Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supplementary Information

for

Synthesis of poly(bicyclohexyldimethylene terephthalate): Effect of regioisomer ratios on physical properties

Tiffany N. Thompson,[a] Alexander S. Coley[a] and Michael D. Schulz[*,a]*

Department of Chemistry, Macromolecules Innovation Institute (MII), Virginia Tech, Blacksburg, Virginia 24061, United States

Tel: 540-231-8244; Email: mdschulz@vt.edu

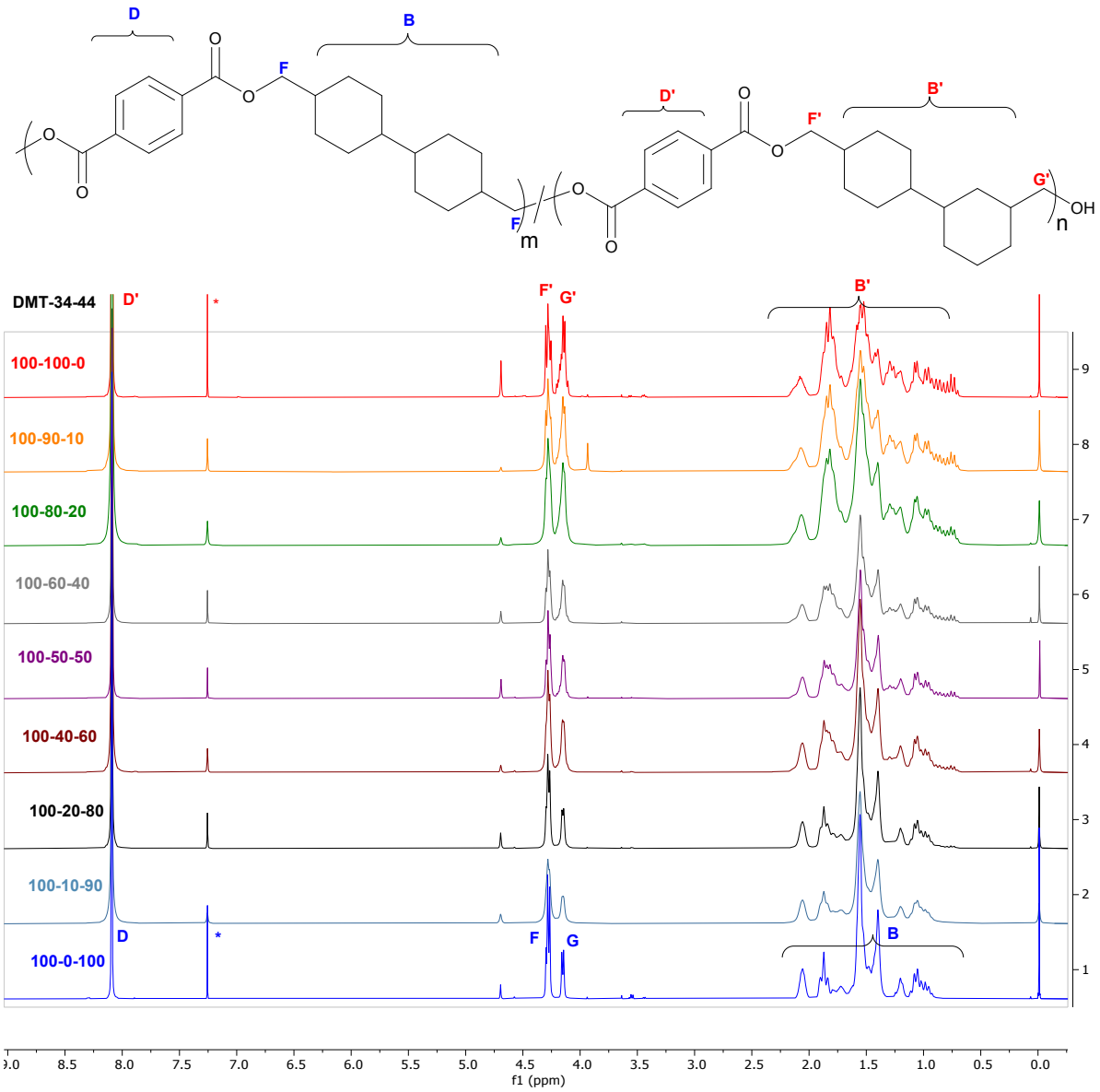

Fig. S1 ^{1}H NMR spectra of poly(bicyclohexyldimethylene terephthalate) polyester series. * - $CDCl_3$

