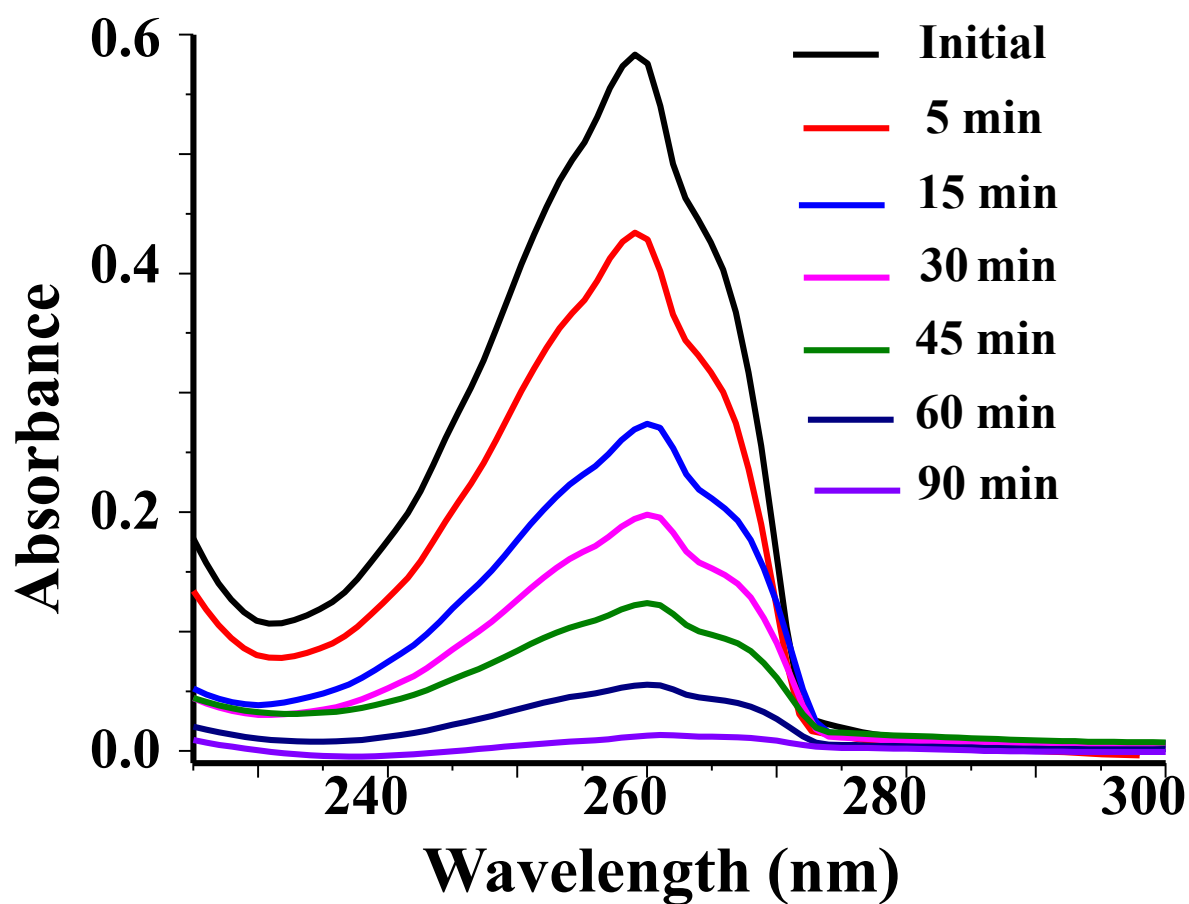


Figure S4: Monitoring the removal of toluene from toluene-methanol-water azeotrope (1.15:0.19:0.06, vol:vol) by TEOC-PTMO-PTE film through UV-Vis spectroscopy.

