Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Hydrophobic functional liquids based on trioctylphosphine oxide (TOPO) and carboxylic acids

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1. NMR physical characterisation starting materials (checking purity)

1.1. TOPO

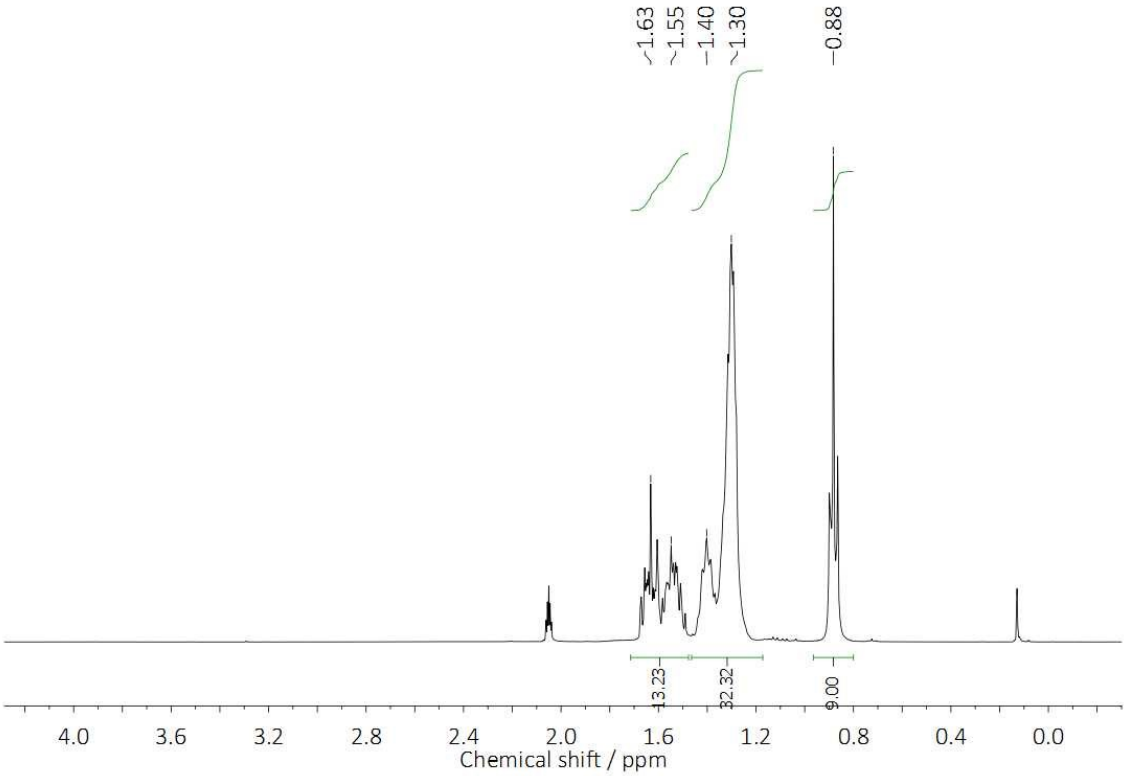

Figure S1. ^{1}H spectrum of TOPO used for physical characterisation experiments. NMR solvent: d_6-acetone

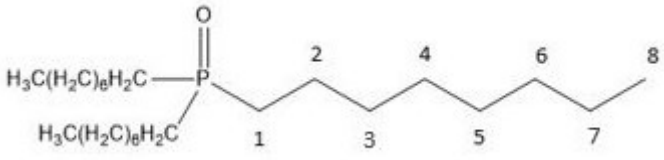

Figure S2. ^{1}H assignment of TOPO peaks

Table S1. ^{1}H assignment of TOPO peaks

^{1}H δ / ppm	Multiplicity	Assignment
0.88	Triplet	8
1.30	Multiplet[b]	5-7
1.40	Multiplet[b]	3-4
1.55	Multiplet[b]	2
1.63	Multiplet[b]	1

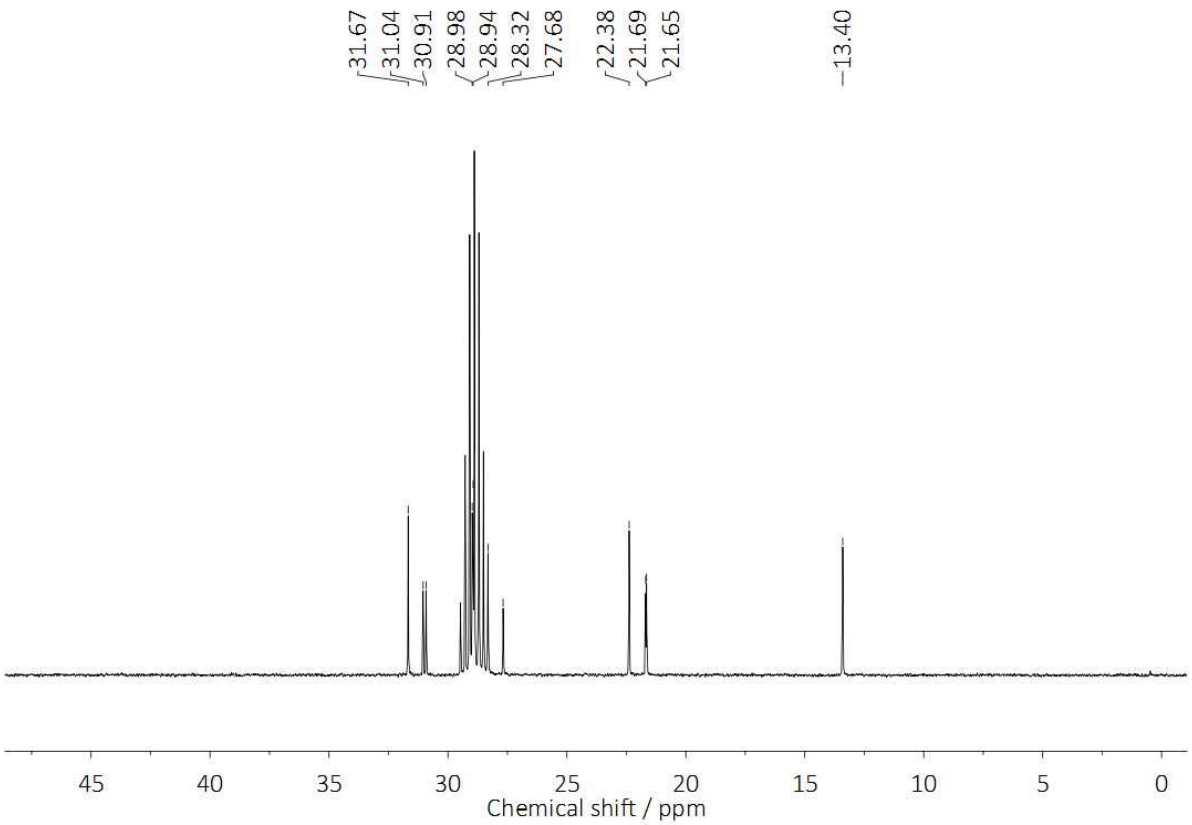

Figure S3. ^{13}C spectrum of TOPO used for physical characterisation experiments. NMR solvent: d_6-acetone

Table S2. ^{13}C assignment of TOPO peaks

^{13}C δ / ppm	Assignment
13.40	8
21.65	3
21.69	
22.38	7
27.68	1
28.32	
28.94	6
28.98	5
30.91	2
31.04	
31.67	4

1.2. Levulinic acid

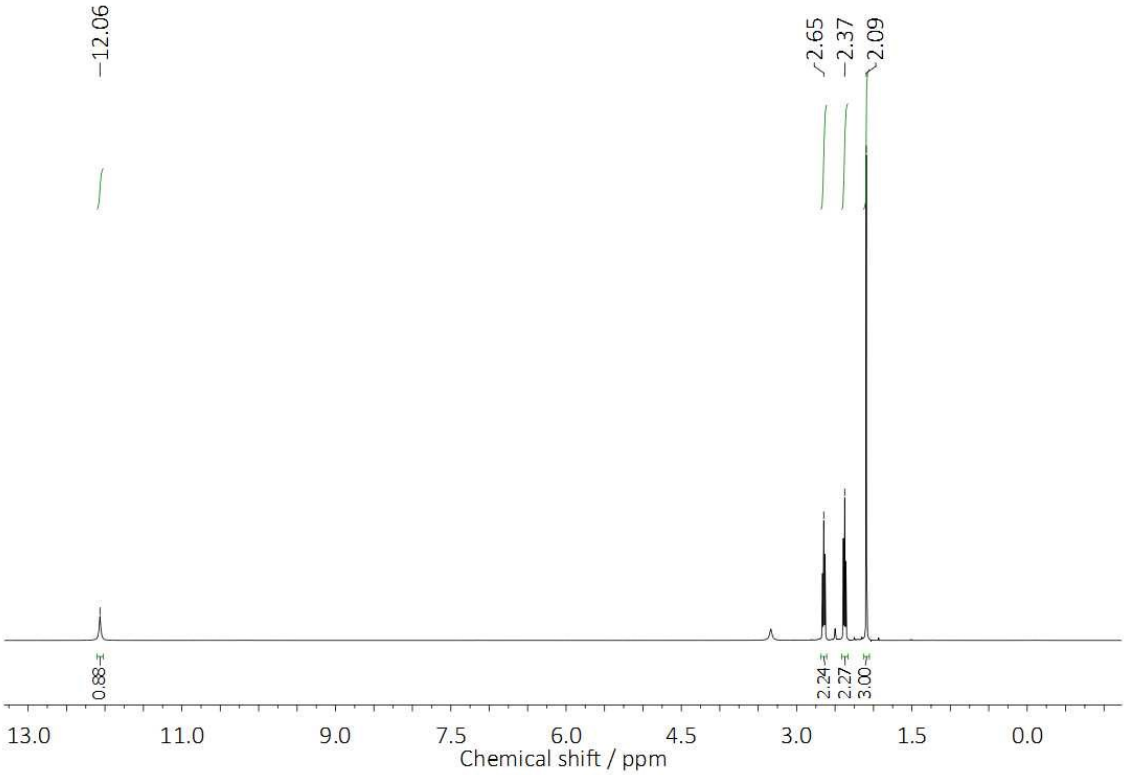

Figure S4. ^{1}H spectrum of levulinic acid used for physical characterisation experiments. NMR solvent: d_6-DMSO

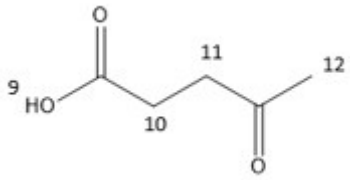

Figure S5. ^{1}H Assignment of levulinic acid

Table S3. ^{1}H assignment of levulinic acid

^{1}H δ / ppm	Multiplicity	Assignment
2.09	Singlet	12
2.37	Triplet	10
2.65	Triplet	11
12.06	Singlet	9

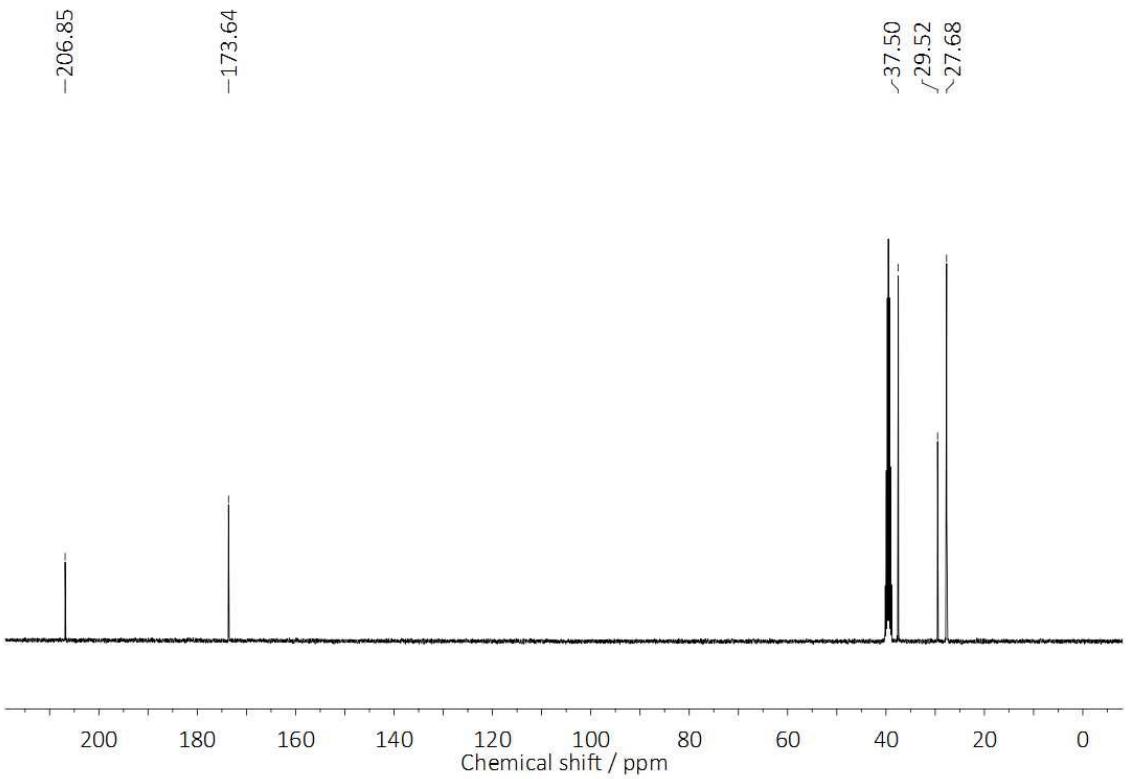

Figure S6. ^{13}C spectrum of levulinic acid used for physical characterisation experiments. NMR solvent: d_6-DMSO

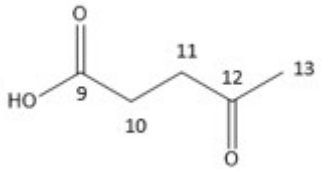

Figure S7. ^{13}C assignment of levulinic acid

Table S4. ^{13}C assignment of levulinic acid

^{13}C δ / ppm	Assignment
27.68	10
29.52	13
37.50	11
173.64	9
206.85	12

1.3. Malonic acid

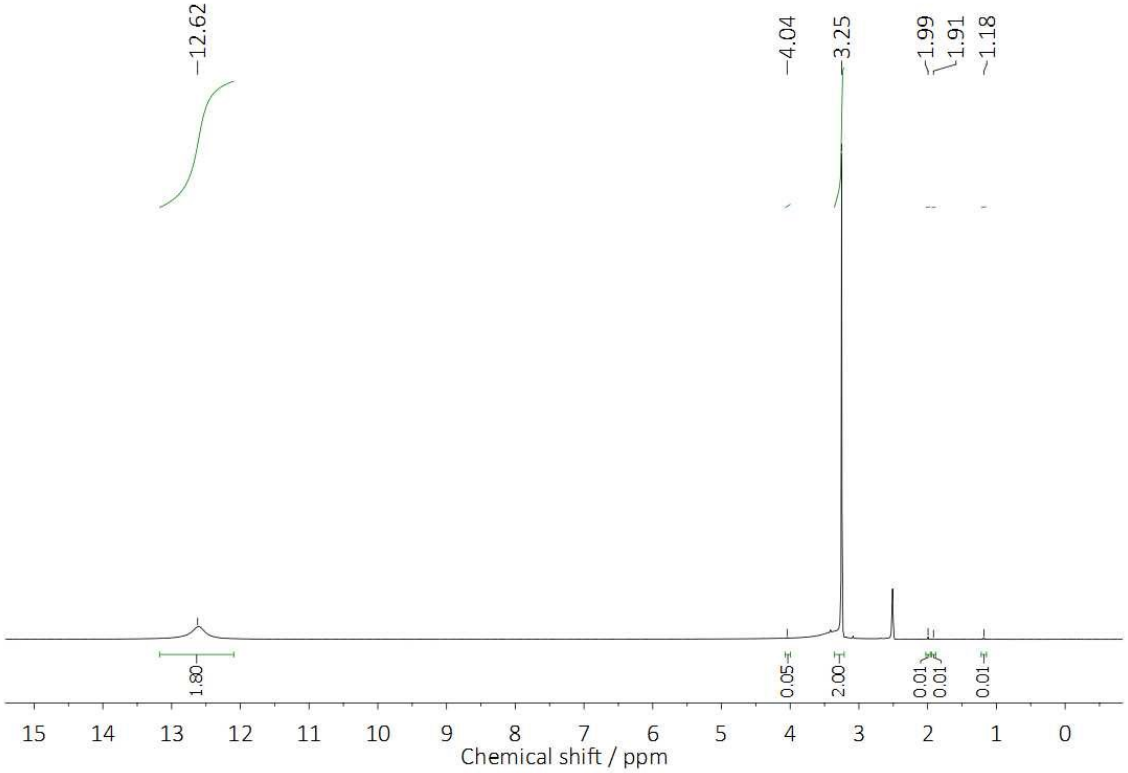

Figure S8. ^{1}H spectrum of malonic acid used for physical characterisation experiments. NMR solvent: d_6-DMSO. Purity >99.5%. Ethyl acetate impurity: 0.28% (0.33 mol%). Acetic acid impurity: 0.19% (0.33 mol%)

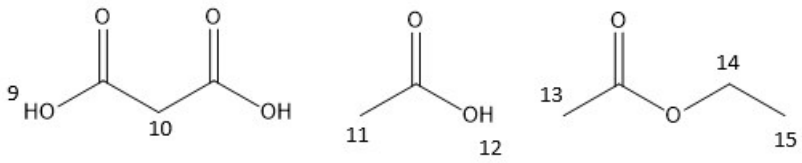

Figure S9. Malonic acid, acetic acid and ethyl acetate ^{1}H assignment

Table S5. ^{1}H assignment of malonic acid with trace acetic acid and ethyl acetate impurities

^{1}H δ / ppm	Multiplicity	Assignment
1.18	Triplet	15
1.91	Singlet	13
1.99	Singlet	11
3.25	Singlet	10
4.04	Quartet	14
12.62	singlet	9,12

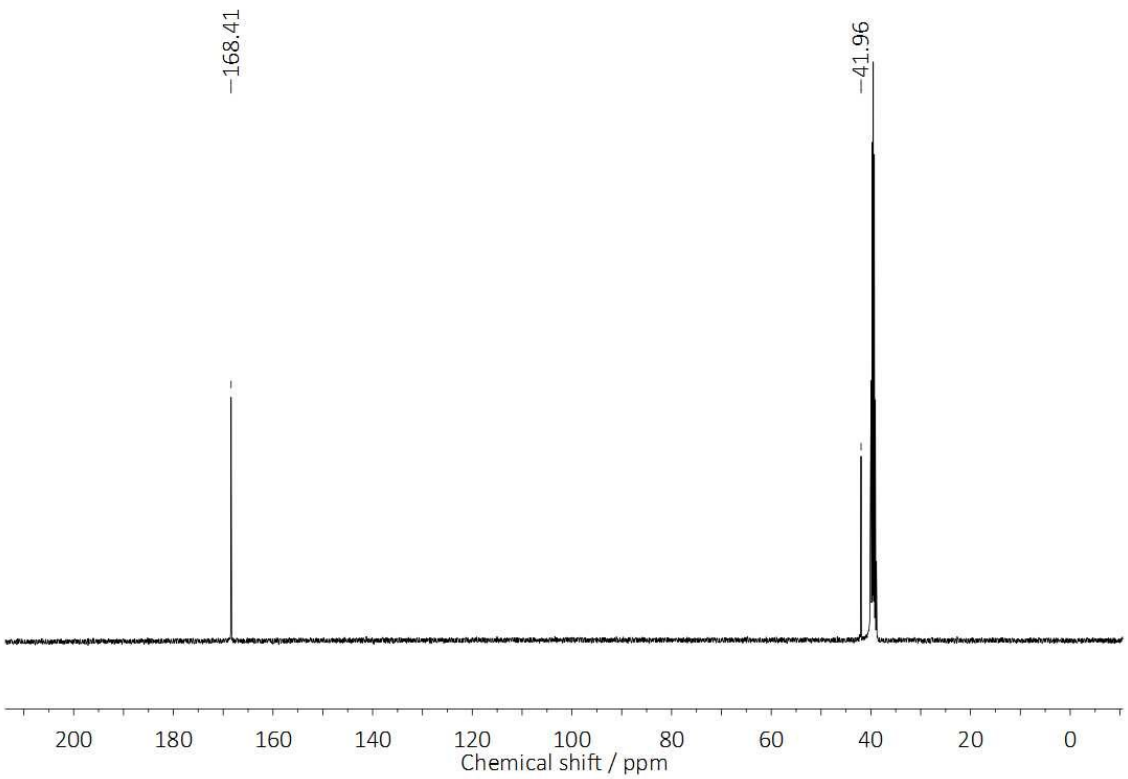

Figure S10. ^{13}C spectrum of malonic acid used for physical characterisation experiments. NMR solvent: d_6-DMSO

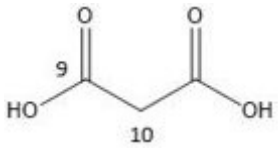

Figure S11. Malonic acid ^{13}C assignment

2. Leaching study FT-IR calibration curve

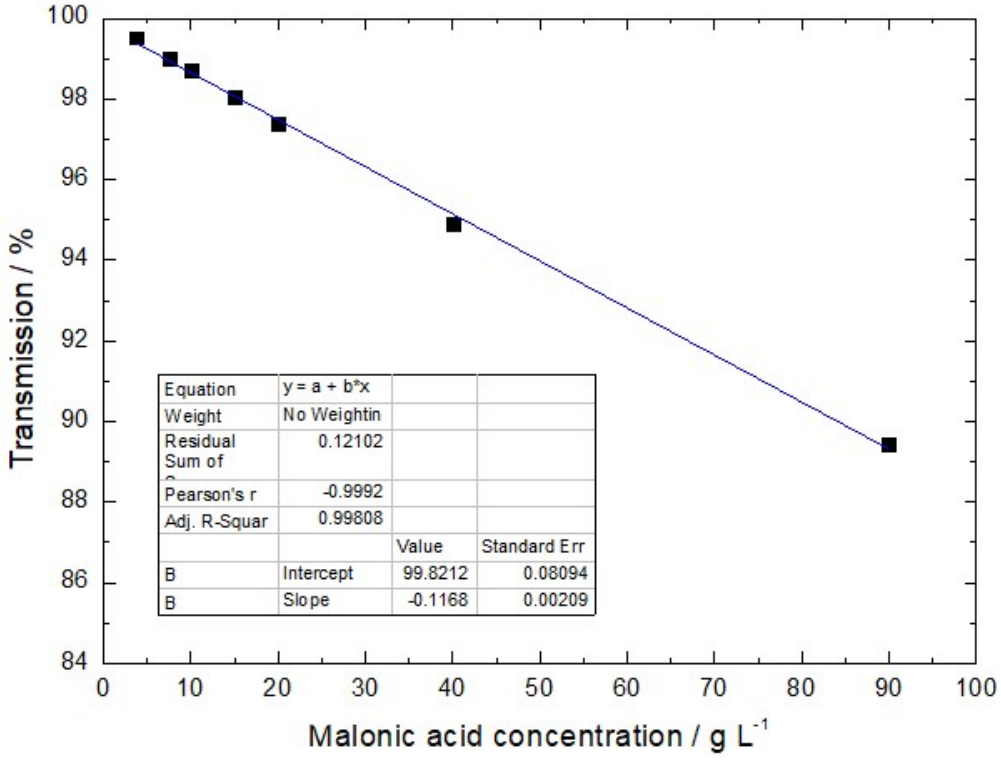

Figure S12. Calibration curve used in leaching studies showing FT-IR transmission as a function of malonic acid concentration. Malonic acid dissolved in de-ionised water at concentrations 3.8-90 g L^{-1}

3. TGA physical characterisation starting materials (checking dryness)

3.1. TOPO

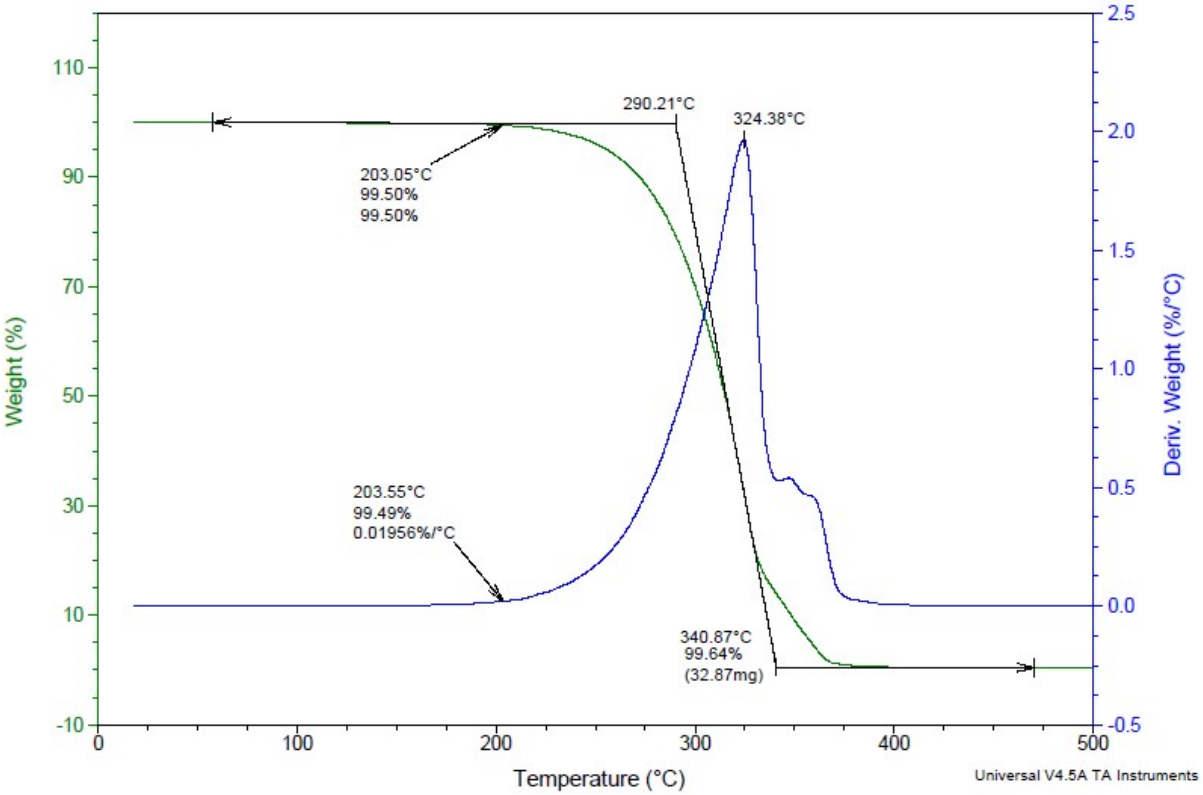

Figure S13. TGA of TOPO under dynamic heating regime (10 °C min^{-1})

