Supporting Information for “Controlled Organocatalytic Ring-Opening Polymerization of ε-Thionocaprolactone”

Partha P. Datta and Matthew K. Kiesewetter

Department of Chemistry, University of Rhode Island, Kingston, RI 02881 USA

Figure S1. MALDI-TOF of the PtnCL resulting from the 1/BEMP catalyzed ROP of tnCL. Minor peaks could not be identified, but they are not consistent with H+, Li+, Na+ or K+ adducts of cyclic or linear PtnCL with benzyl alcohol or BEMP end groups.
Figure S2. (upper) GPC trace of PtnCL resulting from the 1/BEMP catalyzed ROP of tnCL from pyrene butanol. The high weight tail grows in late in the ROP. (middle) GPC traces (UV) showing the evolution of the peak shape as a function of conversion. (lower) GPC traces (UV) of the polymer species resulting from allowing the ROP solution to stir with catalysts after full conversion (5h is full conversion).
Figure S3. Temperature dependent equilibrium constant for the reversible ROP of tnCL catalyzed by TBD from benzyl alcohol.

\[
\ln \frac{1}{[M]_{eq}} = -\frac{\Delta H_p}{RT} + \frac{\Delta S_p}{R}
\]

Figure S4. First order evolution of monomer vs time for the copolymerization of tnCL and VL. Reaction conditions tnCL (1M, 100 mg), VL (1M, 100 mg), 1 mol% benzyl alcohol, 5 mol% BEMP, 5 mol% 1 in C₆D₆.
Figure S5. Titration curve for the binding of tnCL to 1. Observed chemical shift of 1 (o-protons, 5 mM) vs [tnCL] in C₆D₆. Solid line is the fit from the quadratic binding equation.

Figure S6. First order evolution of [tnCL] vs time in the 1/BEMP catalyzed ROP from benzyl alcohol.
Figure S7. The binding of ethyl acetate (or ethyl thionoacetate) to 1 is too low to be measured, and the binding of tnCL to 1 is: $K_{eq} = 1.6$. Because the binding constant of 1 to ethyl thionoacetate is greater than unity, the selectivity of 1 for tnCL must be: $K_{eq(\text{sel.})} \leq 1.6$, or $\Delta G^\neq < 0.27$ kcal/mol if the selectivity at the reagents were to be translated to the transition state. This incongruity suggests other modes of action of 1 upon the reaction that are unique to the transition state.
Figure S8. $^{13}$C NMR (75 MHz, CDCl$_3$) spectrum of the polymer resulting from the ROP of tnCL (2M, toluene) from benzyl alcohol (1 mol%) catalyzed by DBU (5 mol%) at room temperature. The formation of poly(thionocaprolactone) as evidenced by the carbonyl resonance at 223 ppm.
Figure S9. $^{13}$C NMR (75 MHz, CDCl$_3$) spectrum of the polymer resulting from the ROP of tnCL (2M, toluene) from benzyl alcohol (1 mol%) catalyzed by DBU (5 mol%) at 100°C results in the formation of poly(thiono-co-thiocaprolactone) as evidenced by the two carbonyl resonances at 223 ppm and 199 ppm. The most downfield resonance is due to unconverted monomer.
Figure S10. $^{13}$C NMR (75 MHz, CDCl$_3$) spectrum of P(tnCL-co-VL) (50:50).
Figure S11. $^1$H NMR (300 MHz, CDCl$_3$) spectrum of P(tnCL-co-VL) (50:50).
Figure S12. $^1$H NMR (300 MHz, CDCl$_3$) spectrum of tnCL.
Figure S13. $^{13}$C NMR (75 MHz, CDCl$_3$) spectrum of tnCL.
Figure S14. $^1$H NMR (300 MHz, CDCl$_3$) spectrum of PtnCL.
COMPUTATIONAL OUTPUT

Figure S15. Calculated (DFT B3LYP//6-31G**) electrostatic potential of atoms in the C=X bond of 7-membered and s-trans lactones.

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Number of basis functions: 109  
Multiplicity: 1  
Solvation: toluene [SM8]  
Free Energy of Solvation: -22.1872126 kJ/mol  
SCF total energy: -591.3523054 hartrees

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methyl thionoacetate + TU

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Number of basis functions: 553
Multiplicity: 1
Solvation: toluene [SM8]
Free Energy of Solvation : -60.5273905 kJ/mol
SCF total energy: -2279.4107961 hartrees

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methyl acetate

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Number of basis functions: 105
Multiplicity: 1
Solvation: toluene [SM8]
Free Energy of Solvation: -12.7057187 kJ/mol
SCF total energy: -268.4015947 hartrees

Cartesian Coordinates (Angstroms)

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Number of shells: 62
Number of basis functions: 170
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Solvation: toluene [SM8]
Free Energy of Solvation: -27.6012335 kJ/mol
SCF total energy: -385.1315410 hartrees

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**Method:** RB3LYP  
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**Number of shells:** 207  
**Number of basis functions:** 614  
**Multiplicity:** 1
Solvation: toluene [SM8]

Free Energy of Solvation: -67.1539901 kJ/mol
SCF total energy: -2073.2133692 hartrees

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37 C19 : -0.263  -0.158  -0.475
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39 H20 : +0.092  +0.098  +0.234
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44 H25 : +0.090  +0.091  +0.245
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57 F6  : -0.160  -0.263  -0.364
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Method: RB3LYP
Basis set: 6-31G**
Number of shells: 63
Number of basis functions: 174
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Solvation: toluene [SM8]

Free Energy of Solvation: \(-38.5515024\) kJ/mol

SCF total energy: \(-708.0828269\) hartrees

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Free Energy of Solvation: -75.7255567 kJ/mol  
SCF total energy: -2396.1542883 hartrees

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Number of shells: 63
Number of basis functions: 174
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Solvation: toluene [SM8]
Free Energy of Solvation: -30.4982395 kJ/mol
SCF total energy: -708.1027241 hartrees

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**tCL + TU**

Method: RB3LYP
Basis set: 6-31G**
Number of shells: 208
Number of basis functions: 618
Multiplicity: 1
Solvation: toluene [SM8]
Free Energy of Solvation:  -69.9213362 kJ/mol
SCF total energy: -2396.1749852 hartrees

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