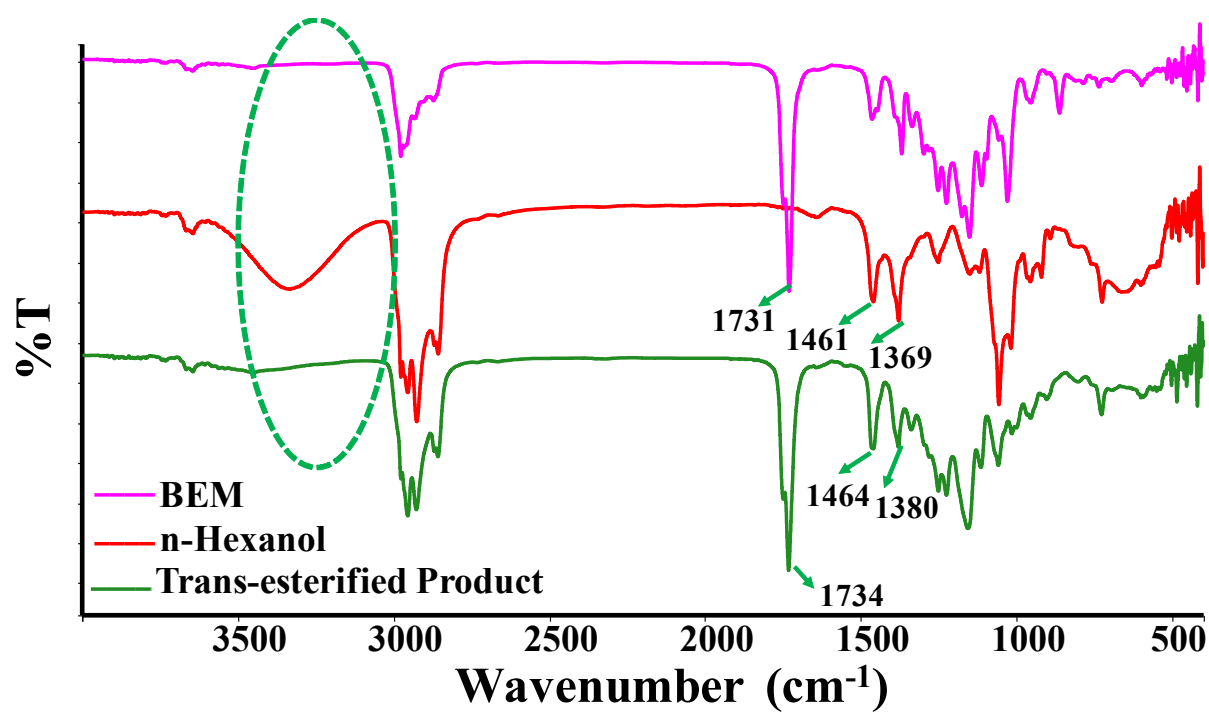


Figure S5: FTIR spectra of BEM, n-hexanol and exchange product of BEM with n-hexanol.