3.2. Levulinic acid

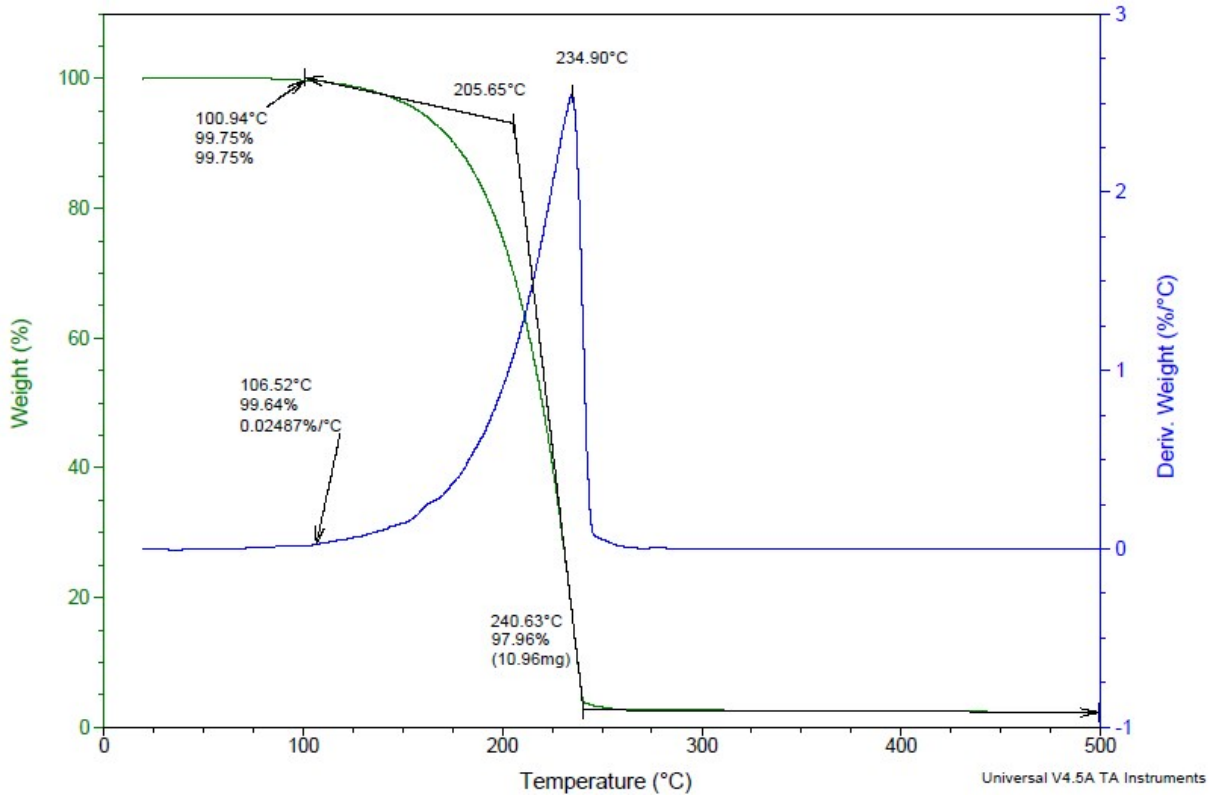

Figure S14. TGA of levulinic acid under dynamic heating regime (10 °C min^{-1})

3.3. Malonic acid

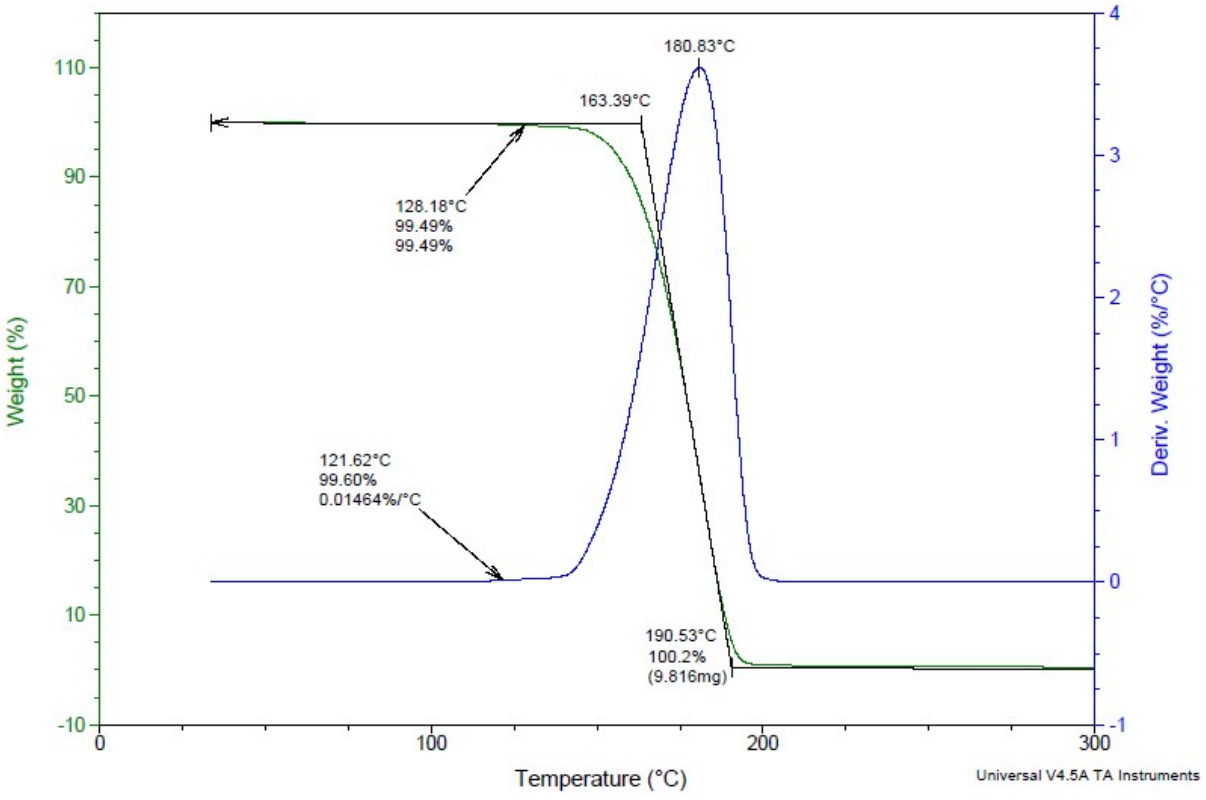

Figure S15. TGA of malonic acid under dynamic heating regime (10 °C min^{-1})

4. Thermal behaviour

4.1. Isothermal TGA TOPO:Malonic acid at 90 °C

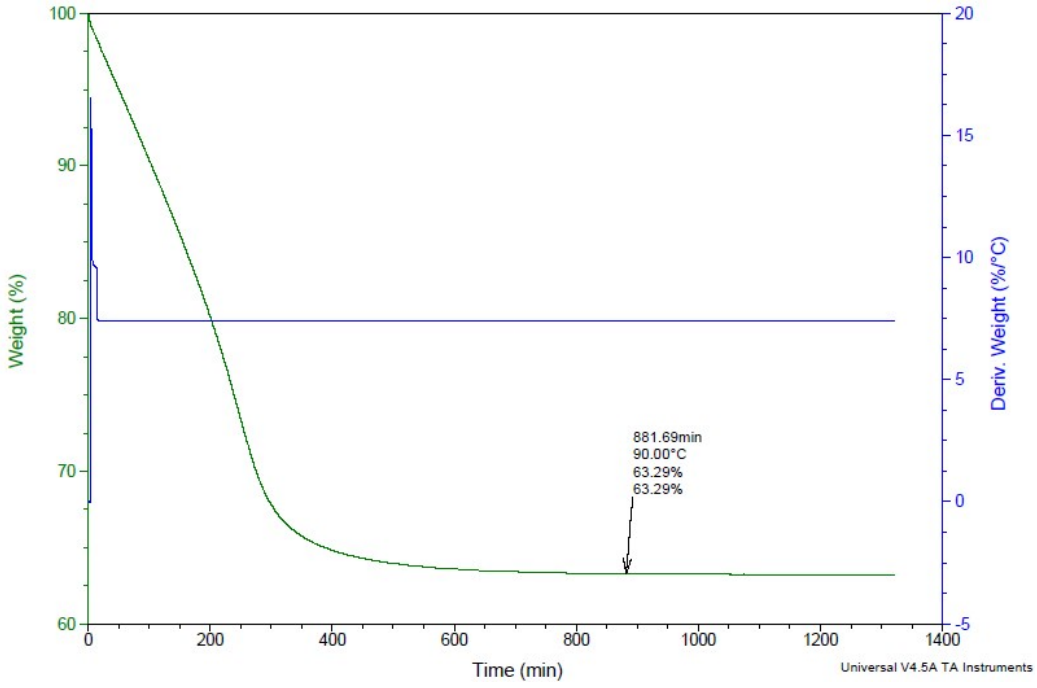

Figure S16. χ_{TOPO} = 0.33 TOPO:malonic acid held isothermally at 90 °C. Blue line = temperature derivative.

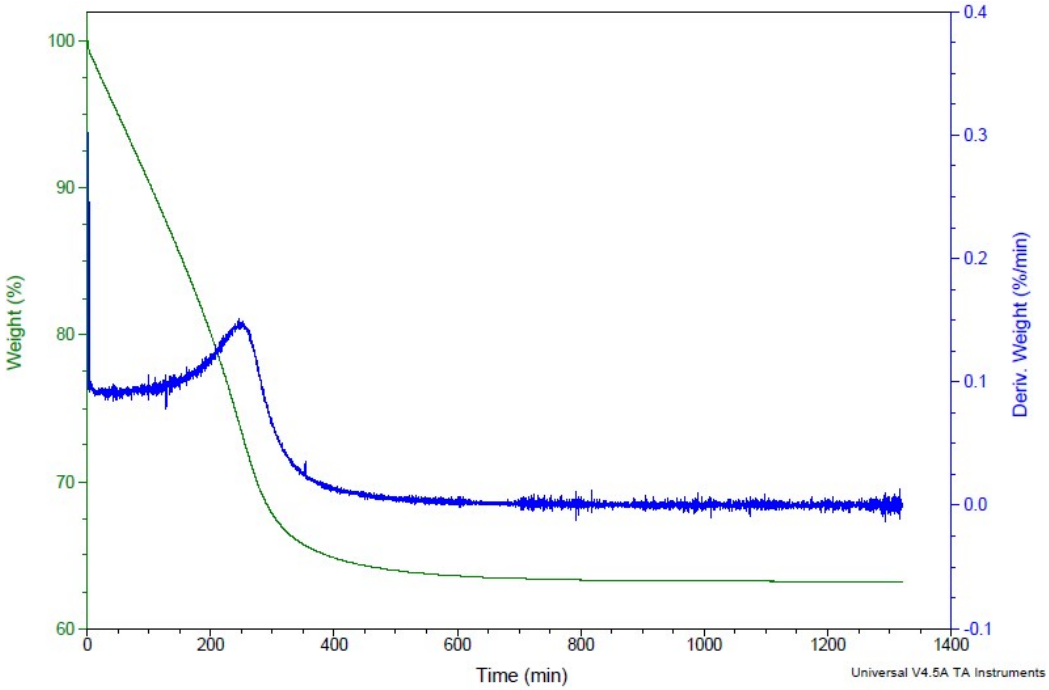

Figure S17. χ_{TOPO} = 0.33 TOPO:malonic acid held isothermally at 90 °C. Blue line = time derivative.

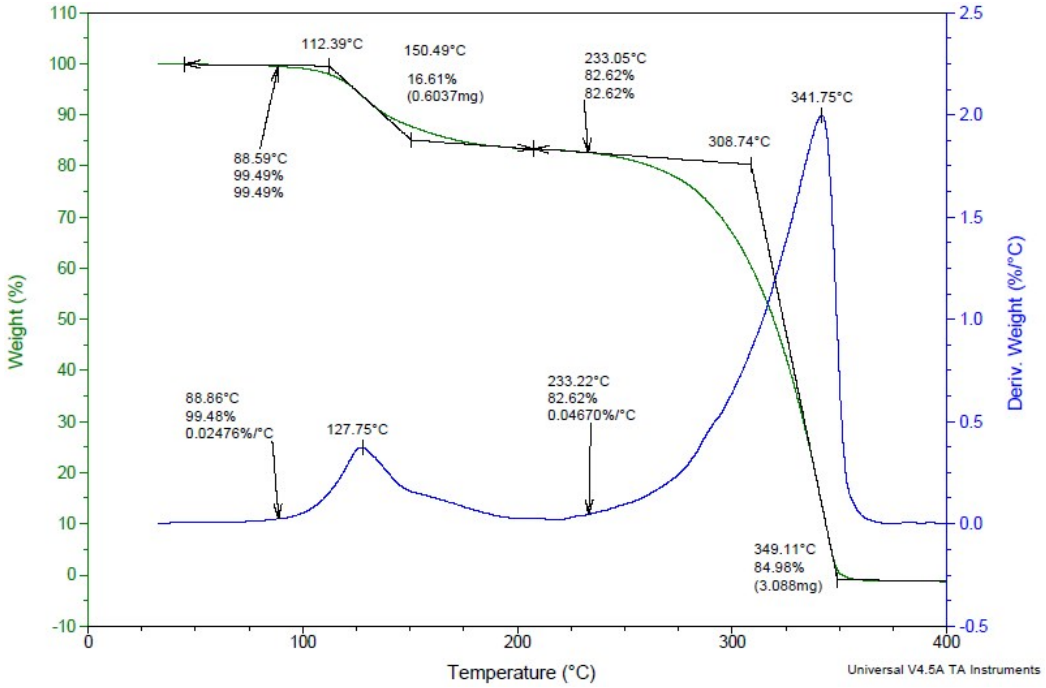

Figure S18. χ_{TOPO} = 0.60 TOPO:malonic acid. Heating rate 10 °C min^{-1}. Shows two stage decomposition with well resolved peaks.

4.2. Evolved gas analysis TOPO:malonic acid at 90 °C

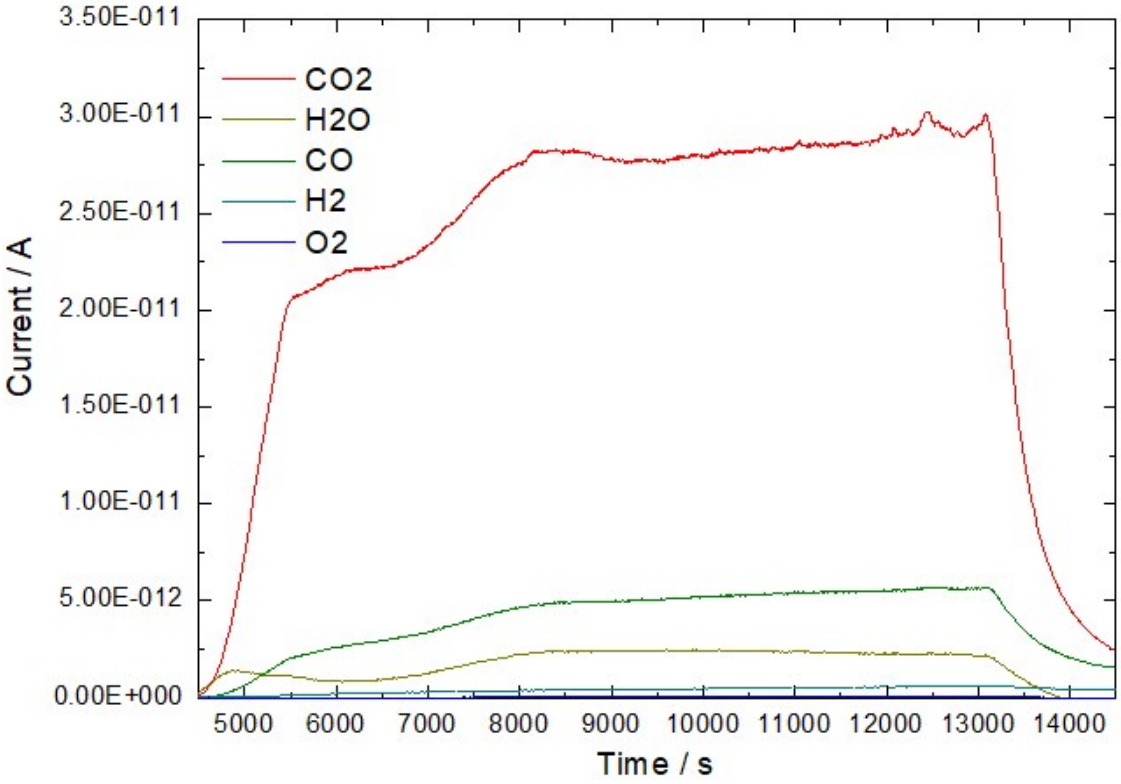

Figure S19. *In situ* GC-MS evolved gas analysis of χ_{TOPO} = 0.33 TOPO:malonic acid held at isothermally 90 °C

4.3. ^{13}C analysis of the TOPO:malonic acid liquid phase before/after decomposition

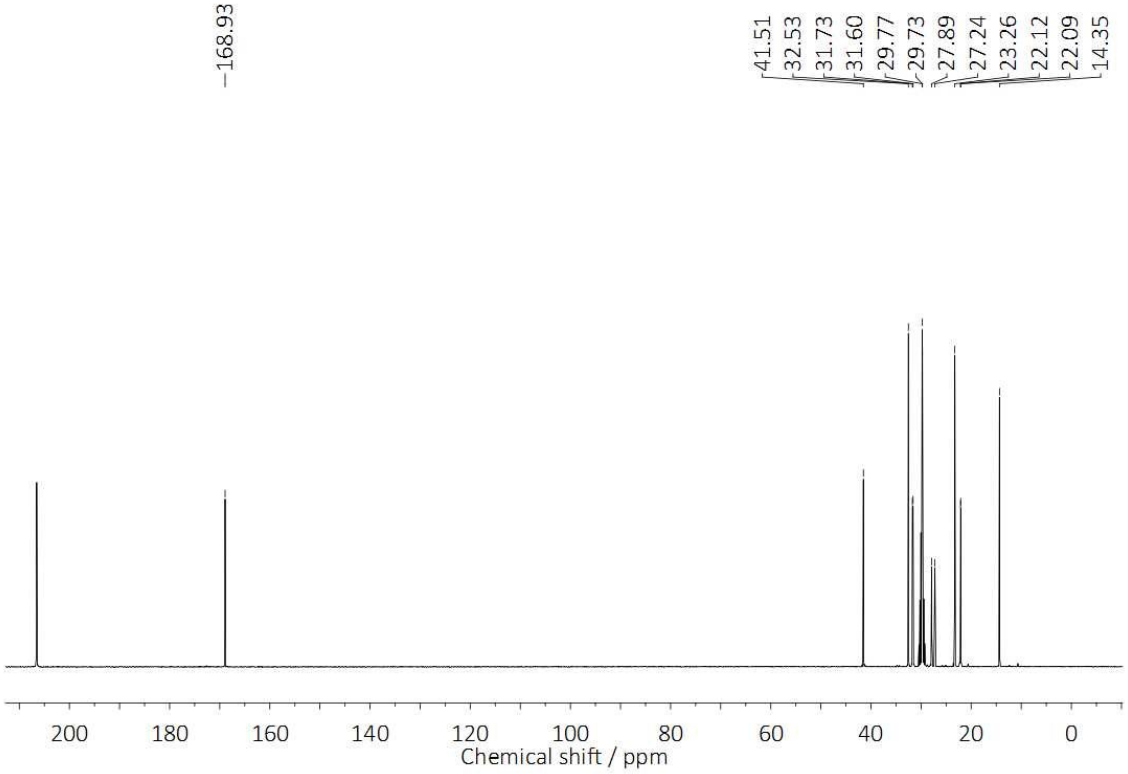

Figure S20. ^{13}C NMR spectrum of χ_{TOPO} = 0.33 TOPO:malonic acid before held isothermally at 90 C. NMR solvent: d_6-acetone

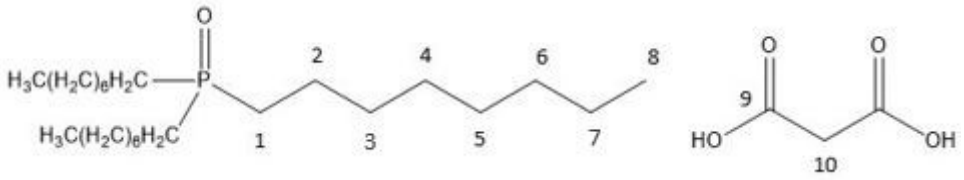

Figure S21. ^{13}C NMR peak assignment χ_{TOPO} = 0.33 TOPO:malonic acid before held isothermally at 90 °C

Table S6. ^{13}C peak assignment χ_{TOPO} = 0.33 TOPO:malonic acid before decomposition, d_6-acetone. TOPO peaks in agreement with literature (d^3-acetonitrile)[1]

^{13}C δ / ppm	Assignment
14.35	8
22.09	3
22.12	
23.26	7
27.24	1
27.89	
29.73	6
29.77	5
31.60	2
31.73	
32.53	4
41.51	10
168.93	9

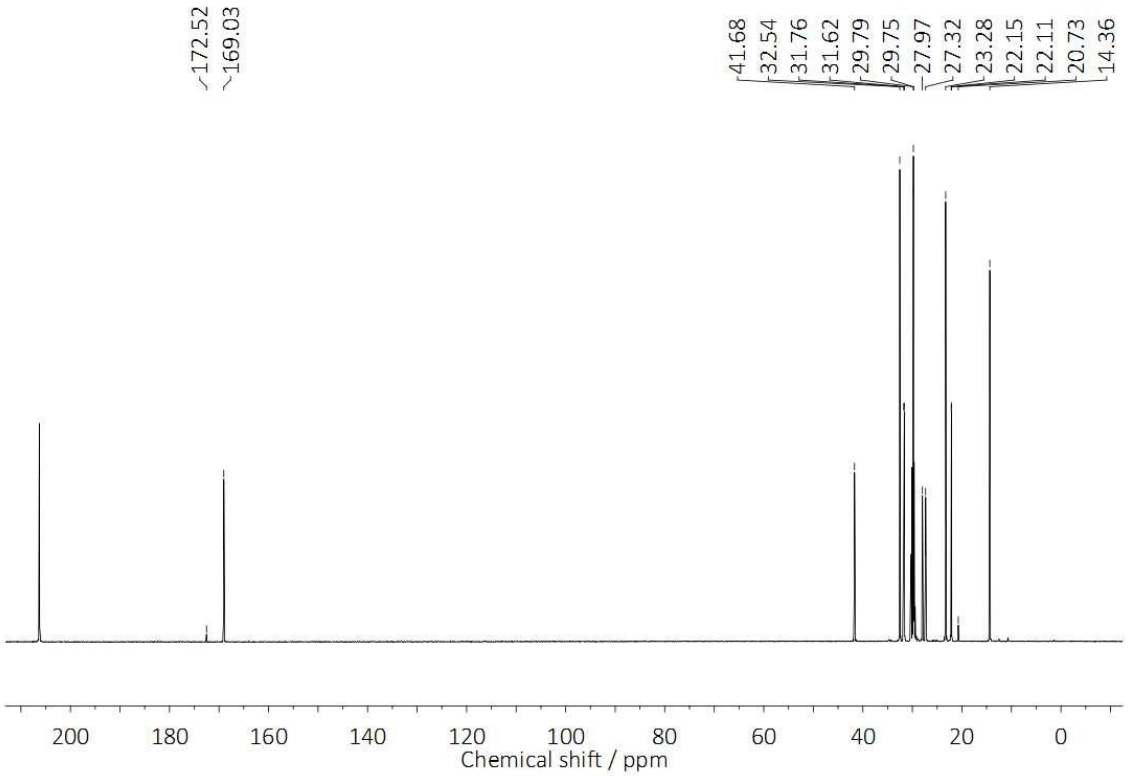

Figure S22. ^{13}C NMR spectrum of χ_{TOPO} = 0.33 TOPO:malonic acid after held isothermally at 90 °C. NMR solvent: d_6-acetone