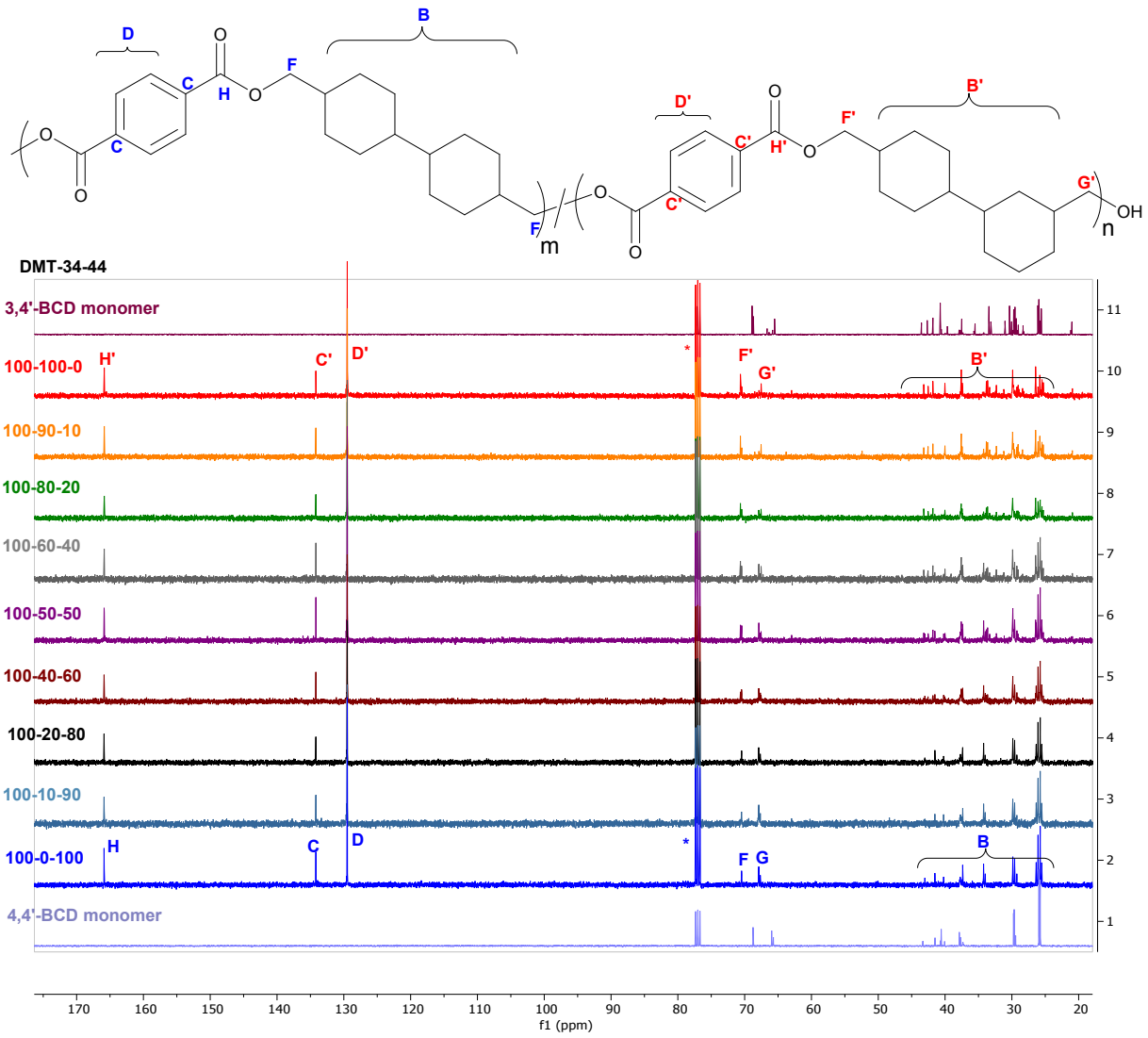

Fig. S2 ^{13}C NMR spectra of poly(bicyclohexyldimethylene terephthalate) polyester series. * - $CDCl_3$

Table S1 Summary of T_g first heat (DSC) and glassy modulus (DMA) of poly(bicyclohexyldimethylene terephthalate) polysester series.