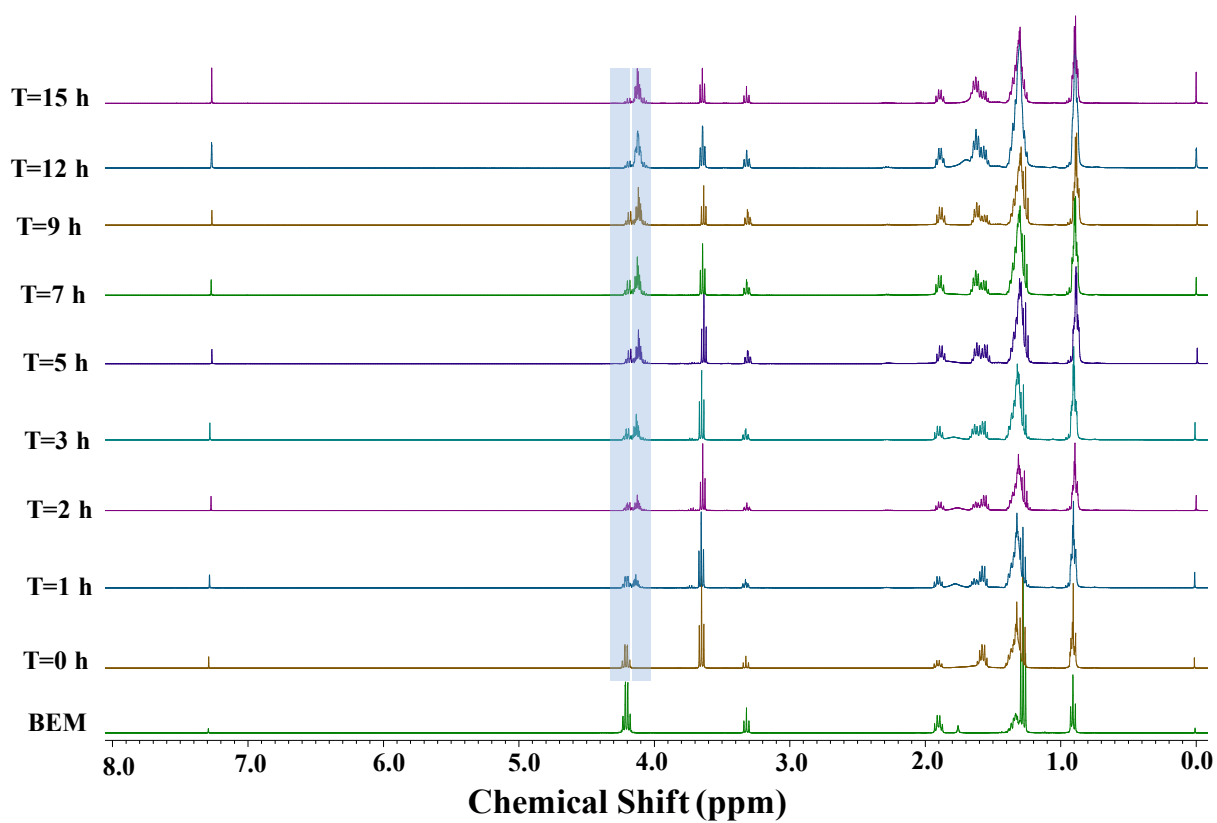


Figure S6: ^1H NMR spectra of BEM & n-hexanol mixture at different time intervals at 130 °C for kinetics study.