Figure S23. ^{13}C NMR peak assignment χ_{TOPO} = 0.33 TOPO:malonic acid after held isothermally at 90 °C. Acetic acid also assigned. NMR solvent: d_6-acetone

Table S7.[13]C peak assignment χ_{TOPO} = 0.33 TOPO:malonic acid after held isothermally at 90 °C. NMR solvent: d_6-acetone. Acetic acid present. TOPO peaks in agreement with literature (d_3-acetonitrile)[1]

^{13}C δ / ppm	Assignment
14.36	8
20.73	11
22.11	3
22.15	
23.28	7
27.32	1
27.97	
29.75	6
29.79	5
31.62	2
31.76	
32.54	4
41.68	10
169.03	9
172.52	12

4.4. Sublimation and deposition of malonic acid from bulk of the mixture

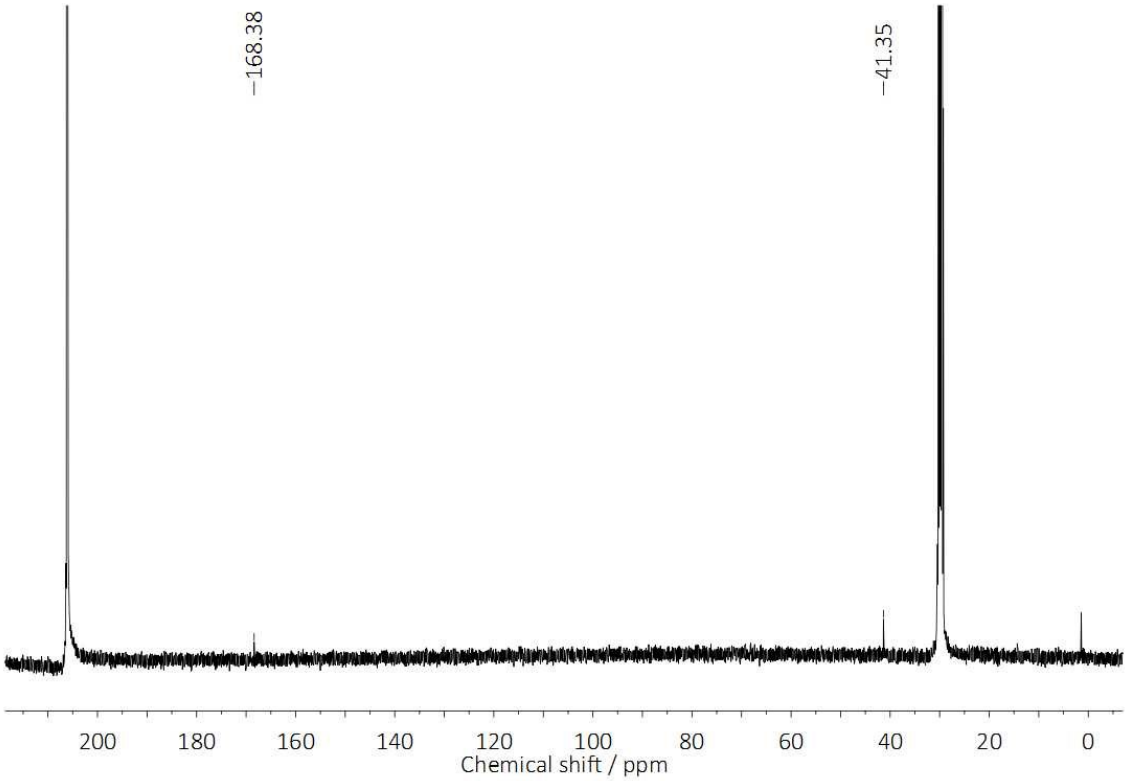

Figure S24.[13]C NMR spectrum of malonic acid sublimed from χ_{TOPO} = 0.33 TOPO:malonic acid held at 90 °C. NMR solvent: d_6-acetone

Table S8. ^{13}C peak assignment of malonic acid sublimed from χ_{TOPO} = 0.33 TOPO:malonic acid held isothermally at 90 °C. NMR solvent: d_6-acetone.

^{13}C δ / ppm	Assignment
41.35	10
168.38	9

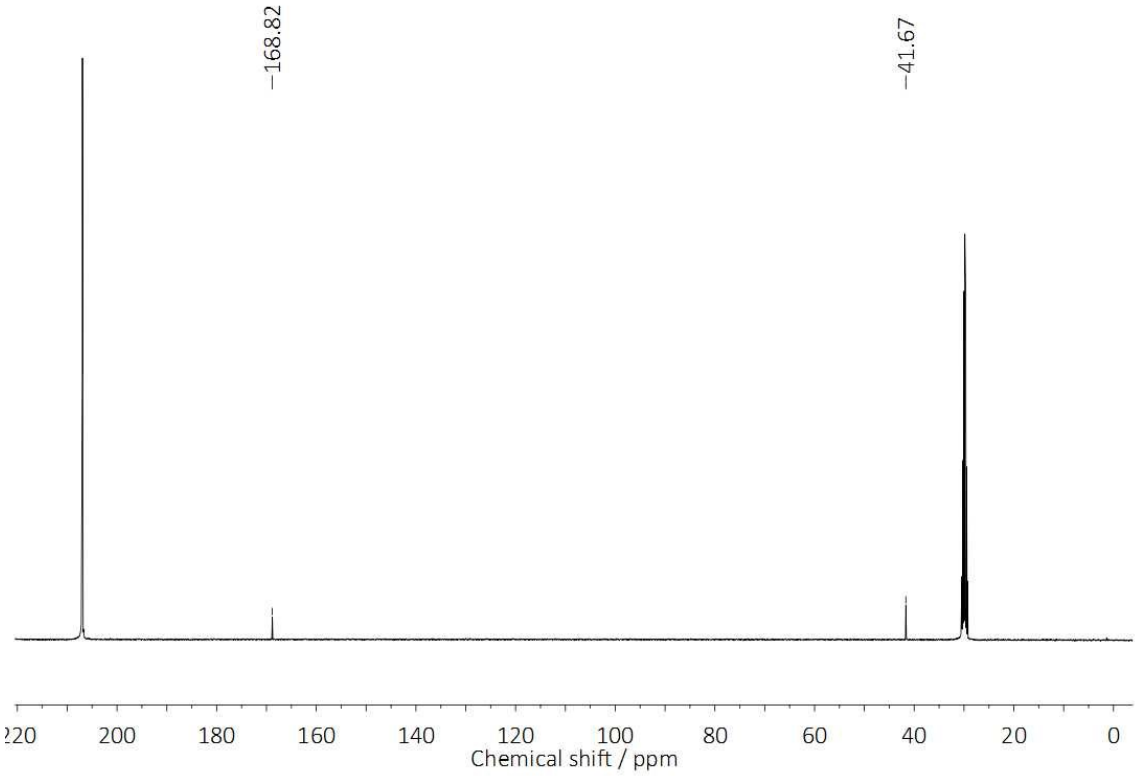

Figure S25. ^{13}C NMR spectrum of malonic acid deposition from χ_{TOPO} = 0.33 TOPO:malonic acid held at 90 °C. NMR solvent: d_6-acetone

Table S9. ^{13}C peak assignment of malonic acid deposited from χ_{TOPO} = 0.33 TOPO:malonic acid held isothermally at 90 °C. NMR solvent: d_6-acetone.

^{13}C δ / ppm	Assignment
41.67	10
168.82	9

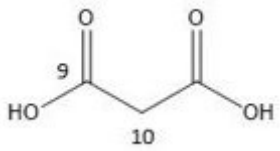

Figure S26.^{13}C NMR peak assignment of malonic acid sublimed and deposited from χ_{TOPO} = 0.33 TOPO:malonic acid held isothermally at 90 °C. NMR solvent: d_6-acetone

4.5. Dynamic heating TGA TOPO:levulinic acid 10 °C min^{-1}

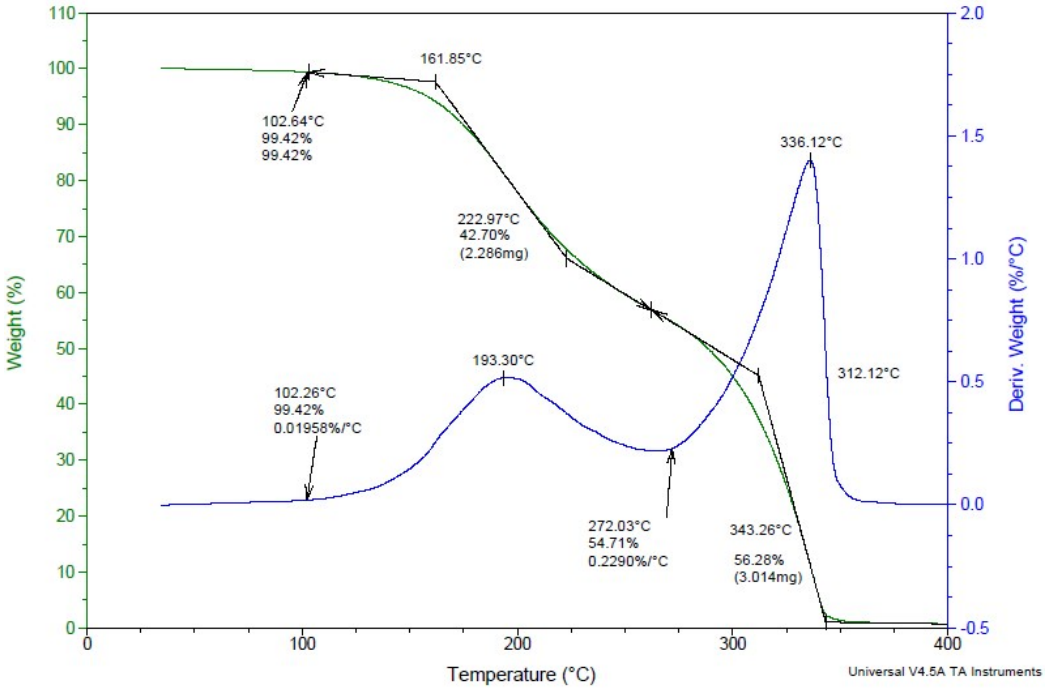

Figure S27. χ_{TOPO} = 0.30 TOPO:levulinic acid. Heating rate 10 °C min^{-1}. Shows two stage decomposition.

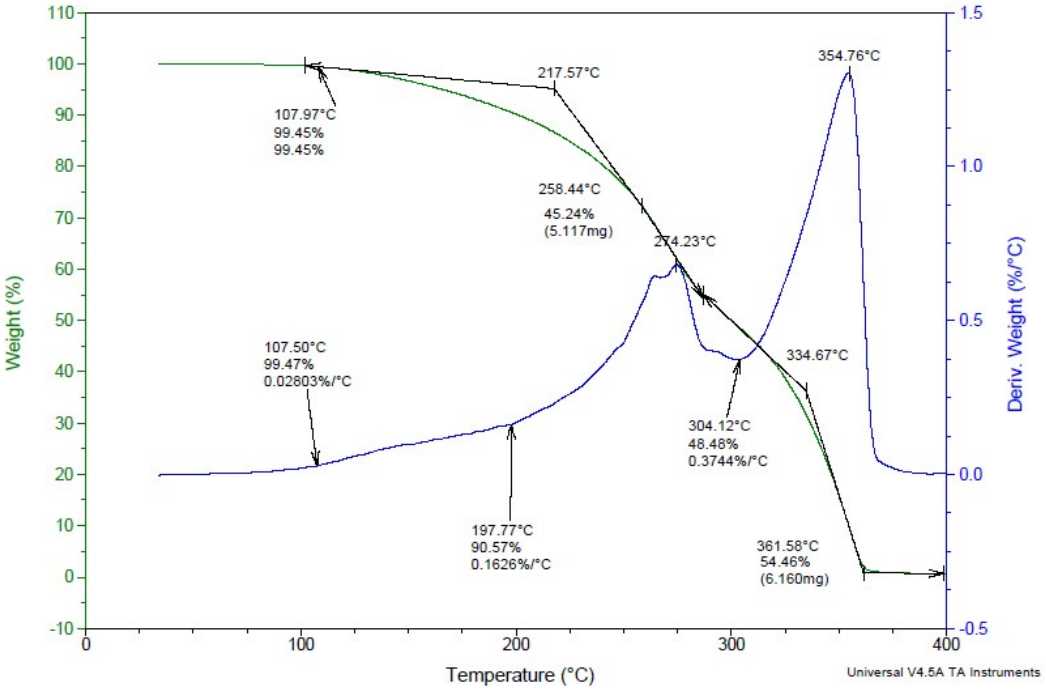

Figure S28. χ_{TOPO} = 0.40 TOPO:levulinic acid. Heating rate 10 °C min^{-1}. Shows three stage decomposition.

4.6. Dynamic heating TGA TOPO:Levulinic acid 1 °C min^{-1}

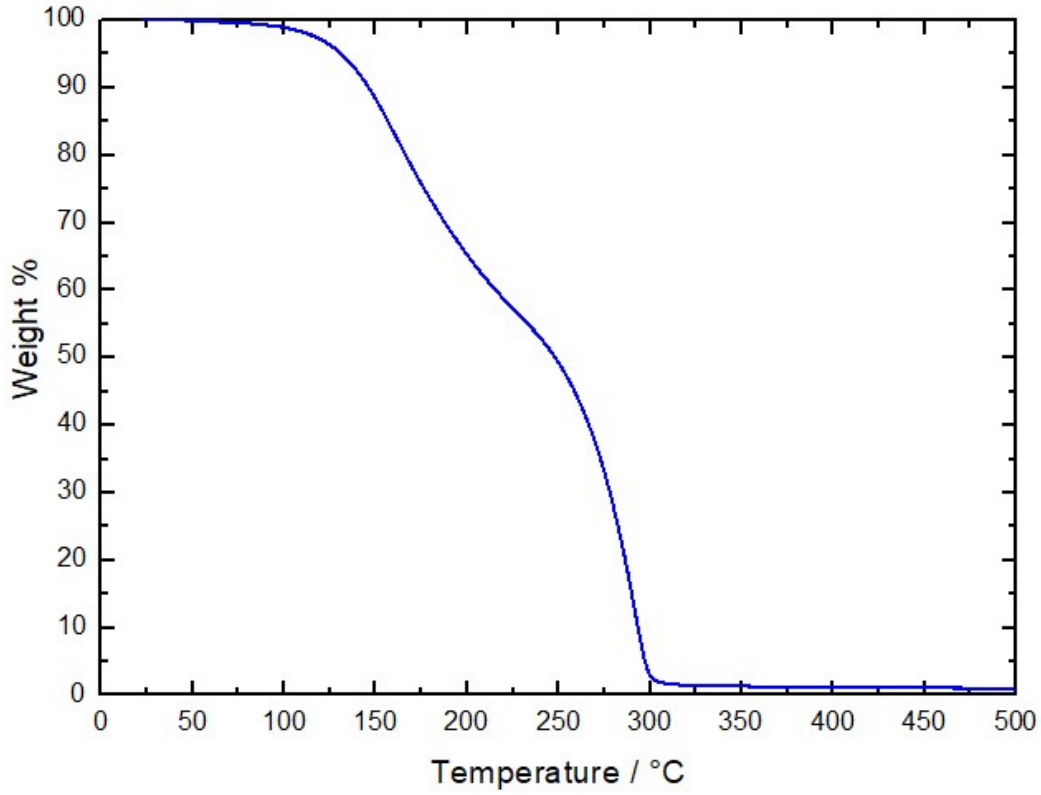

Figure S29. χ_{TOPO} = 0.33 TOPO:levulinic acid. Heating rate 1°C min^{-1}

4.7. Isothermal TGA TOPO:Levulinic acid 90 and 140 °C

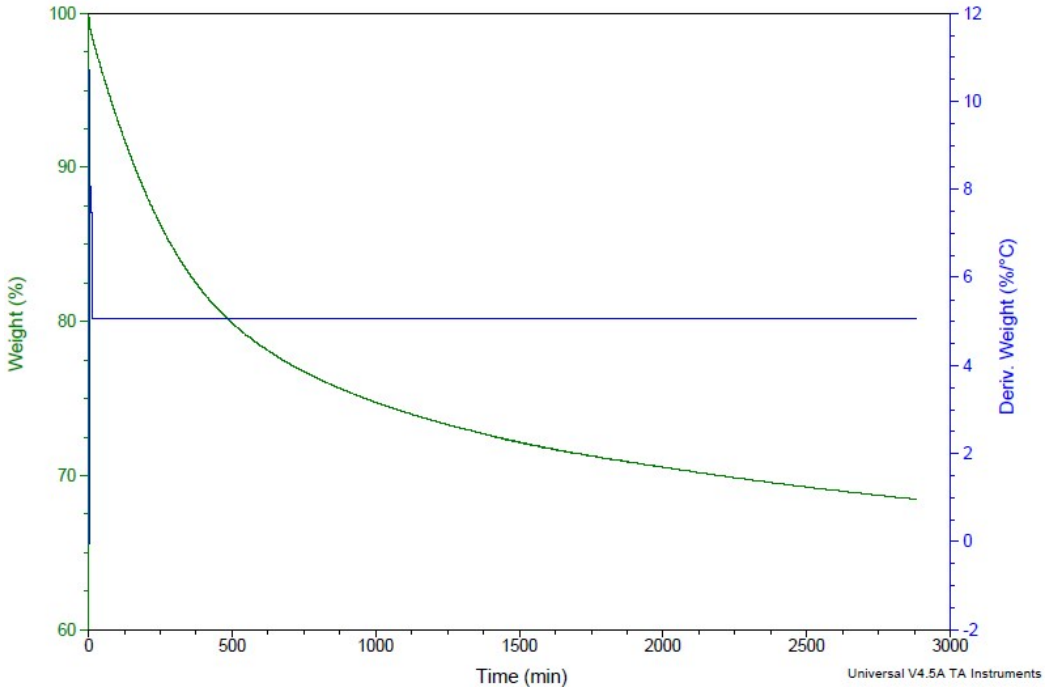

Figure S30. χ_{TOPO} = 0.33 TOPO:levulinic acid held isothermally at 90 °C. Blue line = temperature derivative. Initial ramping rate to isothermal = 50 °C min^{-1}.

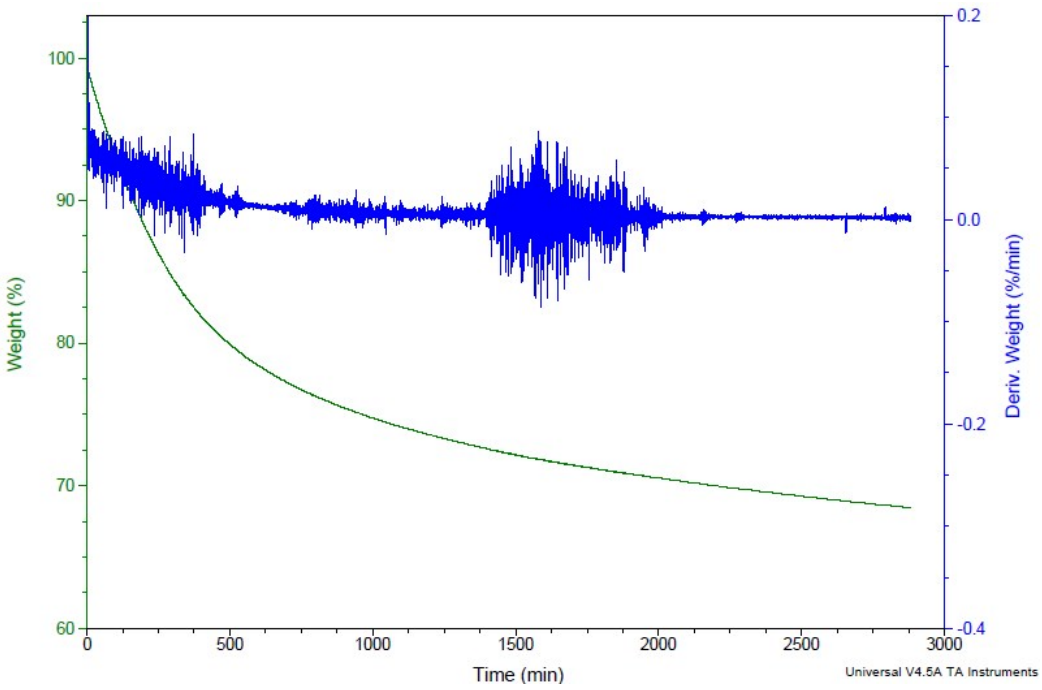

Figure S31. χ_{TOPO} = 0.33 TOPO:levulinic acid held isothermally at 90 °C. Blue line = time derivative. Initial ramping rate to isothermal = 50 °C min^{-1}.

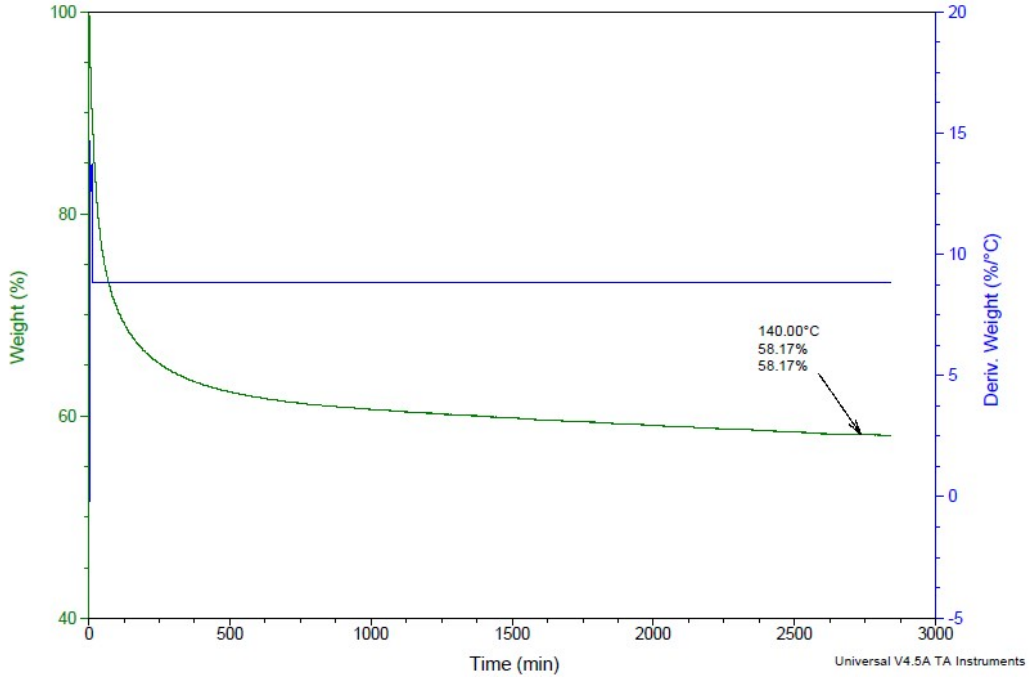

Figure S32. χ_{TOPO} = 0.33 TOPO:levulinic acid held isothermally at 140 °C. Blue line = temperature derivative Initial ramping rate to isothermal = 50 °C min^{-1}.

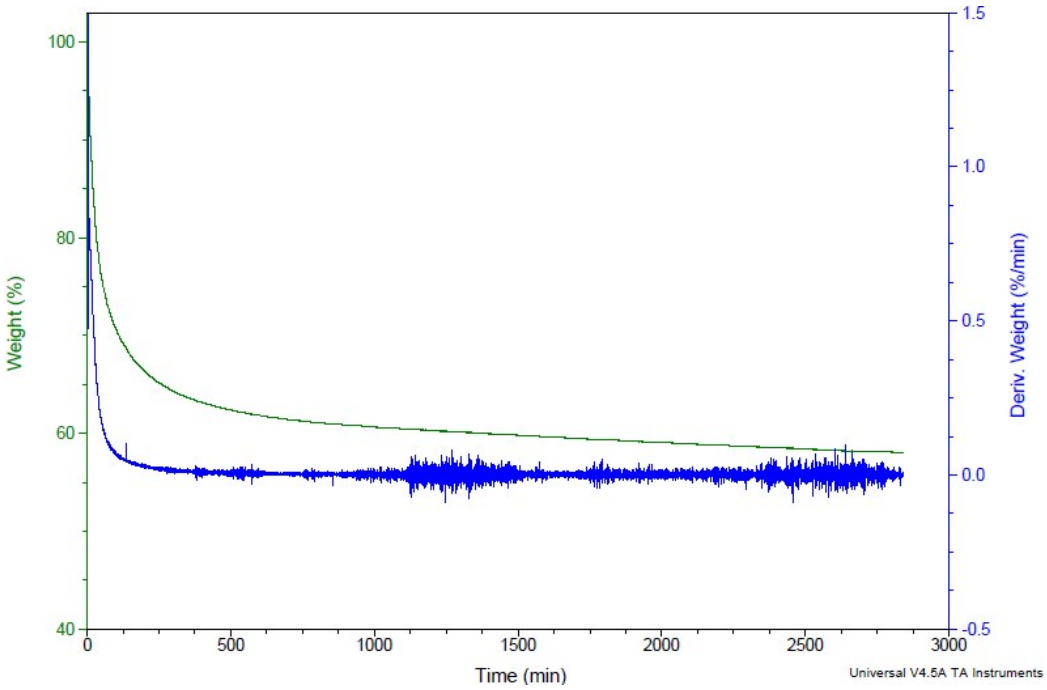

Figure S33. χ_{TOPO} = 0.33 TOPO:levulinic acid held isothermally at 140 °C. Blue line = time derivative Initial ramping rate to isothermal = 50 °C min^{-1}.

