Supporting Information Appendix for

Computational and Experimental Investigations of One-step Conversion of Poly(carbonate)s into Value-Added Poly(aryl ether sulfone)s

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Part I: Experimental Procedures

Materials and Methods. Anhydrous N-cyclohexyl-2-pyrrolidone (CHP) and poly(bisphenol A carbonate) (PC) were used as received from Aldrich. 4,4'-Difluorodiphenylsulfone was purchased from Aldrich, recrystallized from ethanol and dried in a vacuum oven overnight prior to use and potassium carbonate (K_2CO_3) was purchased from Aldrich, ground with a mortar and pestle and dried in a vacuum oven prior to use. d_6-DMSO was purchased from Cambridge Isotope Laboratories (CIL) and used as received. ^{1}H NMR spectra were recorded on a Bruker Avance 400 spectrometer (400 MHz). Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (d_6-DMSO: δ 2.50 ppm). ^{13}C NMR spectra were recorded on a Bruker Avance 400 spectrometer (100 MHz) and chemical shifts are reported in ppm with the solvent resonance as the internal standard (d_6-DMSO: δ 39.51 ppm). Infrared (IR) spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR Alpha spectrophotometer using a Nicolet OMNI-Sampler ATR Smart-Accessory, ν_{max} in cm^{-1}. Gel permeation chromatography (GPC) was performed in THF using a Waters system equipped with four 5-μm Waters columns (300 mm × 7.7 mm) connected in series with an increasing pore size (100, 1000, 10^5, 10^6 Å), a Waters 410 differential refractometer, and a 996 photodiode array detector. The system was calibrated with polystyrene standards. Differential scanning calorimetry (DSC) analyses were performed on a TA Instruments Q2000. The samples (~5 mg) were scanned from 22 °C to 300 °C at a 5 °C/min

heating rate in aluminum closed pans. For absolute molecular weight determination, a GPC system was equipped with a Waters Corp. - 717 auto sampler, 515 HPLC pump, and Styragel High Resolution GPC column bank (Styragel HR1, HR2, HR4E, and HR5E). Elution solvent used was THF (HPLC grade) with flow rate of 1 mL/min at ambient temperature. Light Scattering and refractive index was measured with detectors by Wyatt Technology – Dawn Hellos-II MALS (multi-angle light scattering) with QELS (Quasi-Elastic light scattering) dynamic light scattering module, and Optilab DSP Interferometic refractometer (RI - concentration detector).

Representative Procedure for one-pot depolymerization of PC to PSU: Poly(bisphenol A carbonate) pellets (M_w ~ 32,800 Da, M_n ~ 11,600 Da; 0.256 g, 1.0 mmol, 1.0 equiv.), 4,4'-difluorodiphenylsulfone (0.254 g, 1.0 mmol, 1.0 equiv.), potassium carbonate (0.145 g, 0.105 mmol, 1.05 equiv.), and CHP (3.0 g, ~21 wt % solids) were weighed into pre-dried 20 mL vial in the glovebox equipped with stirbar. The vial was capped and removed from the glovebox, and a septum was attached, sealed with Teflon and electrical tape, and a nitrogen inlet needle and an exit needle was inserted into the septum so that the solution slowly concentrated over the course of the polymerization. The reaction mixture was allowed to heat at 190 °C for 18 hours before removing from heat, allowing to cool, and adding 5 mL CH_2Cl_2. The viscous polymer solution was added dropwise to 50 mL of benchtop methanol at room temperature and an off-white precipitate formed. The polymer precipitate was filtered and dried in a vacuum oven overnight to yield 0.373 g of an off-white powder (M_w ~ 15,500 Da, M_n ~7,400 Da, PDI ~2.09 by GPC, T_g ~ 180 °C, T_d[1%] ~350 °C, 94% yield). IR (cm^{-1}): 3066 (w), 2967 (m), 2872 (w), 1586 (s), 1502 (s), 1488 (s), 1323 (m), 1294 (m), 1244 (s), 1169 (s), 1151 (s). ^{1}H NMR (d_6-DMSO): δ 7.88 (br s, 4 H), 7.27 (br s, 4 H), 7.03 (br s, 8 H), 1.63 (br s, 6 H) ppm. ^{13}C NMR (d_6-DMSO): δ 130.2, 128.4, 120.2, 117.8, 30.3 ppm.

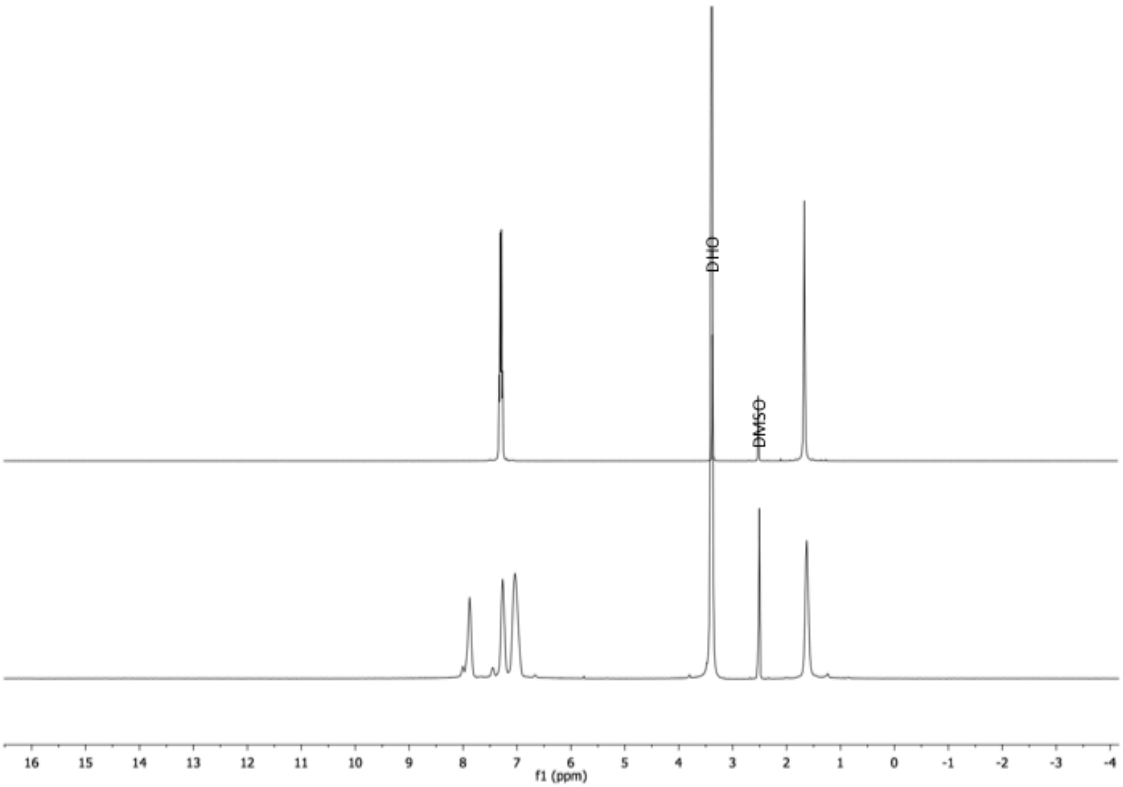


Figure S1. ^{1}H NMR Overlay of commercial PC (top trace) before depolymerization and PSU post-polymerization (d_6-DMSO).

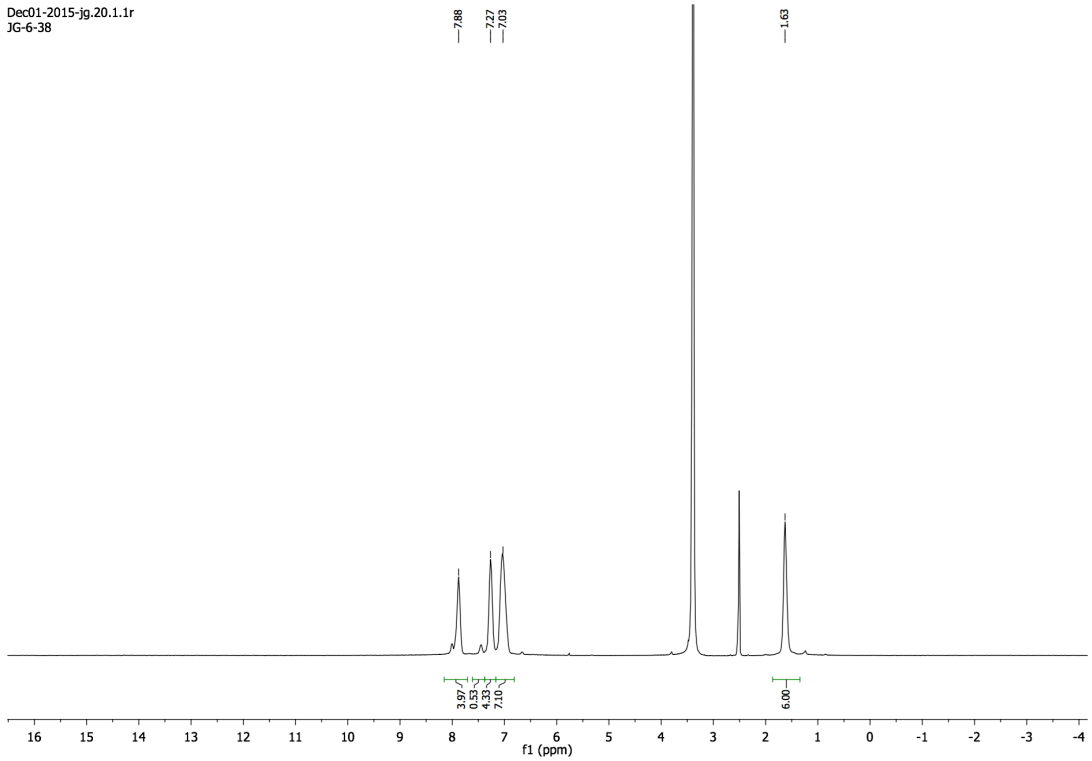


Figure S2. ^{1}H NMR of isolated PSU after *in-situ* repolymerization sequence.

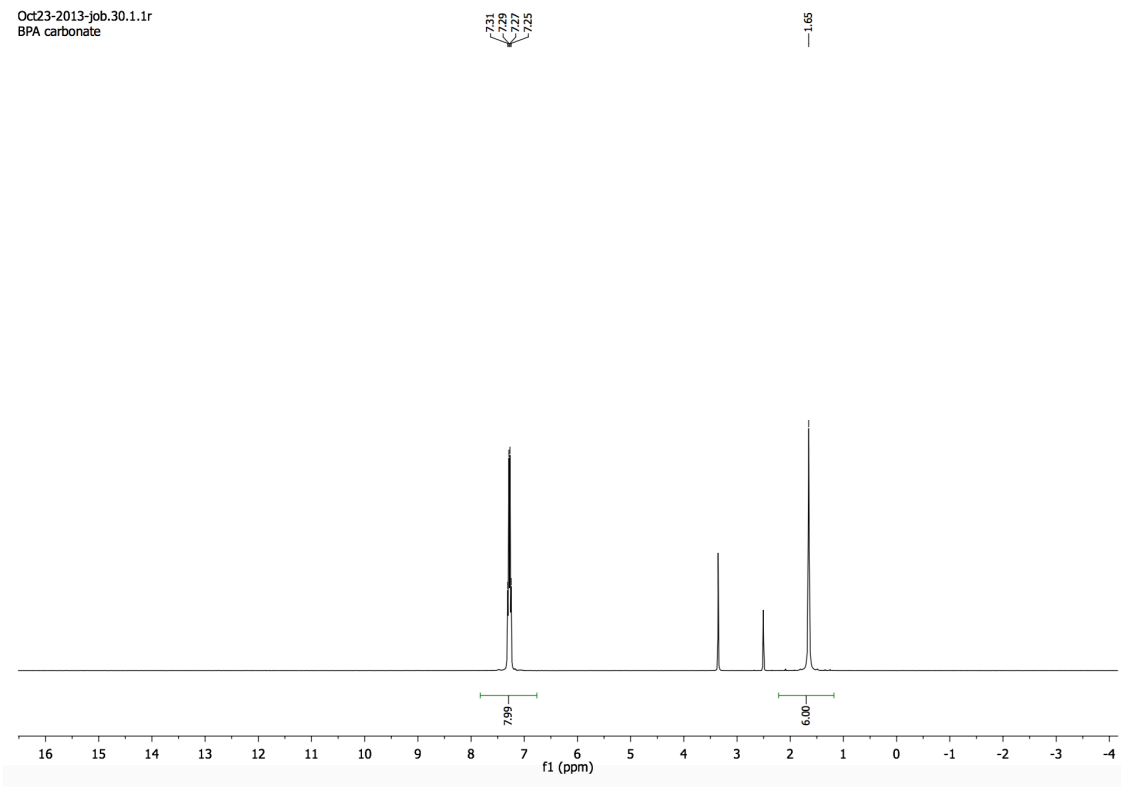


Figure S3. ^{1}H NMR of commercial poly(BPA carbonate) (PC) prior to depolymerization.

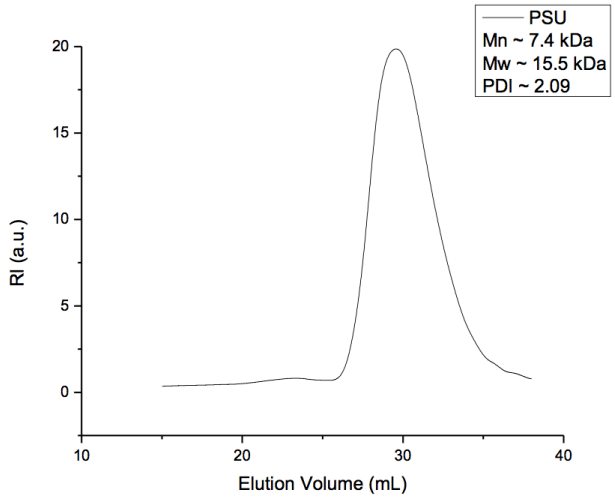


Figure S4. GPC trace of PSU after isolation (Mn ~7.4 kDa, Mw ~15.5 kDa, PDI ~ 2.09 in THF, calibrated with polystyrene standards, elution rate = 1 mL/min).

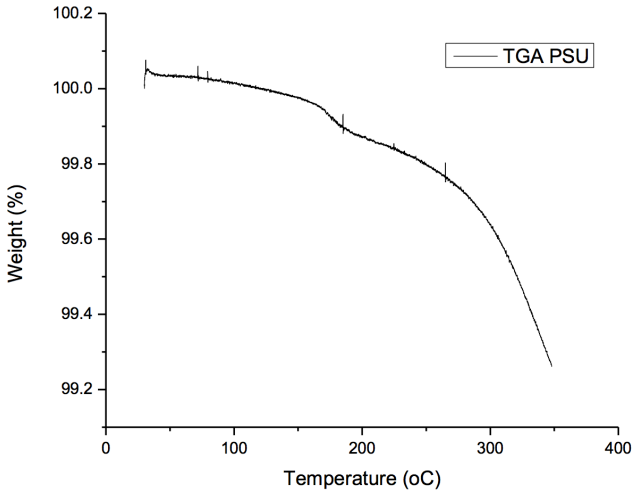


Figure S5. TGA trace of PSU derived from PC (T_d[1%] ~350 °C).

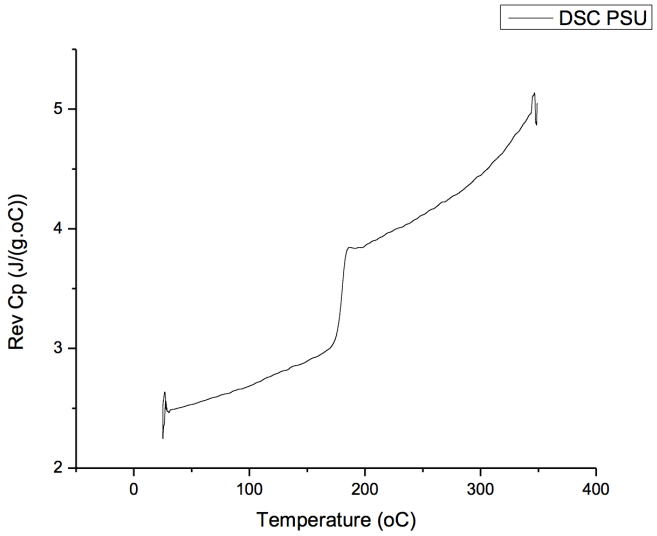


Figure S6. DSC trace of PSU derived from PC (T_g =180.73 °C).