3,4'-BCD:4,4'-BCD	[a]T_g DSC (°C)	[b]DMA Glassy Modulus (MPa) (x 10^3)
100: 0	93	3.70
90:10	95	3.77
80:20	98	3.69
60:40	95	6.15
50:50	96	2.86
40:60	96	3.27
20:80	93	3.51
10:90	96	3.27
0:100	91	6.78

[a]First heat data at a ramp rate of 10 °C min^{-1}. [b]Ramp at 3 °C min^{-1} from -140 to 150 °C at an oscillation amplitude of 15 µm and a frequency of 1Hz.

Table S2 Compilation of mechanical property data for individual runs for the poly(bicyclohexyldimethylene terephthalate) polyester series.

3,4'-BCD:4,4'-BCD	Run	Young's Modulus (MPa) (x 10^3)	Yield Strength (MPa)	Elongation at Break (%)
100:0	1	2.10	35[a]	1
	2	1.92	23[a]	0
	3	1.92	18[a]	8
80:20	1	2.04	40	7
	2	1.97	46	5
	3	1.91	39	4
50:50	1	1.66	46	34
	2	1.01	46	45
	3	1.90	46	25
	4	1.85	46	18
	5	1.93	46	42
20:80	1	1.71	47	12
	2	1.74	40	20
	3	1.58	40	5
	4	1.48	41	24
0:100	1	1.57	--	1
	2	1.48	35[a]	4
	3	1.4 1	21[a]	11

Compression molded films ~ 200 µm thick. Average 3-5 runs per composition. [a]Strength at break.