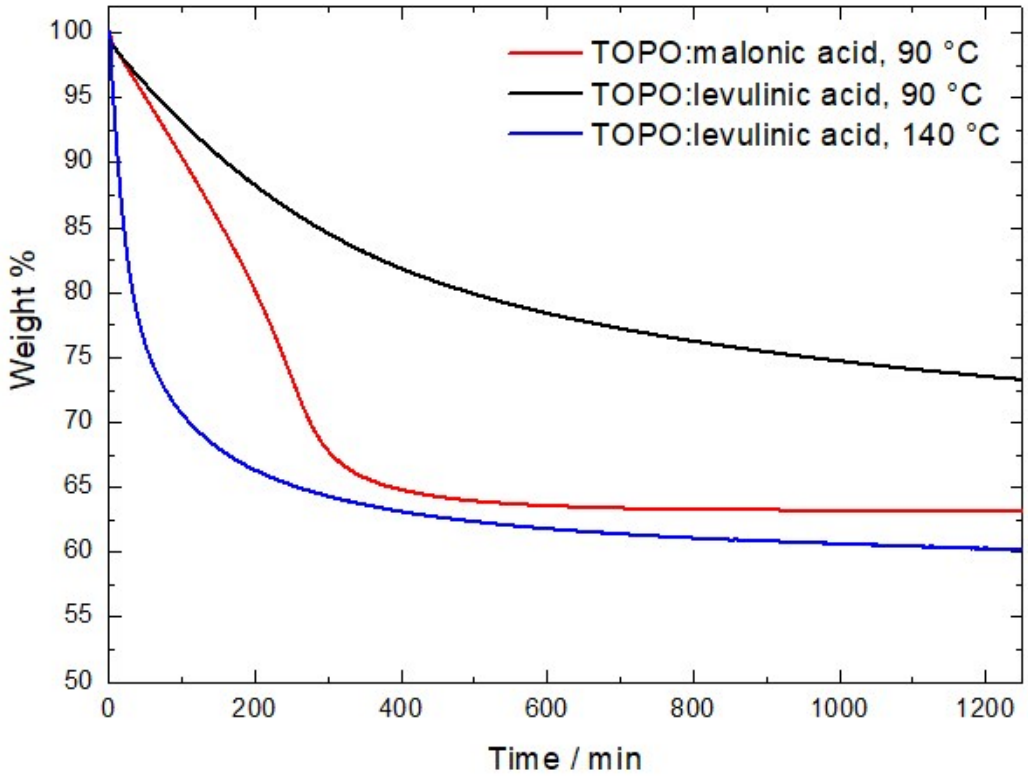

Figure S34. χ_{TOPO} = 0.33 TOPO:malonic acid and TOPO:levulinic acid held isothermally at 90 °C and 140 °C. Initial ramping rate to isothermal = 50 °C min^{-1}

4.8. Evolved gas analysis TOPO:levulinic acid during heating

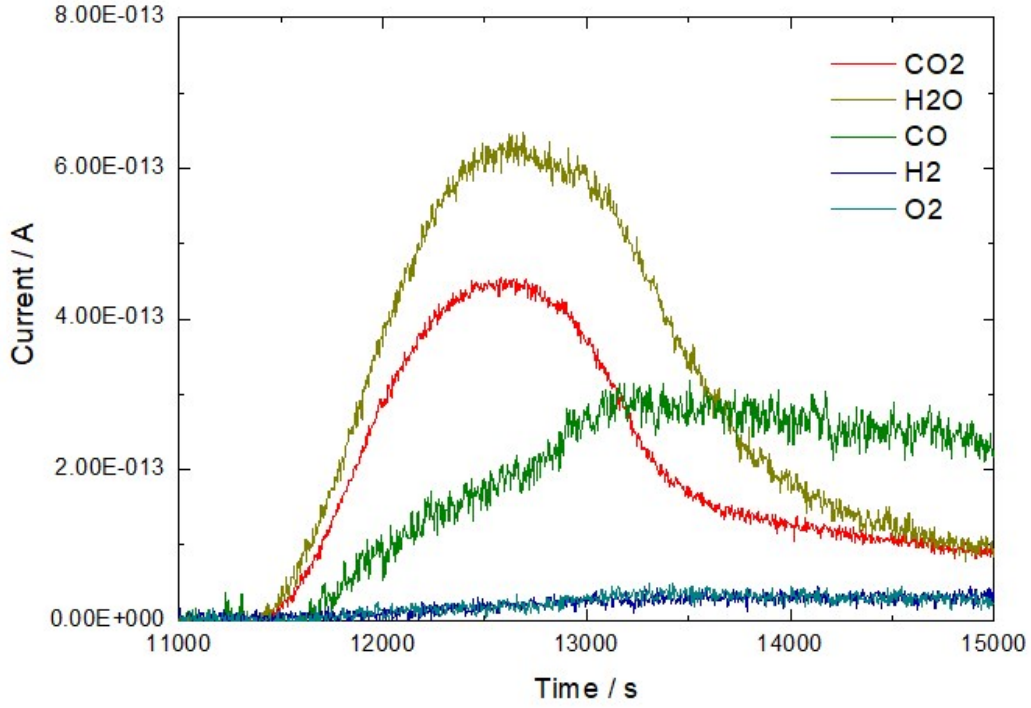

Figure S35. *In situ* GC-MS evolved gas analysis of χ_{TOPO} = 0.33 TOPO:levulinic acid held isothermally at 125 °C

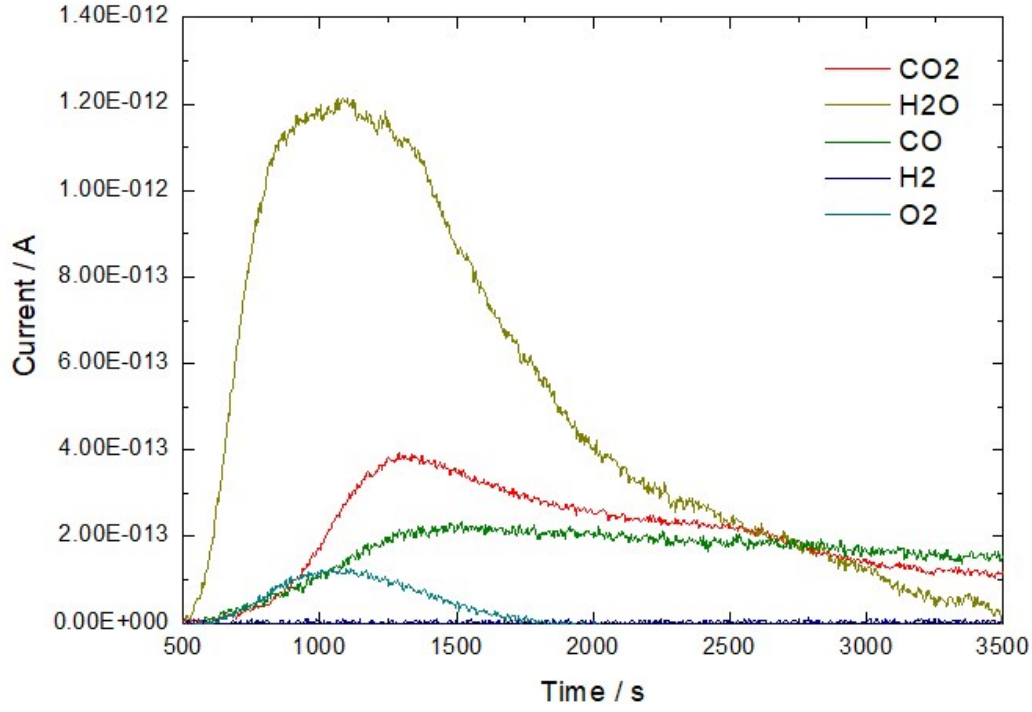

Figure S36. *In situ* GC-MS evolved gas analysis of χ_{TOPO} = 0.33 TOPO:levulinic acid held isothermally at 140 °C

4.9. Analysis of the χ_{TOPO} = 0.33 TOPO:levulinic acid liquid phase before/after decomposition

4.9.1. ^{13}C NMR

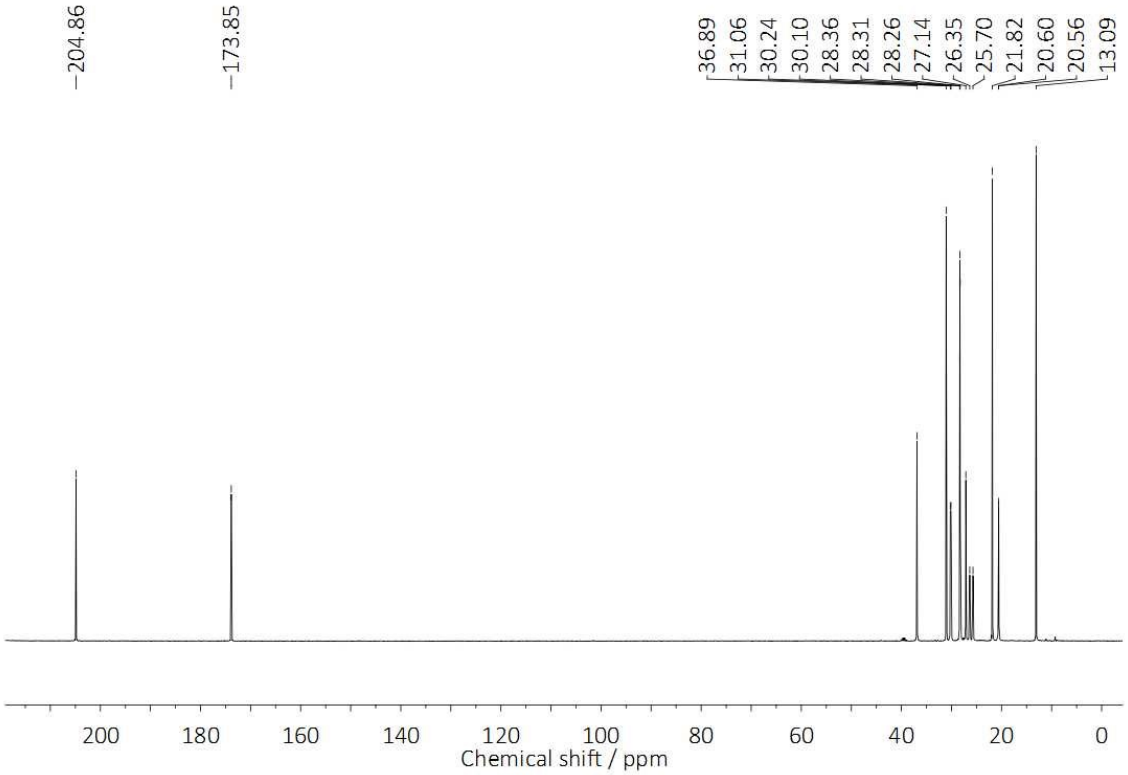

Figure S37. ^{13}C NMR spectrum of χ_{TOPO} = 0.33 TOPO:levulinic acid before held isothermally at 140 °C, neat. NMR solvent: d_6-DMSO (capillary)

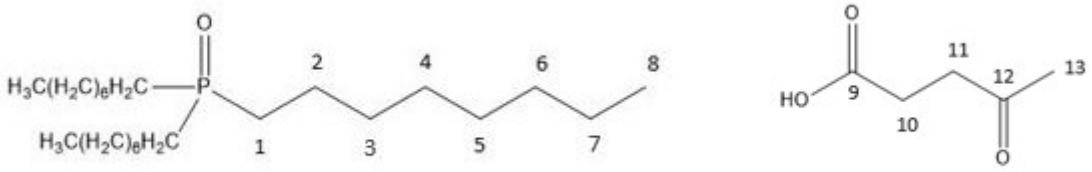

Figure S38. ^{13}C NMR peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid before held isothermally at 140 °C

Table S10. ^{13}C NMR peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid before held isothermally at 140 °C, neat. NMR solvent: d6-DMSO (capillary)

^{13}C δ / ppm	Assignment
13.09	8
20.56	3
20.60	
21.82	7
25.70	1
26.35	
27.14	10
28.26	6
28.31	5
28.36	13
30.10	2
30.24	
31.06	4
36.89	11
173.85	9
204.86	12

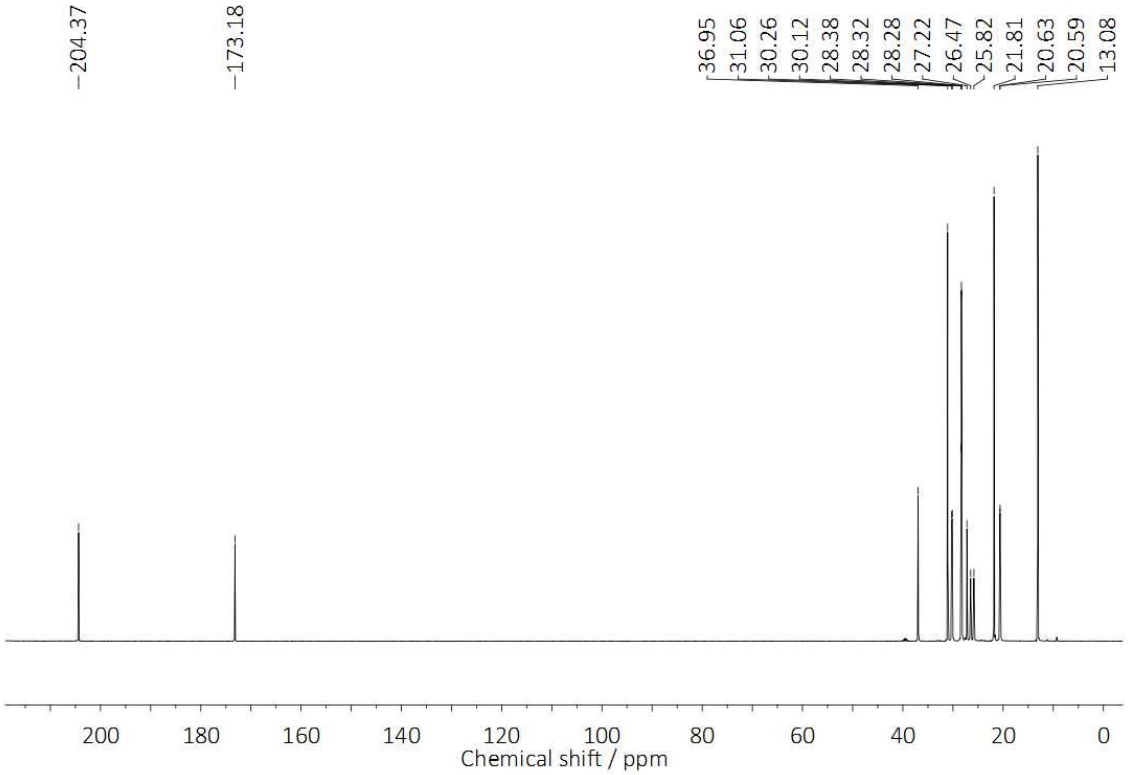

Figure S39. ^{13}C NMR spectrum of χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C, neat. NMR solvent: d_6-DMSO (capillary)

Figure S40. ^{13}C NMR peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C

Table S11. ^{13}C NMR peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid before held isothermally at 140 °C, neat. NMR solvent: d_6-DMSO (capillary)

^{13}C δ / ppm	Assignment
13.08	8
20.59	3
20.63	
21.81	7
25.82	1
26.47	
27.22	10
28.28	6
28.32	5
28.38	13
30.12	2
30.26	
31.06	4
36.95	11
173.18	9
204.37	12

4.9.2. ^{1}H NMR

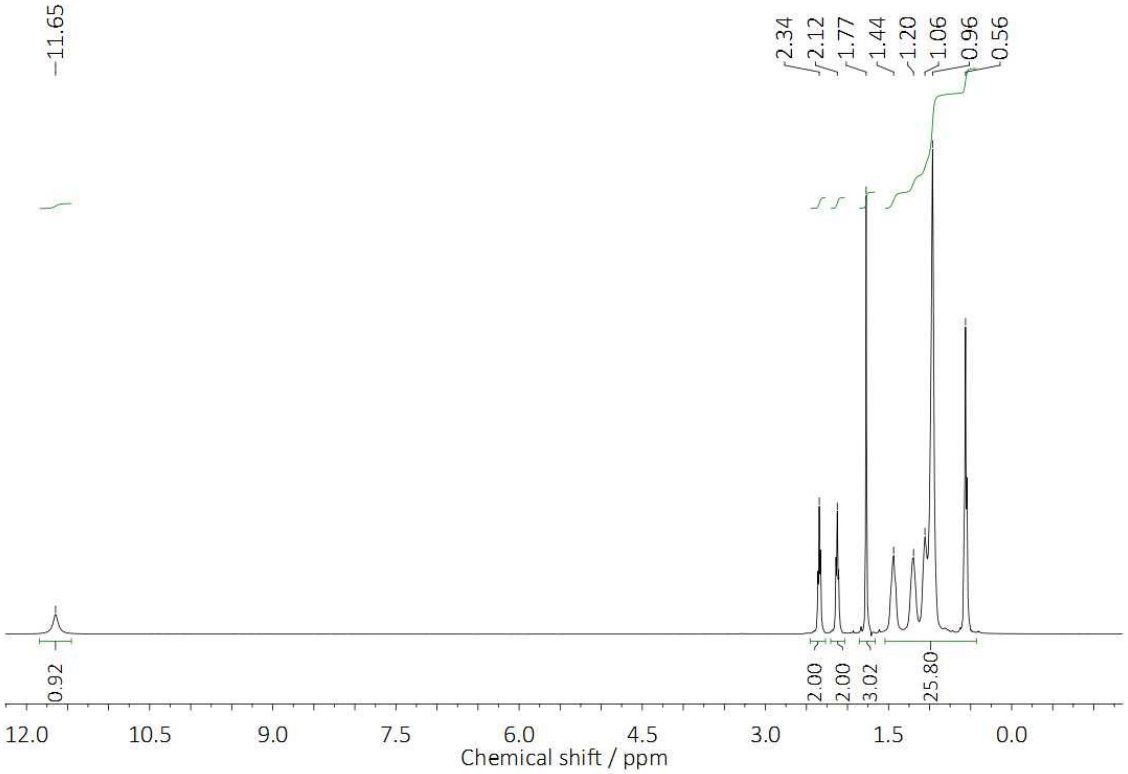

Figure S41. ^{1}H NMR spectrum of χ_{TOPO} = 0.33 TOPO:levulinic acid before held isothermally at 140 °C, neat. NMR solvent: d_6-DMSO (capillary)

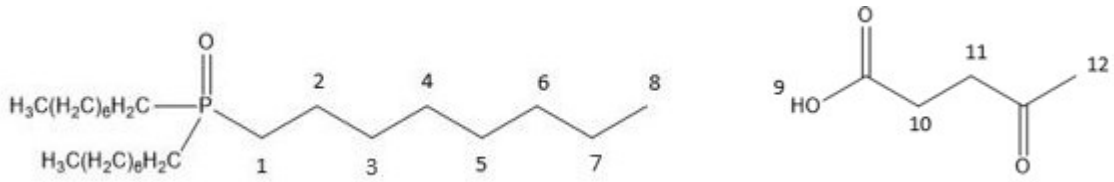

Figure S42.^{1}H NMR peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid before held isothermally at 140 °C. NMR solvent: d_6-DMSO (capillary)

Table S12. ^{1}H peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid before decomposition, d_6-DMSO capillary, (neat). TOPO peaks in agreement with literature (d_3-acetonitrile)[1]. [b]Broad peak

^{1}H δ / ppm	Multiplicity	Assignment
0.56	Triplet	8
0.96	Multiplet[b]	5-7
1.06	Multiplet[b]	4
1.20	Multiplet[b]	3
1.44	Multiplet[b]	1-2
1.77	Singlet	12
2.12	Triplet	10
2.34	Triplet	11
11.65	Singlet	9

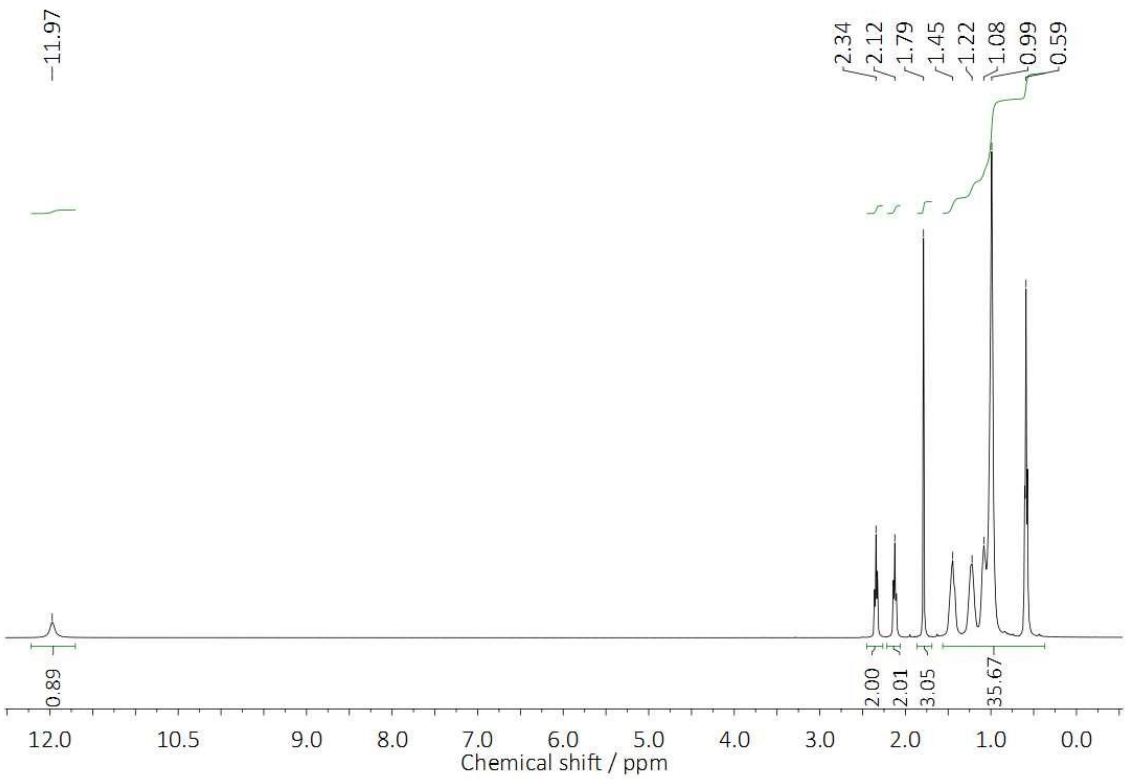

Figure S43. ^{1}H NMR spectrum of χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C, neat. NMR solvent: d_6-DMSO (capillary)

Figure S44. ^{1}H NMR peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C

Table S13.^{1}H peak assignment χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C, neat. NMR solvent: d_6-DMSO capillary. TOPO peaks in agreement with literature (d_3-acetonitrile)[1]. [b]Broad peak

^{1}H δ / ppm	Multiplicity	Assignment
0.59	Triplet	8
0.99	Multiplet[b]	5-7
1.08	Multiplet[b]	4
1.22	Multiplet[b]	3
1.45	Multiplet[b]	1-2
1.79	Singlet	12
2.12	Triplet	10
2.34	Triplet	11
11.97	Singlet	9

4.10. Sublimation/evaporation of levulinic acid

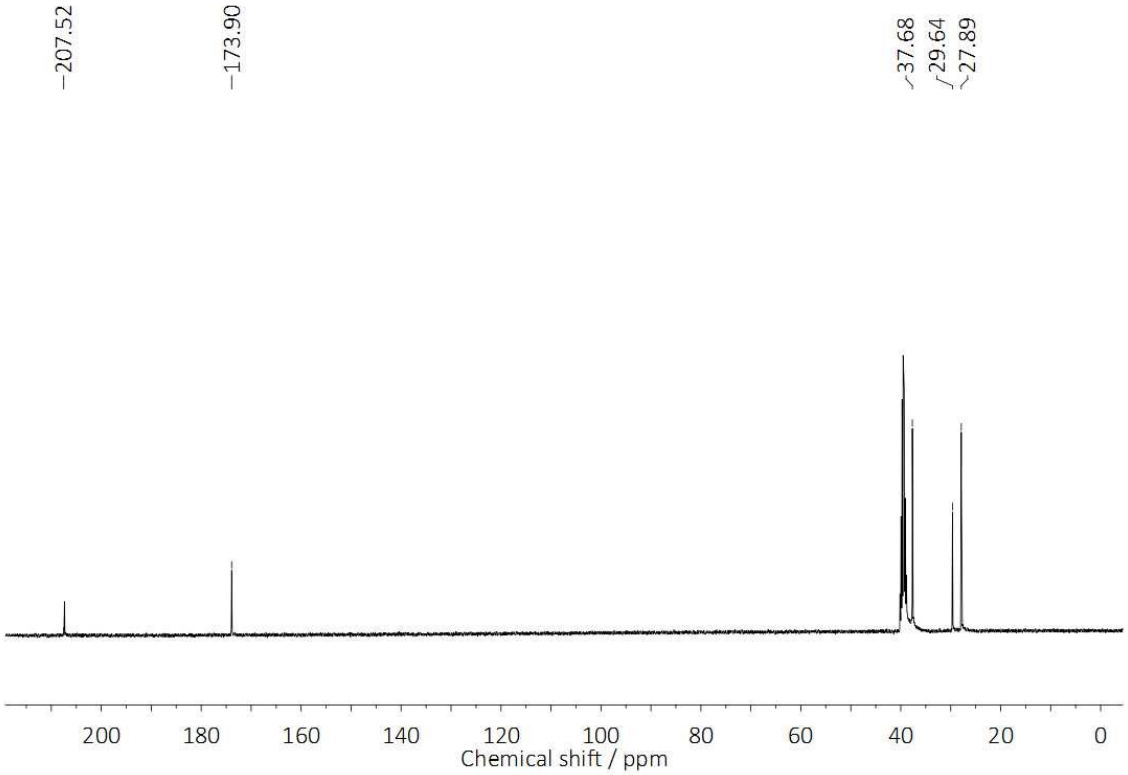

Figure S45. ^{13}C NMR spectrum of levulinic acid sublimed/evaporated from χ_{TOPO} = 0.33 TOPO:malonic acid held at 140 °C. NMR solvent: d_6-DMSO