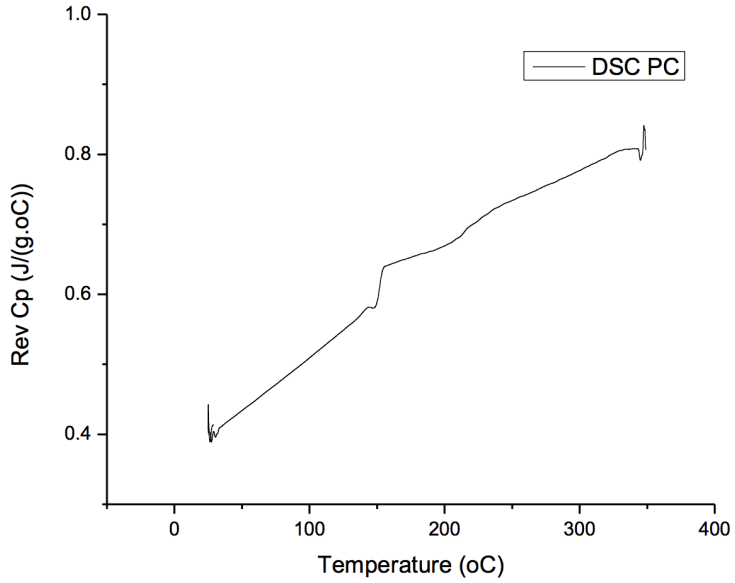


Figure S7. DSC trace of PC starting material (T_g =151.37 °C).

PSU synthesis from BPA (control): Bisphenol A (0.228 g, 1.0 mmol, 1.0 equiv.), 4,4'-difluorodiphenylsulfone (0.254 g, 1.0 mmol, 1.0 equiv.), potassium carbonate (0.145, 0.105 mmol, 1.05 equiv.), and CHP (3.0 g, ~21 wt % solids) were weighed into pre-dried 20 mL vial in the glovebox equipped with stirbar and identical procedure was followed as for the one-pot depolymerization/repolymerization (M_w = 69.5 kDa, M_n = 42.5 kDa, PDI = 1.63 by GPC). Intrinsic viscosity (η) = 0.3943, T_g ~ 187 °C.

Depolymerization studies:

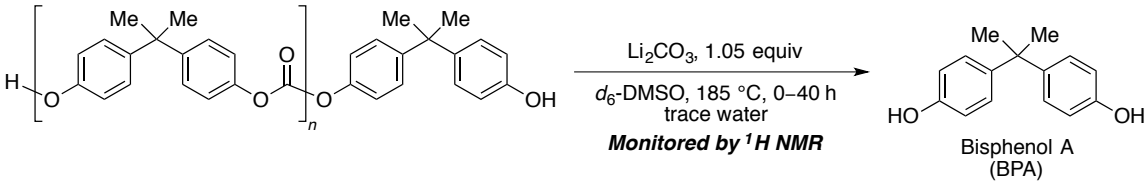


Figure S8. *In-situ* monitoring of base-mediated depolymerization of PC to BPA.

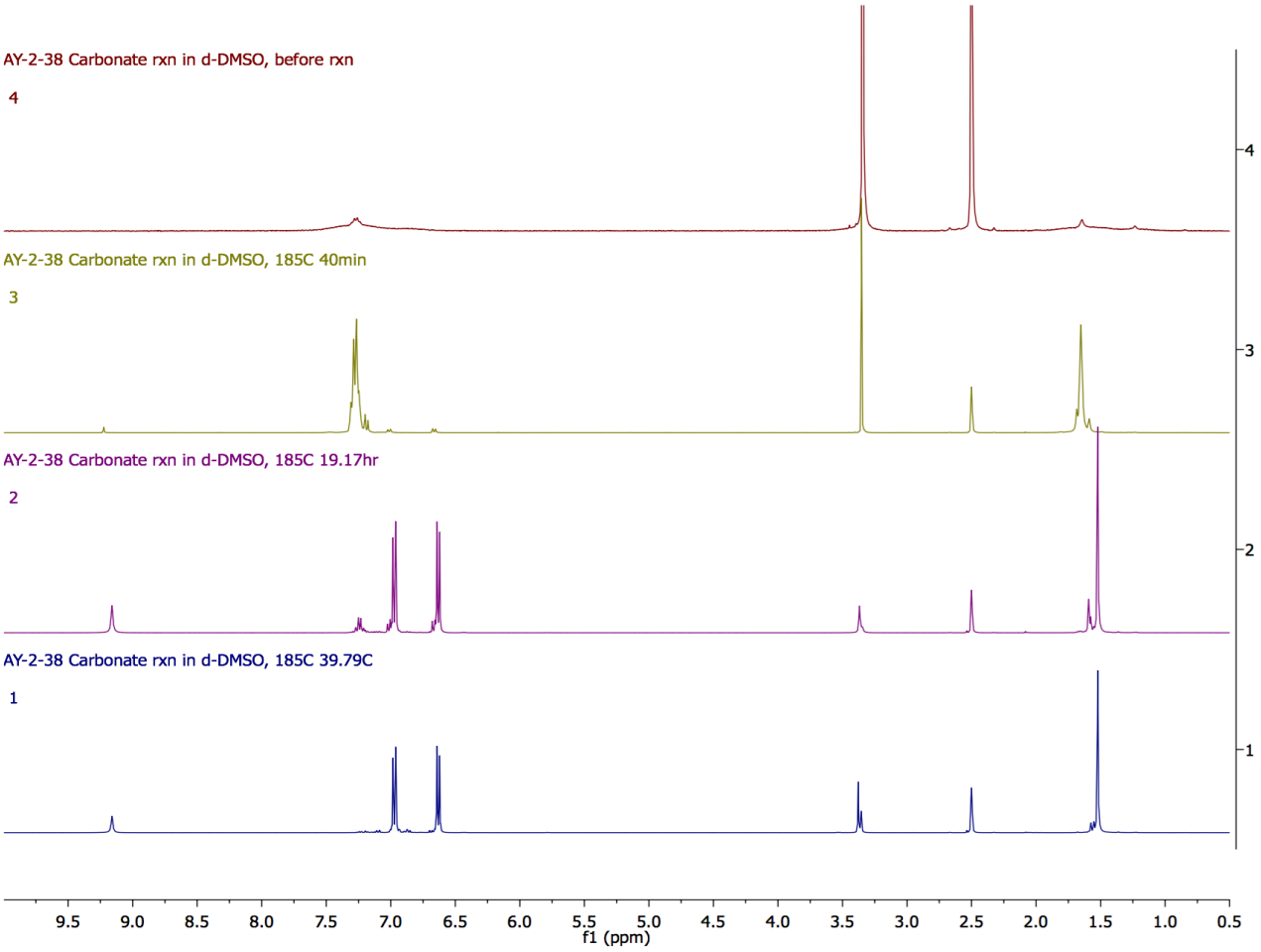


Figure S9. ^{1}H NMR Study of the depolymerization of commercial PC with stoichiometric Li_2CO_3 at 185 °C in d_6-DMSO over 40 h.

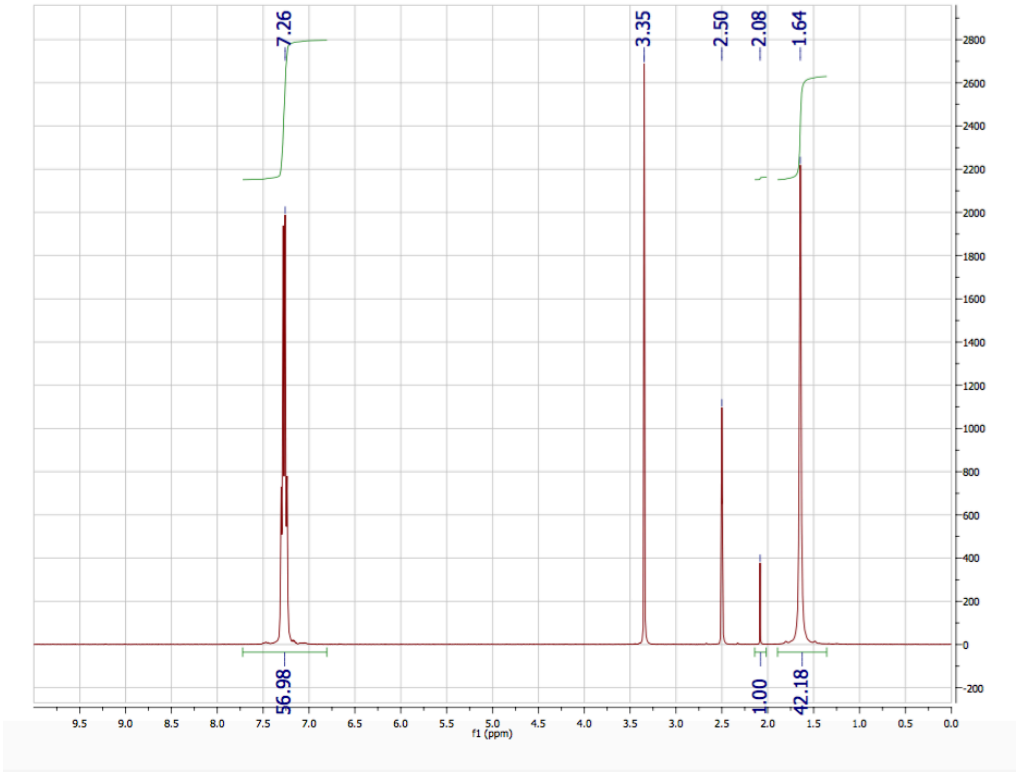
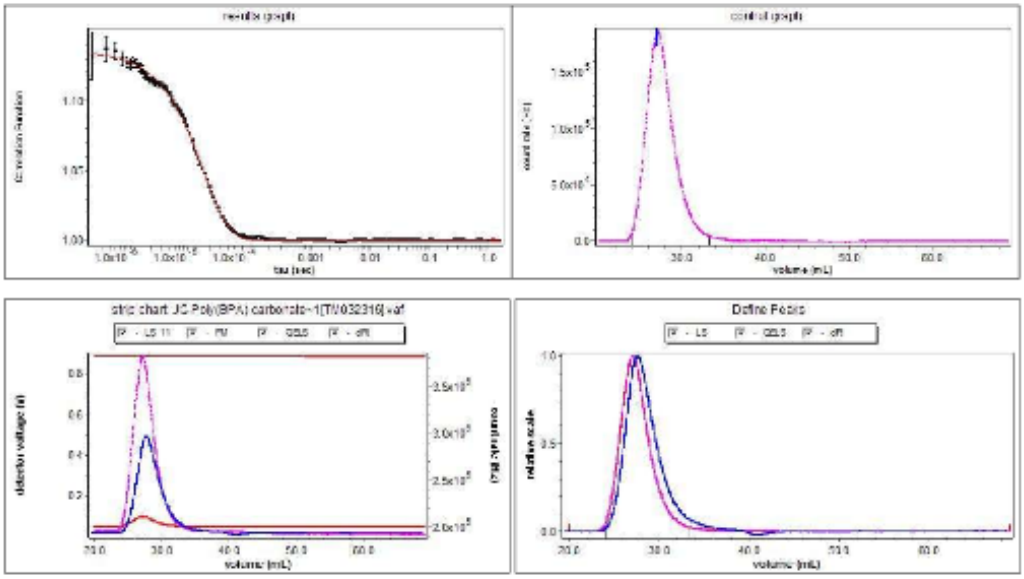


Figure S10. ^{1}H NMR spectra of PC after heating in d_6-DMSO for 3.5 h. No depolymerization of PC was observed within this timeframe.

ASTRA 5.3.4 Summary Report for JG Poly(BPA) carbonate~1[TM032316].vaf

Experiment name: C:\Documents and Settings\Administrator\My Documents\ASTRA V\Data\ JG Poly(BPA) carbonate~1[TM032316].vaf
Sample: JG Poly(BPA) carbonate (JG Poly(BPA) carbonate)
Processing Operator: Thermal Lab
Collection Operator: Thermal Lab
Collection Astra Version: 5.3.4.20



CONFIGURATION

Light scattering instrument: DAWN HELEOS
- **Cell type:** X5
- **Laser wavelength:** 658.0 nm
- **Calibration constant:** 5.0353e-5 1/(V cm)
- **Replaced detector:** 12
- **Temperature control:** n/a
- **Temperature:** n/a

RI instrument: Optilab DSP
UV instrument: n/a
QELS instrument:
- **Model:** Wyatt QELS+
- **Use temperature probe:** yes

Solvent: thf
- **Refractive index:** 1.402
- **Viscosity:** 4.5600e-3 g/(cm sec) (valid if QELS temperature not used)

Flow rate: 1.000 mL/min

PROCESSING

Processing time: Thursday March 24, 2016 10:08 AM Pacific Daylight Time
Collection time: Wednesday March 23, 2016 06:42 PM Pacific Daylight Time
QELS delay time range: 2.00e-7 to 1.00 sec
QELS threshold values: 1.0 to 300.0 nm
Detectors used: 4 5 6 7 8 9 10 11 13 14 15 16 17 18
Concentration detector: RI
Mass results fitting: none (fit degree: n/a)
Radius results fitting: none (fit degree: n/a)

	Peak 1
Peak limits (mL)	24.097 - 33.324
dn/dc (mL/g)	0.156
A_2 (mol mL/g^2)	0.000
UV ext. (mL/(g cm))	0.000
Model	Zimm
Fit degree	1
Injected mass (g)	0.0000

JG Poly(BPA) carbonate~1[TM032316].vaf

Calc. mass (g) 2.2640e-3

RESULTS

	Peak 1
Polydispersity	
Mw/Mn	1.161 (1%)
Mz/Mn	1.372 (1%)
Molar mass moments (g/mol)	
Mn	2.014e+4 (1%)
Mp	2.341e+4 (0.2%)
Mv	n/a
Mw	2.338e+4 (0.6%)
Mz	2.763e+4 (1%)
rms radius moments (nm)	
Rn	15.7 (17%)
Rw	14.3 (15%)
Rz	15.4 (12%)
Hydrodynamic radius moments (nm)	
Rh(n)	6.5 (74%)
Rh(w)	6.7 (45%)
Rh(z)	6.5 (30%)
Translational diffusion moments (cm²/sec)	
Dt(n)	9.92e-7 (25%)
Dt(w)	9.56e-7 (22%)
Dt(z)	9.71e-7 (17%)

Figure S11. Absolute molecular weight determination of PC starting polymer through the use of light scattering detection and GPC.

ASTRA 5.3.4 Summary Report for JG 6-38~1[TM032316].vaf

Experiment name: C:\Documents and Settings\Administrator\My Documents\ASTRA V\Data\JG 6-38~1[TM032316].vaf
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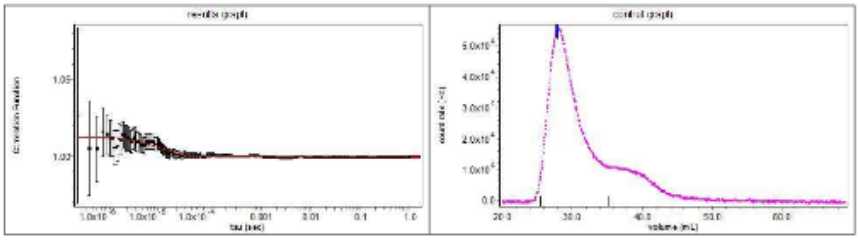
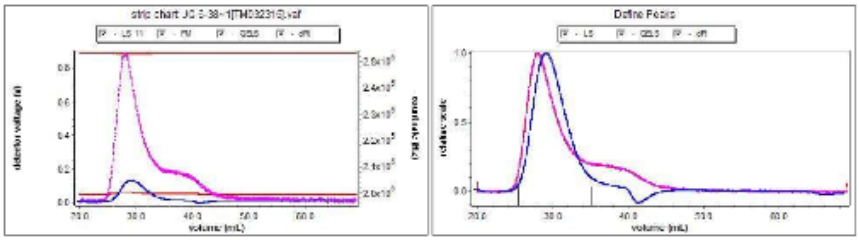
Processing Operator: Thermal Lab
Collection Operator: Thermal Lab
Collection Astra Version: 5.3.4.20





CONFIGURATION

Light scattering instrument: DAWN HELEOS
- **Cell type:** X5
- **Laser wavelength:** 658.0 nm
- **Calibration constant:** 3.0353e-5 1/(V cm)
- **Replaced detector:** 12
- **Temperature control:** n/a
- **Temperature:** n/a

RI instrument: Optilab DSP
UV instrument: n/a
QELS instrument:
- **Model:** Wyatt QELS+
- **Use temperature probe:** yes

Solvent: thf
- **Refractive index:** 1.402
- **Viscosity:** 4.5600e-3 g/(cm sec) (valid if QELS temperature not used)

Flow rate: 1.000 mL/min

PROCESSING

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Collection time: Wednesday March 23, 2016 05:31 PM Pacific Daylight Time
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QELS threshold values: 1.0 to 300.0 nm
Detectors used: 6 7 8 9 10 11 13 14 15 16
Concentration detector: RI
Mass results fitting: none (fit degree: n/a)
Radius results fitting: none (fit degree: n/a)

	Peak 1
Peak limits (mL)	25.472 - 35.072
dn/dc (mL/g)	0.156
A_2 (mol mL/g^2)	0.000
UV ext. (mL/(g cm))	0.000
Model	Zimm
Fit degree	1
Injected mass (g)	0.0000

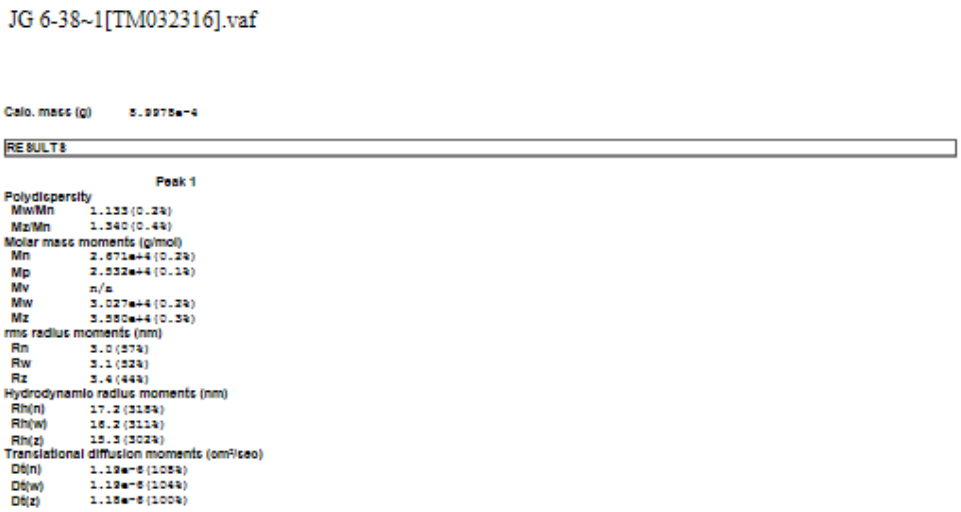

Figure S12. Absolute molecular weight determination by light scattering detection for PSU after depolymerization/repolymerization sequence.