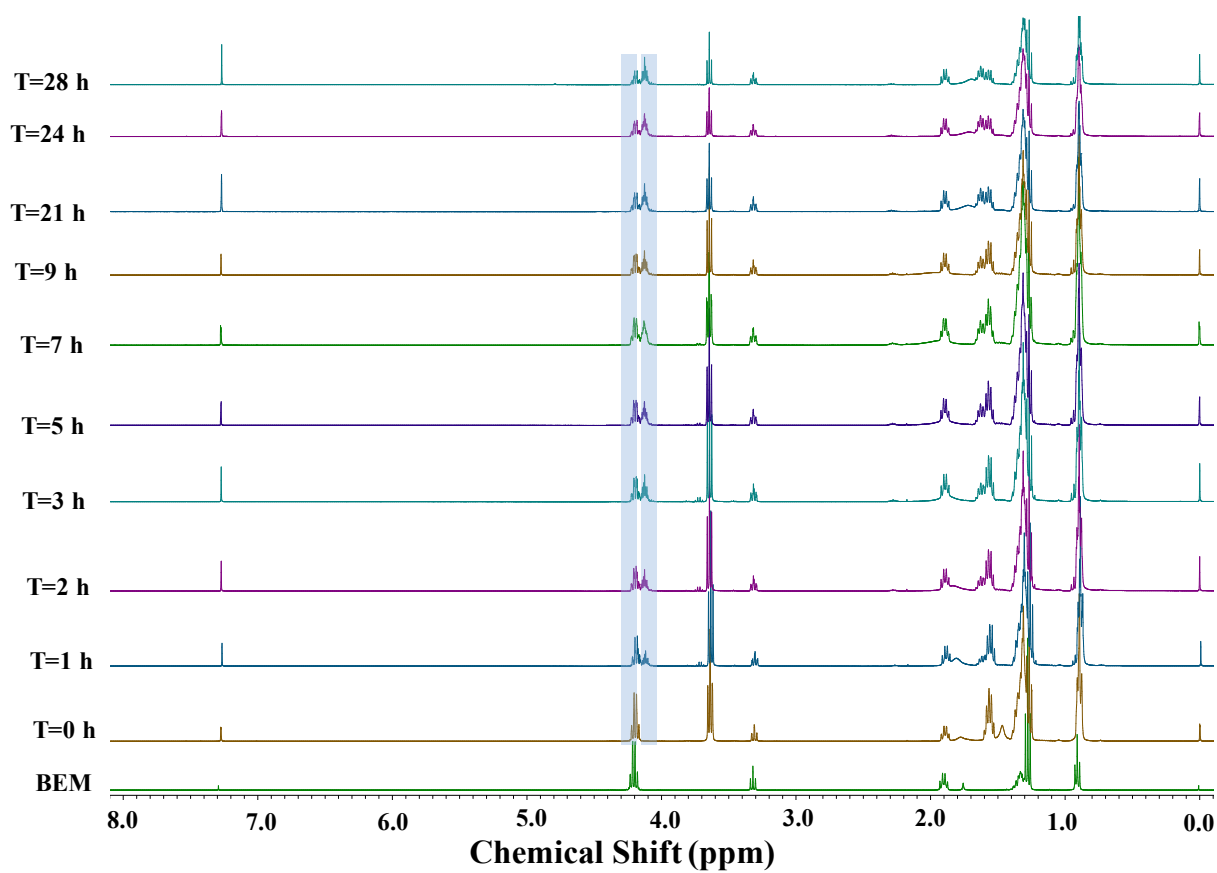


Figure S7: ^1H NMR spectra of BEM & n-Hexanol mixture at different time intervals at 120 °C for kinetics study.