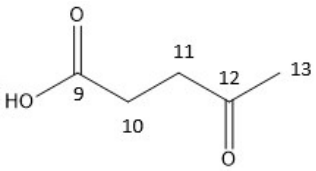

Figure S46. ^{13}C NMR peak assignment of levulinic acid sublimed from χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C

Table S14. ^{13}C NMR peak assignment of levulinic acid sublimed from χ_{TOPO} = 0.33 TOPO:levulinic acid after held isothermally at 140 °C

^{13}C δ / ppm	Assignment
27.89	10
29.64	13
37.68	11
173.90	9
207.52	12

4.11. Comparison of thermal decomposition onset

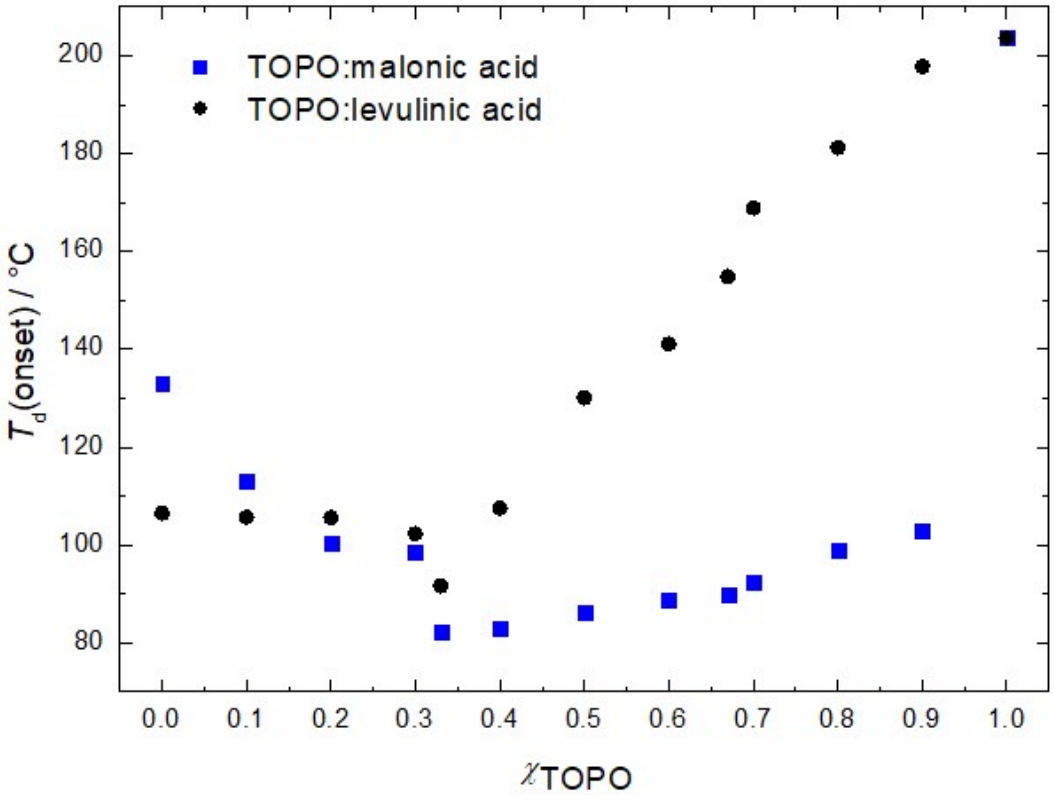

Figure S47. Thermal decomposition (onset) as a function of TOPO mole ratio under TGA dynamic heating at 10 °C min^{-1}