Multi-gram synthesis of PSU from PC: Poly(bisphenol A carbonate) pellets (M_w ~ 32,800 Da, M_n ~ 11,600 Da; 2.53 g, 9.9 mmol, 1.0 equiv.), 4,4'-difluorodiphenylsulfone (2.52 g, 9.9 mmol, 1.0 equiv.), and CHP (21.5 g, ~30 wt % solids) were weighed into a 100-mL container in the glovebox equipped with stirbar. The solution was heated until homogenous and removed from the glove box. The solution was transferred to a 100-mL round bottom flask with stir bar and septa under an active nitrogen flow through an inlet and exit needle. Potassium carbonate (1.44 g, 10.4 mmol, 1.05 equiv.), was added in one portion and the viscous solution was allowed to heat for 18 h at 190 °C before precipitation of the polymer in methanol. An off-white solid was collected and analyzed by GPC (see Figure S13, M_w ~ 20 kDa, M_n ~ 10 kDa, PDI = 1.94).

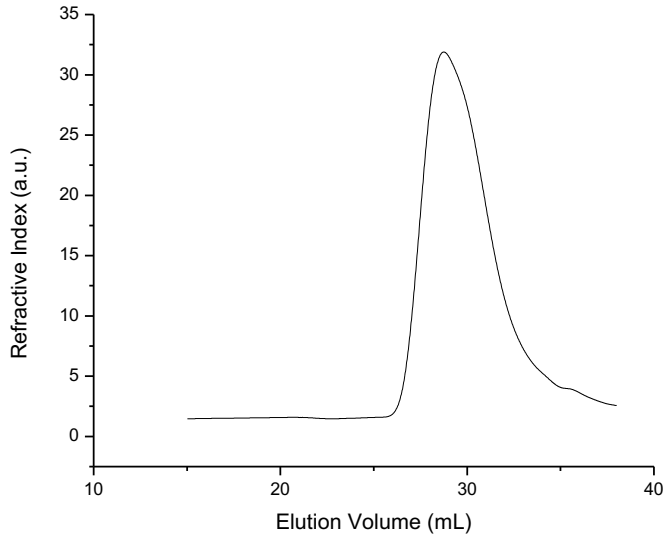

Figure S13. GPC trace of PSU isolated from multi-gram scale depolymerization/repolymerization reaction (M_w = 19,885 Da, M_n = 10,262 Da, PDI = 1.94 in THF calibrated with polystyrene standards, elution rate = 1 mL/min).

Synthesis of PSU from PC with catalytic K_2CO_3: Poly(bisphenol A carbonate) pellets (M_w ~ 32,800 Da, M_n ~ 11,600 Da; 0.304 g, 1.18 mmol, 1.0 equiv.), 4,4'-difluorodiphenylsulfone (0.301 g, 1.18 mmol, 1.0 equiv.), potassium carbonate (0.020 g, 0.144 mmol, 0.12 equiv.), and NMP (3.0 g, ~ 21 wt % solids) were weighed into pre-dried 20 mL vial in the glovebox equipped with stirbar and identical procedure was followed as for the one-pot depolymerization/repolymerization. A crude sample was first analyzed by NMR (Figures S15B and S16A) and GPC (Figure S14, M_w ~ 6.0 kDa, M_n = 3.7 kDa, PDI = 1.64). Macromolecular species were then isolated by precipitation into 15 mL *i*-PrOH and analyzed by NMR (Figures S15A and S16B) and GPC (Figure S14, M_w ~ 6.5 kDa, M_n ~ 4.1 kDa, PDI = 1.57).

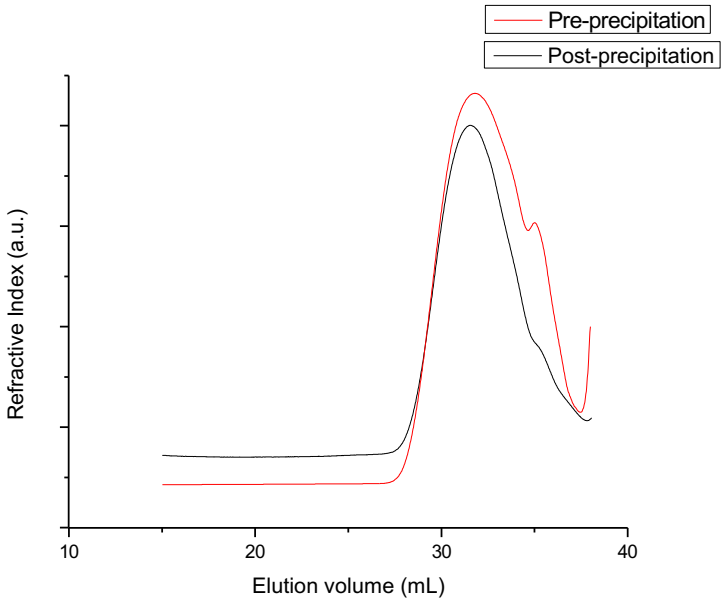

Figure S14. Overlay of GPC data from catalytic reaction with 12 mol % K_2CO_3. Red and black traces are before and after fractional precipitation, respectively. Prior to precipitation: M_n = 3,672 Da, M_w = 6,024 Da, PDI = 1.64. After precipitation: M_n = 4,100 Da, M_w = 6,451 Da, PDI = 1.57.

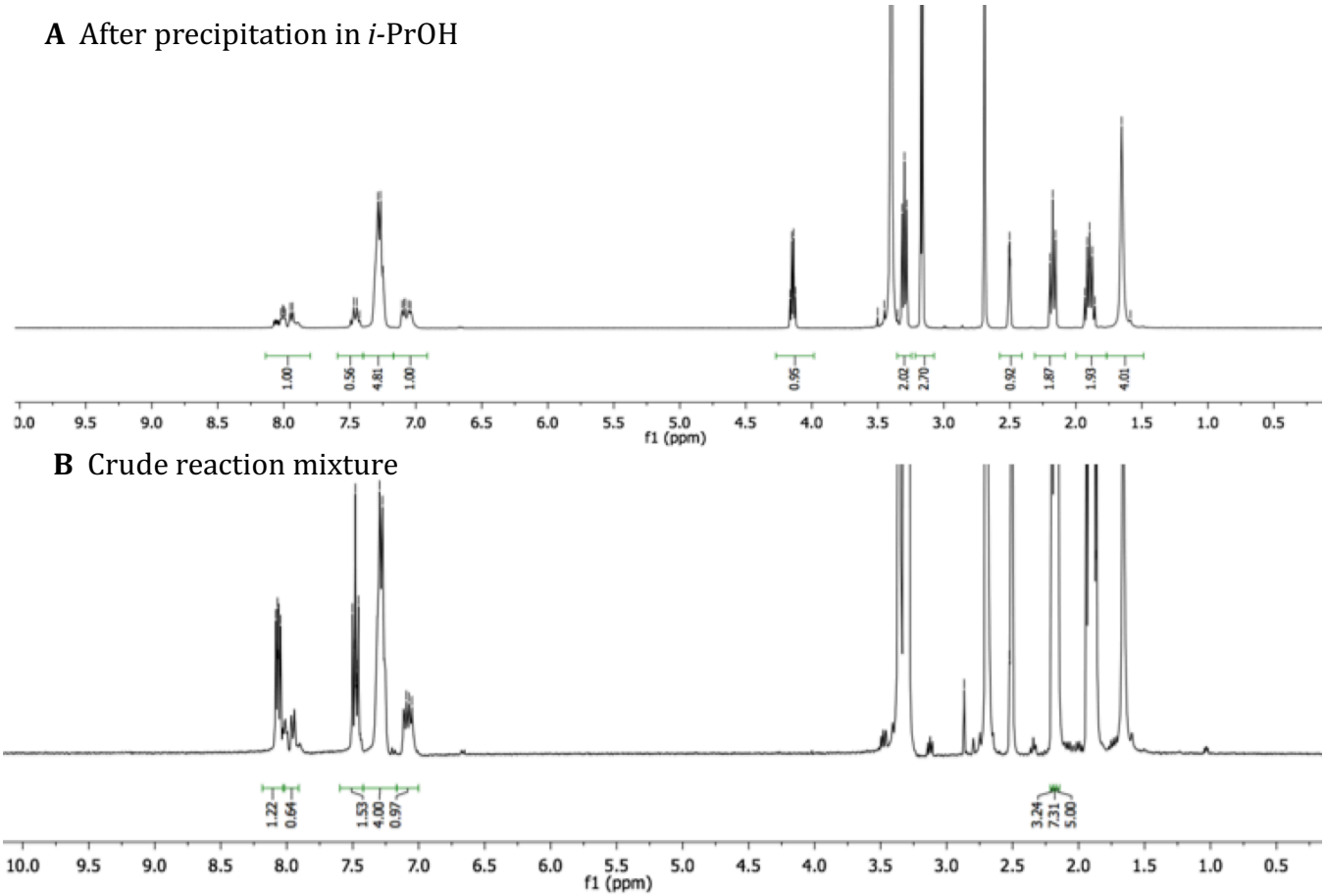

Figure S15. ^{1}H NMR spectra of product (**A**) after precipitation in IPA from the reaction with PC with 4,4'-difluorodiphenylsulfone with 12 mol % K_2CO_3 in NMP (25 wt % solids) and (B) the crude mixture before purification. Approximately 30% of 4,4'-difluorosulfone reacted to form ether linkages.

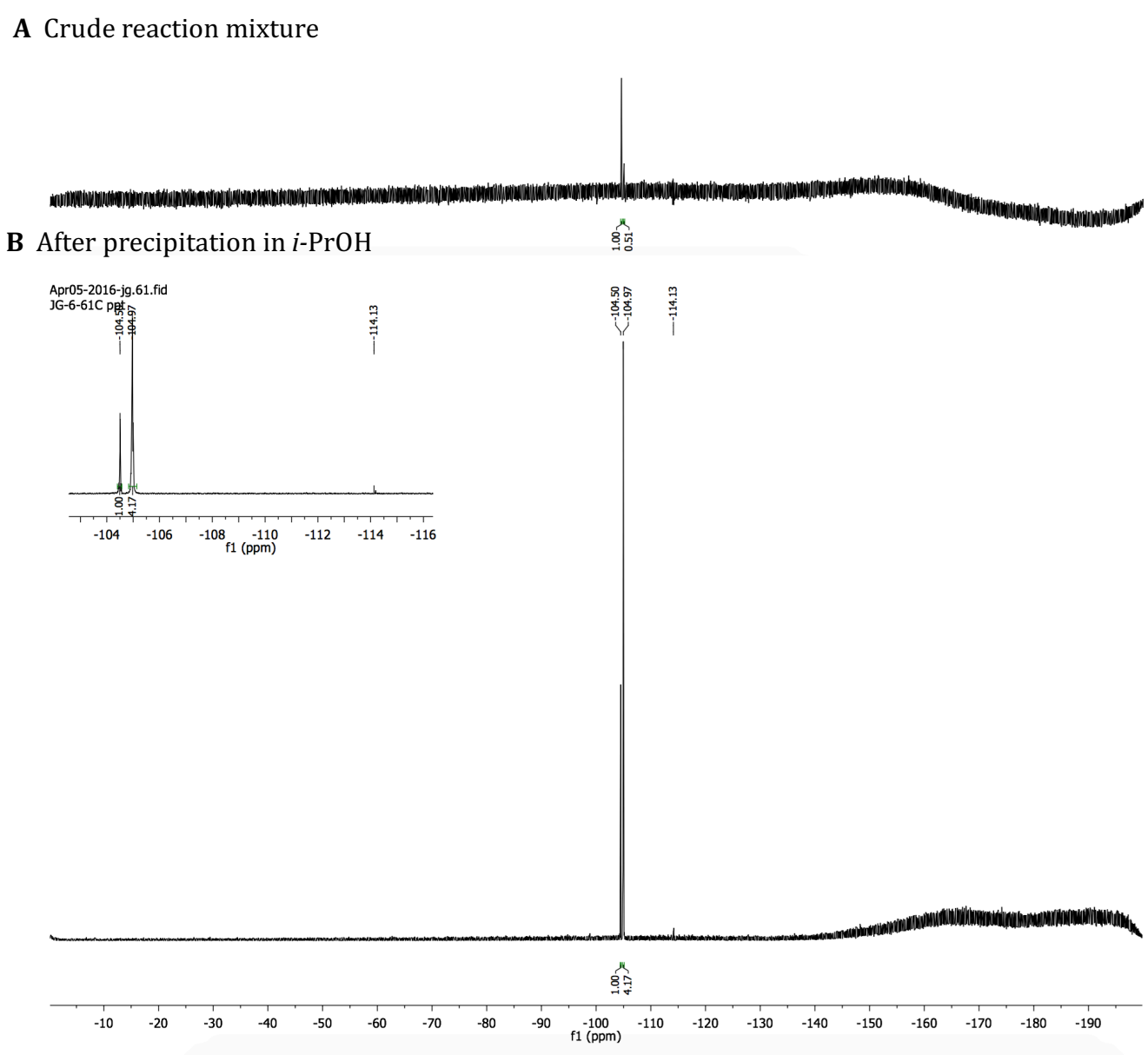

Figure S16. ^{19}F NMR spectra of (**A**) crude mixture before and (**B**) after products after purification by precipitation in IPA from the reaction of PC with 4,4'-difluorodiphenylsulfone with 12 mol % K_2CO_3. Signal at ~-114 ppm corresponds to F^- in the reaction mixture.