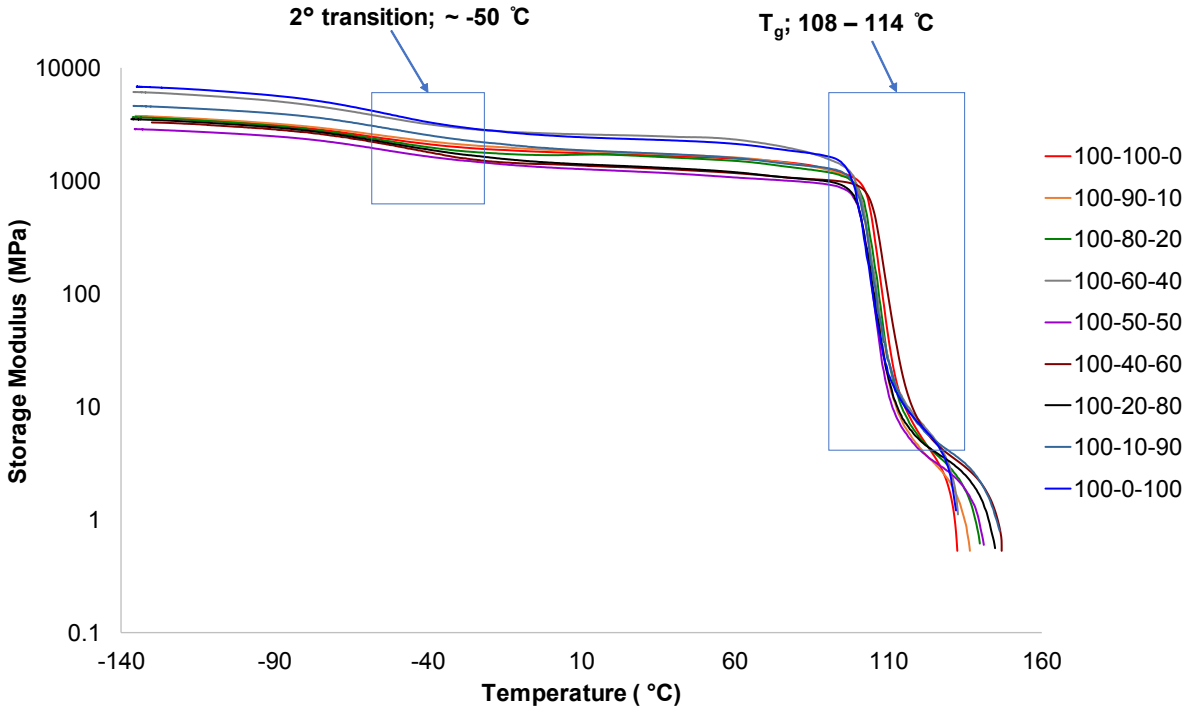

Fig. S3 DMA storage modulus vs. temperature thermogram of poly(bicyclohexyldimethylene terephthalate) polyester series at a ramp rate of 3 °C min^{-1} from -140 to 150°C at an oscillation amplitude of 15 µm and a frequency of 1Hz.

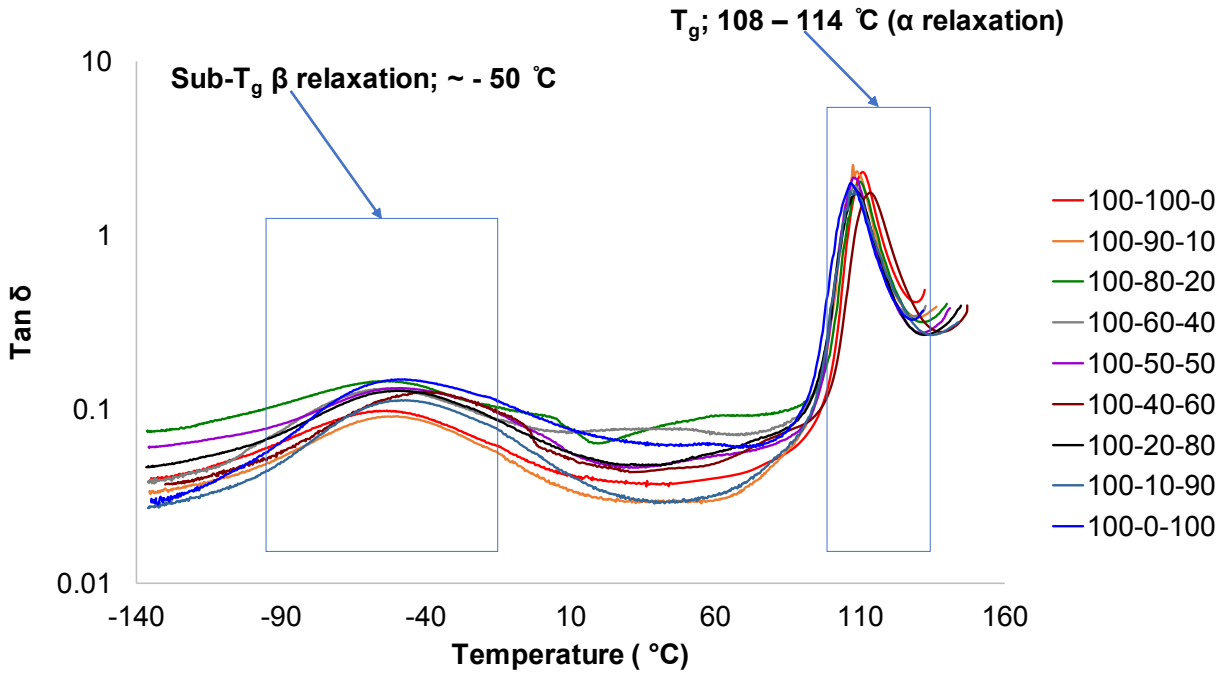

Fig. S4 DMA tan δ vs. temperature thermogram of poly(bicyclohexyldimethylene terephthalate) polyester series at a ramp rate of 3°C min-1 from -140 to 150°C at an oscillation amplitude of 15 µm and a frequency of 1Hz.