5. Phase behaviour

5.1. TOPO:malonic acid

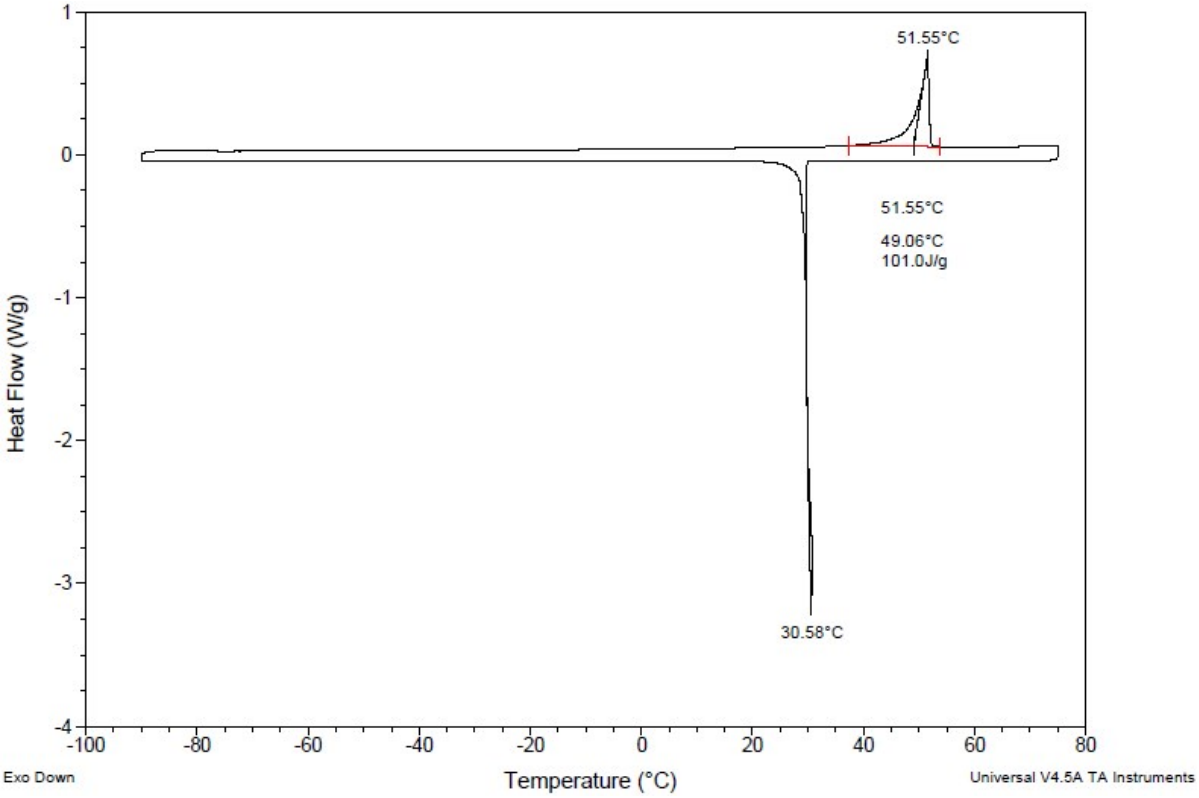

Figure S48. DSC Pure TOPO

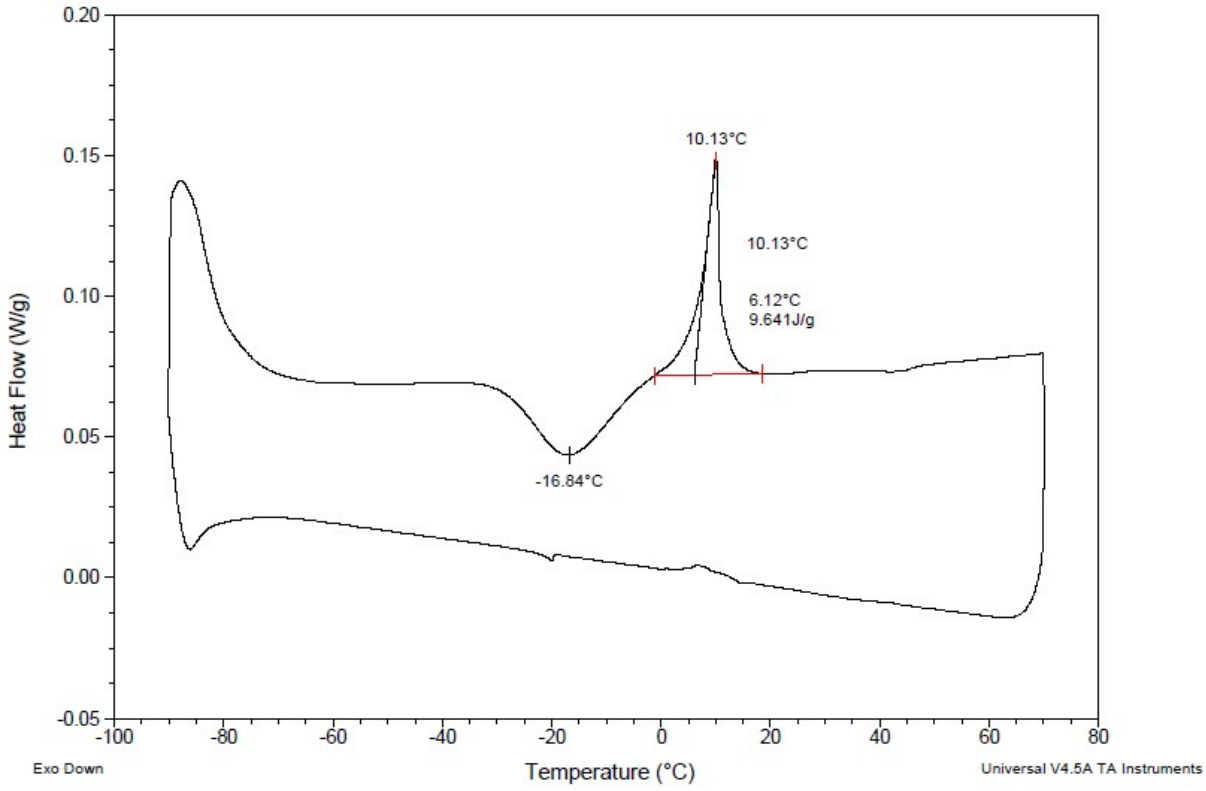

Figure S49. DSC χ_{TOPO} = 0.10 TOPO:malonic acid

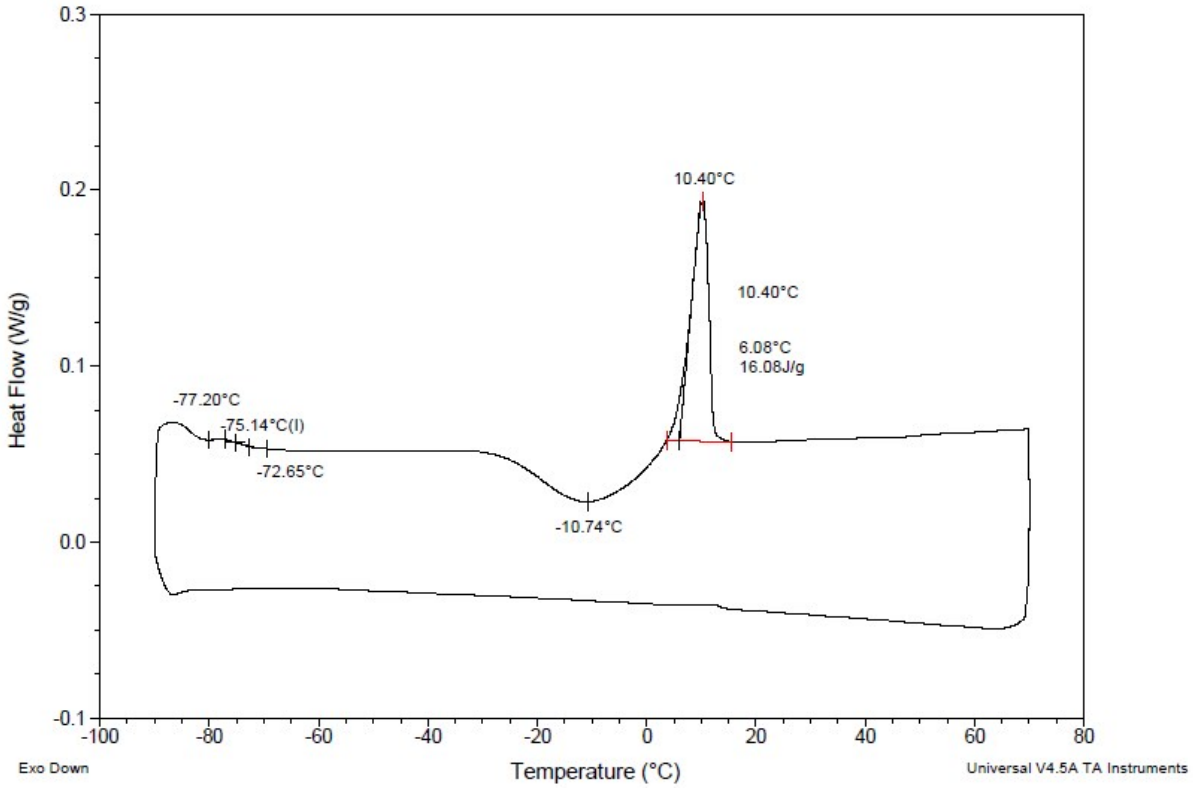

Figure S50. DSC χ_{TOPO} = 0.20 TOPO:malonic acid

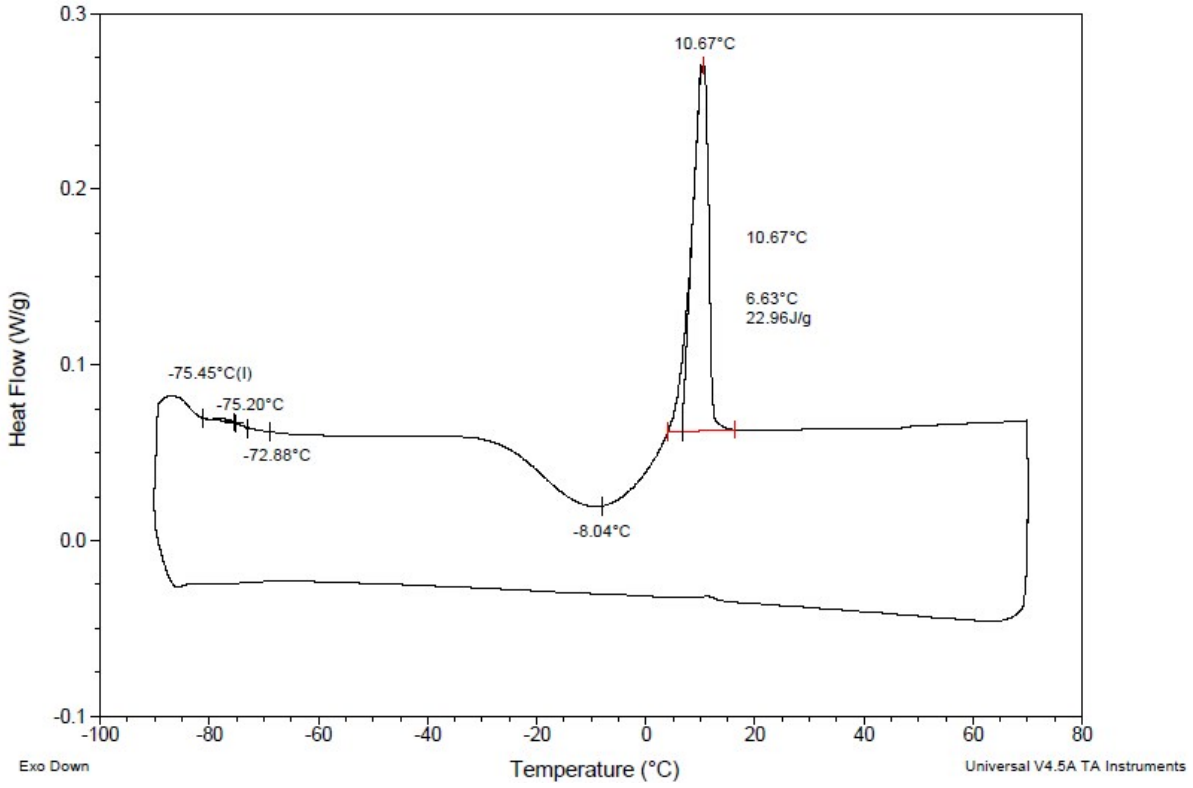

Figure S51. DSC χ_{TOPO} = 0.30 TOPO:malonic acid

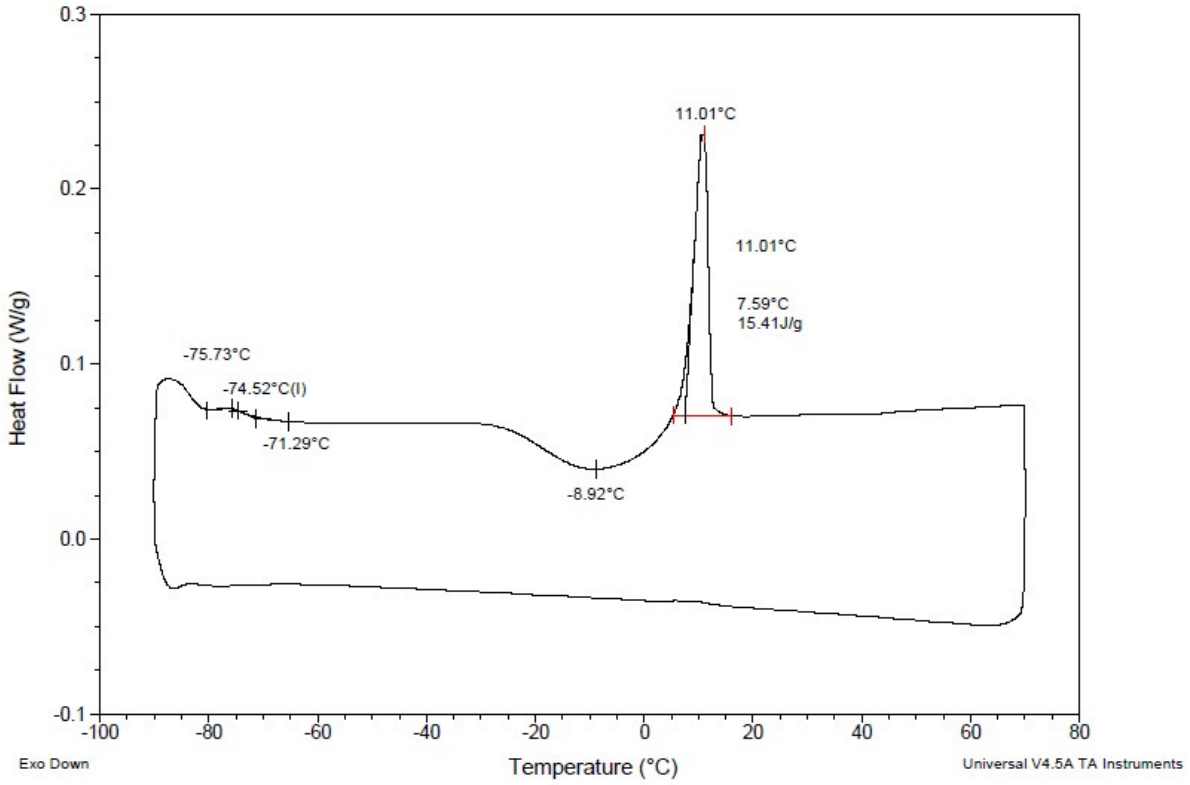

Figure S52. DSC χ_{TOPO} = 0.33 TOPO:malonic acid

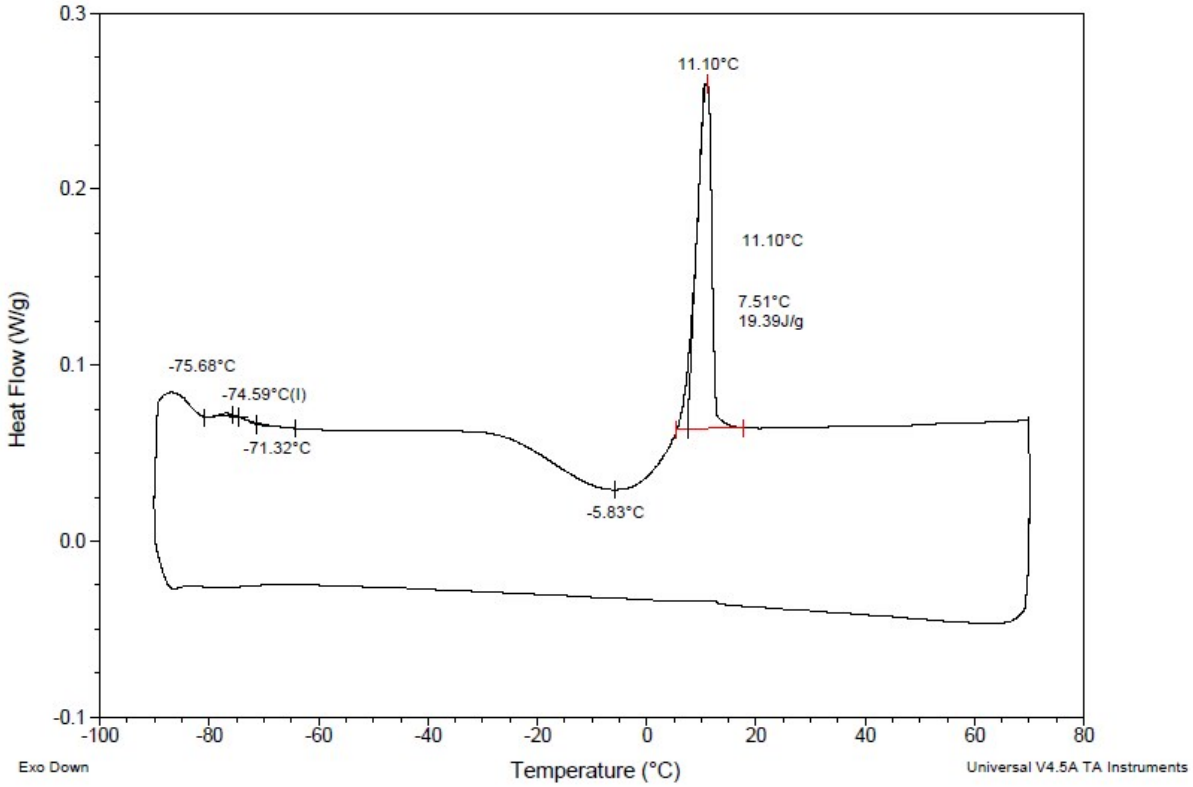

Figure S53. DSC χ_{TOPO} = 0.40 TOPO:malonic acid

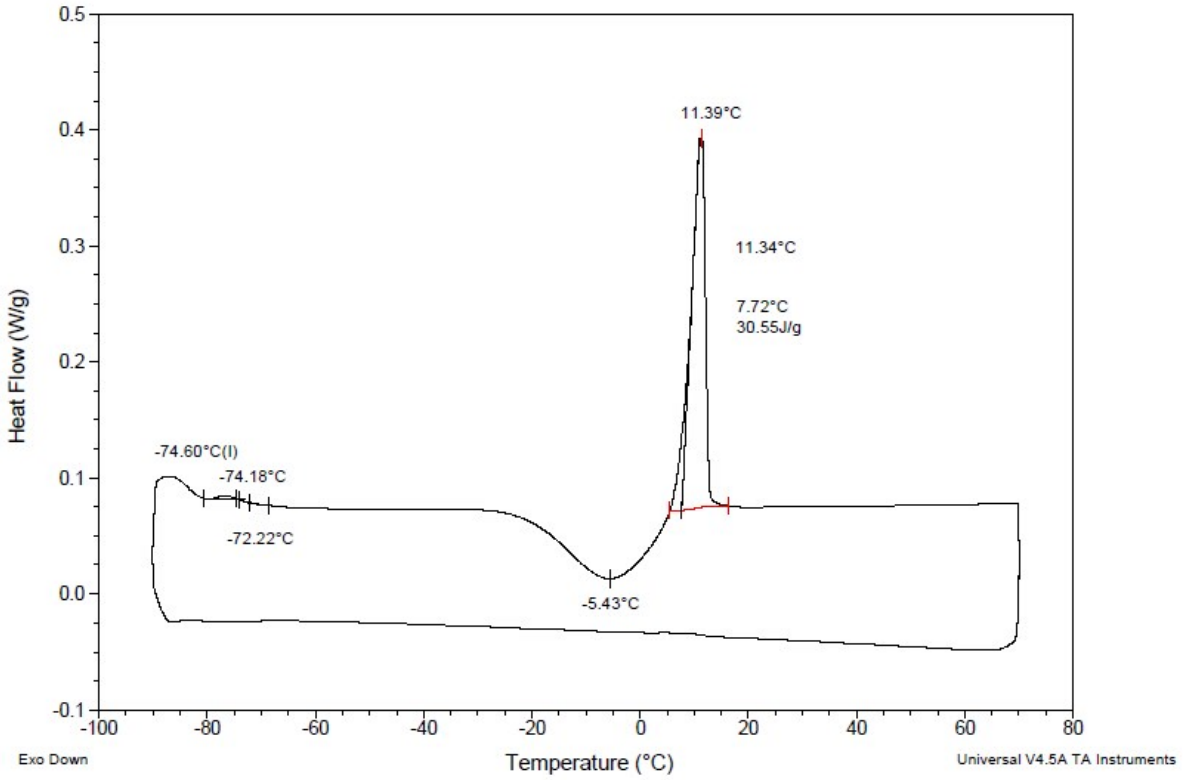

Figure S54. DSC χ_{TOPO} = 0.50 TOPO:malonic acid

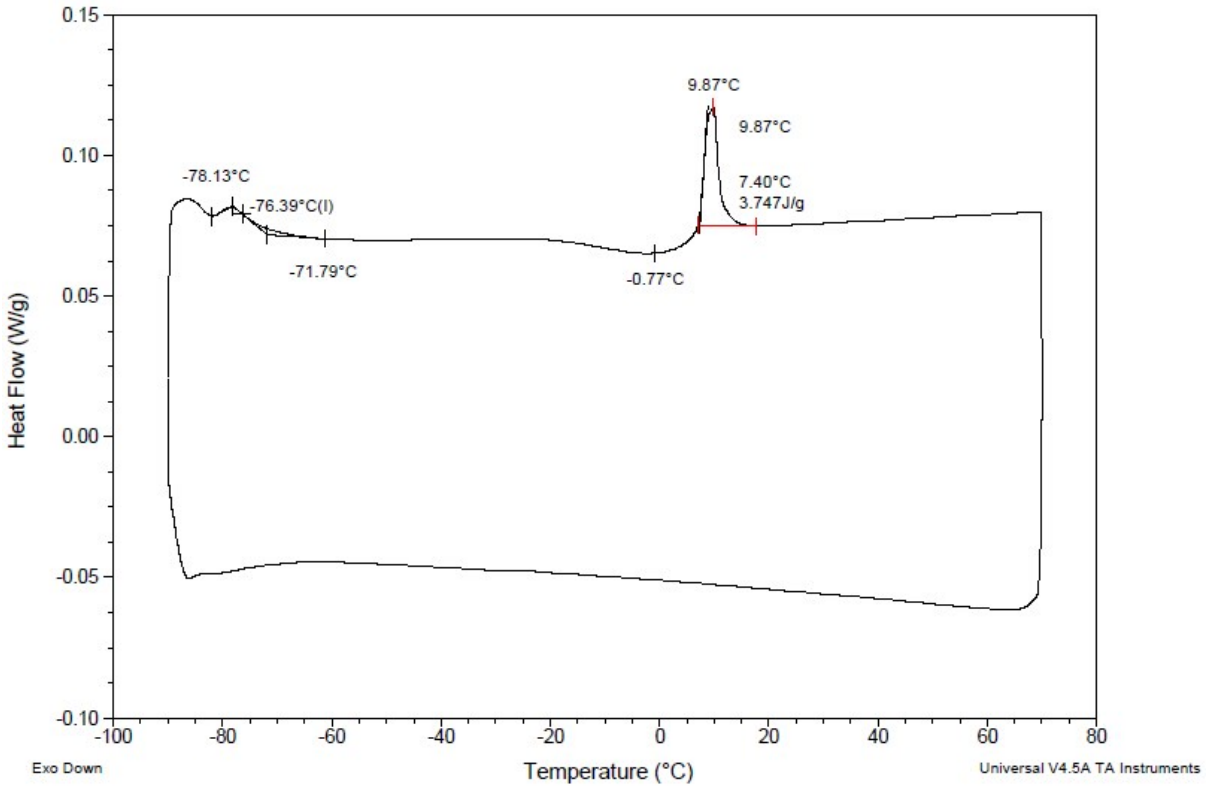

Figure S55. DSC χ_{TOPO} = 0.55 TOPO:malonic acid

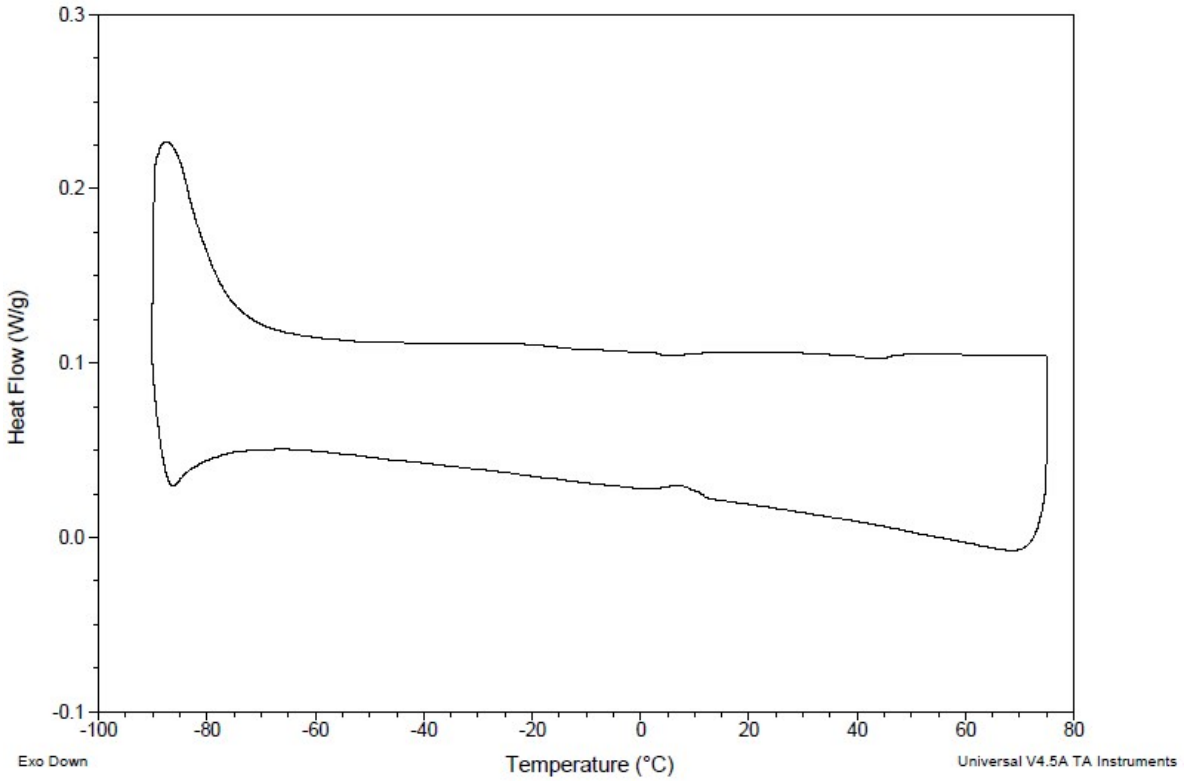

Figure S56. DSC χ_{TOPO} = 0.60 TOPO:malonic acid

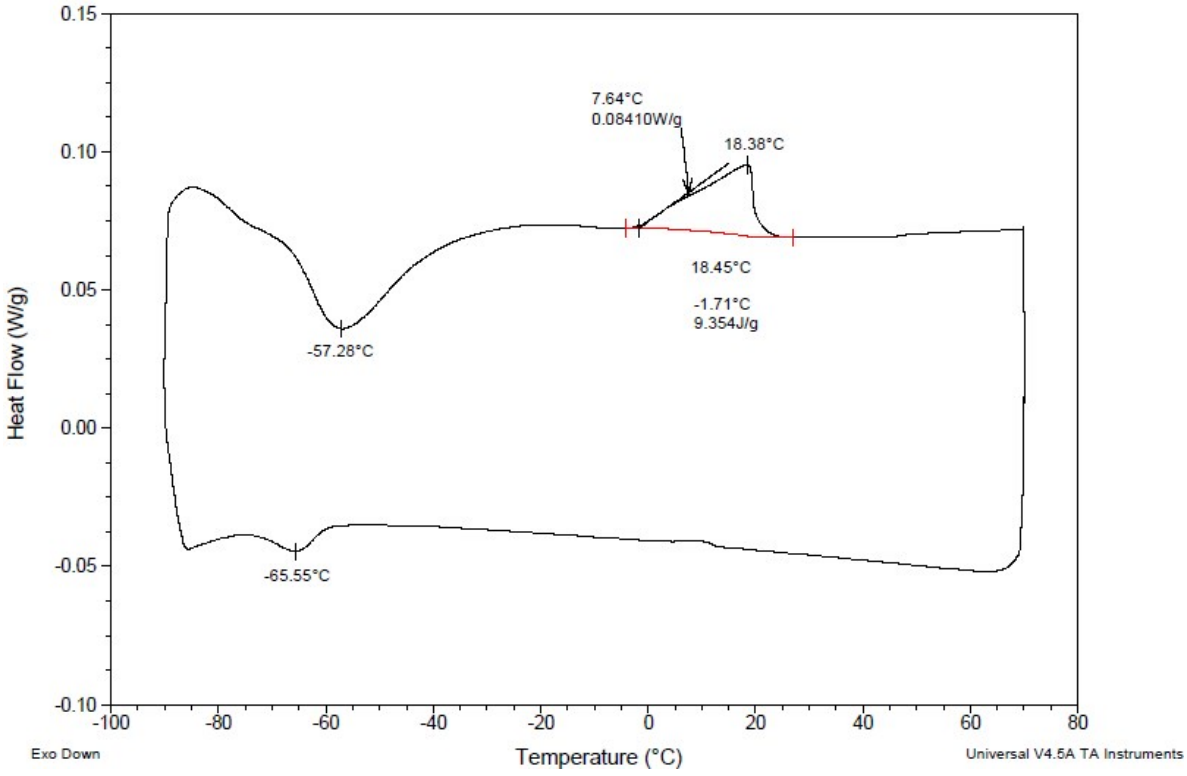

Figure S57. DSC χ_{TOPO} = 0.67 TOPO:malonic acid

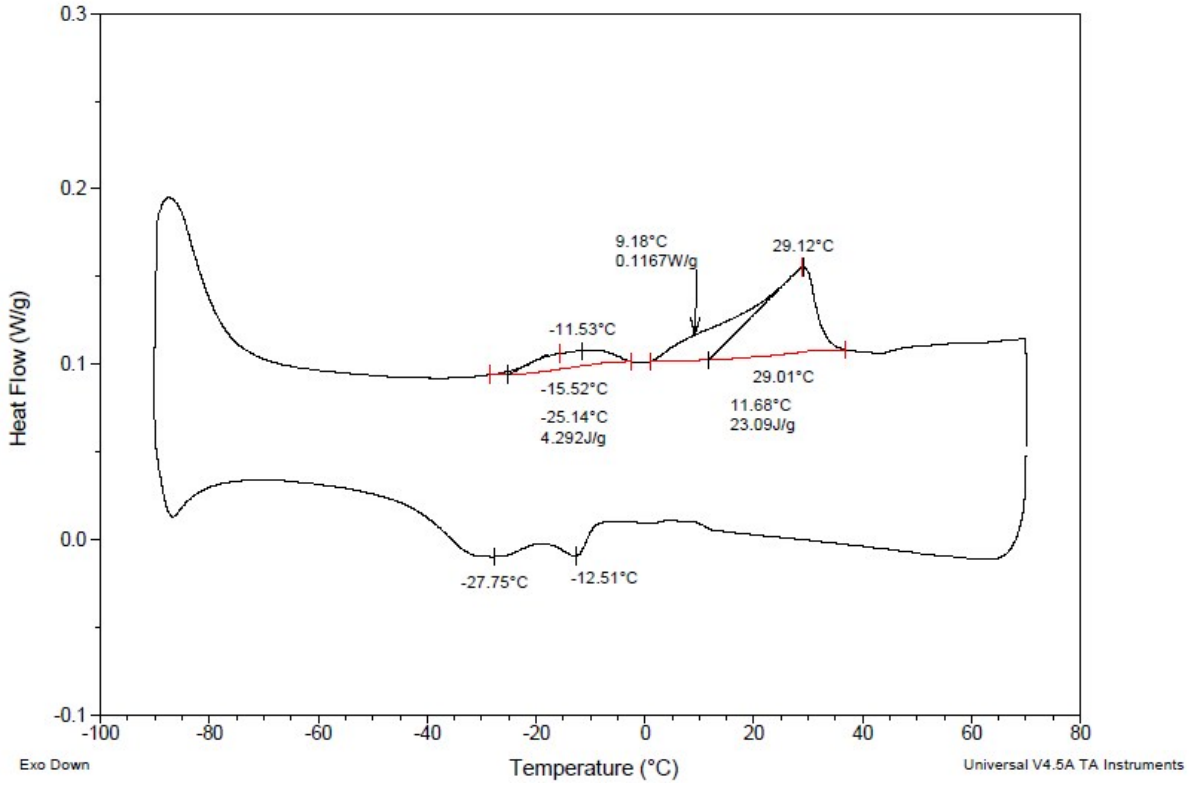

Figure S58. DSC χ_{TOPO} = 0.70 TOPO:malonic acid

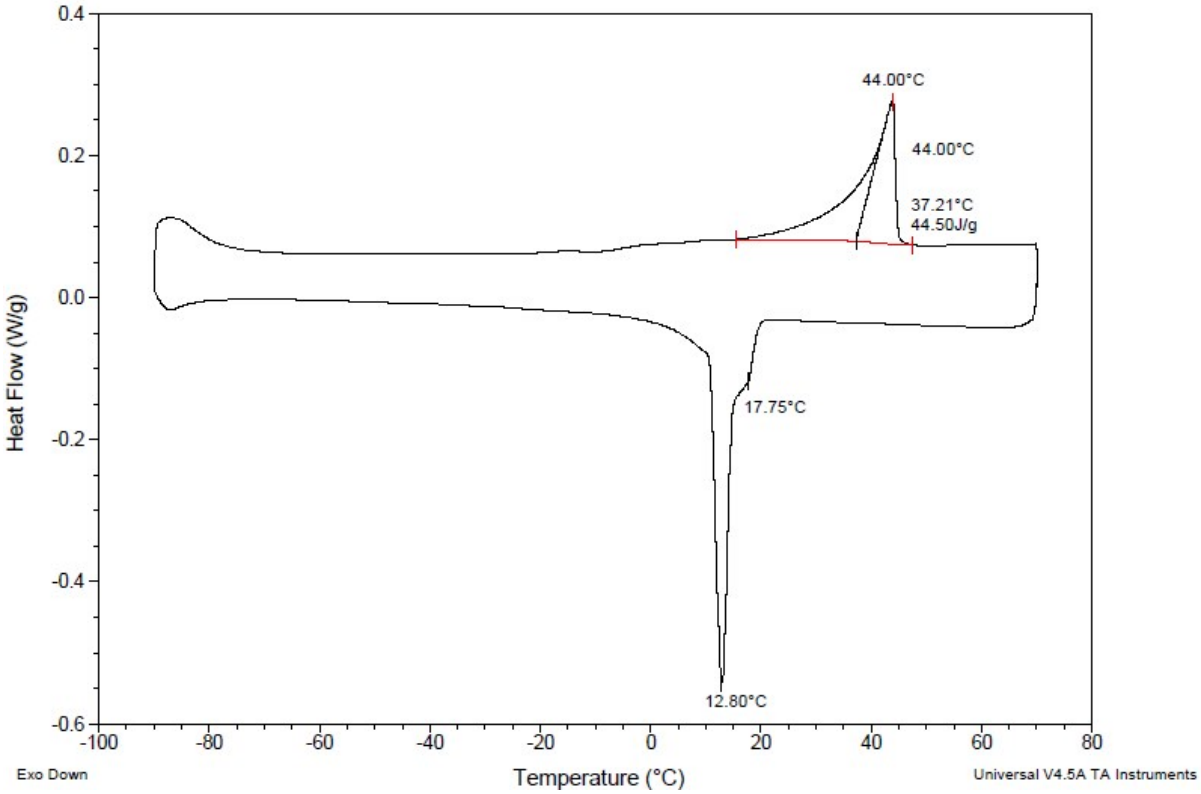

Figure S59. DSC χ_{TOPO} = 0.80 TOPO:malonic acid

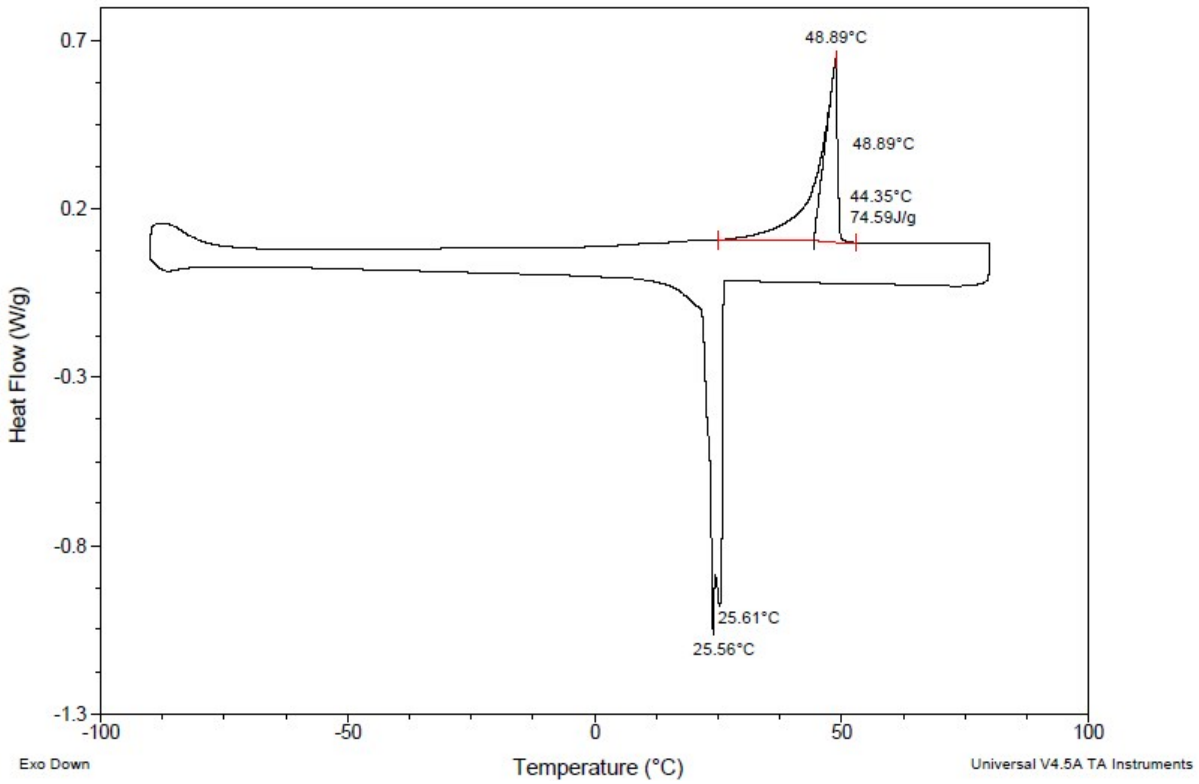

Figure S60. DSC χ_{TOPO} = 0.90 TOPO:malonic acid

5.2. TOPO:levulinic acid

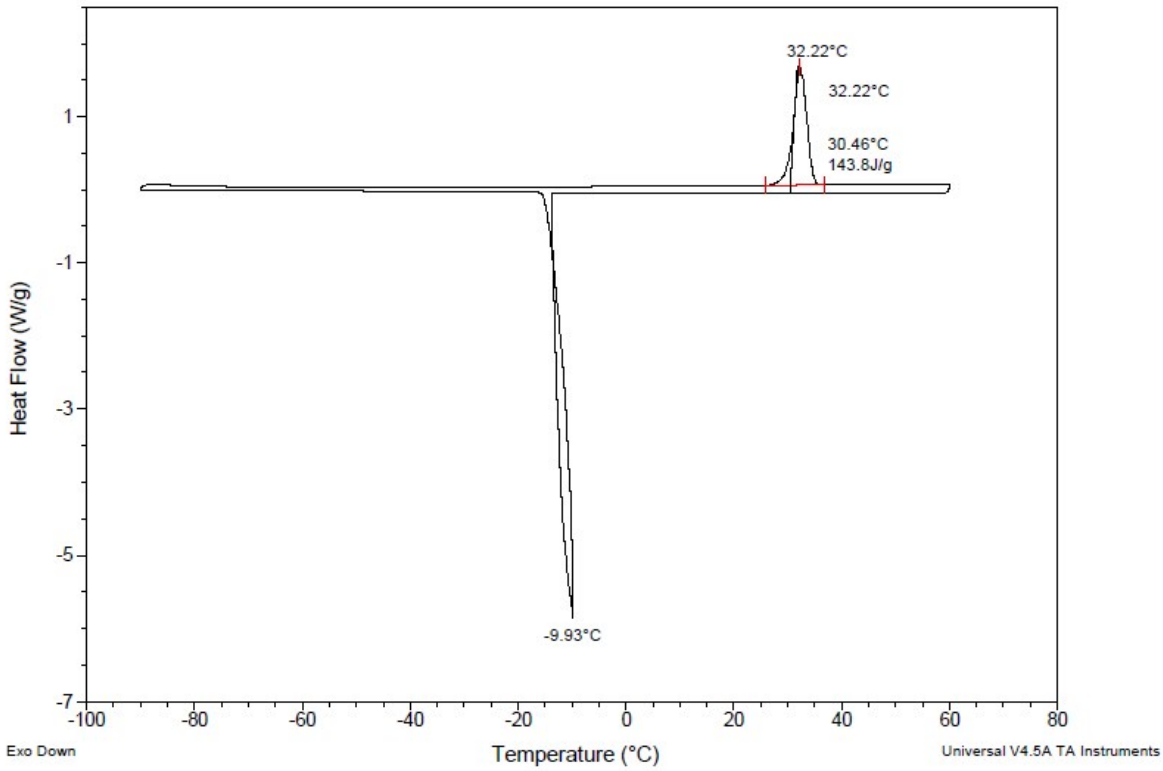

Figure S61. DSC Pure levulinic acid

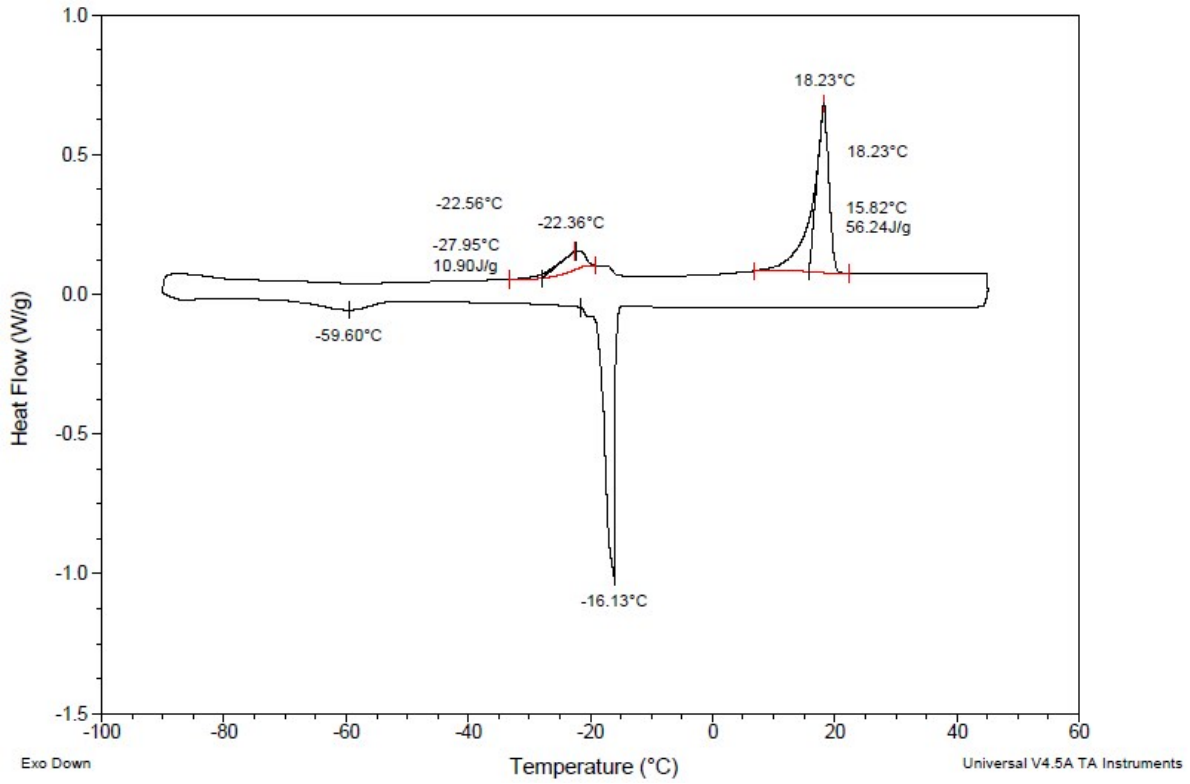

Figure S62. DSC χ_{TOPO} = 0.10 TOPO:levulinic acid

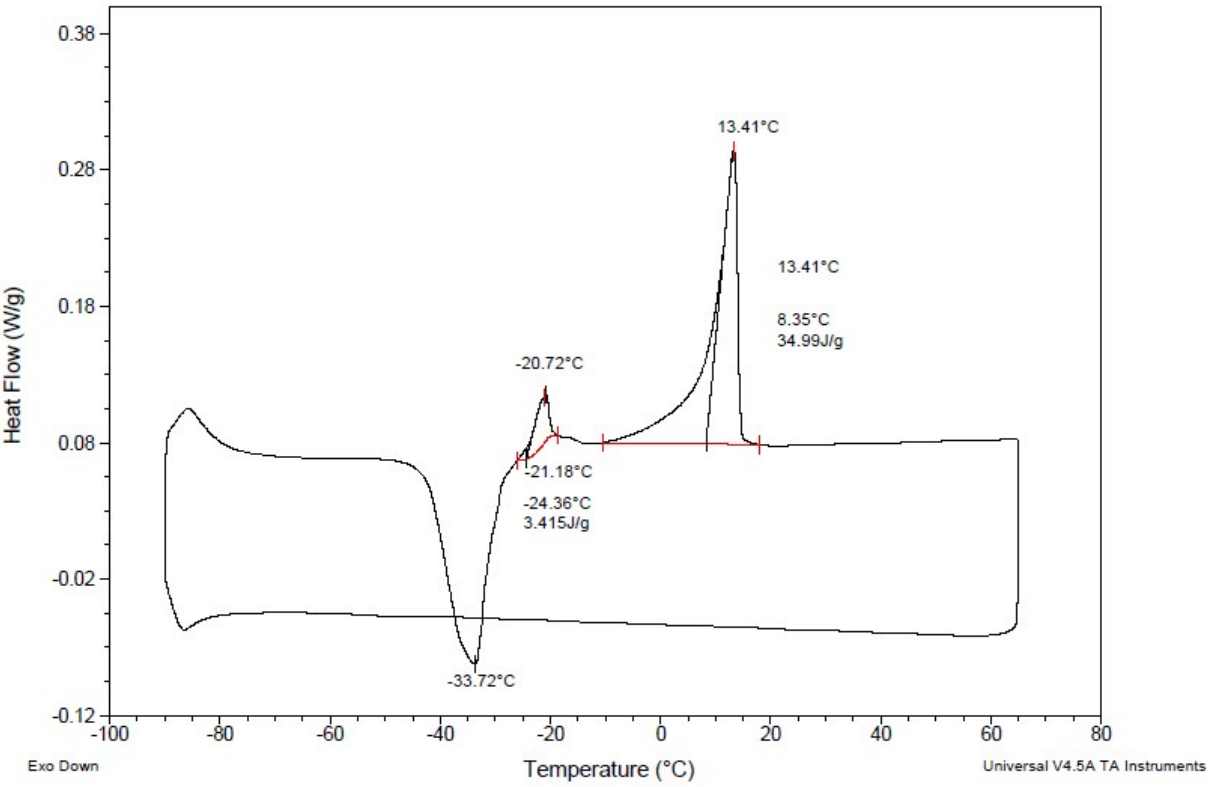

Figure S63. DSC χ_{TOPO} = 0.20 TOPO:levulinic acid

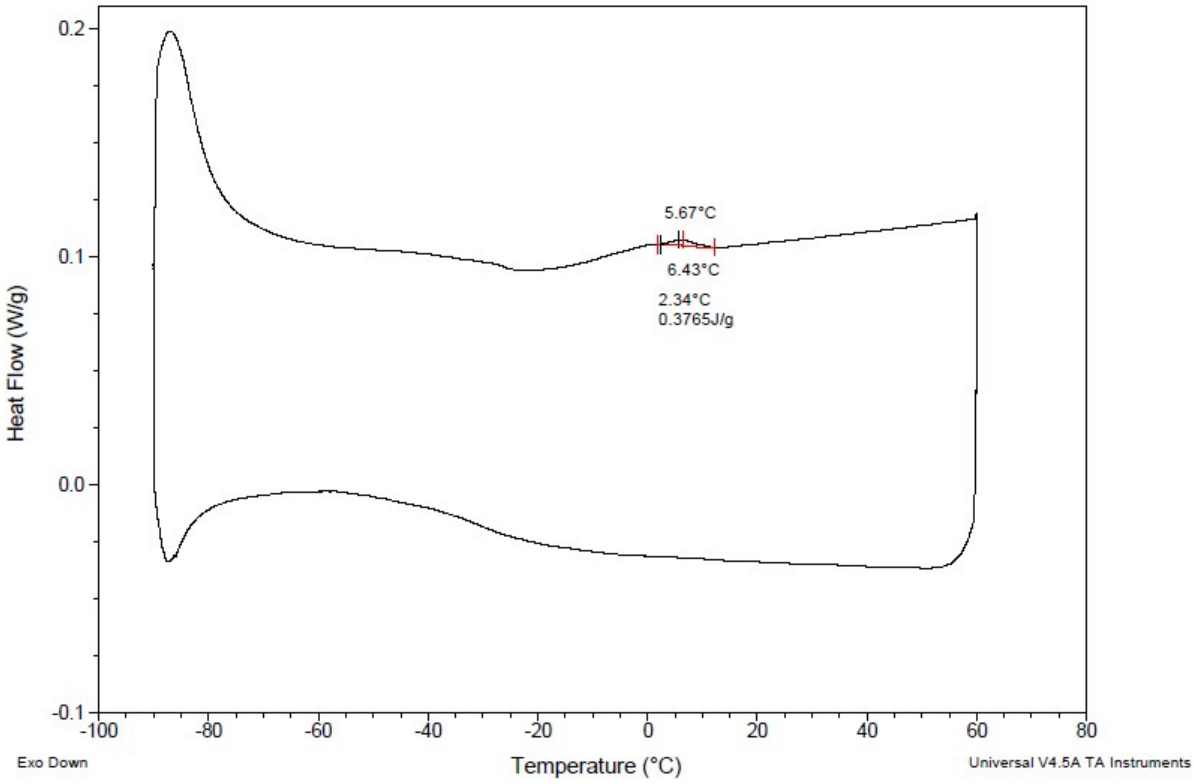

Figure S64. DSC χ_{TOPO} = 0.30 TOPO:levulinic acid

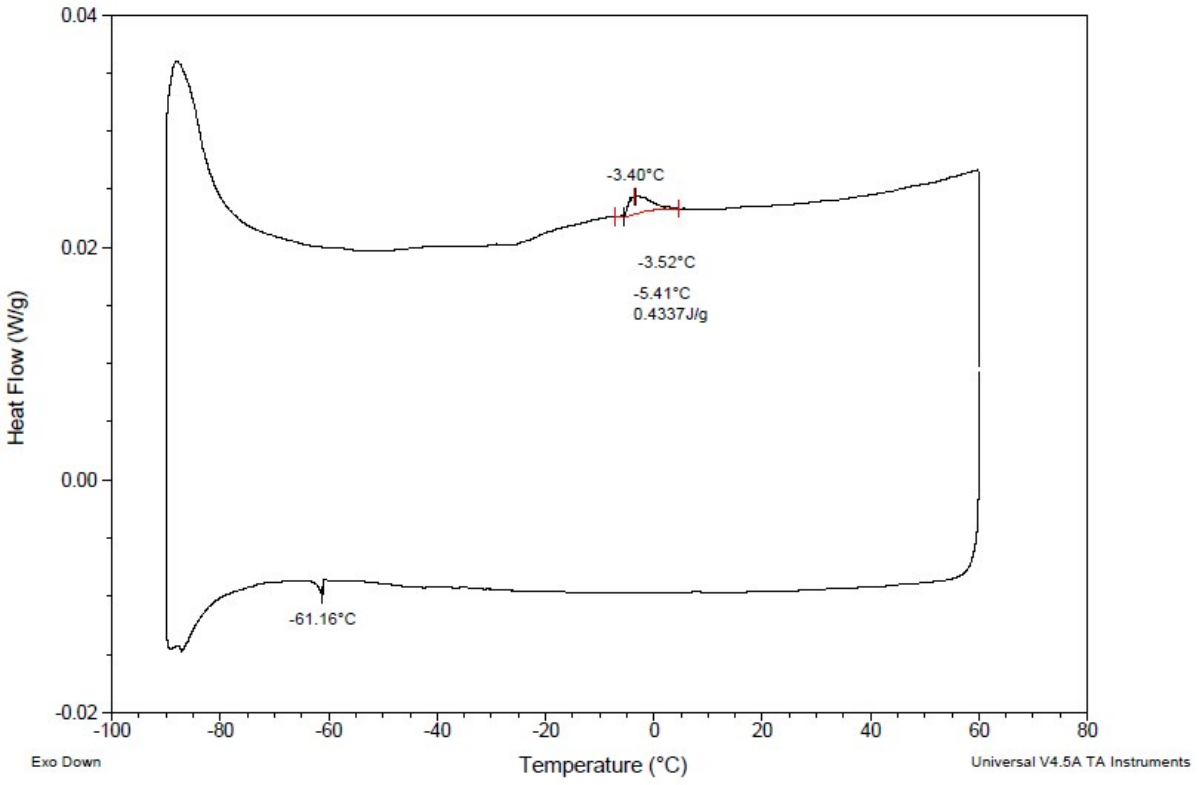

Figure S65. DSC χ_{TOPO} = 0.33 TOPO:levulinic acid

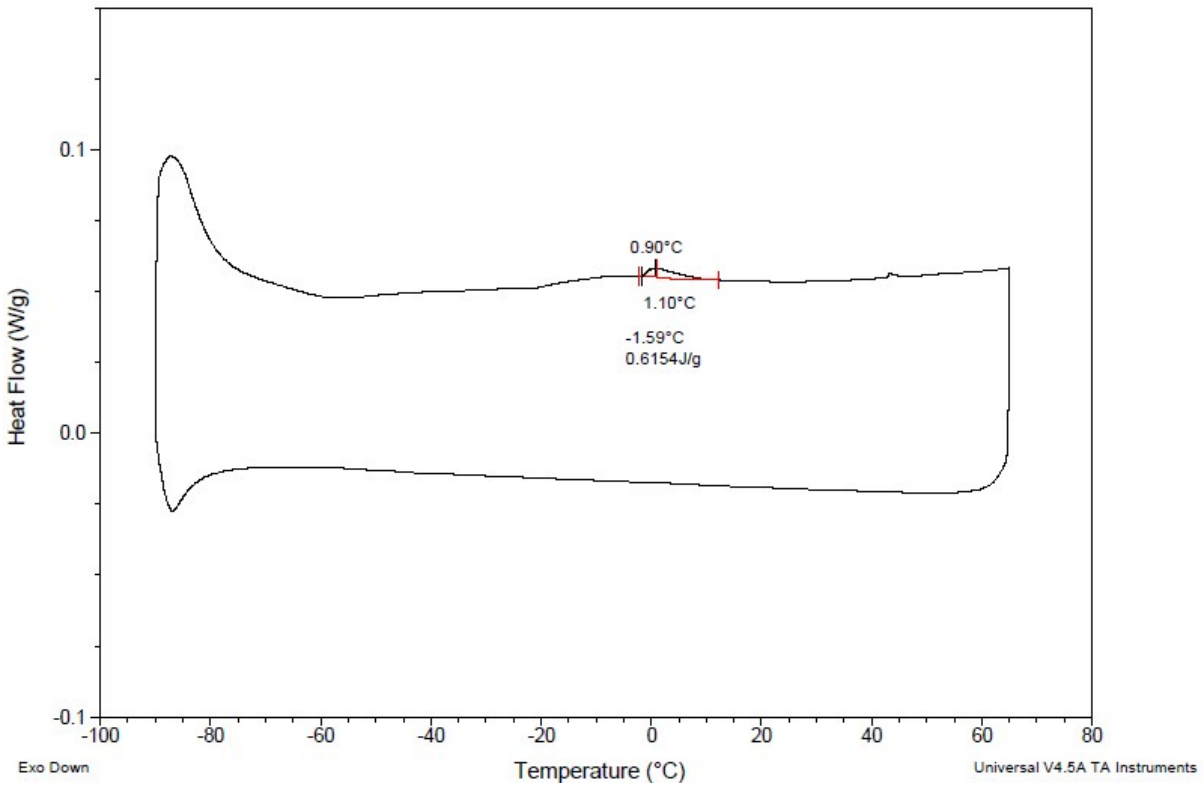

Figure S66. DSC χ_{TOPO} = 0.40 TOPO:levulinic acid

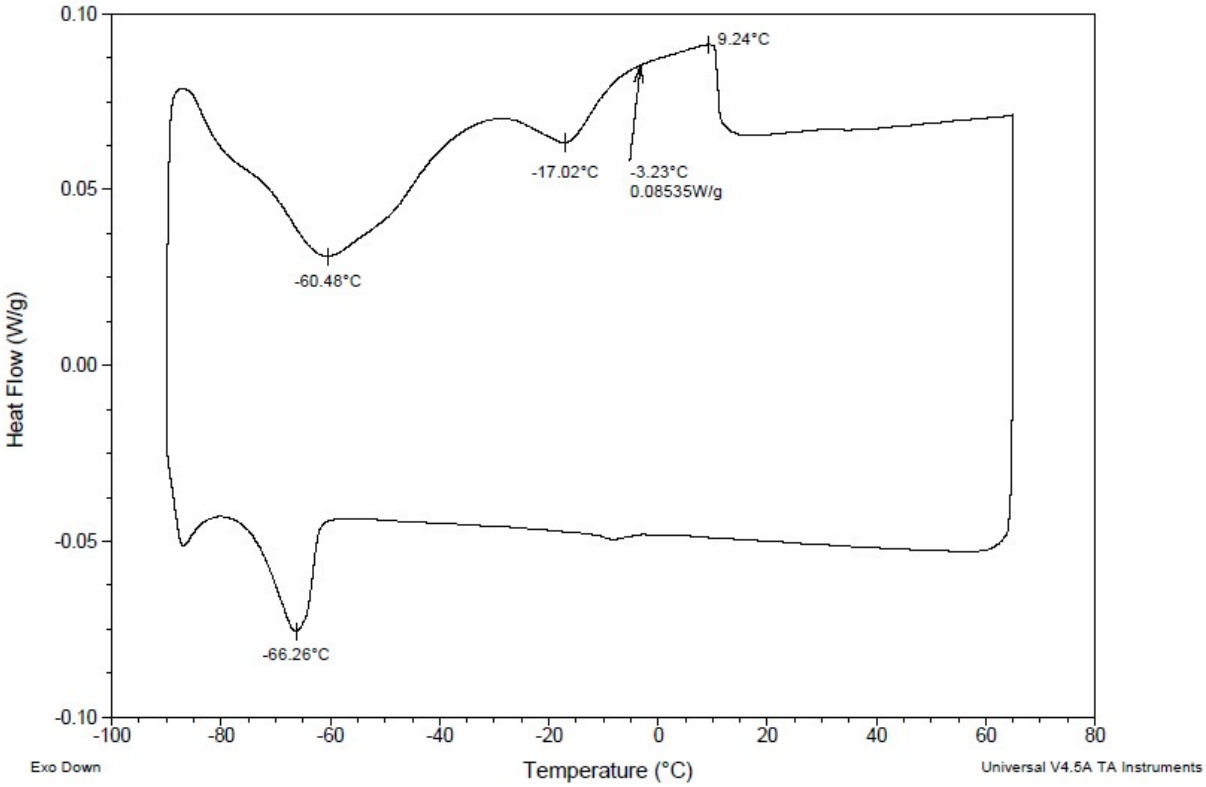

Figure S67. DSC χ_{TOPO} = 0.50 TOPO:levulinic acid

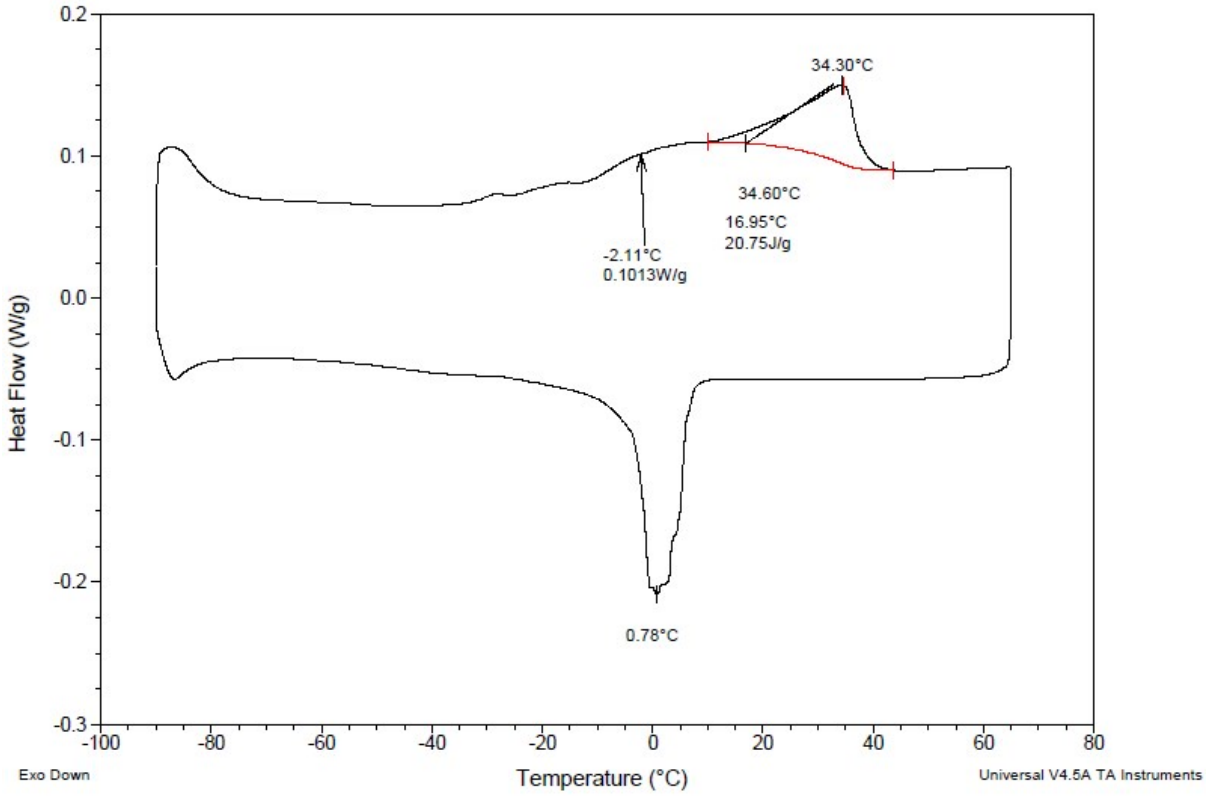

Figure S68. DSC χ_{TOPO} = 0.60 TOPO:levulinic acid

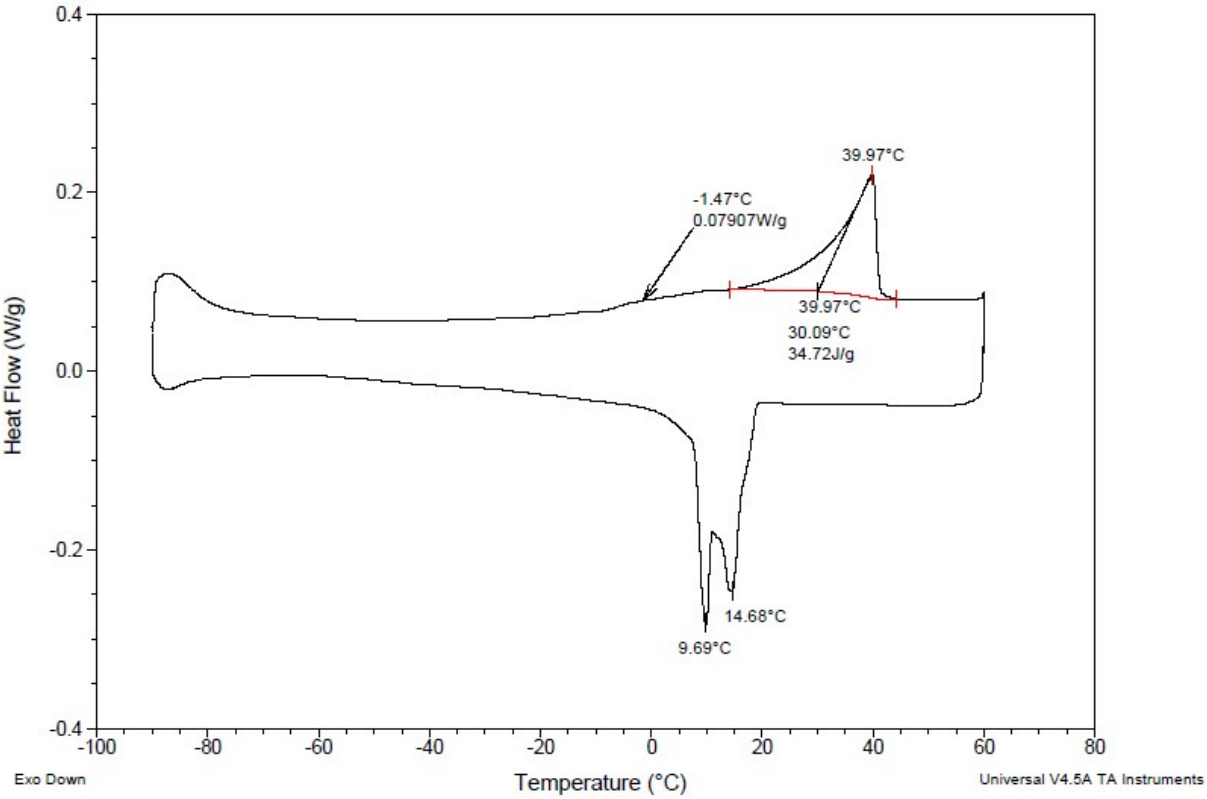

Figure S69. DSC χ_{TOPO} = 0.67 TOPO:levulinic acid

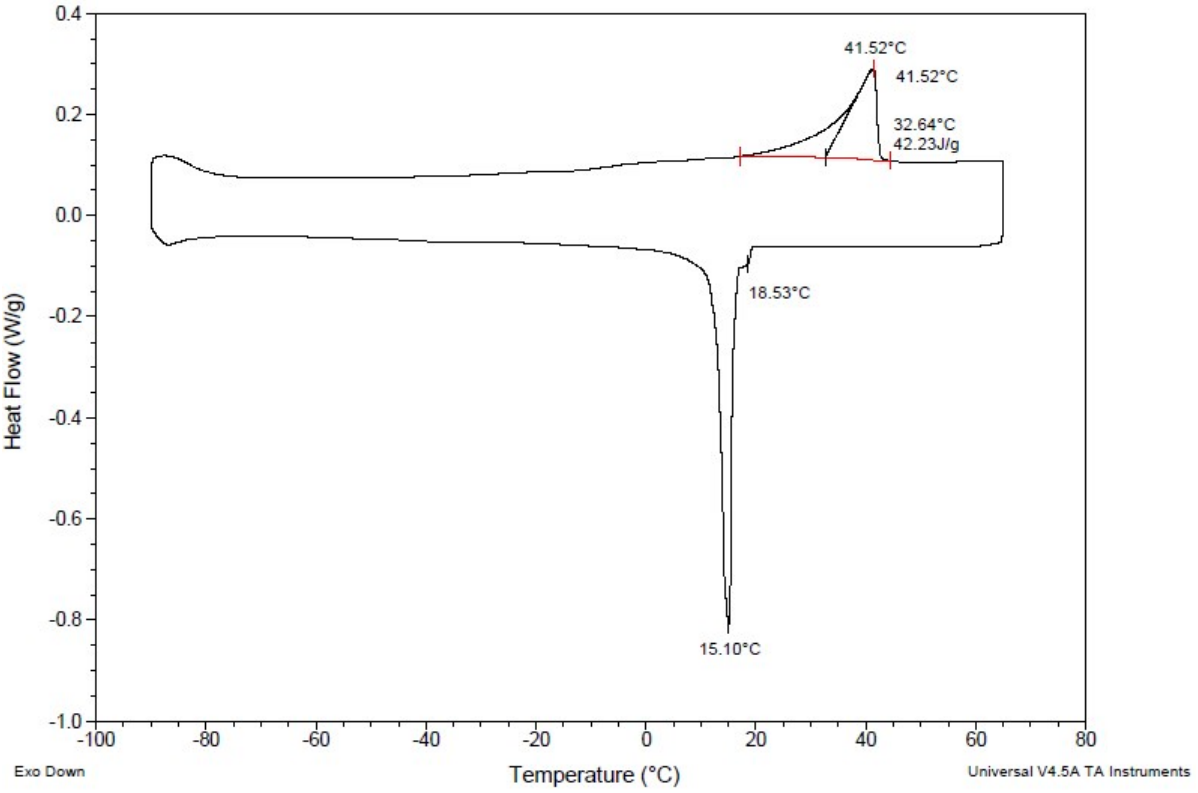

Figure S70. DSC χ_{TOPO} = 0.70 TOPO:levulinic acid

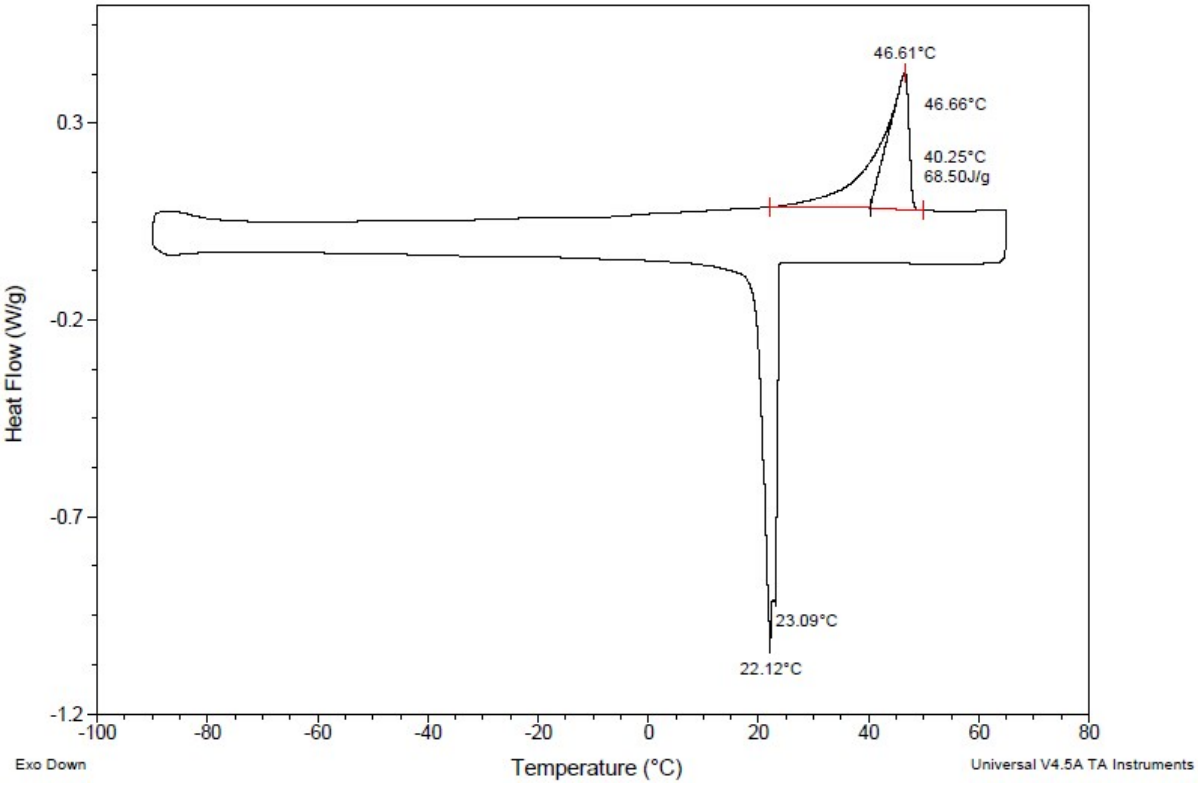

Figure S71. DSC χ_{TOPO} = 0.80 TOPO:levulinic acid

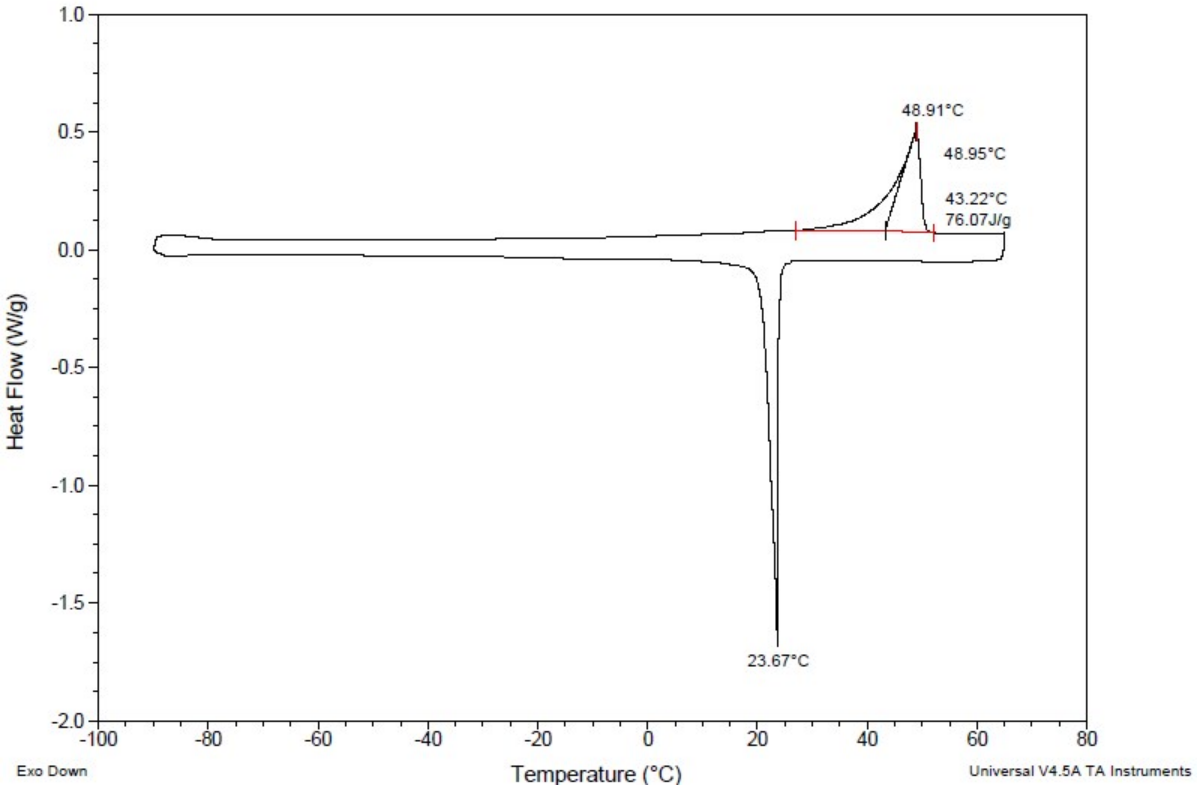

Figure S72. DSC χ_{TOPO} = 0.90 TOPO:levulinic acid