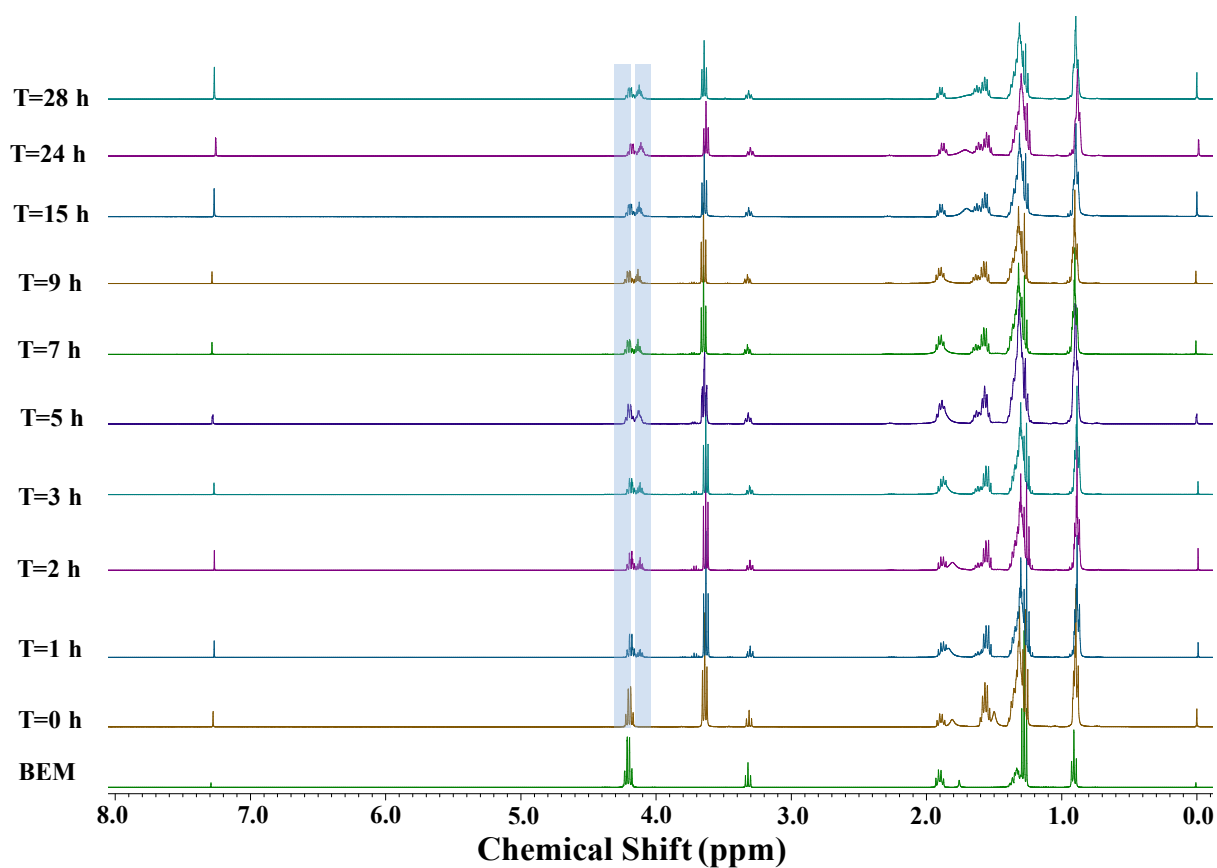


Figure S8: ^1H NMR spectra of BEM & n-Hexanol mixture at different time intervals at 110 °C for kinetics study.

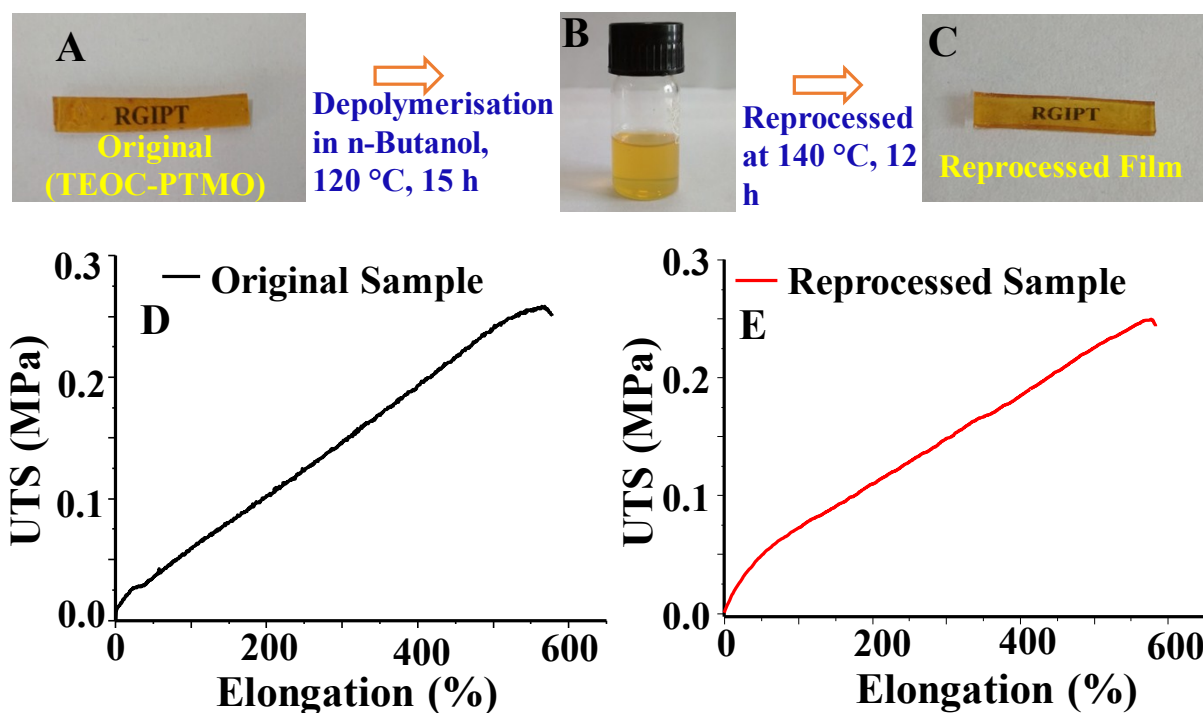


Figure S9: (A) Original sample of TEOC-PTMO, (B) sample after depolymerization, (C) reprocessed sample, (D) tensile data of original and (E) reprocessed sample.