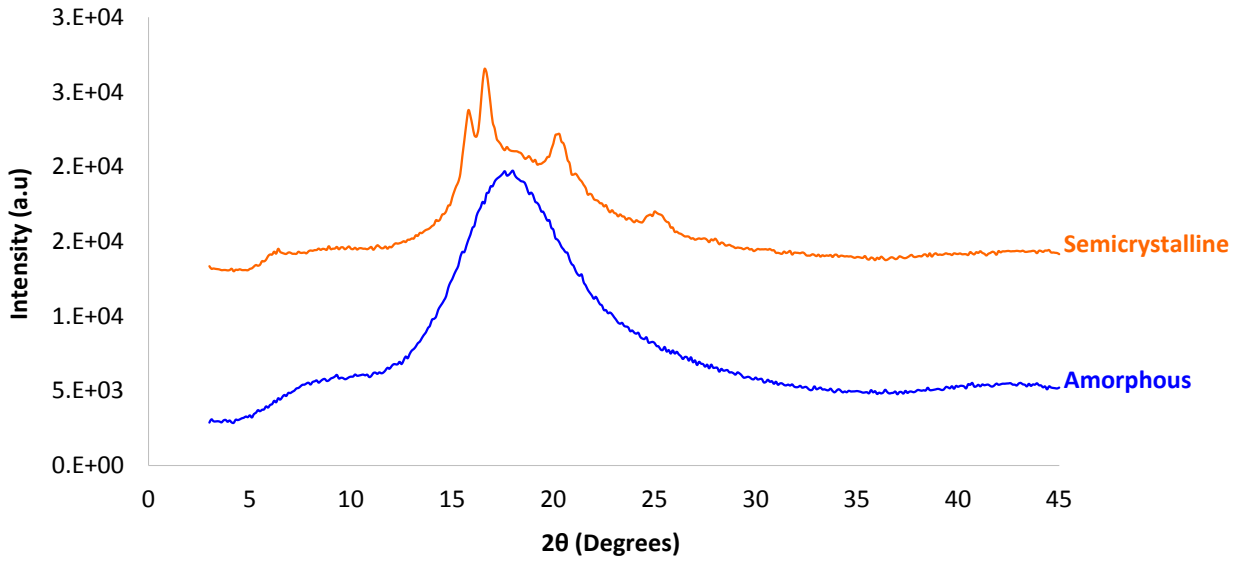

Fig. S5 X-ray diffraction patterns of amorphous and semicrystalline 4,4’-BCD hompolymer.