Table S15. Temperature (T_f) and enthalpy of fusion (ΔH_f) data for pure components in this work and in literature references. In this work, ΔH_f Determined from integration of DSC melting peak. [a] T_f determined from solid-liquid cell apparatus and ΔH_f not reported as sample decomposed at its melting point. [b] A higher ΔH_f value reported here is thought to be due to a greater degree of crystallinity given that the melting point agrees well with the literature.

Component	T_f / °C	ΔH_f / kJ mol^{-1}	Reference
TOPO	52	39.0	This work.
	53	53.5[b]	*Sep. Purif. Technol*., 2019, **216**, 147.
Malonic acid	137[a]	-[a]	This work.
	134	23.1	*J. Phys. Chem. A*, 2004, **108**, 3457.
	136	-	Lide, D. R., Ed. *CRC Handbook of Chemistry and Physics*, 74th ed.; CRC Press: Boca Raton, FL, 1993; p 3-311.
	136	-	*Tetrahedron*, 1963, **19**, 2061.
Levulinic acid	32	16.7[b]	This work
	33	9.2	*Thermochim. Acta*, 1991, **189**, 37.

6. ^{31}P NMR of liquid samples

6.1. TOPO:malonic acid

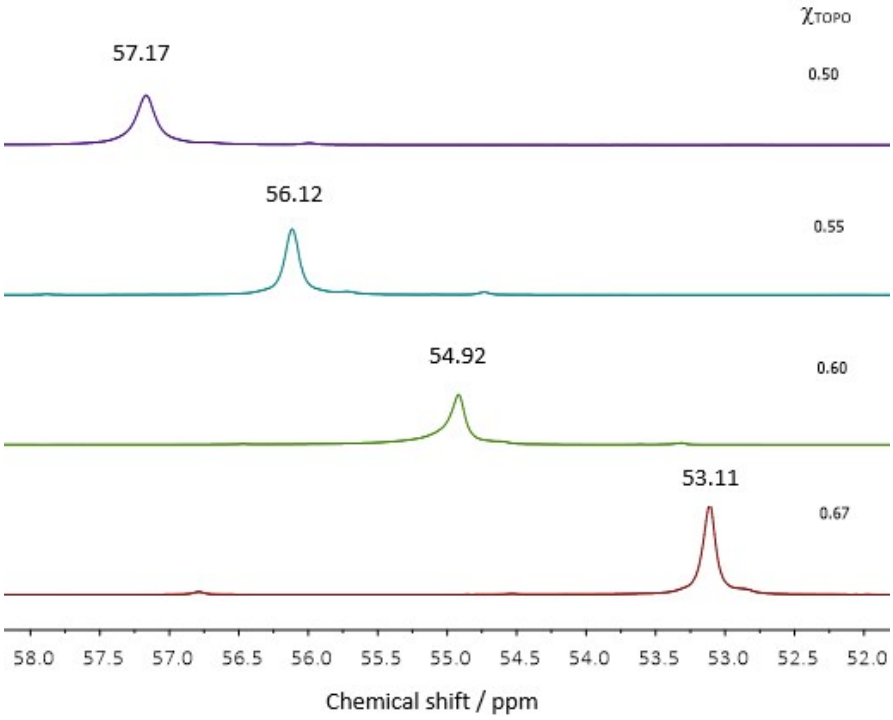

Figure S73. ^{31}P NMR spectra of liquid TOPO:malonic acid samples (neat). NMR solvent: D_3PO_4 (capillary), D_2O lock

6.2. TOPO:levulinic acid

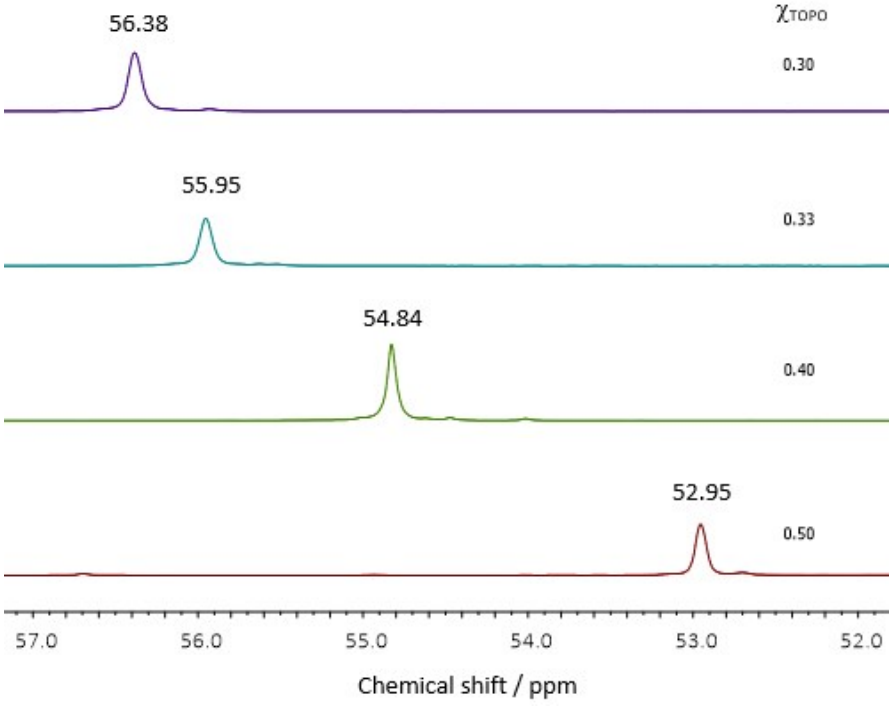

Figure S74. ^{31}P NMR spectra of liquid TOPO:levulinic acid samples (neat). NMR solvent: D_3PO_4 (capillary), D_2O lock

7. TOPO:organic acid density and molar volume

Table S16. Density of TOPO:organic acid mixtures as a function of TOPO molar ratio (χ_{TOPO}) and temperature (°C) as shown in Figures 15 and 16.

χ_{TOPO}	Density (g cm^{-3}) at temperature / °C						
	20	**25**	**30**	**35**	**40**	**45**	**50**
TOPO:malonic acid							
0.50	0.95566	0.95249	0.94917	0.94574	0.94219	0.93832	0.93393
0.55	0.94441	0.94106	0.93770	0.93432	0.93094	0.92752	0.92405
0.60	0.93282	0.92951	0.92618	0.92282	0.91941	0.91596	0.91236
0.67	0.92060	0.91732	0.91401	0.91069	0.90736	0.90399	0.90061
TOPO:levulinic acid							
0.10	1.04842	1.04448	1.04050	1.03652	1.03253	1.02854	1.02456
0.20	0.97337	0.96961	0.96584	0.96209	0.95836	0.95461	0.95089
0.30	0.96738	0.96373	0.96009	0.95644	0.95280	0.94918	0.94555
0.33	0.95942	0.95581	0.95220	0.94859	0.94499	0.94139	0.93780
0.40	0.94370	0.94015	0.93660	0.93306	0.92953	0.92600	0.92247
0.50	0.92604	0.92258	0.91911	0.91564	0.91218	0.90873	0.90527

Table S17. Molar volume of TOPO:organic acid mixtures as a function of TOPO molar ratio (χ_{TOPO}) and temperature (°C) as shown in Figures 15 and 16.

χ_{TOPO}	Molar volume (cm^3 mol^{-1}) at temperature / °C						
	20	**25**	**30**	**35**	**40**	**45**	**50**
