*Supporting information for*

# Preparation of Multiblock Copolymers via Step-wise Addition Polymerization of L-lactide and Trimethylene Carbonate

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## NMR Spectroscopy

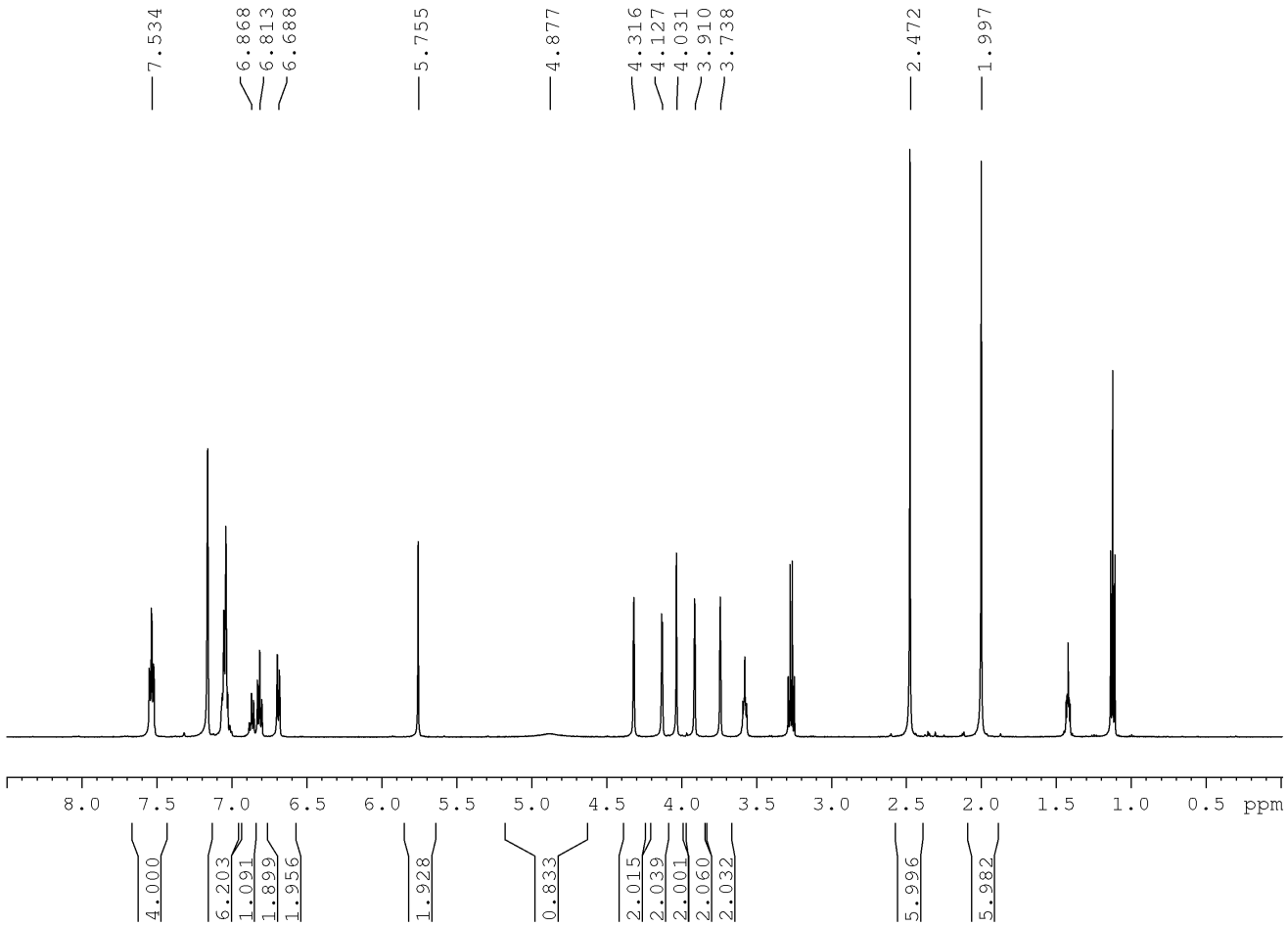



**Figure S1.** $^{1}$H NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: δ (ppm) 2.00 (s, 6H, C*H*$_3$), 2.47 (s, 6H, C*H*$_3$), 3.74 (t, 2H, Cp-*H*), 3.91 (t, 2H, Cp-*H*), 4.03 (s, 2H, OC*H*$_2$Ph), 4.13 (q, 2H, Cp-*H*), 4.32 (t, 2H, Cp-*H*), 4.88 (br s, 1H, B*H*), 5.76 (s, 2H, C*H*), 6.69 (m, 2H, *o*-Ph), 6.81 (m, 2H, *m*-Ph), 6.87 (m, 1H, *p*-Ph), 7.04 (m, 6H, *m*-Ph, *p*-Ph), 7.53 (m, 4H, *o*-Ph). Peaks at 1.12 ppm and 3.27 ppm are attributed to residual diethyl ether. Peaks at 1.42 ppm and 3.58 ppm are attributed to residual tetrahydrofuran.