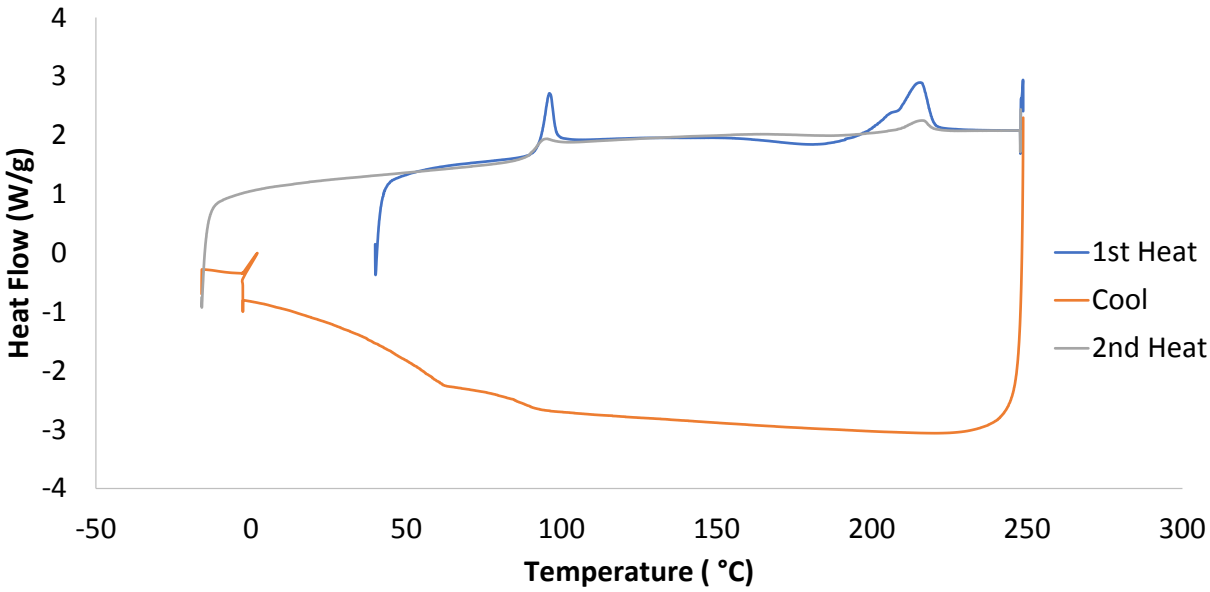

Fig. S6 DSC thermogram of heat-cool-heat cycle of 4,4'-BCD homopolymer after synthesis. Samples in ground state. Heating and cooling cycles conducted at a ramp rate of 10 °C min^{-1}.

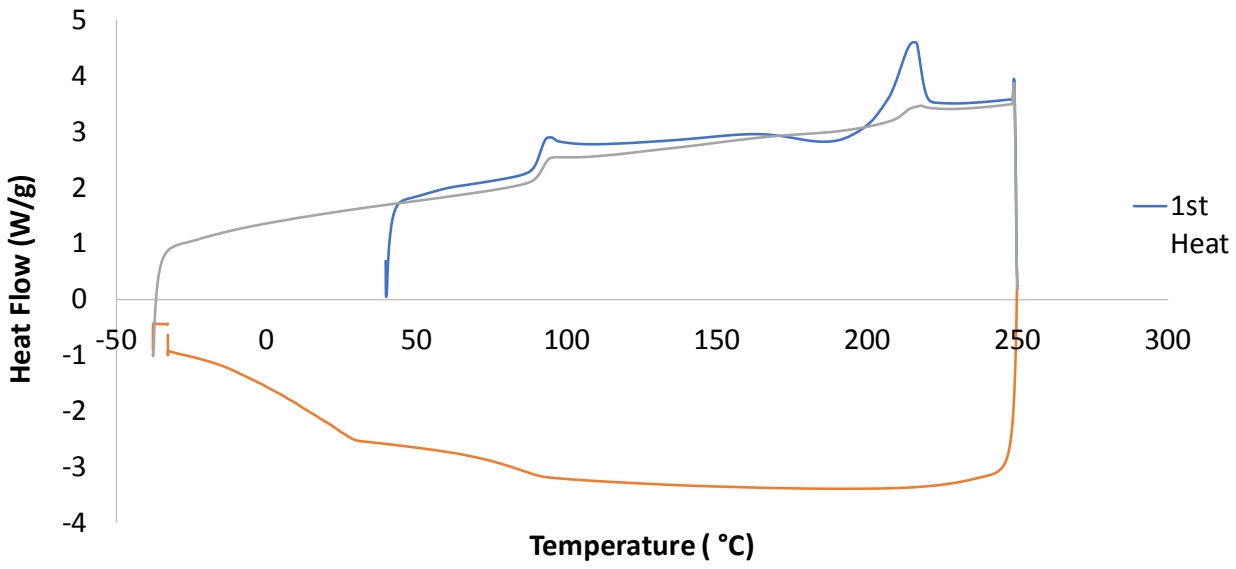

Fig. S7 DSC thermogram of heat-cool-heat cycle of 4,4'-BCD homopolymer after compression into a film. Film Sample. Heating and cooling cycles conducted at a ramp rate of 10 °C min^{-1}.