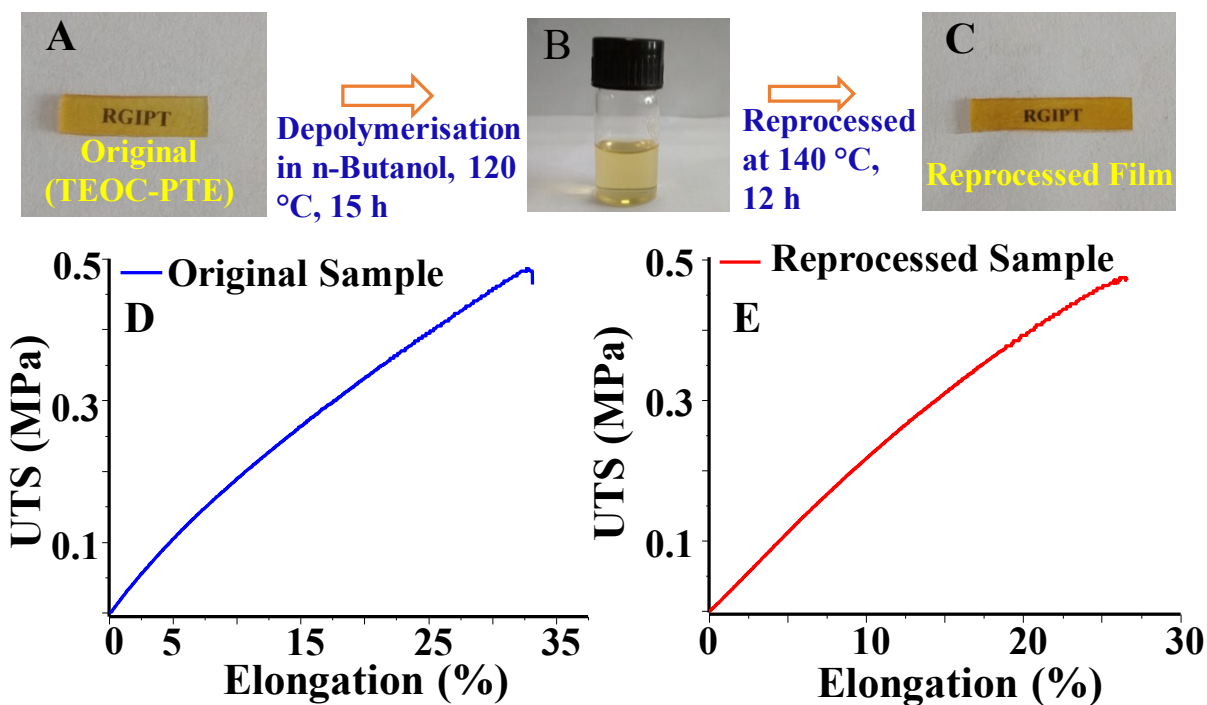


Figure S10: (A) Original sample of TEOC-PTE, (B) sample after depolymerization, (C) reprocessed sample, (D) tensile data of original and (E) reprocessed sample.