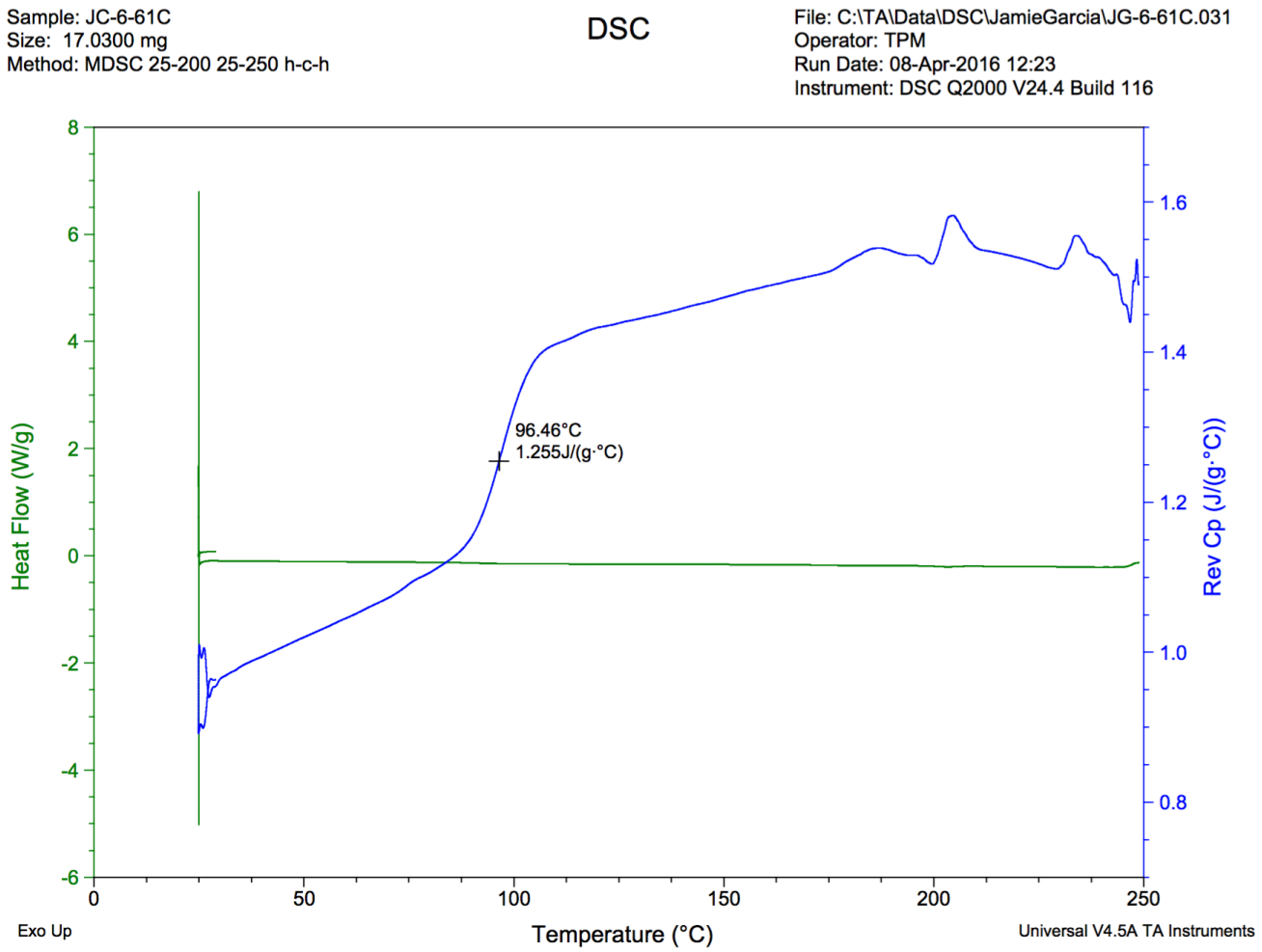

Figure S17. Differential scanning calorimetry (DSC) of product isolated from catalytic reaction. A single T_g is observed at ~100 °C.

Depolymerization of PC with substoichiometric LiF: Poly(bisphenol A carbonate) pellets (M_w ~ 32,800 Da, M_n ~ 11,600 Da; 0.068 g, 0.265 mmol, 1.0 equiv.) and lithium fluoride (0.005 g, 0.187 mmol, 0.71 equiv.) were weighed into a pre-dried vial in an Ar-filled glovebox. The vial was capped and removed from the glovebox and charged with d_6-DMSO (1.0 mL, 1.0 M) and allowed to heat until homogenous. Once the solution was homogeneous, the solution was transferred to an NMR tube with screwcap and allowed to reflux. The NMR tube was removed from heat and allowed to cool to ambient temperature prior to ^{1}H NMR analysis at each time point in Figure S120.

The reaction is believed to involve the formation of carbonofluoridic acids and esters (Figure S18), which are broken down by water present in the DMSO solvent into carbonic acid and eventually into carbon dioxide gas.

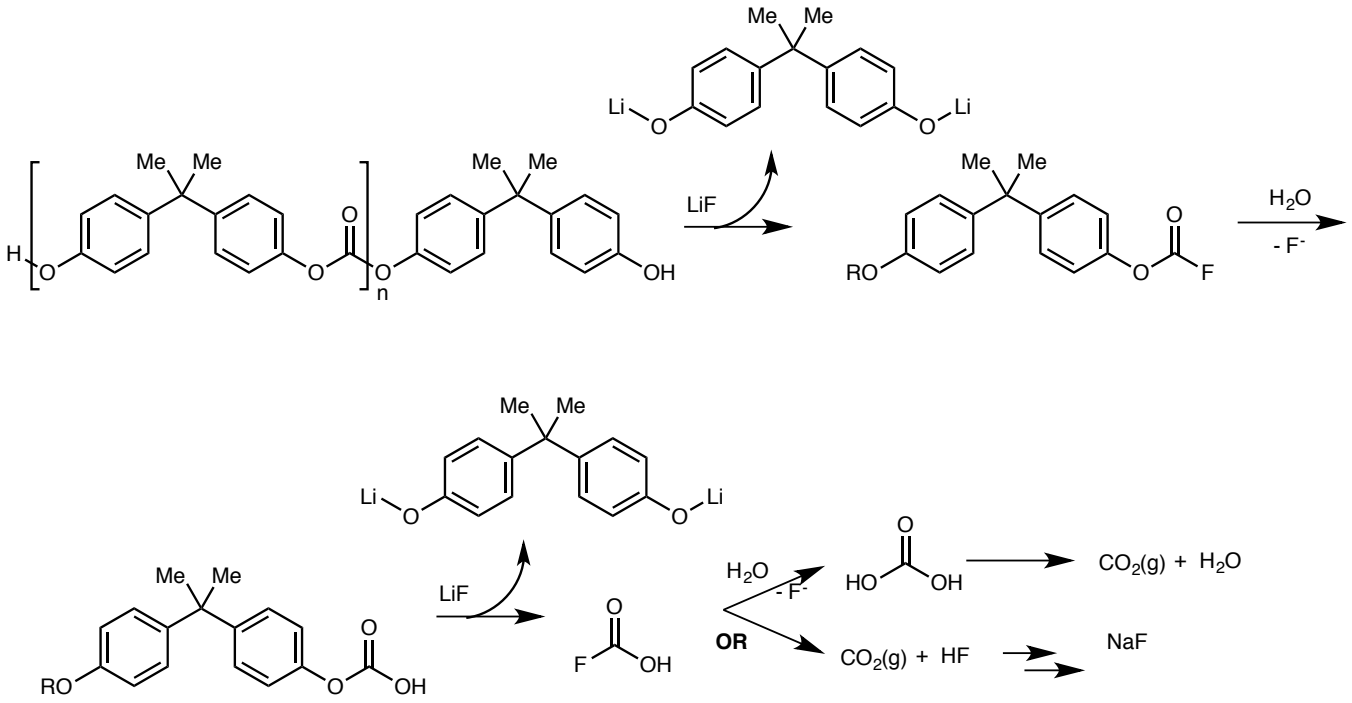

Figure S18. Key intermediates in the depolymerization of PC with LiF.

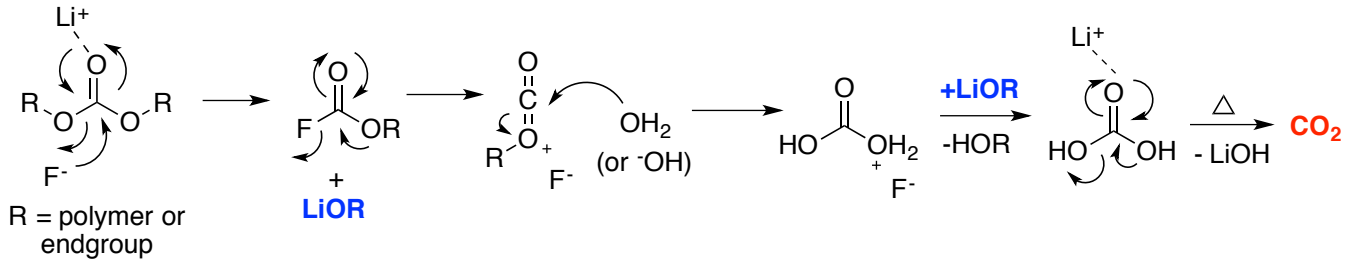

Figure S19. Arrow-pushing mechanism for formation of CO_2 from PC depolymerization.

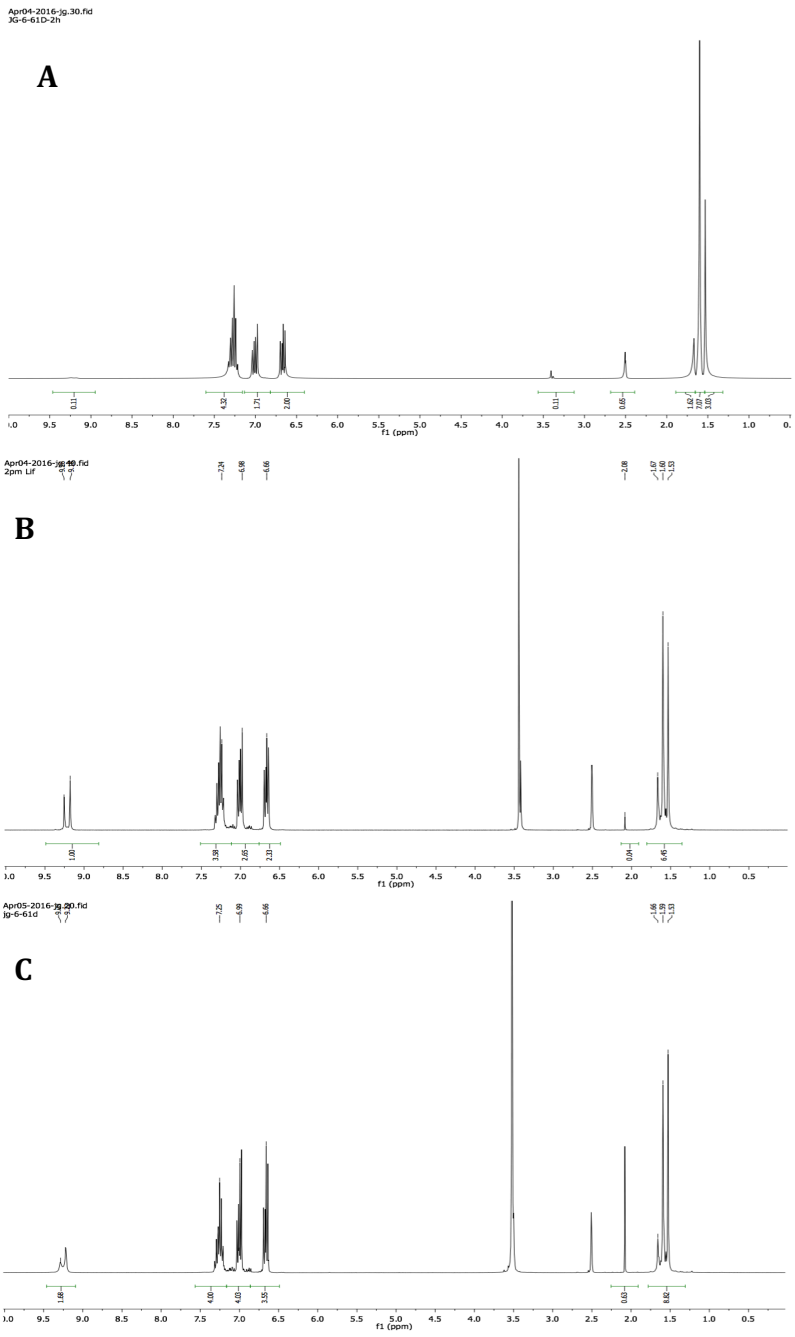

Figure S20. ^{1}H NMR spectra for depolymerization of PC with LiF (0.71 equiv. LiF wrt PC) in d_6-DMSO at 150 °C from 2 to 24 h. (**A**) 2 h, ~46% depolymerization of PC. (**B**) 4 h, ~58% depolymerization of PC. (**C**) After 24 h, ~67% depolymerization of PC. Notably, phenolic protons are observed, likely from protonation of alkoxides with water present in solvent.

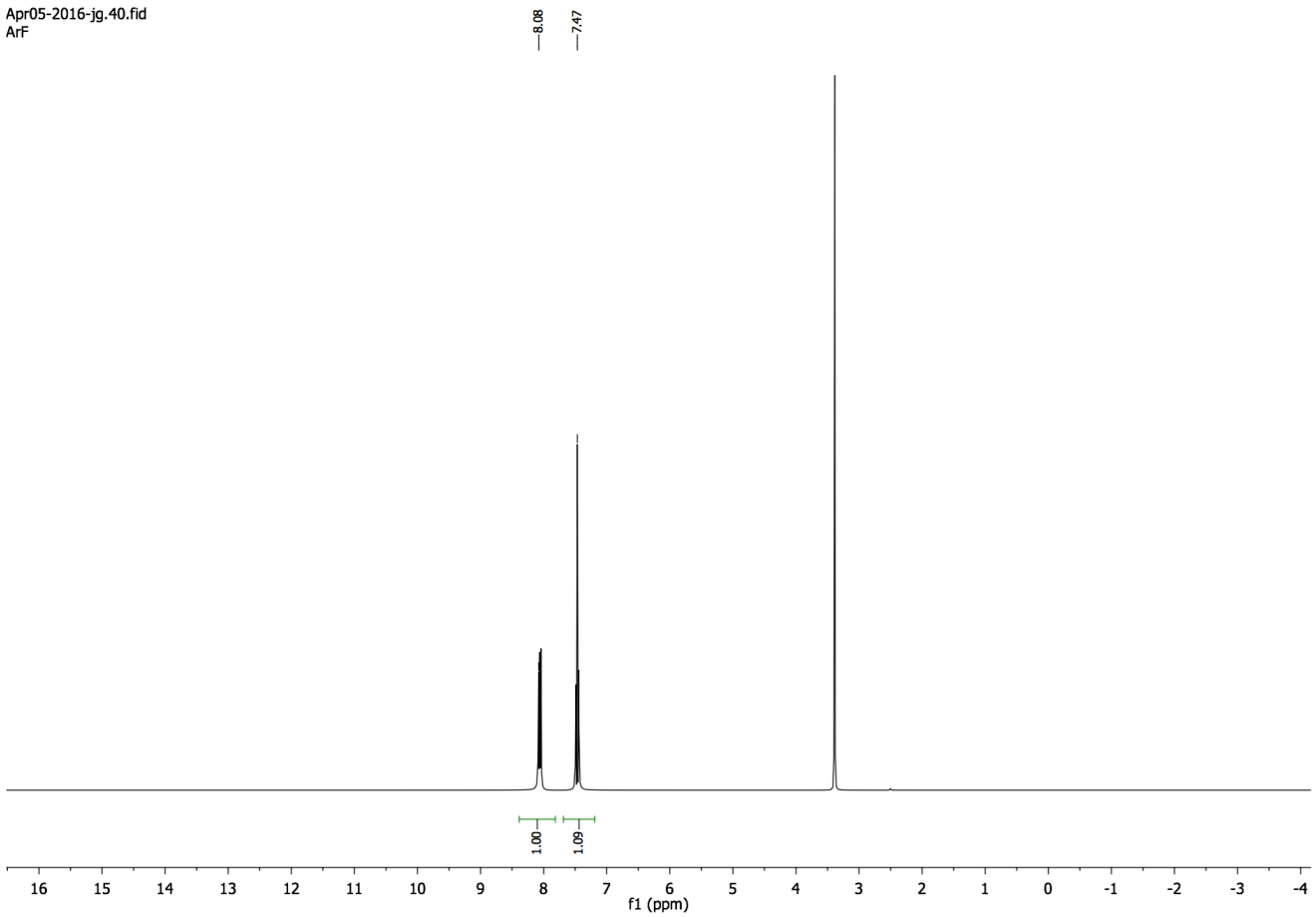

Figure S21. ^{1}H NMR of recrystallized 4,4'-difluorodiphenylsulfone in d_6-DMSO.