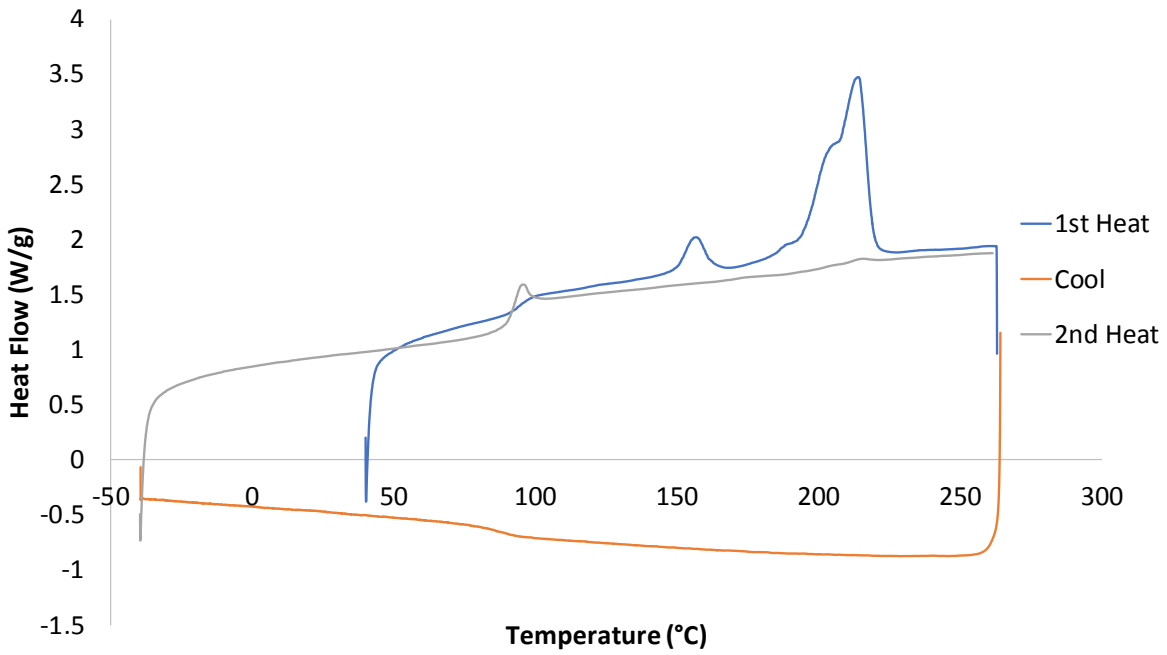

Fig. S8 DSC thermogram of heat-cool-heat cycle of 4,4'-BCD homopolymer after oven annealing of melt compressed film at 145 °C for 1h. Film Sample. Heating and cooling cycles conducted at a ramp rate of 10 °C min^{-1}.

Table S3 Amorphous density measurements of select compositions of the poly(bicyclohexyldimethylene terephthalate) series. All density measurements are in g/cm^3.

3,4'-BCD:4,4'-BCD	Run 1									
	1	2	3	4	5	6	7	8	9	10
100-100-0	1.1622	1.1602	1.1618	1.1604	1.1599	1.157	1.1602	1.1609	1.1568	1.159
100-80-20	1.1569	1.1566	1.1567	1.1573	1.1552	1.1572	1.1548	1.1558	1.1565	1.1564
100-50-50	1.1485	1.1471	1.1475	1.1497	1.1465	1.1467	1.148	1.1485	1.1475	1.1477
100-20-80	1.133	1.1305	1.1341	1.1335	1.1319	1.1321	1.1315	1.1337	1.1318	1.1297
100-0-100	1.1094	1.1096	1.1082	1.1059	1.1054	1.1068	1.1074	1.1042	1.106	1.1029

3,4'-BCD:4,4'-BCD	Run 2									
	1	2	3	4	5	6	7	8	9	10
100-100-0	1.1566	1.1565	1.1569	1.1576	1.1557	1.1551	1.1554	1.1551	1.1553	1.1553
100-80-20	1.1534	1.154	1.1535	1.1517	1.154	1.1541	1.1546	1.1541	1.1544	1.1569
100-50-50	1.1436	1.1441	1.1444	1.1435	1.1451	1.144	1.1449	1.1448	1.1426	1.1426
100-20-80	1.1316	1.1278	1.1302	1.1319	1.13	1.129	1.128	1.1295	1.1301	1.1298
100-0-100	1.1012	1.0999	1.1015	1.1004	1.1022	1.1045	1.0997	1.1014	1.1005	1.1002

3,4'-BCD:4,4'-BCD	Run 3									
	1	2	3	4	5	6	7	8	9	10
100-100-0	1.157	1.1611	1.156	1.1562	1.1563	1.1559	1.1568	1.1541	1.1597	1.1588
100-80-20	1.157	1.1611	1.156	1.1562	1.1563	1.1559	1.1568	1.1541	1.1597	1.1588