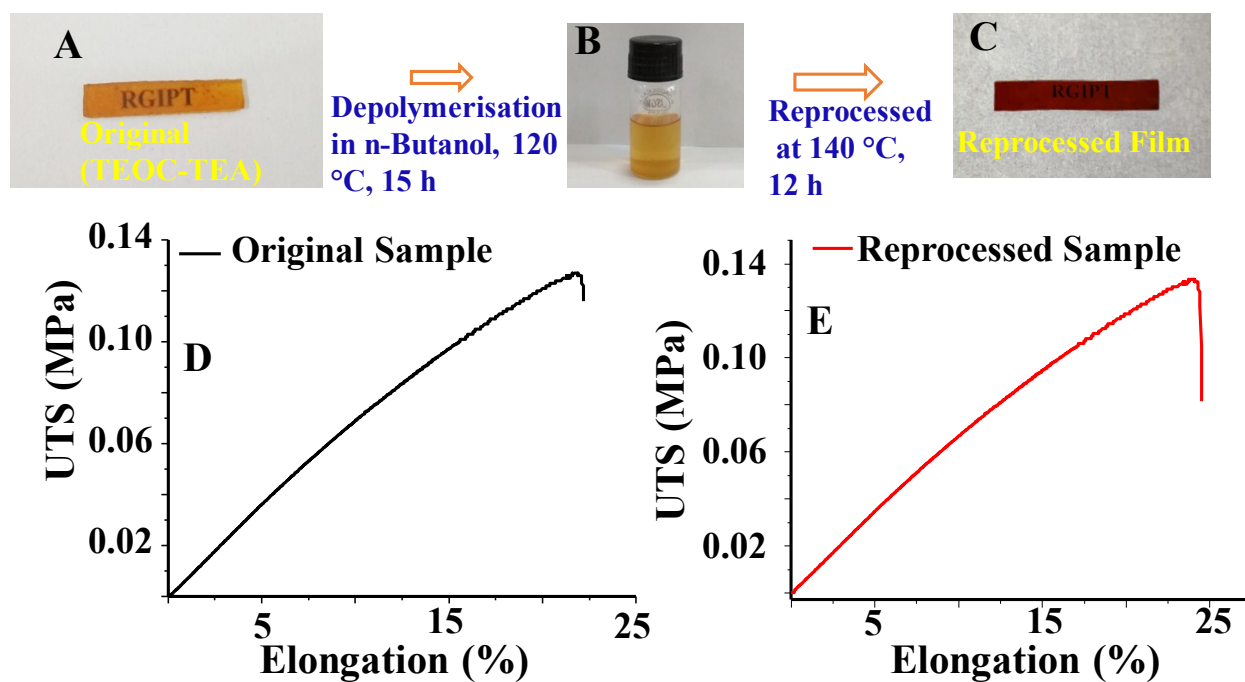


Figure S11: (A) Original sample of TEOC-TEA (B) Sample after depolymerization, (C) reprocessed sample (D) tensile data of original Sample (E) tensile data of reprocessed sample.

Table S1: Molar composition optimization of TEOC and multi-ols in CANs based on their tensile properties

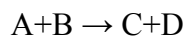
DCNs (Code)	Multi-ol	TEOC (mmol)	Multi-ol (mmol)	UTS (MPa)	ϵ (%)
TEOC-PTE	PTE	4.97	5.96	0.50 ± 0.06	30.0 ± 3.0
TEOC-PTE-1	PTE	4.97	5.46	0.20 ± 0.02	18.0 ± 2.0
TEOC-PTE-2	PTE	4.97	6.46	0.30 ± 0.02	20.0 ± 3.0
TEOC-PTMO-PTE	PTMO/PTE	4.97	6.00	1.10 ± 0.03	283.3 ± 16.0
TEOC-PTMO-PTE-1	PTMO/PTE	4.97	6.23	0.60 ± 0.04	130.0 ± 10.4
TEOC-PTMO-PTE-2	PTMO/PTE	4.97	5.80	0.50 ± 0.03	111.3 ± 9.0

Table S2: Mechanical properties data comparison of original & reprocessed CANs

DCNs	UTS (MPa)	ϵ (%)	E (MPa)
TEOC-PTE (Original)	0.51 ± 0.06	30.0 ± 3.0	1.8 ± 0.04
Reprocessed	0.50 ± 0.05	31.0 ± 3.0	1.8 ± 0.03
TEOC-PTMO (Original)	0.30 ± 0.06	595.0 ± 15.0	0.8 ± 0.01
Reprocessed	0.29 ± 0.04	590.0 ± 9.0	0.7 ± 0.01
TEOC-TEA (Original)	0.14 ± 0.01	23.0 ± 2.2	1.1 ± 0.01
Reprocessed	0.12 ± 0.01	20.0 ± 2.0	1.0 ± 0.01
TEOC-PTMO-PTE (Original)	1.12 ± 0.03	301.3 ± 22.0	0.7 ± 0.03
Reprocessed	1.01 ± 0.02	289.0 ± 20.0	0.6 ± 0.02

Calculations:

We calculated activation energy for 2nd order reaction:



The activation energy was calculated at three different temperatures (413, 403, 393 and 383

°K). The expression for half-life ($t_{1/2}$) is as followed.

By following the 2nd order reaction kinetics;

$$t_{1/2} = \frac{1}{k[A_0]} \dots\dots\dots (\text{Eq. S1})$$

Where k = rate constant of the reaction

$[A_0]$ = initial concentration of the reactant.

The rate constant was obtained by using above equation and the activation energy was obtained.

We know from the Arrhenius Equation

$$k = A e^{-E_a/RT} \dots\dots\dots (\text{Eq S2})$$

Where E_a is activation energy of the reaction,

R = Gas constant in J / mol. °K

T = temperature in °K

A = Arrhenius constant

Slope = E_a/R provides the activation energy