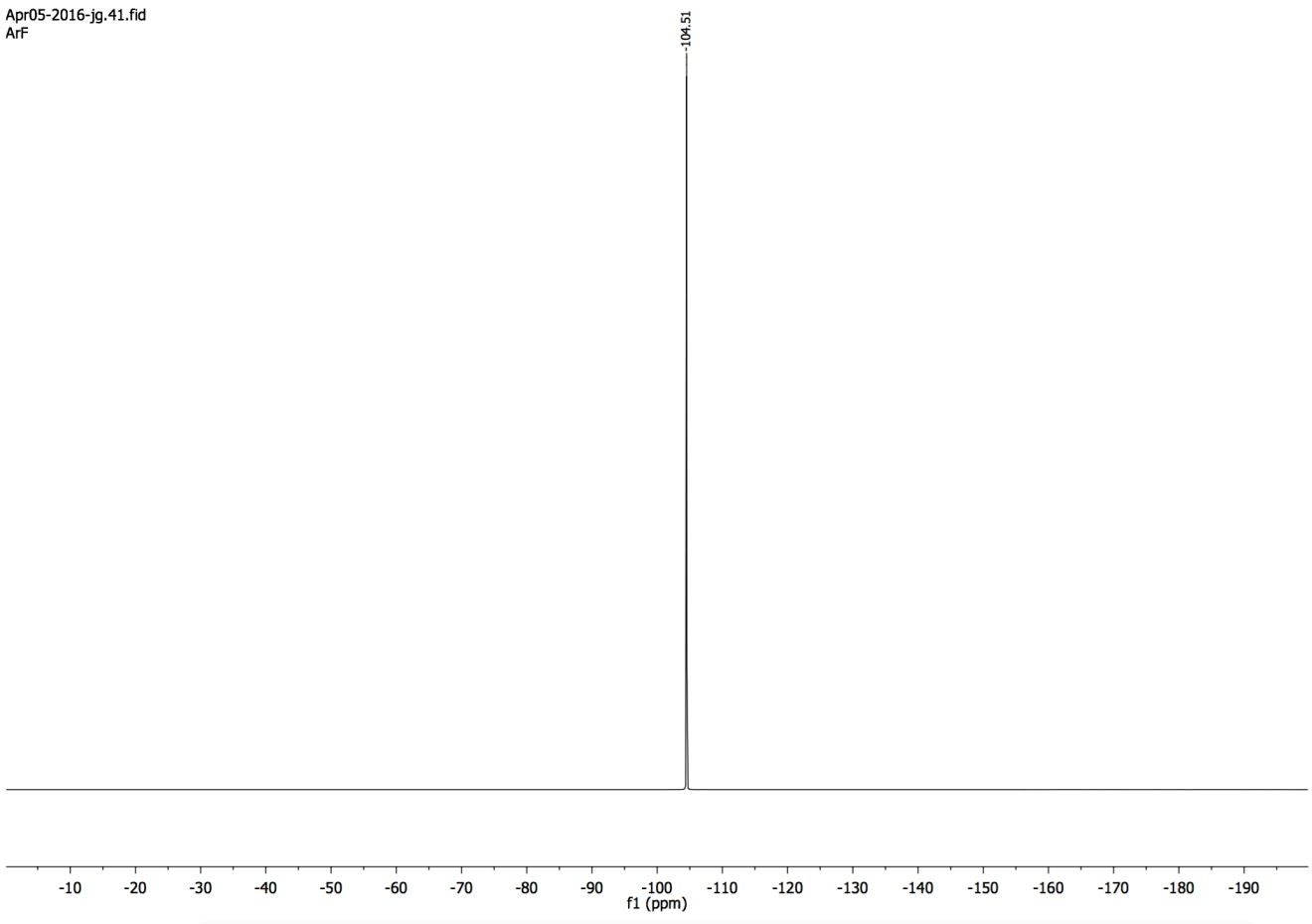

Figure S22. ^{19}F NMR of recrystallized 4,4'-difluorodiphenylsulfone in d_6-DMSO.

Stepwise procedure for depolymerizing PC prior to 4,4'-difluorodiphenylsulfone addition: Poly(bisphenol A carbonate) pellets (M_w ~ 32,800 Da, M_n ~ 11,600 Da; 0.304 g, 1.18 mmol, 1.0 equiv.), potassium carbonate (0.172 g, 1.244 mmol, 1.05 equiv.), and NMP (3.0 g, ~ 26 wt % solids) were weighed into pre-dried 20 mL vial in the glovebox equipped with stirbar. The solution was allowed to stir for 18 h prior to addition of 4,4'-difluorodiphenylsulfone (0.301 g, 1.18 mmol, 1.0 equiv.) in a single portion. The brown solution was allowed to heat for an additional 18 h prior to analysis of the crude mixture by ^{1}H NMR (Figure S23) and GPC. PSU oligomers produced were less than ~1 kDa by GPC analysis.

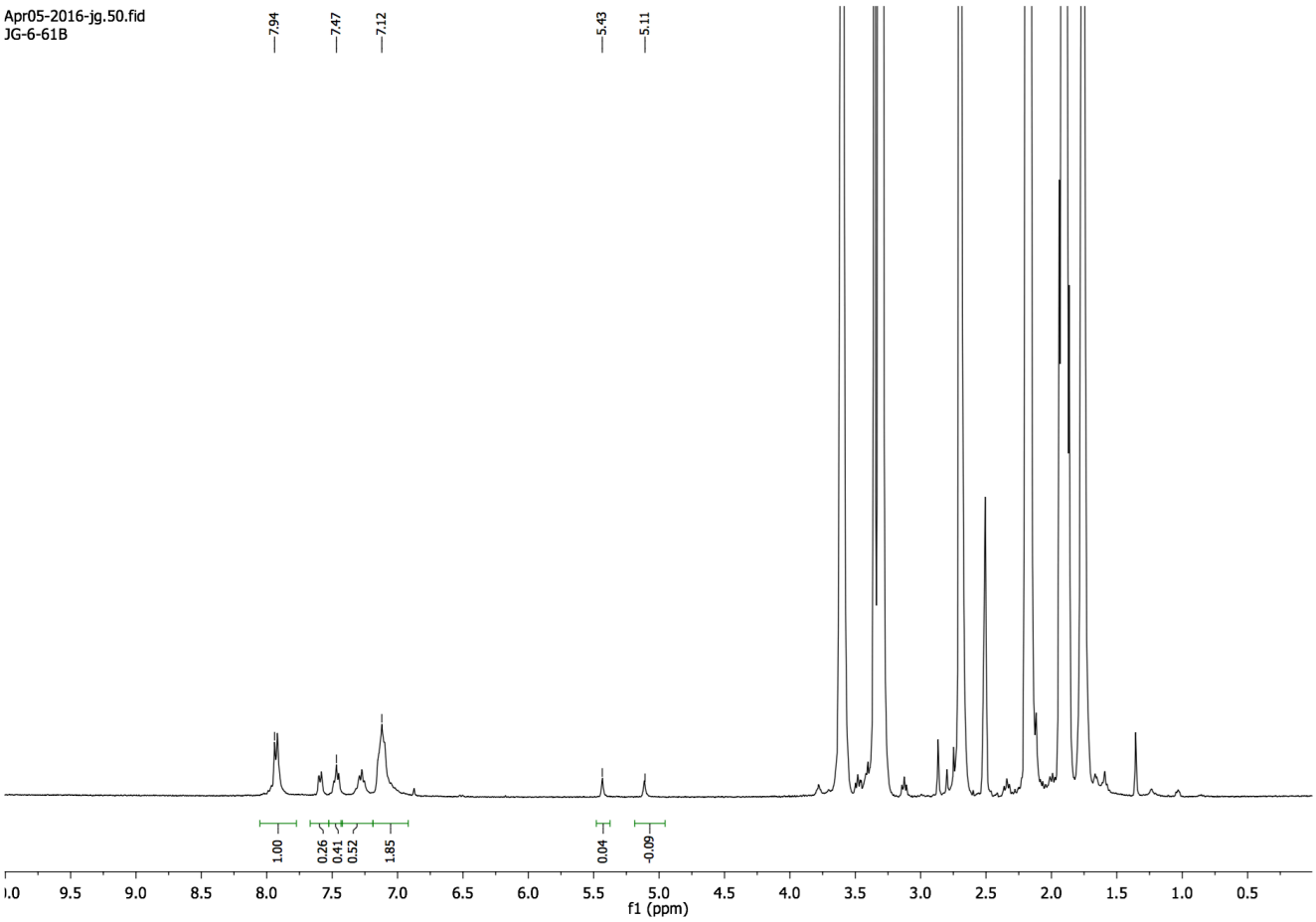

Figure S23. ^{1}H NMR crude reaction mixture after first depolymerizing PC with 1 equiv. K_2CO_3 for at 190 °C for 18 h, followed by addition of 4,4'-difluorodiphenylsulfone in NMP and continued heating for an additional 18 h. PSU oligomers were formed in low molecular weights (~1 kDa and below) and 4,4'-difluorodiphenylsulfone was completely consumed.

Representative Procedure for one-pot depolymerization of PC to PSU with excess K_2CO_3: Poly(bisphenol A carbonate) pellets (M_w ~ 32,800 Da, M_n ~ 11,600 Da; 0.148 g, 0.278 mmol, 1.0 equiv.), 4,4'-difluorodiphenylsulfone (0.147 g, 0.278 mmol, 1.0 equiv.), potassium carbonate (0.290 g, 2.10 mmol, 3.63 equiv.), and NMP (5.0 g, ~12 wt % solids) were weighed into pre-dried 20 mL vial in the glovebox equipped with stirbar. The vial was capped and removed from the glovebox, and a septum was attached, sealed with Teflon and electrical tape, and a nitrogen inlet

needle and an exit needle was inserted into the septum so that the solution slowly concentrated over the course of the polymerization. The reaction mixture was allowed to heat at 190 °C and after approximately 5 minutes, bubbles (CO_2) evolved vigorously. The mixture was allowed to stir at for 190 °C for 18 hours before removing from heat, allowing to cool, and adding 5 mL CH_2Cl_2. The polymer was precipitated in *i*-PrOH and characterized by GPC (M_n = 2.2 kDa, M_w = 4.5 kDa, PDI = 1.73).

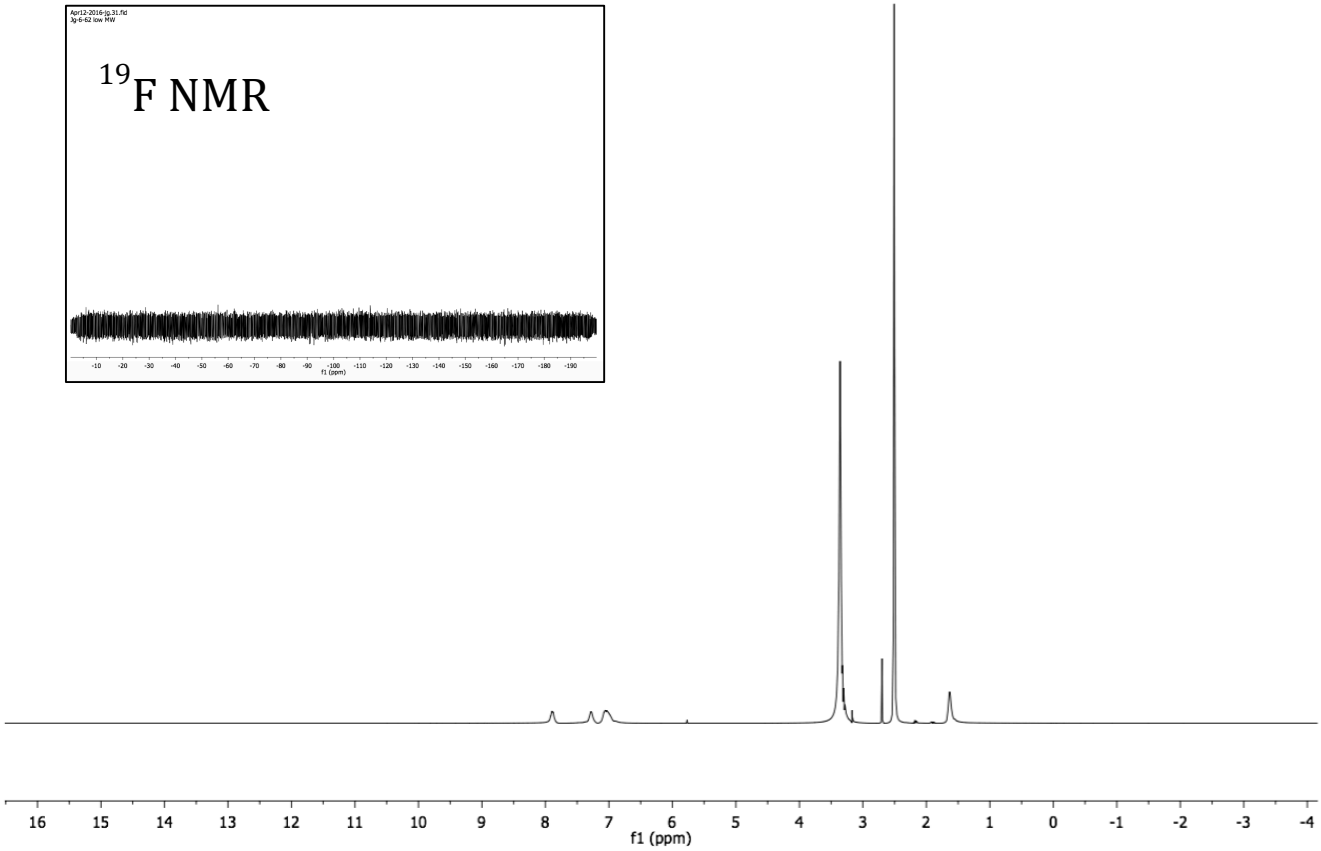

Figure S24. ^1H and ^{19}F NMR of PSU after reaction for 18 h with 3.6 equiv. K_2CO_3. Low concentration of F- containing end groups were observed by ^{19}F NMR (inset).

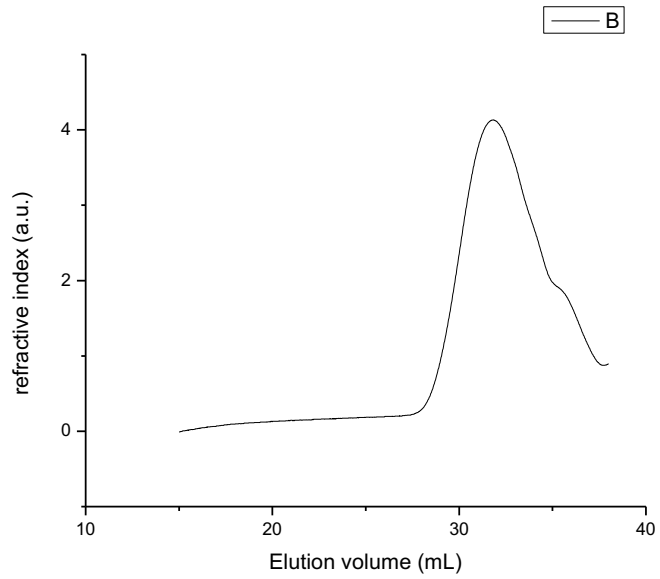

Figure S25. GPC trace of high K_2CO_3-content reaction (M_n = 2,585 Da, M_w = 4,466 Da, PDI = 1.73).

Representative Procedure for one-pot depolymerization of PC to PSU with CD as PC source: Poly(bisphenol A carbonate) in the form of a compact disc (CD) (M_w ~ 19,000 Da, M_n ~ 6,800 Da; 0.255 g, 1.0 mmol, 1.0 equiv.), 4,4'-difluorodiphenylsulfone (0.254 g, 1.0 mmol, 1.0 equiv.), potassium carbonate (0.150 g, 1.09 mmol, 1.09 equiv.), and NMP (3.8 g, ~17 wt % solids) were weighed into pre-dried 20 mL vial in the glovebox equipped with stirbar. The vial was capped and removed from the glovebox, and a septum was attached, sealed with Teflon and electrical tape, and a nitrogen inlet needle and an exit needle was inserted into the septum so that the solution slowly concentrated over the course of the polymerization. The reaction mixture was allowed to heat at 190 °C and after approximately 5 minutes (once the CD pieces had dissolved), bubbles (CO_2) evolved vigorously. The mixture was allowed to stir at for 190 °C for 18 hours before removing from heat, allowing to cool, and adding 10 mL CH_2Cl_2. The polymer was precipitated in 40 mL of MeOH, filtered, isolated and dried *in vacuo*. The off-white powder was characterized by NMR and GPC (M_n = 11 kDa, M_w = 20 kDa, PDI = 1.73). Isolated 0.404 g, 83% yield of PSU.