TOPO:malonic acid							
0.50	256.7	257.6	258.5	259.4	260.4	261.5	262.7
0.55	274.8	275.7	276.7	277.7	278.7	279.8	280.8
0.60	293.3	294.4	295.4	296.5	297.6	298.7	299.9
0.67	318.7	319.8	321.0	322.2	323.3	324.6	325.8
TOPO:levulinic acid							
0.10	136.6	137.1	137.6	138.1	138.7	139.2	139.7
0.20	174.9	175.6	176.2	176.9	177.6	178.3	179.0
0.30	203.9	204.7	205.5	206.3	207.0	207.8	208.6
0.33	214.1	214.9	215.7	216.5	217.3	218.2	219.0
0.40	237.7	238.6	239.5	240.4	241.3	242.3	243.2
0.50	271.5	272.5	273.5	274.5	275.6	276.6	277.7

Table S18. Absolute average deviation of data fitted to linear trendline y = a + b*T* as a function of composition for TOPO:malonic acid and TOPO:levulinic acid mixtures. The units for density and molar volume data are g cm^{-3} and cm^3 mol^{-1} respectively

Mixture	χ_{TOPO}	**Absolute average deviation of the fit / x10^{-5}**	
		Density (ρ)	**Molar volume (V_m)**
TOPO:malonic acid	0.50	0.4658	8.5714
	0.55	-0.4286	-5.2857
	0.60	-0.4648	-14.857
	0.67	0.4296	-4.8571
TOPO:levulinic acid	0.10	0.4658	3.5714
	0.20	0.0015	-14.0000
	0.30	0.2847	5.7143
	0.33	-0.2490	12.1429
	0.40	-0.2158	-9.5714
	0.50	0.5015	13.5714

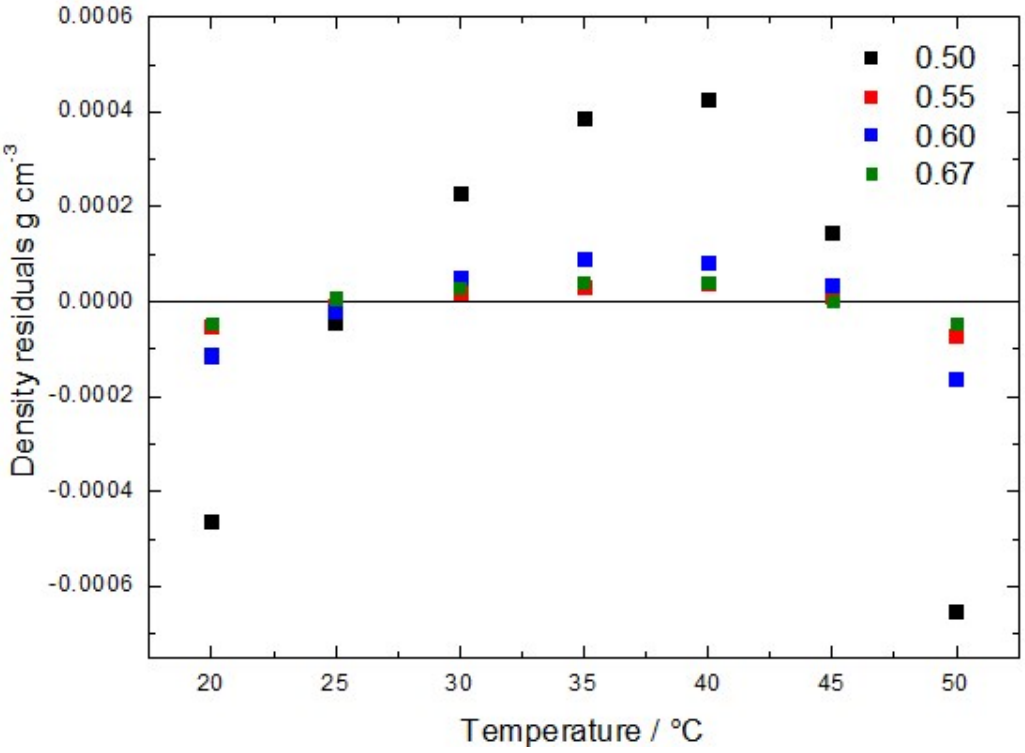

Figure S75. Residual plot of TOPO:malonic acid density data deviation from the linear trendline

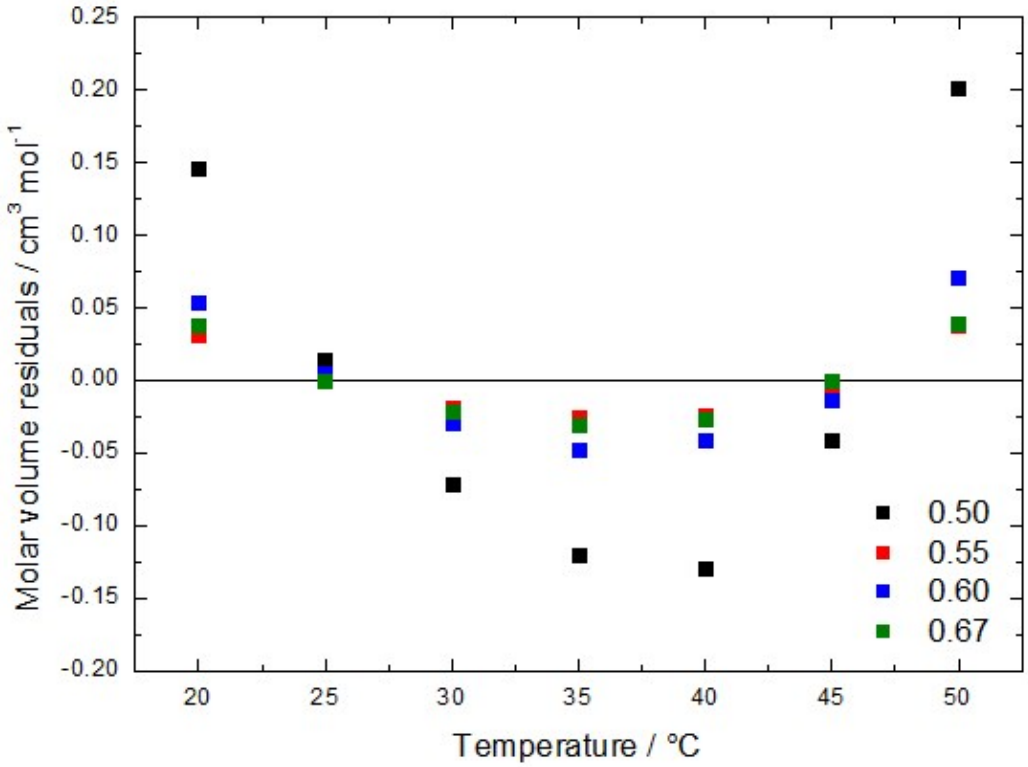

Figure S76. Residual plot of TOPO:malonic acid molar volume data deviation from the linear trendline

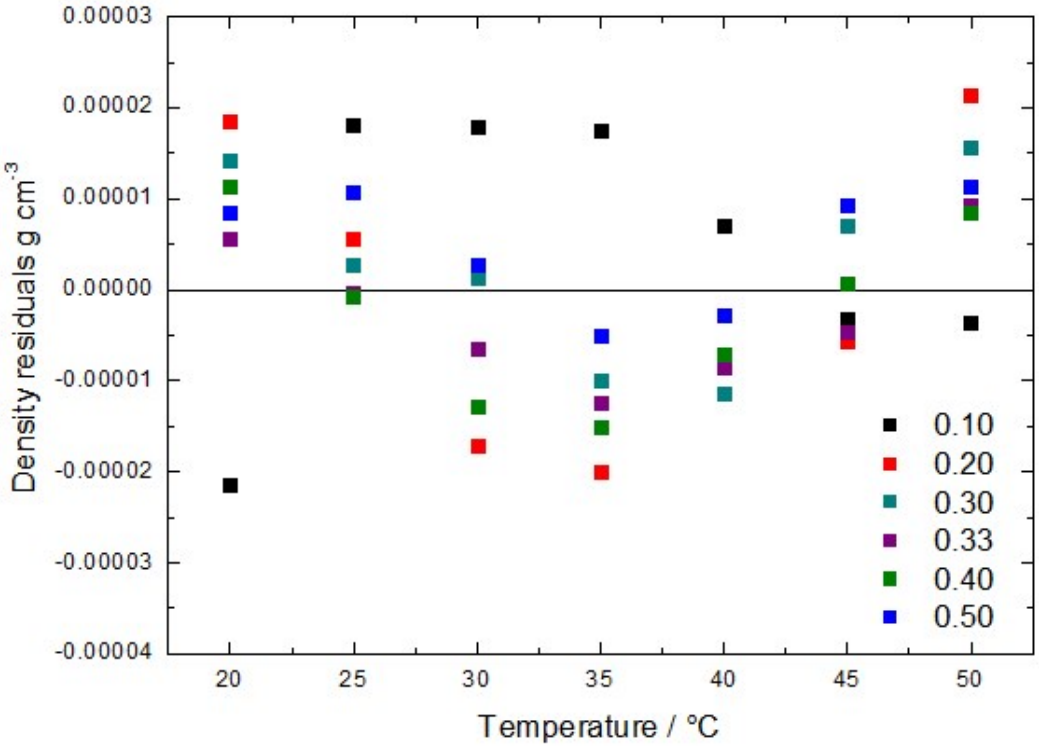

Figure S77. Residual plot of TOPO:levulinic acid density data deviation from the linear trendline

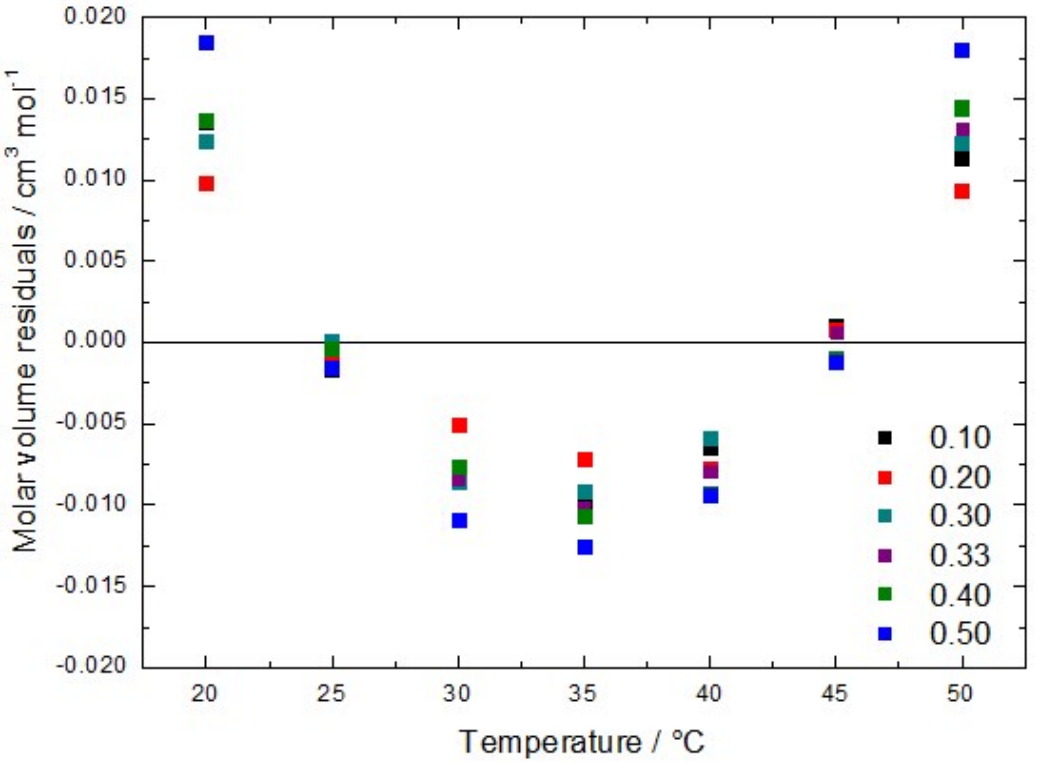

Figure S78. Residual plot of TOPO:malonic acid molar volume data deviation from the linear trendline

8. Leaching studies

Table S19. Changes to the composition of the TOPO:malonic acid eutectic mixture after contact with an equivolume aqueous phase due to malonic acid leaching to the aqueous phase.

[HCl] / M	χ_{TOPO} before contact	χ_{TOPO} after contact	$\Delta\chi_{TOPO}$
0	0.67	0.70	0.03
	0.55	0.66	0.11
6	0.67	0.79	0.12
	0.55	0.76	0.21

9. TOPO:malonic acid extraction efficiency

Table S20. Extraction of gallium from acidic chloride feed across varying HCl concentration using χ_{TOPO} = 0.67 TOPO:malonic acid as shown in Figure 16

HCl concentration / M	Extraction efficiency / %
1	50
2	79
4	100
5	100
6	100
8	100

References

1 J. Kříž, J. Dybal, E. Makrlík, J. Budka and P. Vaňura, *J. Phys. Chem. A*, 2009, **113**, 5896–5905.