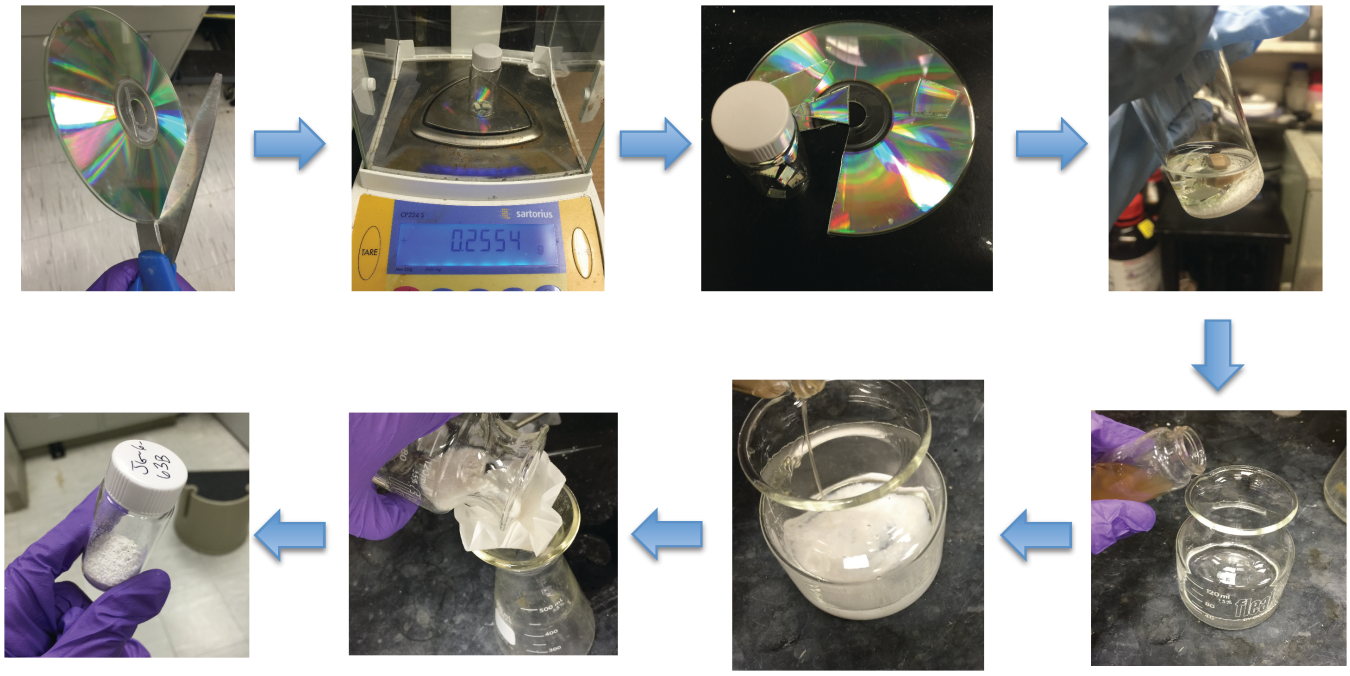

Figure S26. Synthesis of PSU from PC with CD as the PC source. A compact disc was cut into small pieces, weighed, and placed in a vial. The vial was charged with solvent, K_2CO_3, and 4,4'-difluorodiphenyl sulfone. The reaction was allowed to heat for 18 h at 190 °C, the solution was diluted with CH_2Cl_2 and the polymer was precipitated into methanol. The precipitate was filtered, collected in a vial and dried under vacuum to yield PSU as a powder.

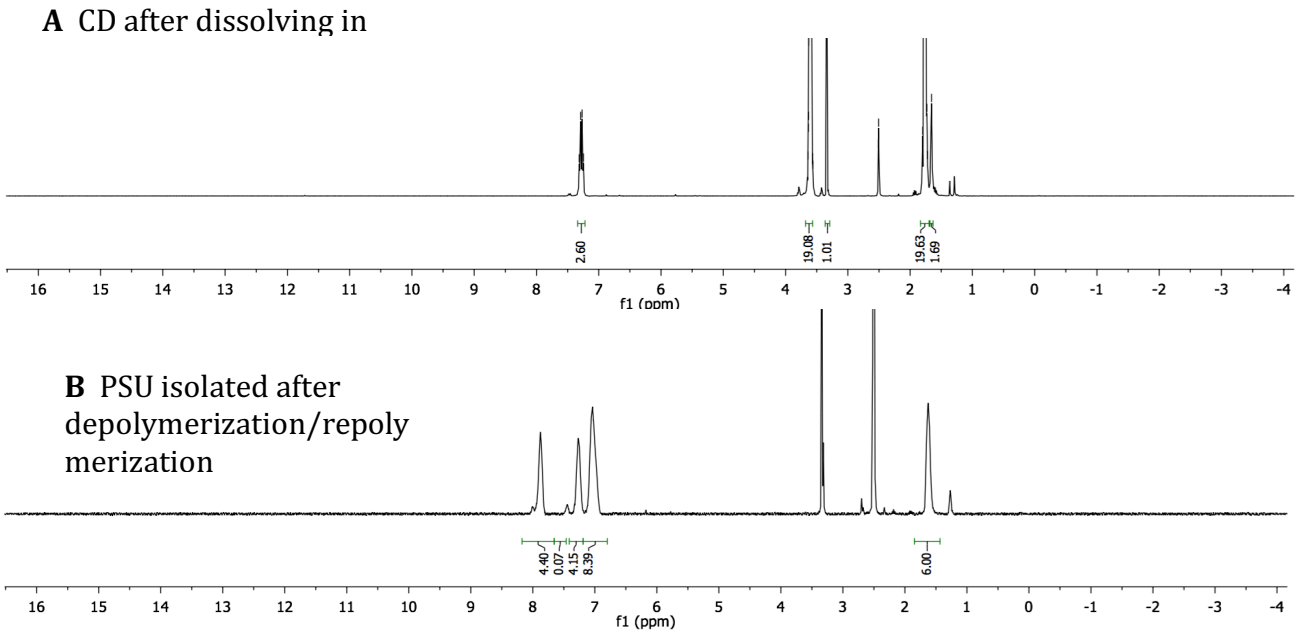

Figure S27. (**A**) ^{1}H NMR spectra of CD material after dissolving in THF and concentrating. (**B**) ^{1}H NMR spectra of the PSU after depolymerization and repolymerization.

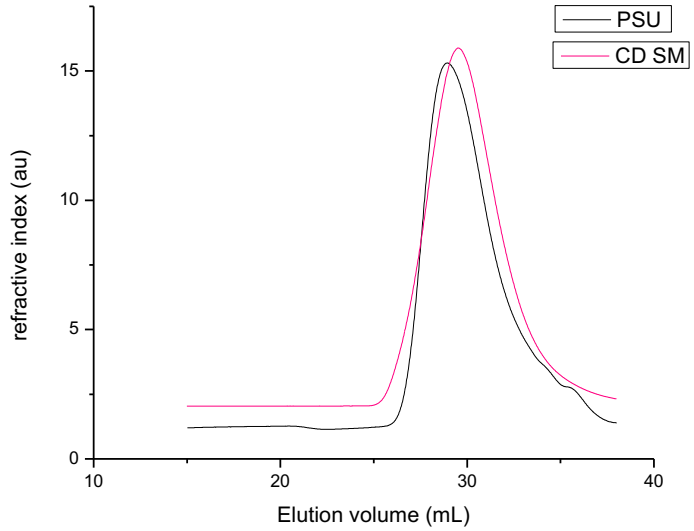

Figure S28. GPC overlay of CD starting material (red trace) with PSU after isolation (black trace). CD starting material M_n = 6,572 Da, M_w = 18,814, PDI = 2.78. Isolated PSU after depolymerization/repolymerization M_n = 11, 444 Da, M_w = 19,791 Da, PDI = 1.73.

Representative Procedure for determination of end group functionality: Poly(aryl ether sulfone) (20.0 mg, 0.041 mmol), and pentafluoroisocyanate (excess, ~20 mg) and d_6-DMSO (1.0 mL, 1.0 M) were weighed into a 20 mL vial. The contents of the vial was transferred to an NMR tube with cap. After 24 h at 22 °C, the solution was analyzed by ^{19}F NMR. The ratio of the signal at ~-63 ppm to the signal at ~-104 ppm was 1:2.5 when number of fluorines per signal were accounted for.

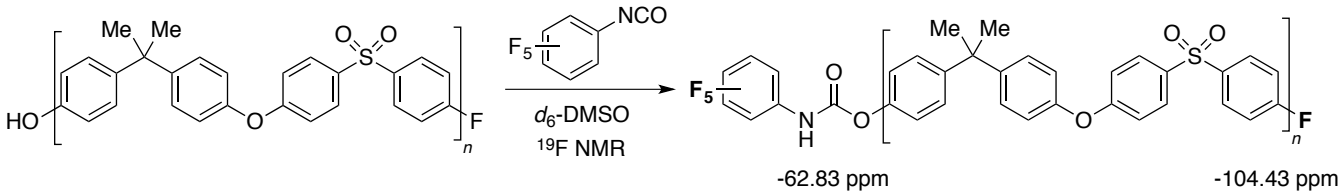

Figure S29. Reaction of isocyanate with free hydroxyl end groups to determine the ratio of hydroxyl- to fluoro-substitution on the terminal aryl ring.

Part II: Computational Methodology

All calculations were performed with the GAMESS-US[1–3] suite of packages using the dispersion-corrected[4] B3LYP[5–8] (B3LYP-D3) density functional theory (DFT) method. Geometry optimizations were performed with the 6-31+G(2d,p)[9] basis set followed by single point energy calculations with the aug-cc-pVTZ[10,11] basis set. A continuum dielectric with the SMD[12] method was utilized to represent reaction conditions and all reported stationary points were optimized in implicit DMA solvent as a model for NMP. Reported energies are free energies in kcal/mol. Only vibrational free energy corrections to the electronic energy at 463 K were used in accordance with recommendations for molecules optimized in implicit solvent.[13] For gaseous CO_2, the translational, vibrational and rotational free energy corrections to the electronic energy at 463 K were used. Normal modes of all structures were examined to verify that equilibrium structures possess no imaginary frequencies and that one imaginary frequency corresponding to bond formation or bond breaking was obtained for transition state structures. Intrinsic reaction coordinate (IRC) calculations were also performed to verify that transition states are connected to reactant complexes and intermediates on the free energy surfaces of reactions. Partial atomic charges have been computed from an electrostatic potential fit that preserves total molecular charge, dipole and quadrupole moments.

The following settings were used in GAMESS-US.

$dft nrad=96 nleb=590 $end

$tescav ntsall=240 $end

$force temp=463 $end

Gradient tolerance [a.u.]: 0.00003 for minima and saddle points

Part III: Cartesian Coordinates and Energies of Stationary Points

1-fluoro-4-(methylsulfonyl)benzene
E [6-311+G(2d,p); Hartrees] = -919.6311258231
E [aug-cc-pVTZ; Hartrees] = -919.6889667221
Gvib [kcal/mol] = 72.852

H	1.20394919	-2.95930093	0.86129671
C	0.97221769	-1.90241304	0.88675096
C	0.60676920	-1.20877880	-0.25891822
H	0.55359804	-1.72025584	-1.21087948
C	0.32369900	0.15130049	-0.17348684
C	0.39809209	0.83493067	1.03625937
H	0.18372156	1.89451605	1.07955606
C	0.76472200	0.14809764	2.18584028
H	0.84015794	0.64536206	3.14415811
C	1.04091247	-1.20387282	2.07993571
F	1.40128254	-1.87613201	3.19957559
S	-0.15065357	1.04032310	-1.65319962
O	0.43575748	0.35572244	-2.80209343
O	0.13835361	2.45618139	-1.44326686
C	-1.92814741	0.84037281	-1.73461353
H	-2.37374075	1.27315277	-0.84022617
H	-2.25982314	1.37424124	-2.62628561
H	-2.16076856	-0.22035817	-1.81486447

co2
E [6-311+G(2d,p); Hartrees] = -188.6528422033
E [aug-cc-pVTZ; Hartrees] = -188.6635661410
Gvib, rot, trans [kcal/mol] = -17.139

C	0.00000001	-0.00000000	-0.00000005
O	0.00377999	0.00213023	-1.16035029
O	-0.00378000	-0.00213023	1.16035034

di-p-tolyl carbonate
E [6-311+G(2d,p); Hartrees] = -806.0101314762
E [aug-cc-pVTZ; Hartrees] = -806.0573170539
Gvib [kcal/mol] = 141.697

C	-1.40907905	-1.12955043	-1.69051360
O	-0.21702645	-0.38396627	-1.74789615

C	0.26652880	0.07408839	-0.58049181
C	-5.04209534	-3.40865128	-1.73151099
C	-3.76107975	-2.61642021	-1.71519948
C	-2.52030272	-3.24129264	-1.58025827
C	-1.33873278	-2.50426839	-1.56779361
C	-2.62124244	-0.47355805	-1.82835621
C	-3.79073041	-1.22316177	-1.83872483
H	-5.59103754	-3.25129144	-2.66428543
H	-4.85475371	-4.47881376	-1.63007807
H	-5.70345072	-3.10529567	-0.91485839
H	-2.46843346	-4.32008458	-1.48464645
H	-0.37612885	-2.98994969	-1.46369342
H	-2.64501126	0.60518658	-1.92480625
H	-4.74305359	-0.71508783	-1.94608505
O	-0.21309987	-0.08859202	0.50745418
O	1.39197671	0.75005752	-0.86889662
C	2.07629852	1.33023903	0.21509326
C	1.78967073	2.63847929	0.56815431
C	2.51391781	3.22897323	1.59594944
C	3.51874450	2.52787336	2.27137957
C	3.77983964	1.21220295	1.88524569
C	3.06304613	0.60586105	0.85676936
H	1.01127312	3.18128665	0.04565971
H	2.29334866	4.25322261	1.87698610
C	4.29225260	3.18826475	3.38247820
H	4.55444142	0.64676817	2.39115459
H	3.26621566	-0.41547501	0.55820777
H	4.81013453	4.08288296	3.02507310
H	5.03995921	2.51623431	3.80671558
H	3.62760989	3.50383821	4.19177378

ether product
E [6-311+G(2d,p); Hartrees] = -1166.0638511029
E [aug-cc-pVTZ; Hartrees] = -1166.1368489152
Gvib [kcal/mol] = 139.442

C	1.64547159	0.87288848	-2.47248501
C	0.43212756	1.36287105	-2.95388051
C	1.70475413	0.18169082	-1.26795725
H	2.64932505	-0.20348822	-0.90609255
H	0.39177456	1.88983998	-3.89836153
C	-2.15822718	-2.51740950	4.56972546
C	-2.06251183	-1.78163824	3.25876446
C	-1.83346604	-0.40170677	3.23790599
C	-1.74400582	0.29655832	2.04016777
C	-1.88680038	-0.39293538	0.84418977
O	-1.85698829	0.31076234	-0.36048837
C	-0.66790404	0.46452287	-1.01177327
C	-0.72428154	1.15814092	-2.22381471
C	0.54677363	-0.02744123	-0.53180035

C	-2.11632371	-1.75862777	0.82994370
C	-2.20332103	-2.44467238	2.03869042
H	-1.24678275	-2.39065856	5.16077679
H	-2.98767480	-2.13919481	5.17427673
H	-2.31430992	-3.58706600	4.42074582
H	-1.72358840	0.13638222	4.17348102
H	-1.56519667	1.36498396	2.02702013
H	-1.67897509	1.52403375	-2.58044697
H	0.59157006	-0.57001678	0.40207999
H	-2.22389734	-2.27605918	-0.11573768
H	-2.38412131	-3.51377089	2.02535967
C	3.75807081	2.71798366	-2.77131825
S	3.14130516	1.15781788	-3.39923183
O	2.78279405	1.34725612	-4.80322504
O	4.10637034	0.11843785	-3.04750592
H	4.68029559	2.93263907	-3.31315638
H	3.01402021	3.49090090	-2.95833910
H	3.95445297	2.61345942	-1.70531075

int1

E [6-311+G(2d,p); Hartrees] = -1394.6904332117

E [aug-cc-pVTZ; Hartrees] = -1394.7752818473

Gvib [kcal/mol] = 143.040

O	-0.42006399	-1.13782086	-1.34544832
C	-0.00188804	-0.63718843	-0.18059103
NA	2.33451289	-0.47164017	-2.36773232
C	-1.63622233	-0.63073179	-1.86418203
C	-5.29914597	0.75283191	-3.59814673
C	-4.01426947	0.27959861	-2.97119793
C	-3.99646144	-0.83822529	-2.13221509
C	-2.80977897	-1.30169984	-1.57398071
C	-1.60720443	0.47867625	-2.68897837
C	-2.80500305	0.92730098	-3.23676179
H	-5.27241079	1.82430107	-3.80636656
H	-5.47957622	0.23957335	-4.54829435
H	-6.15714387	0.55345834	-2.95279204
H	-4.92184216	-1.35736177	-1.90862157
H	-2.79594285	-2.16717148	-0.92274590
H	-0.66738338	0.98204118	-2.87459726
H	-2.79369520	1.79882725	-3.88212089
O	-0.57462721	0.17680535	0.50239714
O	1.16919423	-1.22694731	0.10346106
C	1.74186690	-0.94239777	1.36851014
O	3.49233982	1.31123632	-1.64108336
C	2.38969002	1.87404519	-1.29589290
O	1.25529652	1.34268041	-1.73029622
NA	0.18329746	2.37387344	-0.06460696
O	2.32734132	2.88606831	-0.51594550
C	2.83180008	-0.09783889	1.43489837

C	3.42451663	0.11728701	2.67848389
C	2.93784772	-0.49408078	3.83370626
C	1.83103049	-1.34334510	3.71854941
C	1.22941402	-1.57490091	2.48969995
H	3.21622775	0.38533100	0.54390805
H	4.28151424	0.77839755	2.74112033
C	3.57869636	-0.26156030	5.17656155
H	1.43507039	-1.83231623	4.60197992
H	0.37506118	-2.23470022	2.39878373
H	4.40319497	0.45017788	5.11185604
H	3.97280558	-1.19409938	5.59090708
H	2.85385952	0.12813623	5.89679301

int2

E [6-311+G(2d,p); Hartrees] = -1394.6681609149

E [aug-cc-pVTZ; Hartrees] = -1394.7536963823

Gvib [kcal/mol] = 144.920

O	0.20398700	-0.49583167	-1.22697850
C	1.06753896	0.65357795	-1.00003509
NA	2.93755469	-1.05729013	-2.27457349
C	-1.10805879	-0.25639080	-1.55563717
C	-5.28070955	0.21566779	-2.58280583
C	-3.82899560	0.04842376	-2.21330825
C	-3.41015847	-0.93533331	-1.31730863
C	-2.06625568	-1.08682890	-0.98541925
C	-1.50345044	0.72844394	-2.46168005
C	-2.84932798	0.87515467	-2.77346552
H	-5.60801841	1.25189109	-2.45964253
H	-5.45786332	-0.05352119	-3.62894206
H	-5.92612242	-0.41344454	-1.96670698
H	-4.14211464	-1.59352747	-0.86079333
H	-1.75113084	-1.84513237	-0.27837338
H	-0.75921963	1.36800926	-2.91527339
H	-3.14410862	1.64818247	-3.47638448
O	0.56651962	1.62488654	-0.39136191
O	2.23925897	-0.01682981	-0.33157231
C	2.09160269	-0.27736787	1.01632823
O	3.79298867	0.95519786	-2.93763732
C	2.86153029	1.62217223	-2.45295547
O	1.64092987	0.86814786	-2.33534869
NA	1.15082176	3.61340971	-0.98069316
O	2.83621993	2.81928438	-2.12506966
C	2.45982773	0.68059607	1.95352291
C	2.36086493	0.39230641	3.31077381
C	1.89664145	-0.84816137	3.75703451
C	1.52794233	-1.79424323	2.79709561
C	1.62087675	-1.51611387	1.43739711
H	2.82449183	1.64105849	1.61251574
H	2.65262713	1.14603449	4.03481334

C	1.83141051	-1.16940261	5.22788706
H	1.16147868	-2.76506959	3.11433185
H	1.32266559	-2.25014253	0.69946430
H	1.64256506	-0.27514792	5.82589063
H	2.77533629	-1.60083497	5.57752216
H	1.04361706	-1.89396861	5.44540039

int3

E [6-311+G(2d,p); Hartrees] = -1394.7212544631

E [aug-cc-pVTZ; Hartrees] = -1394.8065299395

Gvib [kcal/mol] = 138.883

O	-0.10626772	0.67688159	-3.10202311
C	0.48302033	1.90668884	-2.71774880
NA	2.05033752	-0.24486020	-2.25818985
C	-1.38239094	0.37331280	-2.62434372
C	-5.27870028	-0.81964689	-1.24915898
C	-3.91088261	-0.40054641	-1.72222570
C	-2.84434241	-0.25470623	-0.83182559
C	-1.58253724	0.12899797	-1.27390594
C	-2.42087411	0.23913167	-3.53263601
C	-3.67658958	-0.14772187	-3.07703521
H	-6.02942330	-0.06063667	-1.48770278
H	-5.59730532	-1.74818490	-1.73177218
H	-5.29887861	-0.98093133	-0.16998559
H	-2.99631123	-0.44532681	0.22501427
H	-0.75818837	0.24458218	-0.58001495
H	-2.24197733	0.43315658	-4.58344806
H	-4.48777635	-0.25481813	-3.78963603
O	-0.21132046	2.75655689	-2.14949217
O	1.98561181	0.69940285	-0.23936234
C	1.97730845	0.15528264	0.96696210
O	4.75445729	0.43179784	-1.49913219
C	4.57755830	1.48974560	-1.05674092
O	1.71118770	1.93040064	-2.96963354
NA	1.61804326	2.86596689	-0.67261923
O	4.45318595	2.56602335	-0.63944540
C	2.62932741	0.75798410	2.06572894
C	2.59528819	0.18733324	3.33365737
C	1.92318523	-1.01190698	3.58559861
C	1.27981342	-1.61723318	2.50220243
C	1.30311046	-1.05807740	1.22986758
H	3.16804239	1.68814105	1.91013454
H	3.10761973	0.69085560	4.14883551
C	1.92037804	-1.64259289	4.95595818
H	0.74222567	-2.54889763	2.65572169
H	0.77935225	-1.54921027	0.41540380
H	1.99881031	-0.88957160	5.74427211
H	2.76077452	-2.33390832	5.08590301
H	1.00512763	-2.21346461	5.13281816

int4
E [6-311+G(2d,p); Hartrees] = -1206.0541057318
E [aug-cc-pVTZ; Hartrees] = -1206.1287668340
Gvib [kcal/mol] = 136.631

O	-0.09637264	0.69444930	-3.12983321
C	0.50523819	1.92661676	-2.78149511
NA	2.18287429	-0.14875495	-2.32925946
C	-1.33184809	0.37652764	-2.56366051
C	-5.10400236	-0.87033845	-0.91333947
C	-3.78017301	-0.43008895	-1.48299934
C	-2.66015632	-0.24807459	-0.66818849
C	-1.43832893	0.15155190	-1.19904456
C	-2.42557309	0.20638021	-3.39852781
C	-3.64055729	-0.19681340	-2.85414816
H	-5.88686780	-0.13324070	-1.11424972
H	-5.43162668	-1.81478326	-1.35756669
H	-5.04933792	-1.01211385	0.16744714
H	-2.73706498	-0.42454222	0.39922979
H	-0.57169293	0.29036159	-0.56425188
H	-2.32159421	0.38480042	-4.46214554
H	-4.49452456	-0.33266046	-3.50960950
O	-0.16379431	2.77885070	-2.18609698
O	2.03297673	0.71183115	-0.29927803
C	1.92831718	0.15213613	0.89297179
O	1.72055829	1.95773239	-3.09047337
NA	1.71316010	2.87138257	-0.76717645
C	2.37138096	0.80474589	2.06690243
C	2.24157734	0.22001524	3.32067241
C	1.67058256	-1.04534582	3.48948027
C	1.23185479	-1.69981803	2.33553550
C	1.35462920	-1.12707987	1.07418670
H	2.83084628	1.78536680	1.97629904
H	2.59675697	0.76328549	4.19211200
C	1.57158451	-1.68692299	4.85106460
H	0.77878145	-2.68355329	2.42149858
H	0.98826758	-1.66508849	0.20489469
H	1.35458411	-0.94945278	5.62851622
H	2.50651078	-2.18426986	5.13341045
H	0.78278967	-2.44259389	4.88139327

int5
E [6-311+G(2d,p); Hartrees] = -1206.0492083613
E [aug-cc-pVTZ; Hartrees] = -1206.1237313304
Gvib [kcal/mol] = 133.191

O	-0.24206641	-0.55197620	-3.65747696
C	0.84196317	2.49059504	-1.45071413
NA	1.41886473	-0.74455578	-2.26562154

C	-1.40967495	-0.43349734	-3.11007332
C	-5.30347700	0.00990452	-1.10033497
C	-3.96014788	-0.13717630	-1.76956696
C	-3.28561191	-1.36729272	-1.80662944
C	-2.06072699	-1.51987937	-2.44910385
C	-2.11656297	0.80582866	-3.07285932
C	-3.34207609	0.93831204	-2.42459855
H	-5.46055909	1.02794594	-0.73571011
H	-6.12339658	-0.21533219	-1.79150350
H	-5.40514005	-0.66768688	-0.24902612
H	-3.72718448	-2.22770401	-1.31175792
H	-1.56267010	-2.48407610	-2.44240430
H	-1.66193545	1.66440927	-3.55602359
H	-3.82833024	1.90973684	-2.42071242
O	-0.13534701	2.85902703	-0.94336096
O	0.65081467	-0.07785618	-0.29779201
C	1.29139080	-0.13187235	0.86243111
O	1.82105089	2.17558424	-1.98714606
NA	-1.50578389	0.30223229	-0.40658271
C	1.34937369	0.97417072	1.73610903
C	2.01516231	0.90185035	2.95717721
C	2.66348590	-0.26164247	3.37456889
C	2.61349188	-1.36178571	2.51059214
C	1.95123825	-1.30602523	1.29140367
H	0.85890654	1.89678205	1.44275720
H	2.02993648	1.77896836	3.59785277
C	3.38008592	-0.34613755	4.69937090
H	3.10250463	-2.28760549	2.80151523
H	1.91780954	-2.18253533	0.65088459
H	3.33856953	0.60387087	5.23681646
H	4.43565438	-0.60688631	4.57268137
H	2.93997298	-1.11011800	5.34857565

int6
E [6-311+G(2d,p); Hartrees] = -1017.3852403738
E [aug-cc-pVTZ; Hartrees] = -1017.4498280267
Gvib [kcal/mol] = 130.022

O	-0.00558565	-1.58219005	0.01957259
NA	-1.51389818	0.00996118	-0.01676577
C	-0.02354145	-2.90055941	0.04051945
C	-0.07436984	-7.27897637	0.08171679
C	-0.06428875	-5.77047332	0.09272982
C	1.08748704	-5.04910313	0.41958228
C	1.11478198	-3.65948868	0.39667422
C	-1.18384421	-3.63920489	-0.28599930
C	-1.19629424	-5.02895778	-0.25699659
H	-1.06835345	-7.67523804	0.30487053
H	0.21966955	-7.67967540	-0.89515201
H	0.61960696	-7.69065821	0.81916655

H	1.98840239	-5.58652369	0.70298318
H	2.02727739	-3.13546822	0.66690140
H	-2.08451014	-3.09967678	-0.56541061
H	-2.11412174	-5.55025910	-0.51505808
O	0.01405451	1.58194867	0.00594346
C	0.03070888	2.90015994	0.02347021
NA	1.52298712	-0.01066370	0.04340792
C	1.20607758	3.63971053	-0.23447344
C	1.21472900	5.03118960	-0.20634150
C	0.06341415	5.77074003	0.07203134
C	-1.10726943	5.04688638	0.32595971
C	-1.13097576	3.65895751	0.30353085
H	2.12227043	3.10192763	-0.46185183
H	2.14580823	5.55262472	-0.41018515
C	0.06881797	7.27900685	0.10390923
H	-2.02546949	5.58436785	0.54779417
H	-2.05901230	3.13353519	0.51108513
H	-0.63767440	7.70200852	-0.61752216
H	1.05729902	7.67932373	-0.13256899
H	-0.21418318	7.66476843	1.08876861

int7
E [6-311+G(2d,p); Hartrees] = -1937.0388331039
E [aug-cc-pVTZ; Hartrees] = -1937.1605534787
Gvib [kcal/mol] = 200.507

O	-5.40152267	0.14041252	0.80352321
C	-6.61025606	-0.28491086	0.48028367
C	-10.60239627	-1.66514086	-0.65641646
C	-9.23093738	-1.19627730	-0.23812989
C	-8.17539618	-2.08970066	-0.04241586
C	-6.90050854	-1.65512373	0.30816370
C	-7.68518406	0.61083265	0.28590787
C	-8.95024613	0.16306092	-0.06827946
H	-11.39010550	-1.07796446	-0.17640208
H	-10.74104564	-1.57128935	-1.73761538
H	-10.76243917	-2.71409323	-0.39477260
H	-8.35121856	-3.15481459	-0.16700296
H	-6.09896660	-2.37557586	0.44426017
H	-7.50092137	1.67368484	0.40769717
H	-9.74118428	0.89114461	-0.22206507
O	-2.57616336	1.22914085	1.69158281
C	-1.43418919	1.75527801	2.09118092
NA	-3.86437285	-0.46394873	2.21907705
C	-0.71133790	1.24195844	3.19068368
C	0.49179842	1.80848098	3.60263814
C	1.04850420	2.91276524	2.95394396
C	0.33963641	3.42929674	1.86357464
C	-0.86089905	2.87438700	1.44015716
H	-1.11277278	0.38555373	3.72481409

H	1.00862737	1.37648295	4.45507356
C	2.35930014	3.52047161	3.39037606
H	0.73795127	4.28839880	1.33027726
H	-1.37725678	3.30412668	0.58622951
H	3.13762681	3.38939712	2.63125802
H	2.72142835	3.06306578	4.31366171
H	2.26566964	4.59621982	3.56779049
C	-8.33602802	0.80887100	-3.52862496
C	-7.28678440	-0.08399903	-3.34621237
C	-8.22117664	2.15592421	-3.19767266
H	-9.05668245	2.83075703	-3.32784067
H	-7.40651881	-1.12936294	-3.59373963
C	-5.99549783	1.72080953	-2.51626965
C	-6.08652222	0.37918839	-2.82323742
C	-7.02233288	2.62797615	-2.68250179
F	-4.81315938	2.18461783	-1.99045139
H	-5.25095929	-0.28345204	-2.64412106
H	-6.89214097	3.66569996	-2.40591389
NA	-4.13102915	1.84586875	0.23370044
C	-9.75690076	0.70577844	-5.96428023
S	-9.86947934	0.23264933	-4.24296745
O	-10.96893133	0.98551318	-3.63683612
O	-9.90494722	-1.22740730	-4.17994570
H	-10.67213442	0.35098560	-6.43999141
H	-9.68470104	1.79021614	-6.02596207
H	-8.88166342	0.22328683	-6.39653981

int8
E [6-311+G(2d,p); Hartrees] = -1937.0480031491
E [aug-cc-pVTZ; Hartrees] = -1937.1677553259
Gvib [kcal/mol] = 198.381

O	-5.93828514	0.73200494	-1.16492022
C	-6.60503147	0.19017264	-0.06454550
C	-8.49824775	-1.41199631	3.45014398
C	-7.81061059	-0.84222844	2.23800805
C	-6.98318822	-1.64308912	1.43682182
C	-6.38041322	-1.13501665	0.28870986
C	-7.41023002	1.01389721	0.70935881
C	-8.00555151	0.49366952	1.85919706
H	-8.67985299	-0.64860218	4.20849926
H	-9.47028863	-1.83021733	3.17025557
H	-7.91783250	-2.21711486	3.90408315
H	-6.80856056	-2.67761243	1.70952448
H	-5.73847432	-1.75563179	-0.32441946
H	-7.56006666	2.04682491	0.42085141
H	-8.63687201	1.13540363	2.46315737
O	-3.57310747	1.21808722	1.58488828
C	-2.42061298	1.58370818	2.13697885
NA	-5.18334291	0.39828424	2.73030611

C	-1.56021958	0.64500860	2.74710662
C	-0.35171299	1.03142101	3.31489825
C	0.07247446	2.36379655	3.30851524
C	-0.77646503	3.29797835	2.70954796
C	-1.99029386	2.92767014	2.13943544
H	-1.85885853	-0.39910921	2.75876888
H	0.27934404	0.27480547	3.77297968
C	1.40437297	2.76560610	3.89163670
H	-0.48542991	4.34446013	2.68885638
H	-2.63277060	3.67914124	1.69077962
H	2.21984333	2.61944775	3.17428687
H	1.64929943	2.17614141	4.77922884
H	1.41391039	3.81960853	4.17996599
C	-7.21808709	-0.00312506	-5.02795235
C	-5.97021395	0.56939470	-4.78779741
C	-8.06122497	-0.34448636	-3.97806543
H	-9.02532140	-0.79408437	-4.17617311
H	-5.31510988	0.81947371	-5.61239096
C	-6.41030620	0.45567109	-2.43785735
C	-5.56054789	0.80343695	-3.48623276
C	-7.65746085	-0.11635285	-2.66854881
F	-2.79255744	1.96737768	-2.48078826
H	-4.58766420	1.24224668	-3.27139951
H	-8.30894661	-0.38523741	-1.84854794
NA	-3.58016948	1.41035387	-0.62762802
C	-8.49067950	1.26749509	-7.20242948
S	-7.74714473	-0.28549482	-6.71051104
O	-8.79384127	-1.30481530	-6.69702926
O	-6.55903909	-0.49708632	-7.53384878
H	-8.82396899	1.14209688	-8.23370320
H	-9.33535296	1.47582111	-6.54753982
H	-7.73968040	2.05330591	-7.13521300

int9

E [6-311+G(2d,p); Hartrees] = -770.9777402929

E [aug-cc-pVTZ; Hartrees] = -771.0252840853

Gvib [kcal/mol] = 64.980

O	-3.43958776	1.45466901	1.66384318
C	-2.27045462	1.72891446	2.21164952
NA	-5.34922354	0.51928464	2.18222101
C	-1.56937940	0.78507405	2.99582753
C	-0.33229885	1.08300295	3.55771097
C	0.27773141	2.32914427	3.38288772
C	-0.41040265	3.26883782	2.60933229
C	-1.64692617	2.98565088	2.03972014
H	-2.01334790	-0.19483438	3.14332355
H	0.17334288	0.32287110	4.14709079
C	1.60155881	2.65739554	4.02935903
H	0.03001041	4.24902763	2.44794442

H	-2.15790917	3.73770749	1.44578029
H	2.15922909	3.39479943	3.44656799
H	2.22907588	1.76830237	4.13054241
H	1.46847087	3.07425660	5.03409328
F	-6.14245522	0.86867582	0.24350258
NA	-4.30320010	1.75086995	-0.33080952

int10
E [6-311+G(2d,p); Hartrees] = -1690.6327043085
E [aug-cc-pVTZ; Hartrees] = -1690.7372136764
Gvib [kcal/mol] = 132.719

F	4.91745450	-0.63258535	1.79714435
NA	6.09070074	-2.40634152	1.90233652
O	6.72920662	-1.93563543	4.00305100
C	6.96059076	-2.78324201	4.98944838
NA	5.40041334	-0.19301612	3.80958756
C	6.51368144	-2.53883486	6.30902331
C	6.71589032	-3.45810770	7.32763309
C	7.38430488	-4.66818978	7.10869767
C	7.84701111	-4.91012747	5.81456613
C	7.64934962	-3.99797253	4.78190227
H	5.97150548	-1.62079739	6.51589684
H	6.33266081	-3.23590168	8.31928749
C	7.59210480	-5.65762189	8.22899336
H	8.37185988	-5.83732256	5.60173386
H	8.01835905	-4.22126654	3.78498879
H	6.64227541	-5.97043812	8.67341785
H	8.19576984	-5.23259749	9.03752448
H	8.10235458	-6.55644283	7.87560589
H	2.96848034	-2.16380925	3.39981420
C	3.19449330	-2.87917022	4.18079194
C	2.69442160	-2.74472578	5.46913400
H	2.07570957	-1.89504419	5.72629188
C	3.00296830	-3.71263377	6.42186080
C	3.79892882	-4.81176069	6.12107896
H	4.03211669	-5.54375425	6.88081648
C	4.31768781	-4.94292162	4.83992918
H	4.96838762	-5.76262839	4.57089816
C	4.00147561	-3.97037059	3.91534790
F	4.53372177	-4.08105536	2.65954618
S	2.35905047	-3.52798596	8.07769073
O	2.32668223	-2.09911665	8.39567191
O	3.10373828	-4.42035359	8.96518388
C	0.67511902	-4.12114164	7.98334883
H	0.69651222	-5.16307572	7.66767605
H	0.26003085	-4.02713077	8.98776587
H	0.12272620	-3.50332783	7.27763306

int11
E [6-311+G(2d,p); Hartrees] = -1690.6485281351
E [aug-cc-pVTZ; Hartrees] = -1690.7511135170
Gvib [kcal/mol] = 132.234

O	-5.94537000	0.70986526	-1.16842621
C	-6.61412195	0.17289747	-0.06670340
C	-8.48255343	-1.40015300	3.47424214
C	-7.80331045	-0.84185533	2.25112857
C	-6.98002779	-1.64822233	1.45168097
C	-6.38510082	-1.14838893	0.29537631
C	-7.41893425	1.00094199	0.70257911
C	-8.00566475	0.48956734	1.86021788
H	-8.62071195	-0.63614381	4.24123286
H	-9.47391394	-1.78288145	3.21293517
H	-7.91727060	-2.22663014	3.90787033
H	-6.80097872	-2.67971199	1.73304443
H	-5.74260236	-1.77086754	-0.31502211
H	-7.57019827	2.03105921	0.40505709
H	-8.63449935	1.13472437	2.46320305
F	-3.66894751	1.18634428	1.51715278
NA	-5.13870532	0.39722204	2.71907857
C	-7.22288456	-0.00207724	-5.03125425
C	-5.97775105	0.57786488	-4.78870558
C	-8.06570773	-0.35613553	-3.98470613
H	-9.02761102	-0.80888258	-4.18536099
H	-5.32413841	0.84002425	-5.61061112
C	-6.41769687	0.44270404	-2.43896206
C	-5.57043407	0.80482945	-3.48584239
C	-7.66174705	-0.13584407	-2.67411649
F	-2.80741996	1.99606181	-2.45804869
H	-4.60128133	1.24889615	-3.26584864
H	-8.31004457	-0.41512941	-1.85518566
NA	-3.57844672	1.43697829	-0.59275146
C	-8.47024859	1.28407995	-7.22233201
S	-7.74963303	-0.27026933	-6.71133700
O	-8.80767948	-1.28304229	-6.71063845
O	-6.56217591	-0.51422286	-7.53403903
H	-8.80027985	1.14884173	-8.25320078
H	-9.31281887	1.50321389	-6.56844736
H	-7.70636235	2.05716776	-7.15699590

int12
E [6-311+G(2d,p); Hartrees] = -524.5700337777
E [aug-cc-pVTZ; Hartrees] = -524.6006691711
Gvib [kcal/mol] = -.950

F	-0.00634865	-1.55671726	0.01967334
NA	-1.44976559	0.00858779	-0.01568465
F	0.01511134	1.55622276	0.00633981
NA	1.45861172	-0.00908114	0.04191600

na2co3
E [6-311+G(2d,p); Hartrees] = -588.6505513272
E [aug-cc-pVTZ; Hartrees] = -588.6886920075
Gvib [kcal/mol] = 6.157

O	1.43536332	-0.21706557	0.57517020
C	0.29634570	-0.36286386	0.00487302
O	-0.54633677	0.66743718	0.00441075
NA	-2.01761095	-0.52772539	-1.08810906
O	-0.07430777	-1.45017873	-0.56463412
NA	0.90654646	1.89039637	1.06828921

ts1
E [6-311+G(2d,p); Hartrees] = -1394.6636015265
E [aug-cc-pVTZ; Hartrees] = -1394.7487086727
Gvib [kcal/mol] = 144.683
Number of imaginary frequencies: 1 [258.92 cm-1]

O	0.05863569	-0.52570279	-1.28790034
C	0.75003470	0.51429004	-0.65240392
NA	2.34115741	-0.84734139	-2.48551131
C	-1.24886602	-0.26323999	-1.70092422
C	-5.30407571	0.28017365	-3.02846864
C	-3.88741572	0.10685998	-2.54617813
C	-3.58988470	-0.72758106	-1.46691250
C	-2.27858178	-0.91309690	-1.04000651
C	-1.51073832	0.57233926	-2.77853630
C	-2.82713206	0.75346737	-3.18866838
H	-5.48505158	1.29745920	-3.38292373
H	-5.51855991	-0.39661913	-3.86208970
H	-6.02602207	0.06378557	-2.23843412
H	-4.39187877	-1.24018627	-0.94663961
H	-2.05006571	-1.55615411	-0.19879049
H	-0.69123416	1.06926866	-3.28028955
H	-3.03103916	1.40818860	-4.02944044
O	0.16458649	1.37627218	-0.00602959
O	1.94597197	-0.08144006	-0.19804474
C	2.01179071	-0.33198985	1.17479796
O	3.65566634	0.98208569	-2.53977095
C	2.75479945	1.74142650	-2.09836903
O	1.45840614	1.25247574	-2.15865361
NA	0.77042205	3.23537258	-1.08841896
O	2.90375695	2.90427192	-1.63769804
C	2.58510247	0.61094310	2.01364582
C	2.69920938	0.33152115	3.37094726
C	2.24653214	-0.87977184	3.90253186
C	1.67046007	-1.80777553	3.03170163
C	1.55026342	-1.54136074	1.67110174
H	2.93450070	1.54900495	1.60145381

H	3.14775625	1.07000312	4.02695149
C	2.40793767	-1.18608648	5.36870319
H	1.30959885	-2.75475732	3.41843165
H	1.10168442	-2.26139629	0.99769783
H	2.29816951	-0.28732960	5.97965947
H	3.40097394	-1.59888764	5.57451822
H	1.67312896	-1.91849230	5.70896088

ts2
E [6-311+G(2d,p); Hartrees] = -1394.6548096396
E [aug-cc-pVTZ; Hartrees] = -1394.7400982440
Gvib [kcal/mol] = 141.184
Number of imaginary frequencies: 1 [245.53 cm-1]

O	0.15810908	-0.35156905	-1.22266416
C	0.98319259	0.93718379	-0.97982888
NA	2.10102309	-0.89336784	-2.39676644
C	-1.15268215	-0.20937504	-1.57512262
C	-5.34739799	-0.06273178	-2.65379778
C	-3.88594678	-0.11043724	-2.28650705
C	-3.37169840	-1.17117171	-1.53402879
C	-2.03083001	-1.22052189	-1.17641925
C	-1.64670774	0.85156299	-2.33470009
C	-2.99725399	0.89290909	-2.67391181
H	-5.57939812	0.81341611	-3.26273443
H	-5.64679669	-0.94965274	-3.22025338
H	-5.98182969	-0.02397332	-1.76287526
H	-4.03329547	-1.96989459	-1.21290573
H	-1.64655382	-2.04144031	-0.58184029
H	-0.97632684	1.63200891	-2.66484089
H	-3.36087752	1.72929105	-3.26262551
O	0.42762169	1.75979303	-0.20854360
O	2.23772382	0.17907248	-0.31856387
C	2.11835324	-0.13774736	1.00234627
O	3.88616150	0.70581754	-2.79982264
C	3.46991380	1.67032082	-2.25768209
O	1.48392843	1.32526023	-2.17423760
NA	1.39478782	3.44397513	-1.23481668
O	3.59021873	2.75412559	-1.79321624
C	2.39455349	0.81483481	1.98331602
C	2.31236142	0.48014391	3.33041819
C	1.95425555	-0.80774431	3.73901150
C	1.67750026	-1.75170435	2.74668683
C	1.75302554	-1.42499305	1.39629080
H	2.67344101	1.81556234	1.67860719
H	2.53163210	1.23602566	4.07808911
C	1.90451149	-1.17418207	5.20039281
H	1.39407349	-2.75998962	3.03186314
H	1.52088525	-2.16425052	0.63920634

H	1.61394635	-0.32095463	5.81785659
H	2.88294537	-1.51359205	5.55711897
H	1.19343014	-1.98201001	5.38750132

ts3

E [6-311+G(2d,p); Hartrees] = -1206.0430266686

E [aug-cc-pVTZ; Hartrees] = -1206.1177180760

Gvib [kcal/mol] = 134.767

Number of imaginary frequencies: 1 [159.34 cm-1]

O	-0.08718812	0.03090646	-3.00755536
C	1.04688413	1.73080392	-2.81702685
NA	1.57626506	-1.08477825	-2.02936562
C	-1.38400035	0.11771728	-2.72912479
C	-5.62166640	0.48510215	-1.74465518
C	-4.15883279	0.34498847	-2.08016280
C	-3.35457699	-0.62329589	-1.48270872
C	-1.99801675	-0.73912742	-1.79001491
C	-2.20669845	1.09357842	-3.33314004
C	-3.55171530	1.19634065	-3.01273999
H	-5.83994760	1.46370210	-1.30556549
H	-6.24807109	0.38914076	-2.63673002
H	-5.94337238	-0.27601805	-1.03092727
H	-3.78665487	-1.30851228	-0.76013008
H	-1.40720535	-1.52108113	-1.32199257
H	-1.76192327	1.76741409	-4.05612372
H	-4.15016536	1.96115091	-3.49930855
O	0.35323578	2.47226588	-2.20692963
O	1.23443223	-0.20050194	-0.05599498
C	1.72831700	-0.45214334	1.14518211
O	2.03593657	1.38106865	-3.34995797
NA	-0.49059464	1.13394327	-0.36688713
C	2.08193838	0.58175792	2.03965270
C	2.57973824	0.30671642	3.30975278
C	2.76164997	-1.00197677	3.76277127
C	2.42556580	-2.03201775	2.87751247
C	1.92485743	-1.77336601	1.60787899
H	1.96954481	1.61218176	1.71429435
H	2.83648827	1.13619477	3.96285145
C	3.26815098	-1.29944701	5.15222017
H	2.55684653	-3.06453460	3.18995559
H	1.66462756	-2.59660535	0.94887259
H	2.45149134	-1.56766389	5.83197388
H	3.77917823	-0.43626322	5.58538392
H	3.97204897	-2.13646573	5.15383294

ts4

E [6-311+G(2d,p); Hartrees] = -1936.9871080243

E [aug-cc-pVTZ; Hartrees] = -1937.1086137437

Gvib [kcal/mol] = 198.358
Number of imaginary frequencies: 1 [294.49 cm-1]

O	-5.47845953	0.96563509	-0.93069221
C	-6.38637028	0.29511923	-0.17467835
C	-9.17046694	-1.84294111	2.36198892
C	-8.19050250	-1.09913896	1.49387467
C	-7.31475322	-1.78496284	0.64597405
C	-6.42540987	-1.10582665	-0.18286479
C	-7.26127176	0.99317654	0.66765902
C	-8.14330308	0.29844201	1.49136592
H	-9.42961511	-1.27124195	3.25535023
H	-10.10026249	-2.03820280	1.81762684
H	-8.77185793	-2.80845639	2.68057655
H	-7.32389290	-2.86963178	0.63208833
H	-5.75165386	-1.64732136	-0.83515178
H	-7.23095367	2.07566413	0.67551642
H	-8.80429198	0.85784518	2.14460411
O	-2.97387984	1.23074130	1.25862524
C	-1.92960603	1.61289902	1.97850610
NA	-4.69579426	0.06884892	1.90652924
C	-1.45934432	0.86701330	3.08014560
C	-0.35882834	1.27982490	3.82638863
C	0.34067831	2.44909193	3.52309321
C	-0.11657497	3.19476499	2.43114848
C	-1.21647070	2.79820269	1.68251183
H	-1.96176667	-0.06074687	3.33969992
H	-0.03682234	0.66842131	4.66451833
C	1.53375315	2.90038769	4.32831603
H	0.39773443	4.11341078	2.16231192
H	-1.54611855	3.41814321	0.85299870
H	2.42778979	3.00058495	3.70467170
H	1.76768135	2.19216818	5.12627455
H	1.36107551	3.87572873	4.79482135
C	-8.38972231	0.67596279	-3.77226385
C	-7.27535597	-0.16887858	-3.87874283
C	-8.27099987	1.88309197	-3.06801695
H	-9.12002982	2.55280307	-3.00114300
H	-7.35229166	-1.09111338	-4.44185713
C	-5.97615914	1.33847873	-2.48255607
C	-6.08614268	0.15638747	-3.27271077
C	-7.08995354	2.22834407	-2.45642055
F	-4.69575926	2.04931088	-2.72037036
H	-5.22586687	-0.49712488	-3.34220666
H	-6.99652865	3.15425174	-1.90354790
NA	-3.42405207	1.82865027	-0.82979836
C	-9.78634924	1.02267965	-6.20901434
S	-9.88767951	0.26970848	-4.58042019
O	-11.00105575	0.92059354	-3.88307156
O	-9.94119163	-1.18076170	-4.78708503
H	-10.71241801	0.78565249	-6.73462744

H	-9.67845146	2.09992228	-6.08996379
H	-8.92915374	0.60427345	-6.73481628

ts5
E [6-311+G(2d,p); Hartrees] = -1690.5881590610
E [aug-cc-pVTZ; Hartrees] = -1690.6924344280
Gvib [kcal/mol] = 131.246
Number of imaginary frequencies: 1 [300.90 cm-1]

O	-5.48353273	1.00510789	-0.91181625
C	-6.38092643	0.31265612	-0.16999006
C	-9.11031305	-1.90020159	2.36658595
C	-8.15296609	-1.13063619	1.49428375
C	-7.23157304	-1.79277016	0.67650367
C	-6.35881949	-1.08940762	-0.15060936
C	-7.30550512	0.98566951	0.64005723
C	-8.17146244	0.26767275	1.46030975
H	-9.39269393	-1.32748581	3.25214257
H	-10.02996779	-2.13398422	1.82063108
H	-8.67745423	-2.84677648	2.69651852
H	-7.19011722	-2.87675838	0.68625180
H	-5.64792807	-1.61129789	-0.77950619
H	-7.32120663	2.06832437	0.62765671
H	-8.87058171	0.80808327	2.08961296
F	-3.05302808	1.19827205	1.26684845
NA	-4.68284211	0.09452319	1.94338743
C	-8.38249342	0.69354093	-3.73020345
C	-7.28179371	-0.17265996	-3.83048759
C	-8.23239409	1.92743498	-3.07584362
H	-9.06682748	2.61583482	-3.02385961
H	-7.37868055	-1.10927145	-4.36589550
C	-5.94140365	1.35810443	-2.50136760
C	-6.07823060	0.15564470	-3.25761387
C	-7.03622054	2.27326536	-2.49889621
F	-4.65525724	2.01550311	-2.72081622
H	-5.22711411	-0.50986028	-3.32335729
H	-6.91543143	3.21717374	-1.98313534
NA	-3.39480107	1.76960664	-0.74354902
C	-9.77425701	0.93262369	-6.19389723
S	-9.88539602	0.29916379	-4.51867433
O	-10.98206641	1.02889413	-3.86326999
O	-10.01143237	-1.16192741	-4.62988604
H	-10.71475657	0.69295771	-6.69140004
H	-9.62461177	2.00997239	-6.14542163
H	-8.93726548	0.44387534	-6.69014260

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