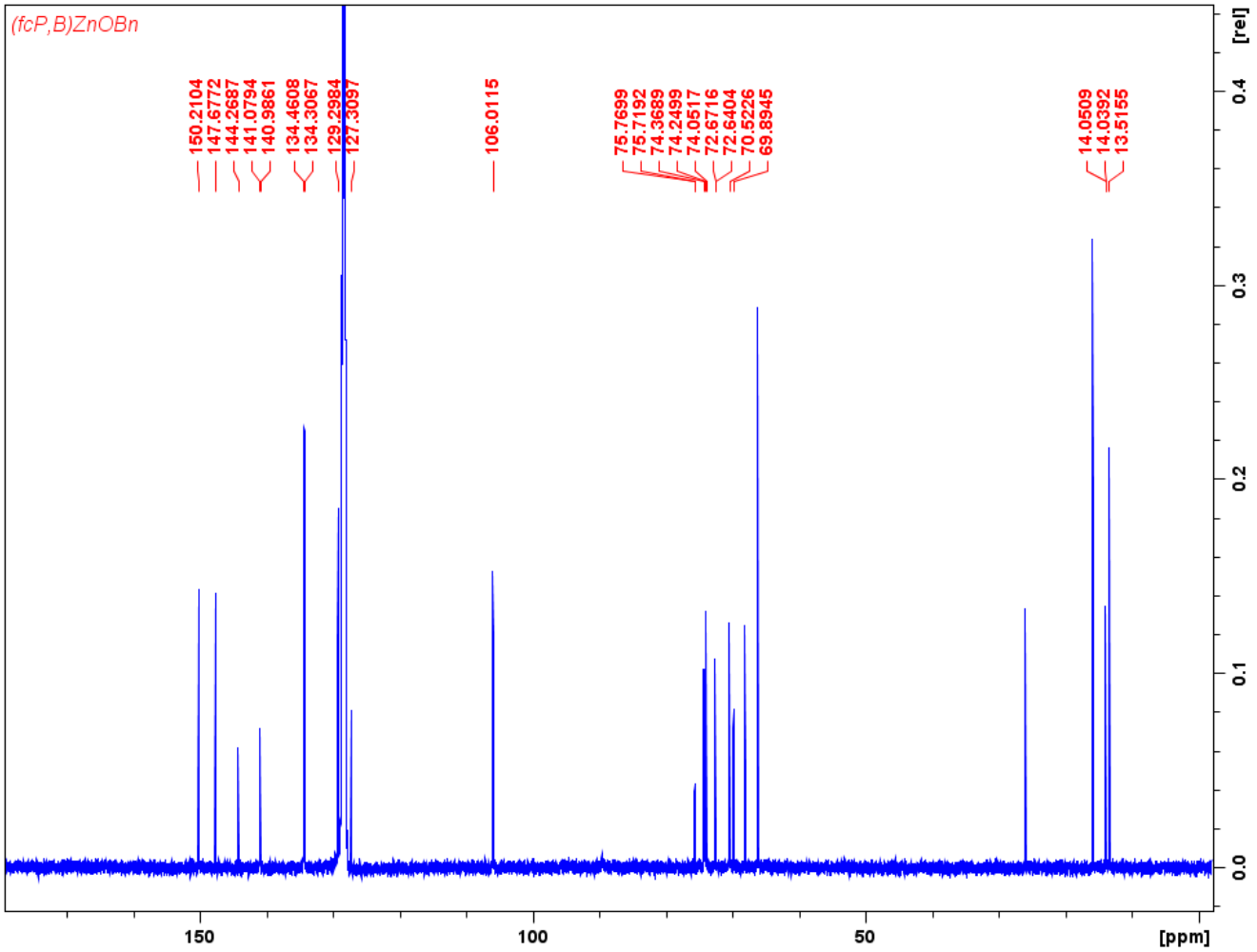



**Figure S2.** $^{13}$C NMR spectrum ($C_6D_6$, 126 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: δ (ppm) 13.5 (s, *C*H$_3$), 14.0 (d, *C*H$_3$), 69.9 (s, Cp-*C*), 70.5 (s, O*C*H$_2$Ph), 72.7 (d, Cp-*C*), 74.1 (s, Cp-*C*), 74.3 (d, Cp-*C*), 75.7 (d, Cp-*C*), 106.0 (s, *C*H), 127.3 (s, aromatic), 129.3 (s, aromatic), 134.4 (d, aromatic), 141.0 (d, aromatic), 144.3 (s, aromatic), 147.7 (s, *C*CH$_3$), 150.2 (s, *C*CH$_3$). Peaks at 15.9 ppm and 66.3 ppm are attributed to residual diethyl ether. Peaks at 26.2 ppm and 68.2 ppm are attributed to residual tetrahydrofuran.

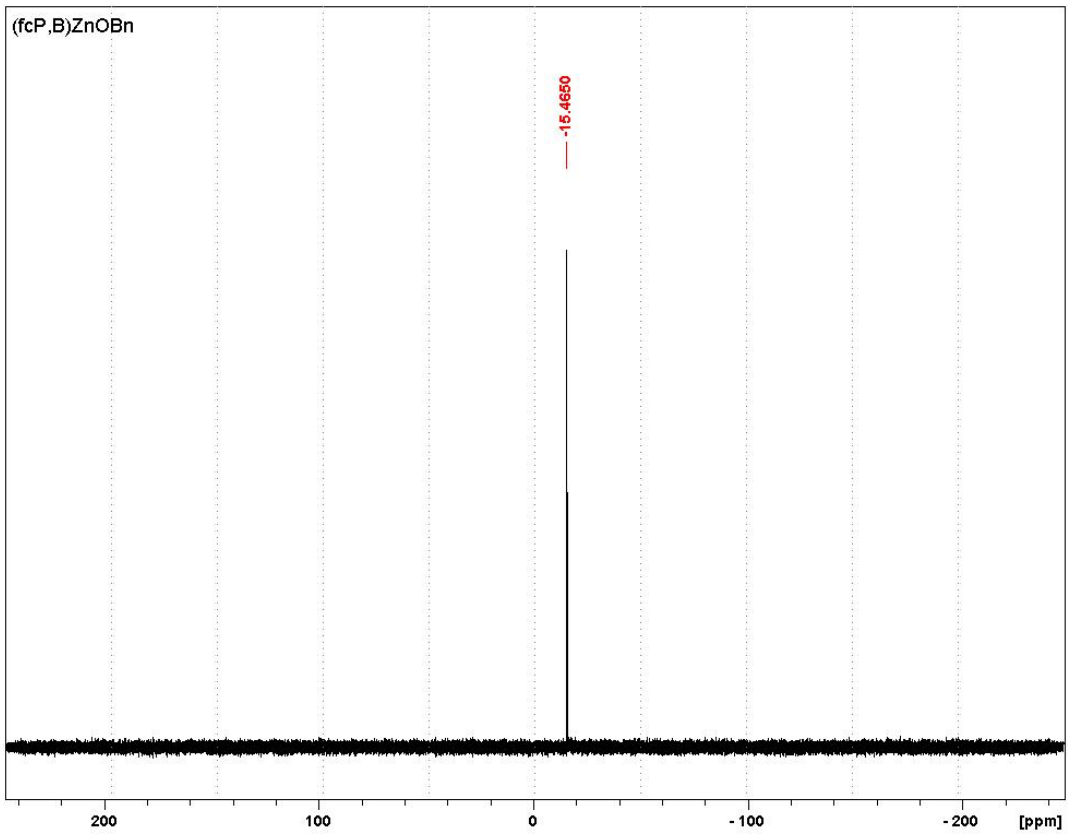



**Figure S3.** $^{31}P\{^{1}H\}$ NMR spectrum ($C_6D_6$, 203 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: δ (ppm) -15.5 (s).

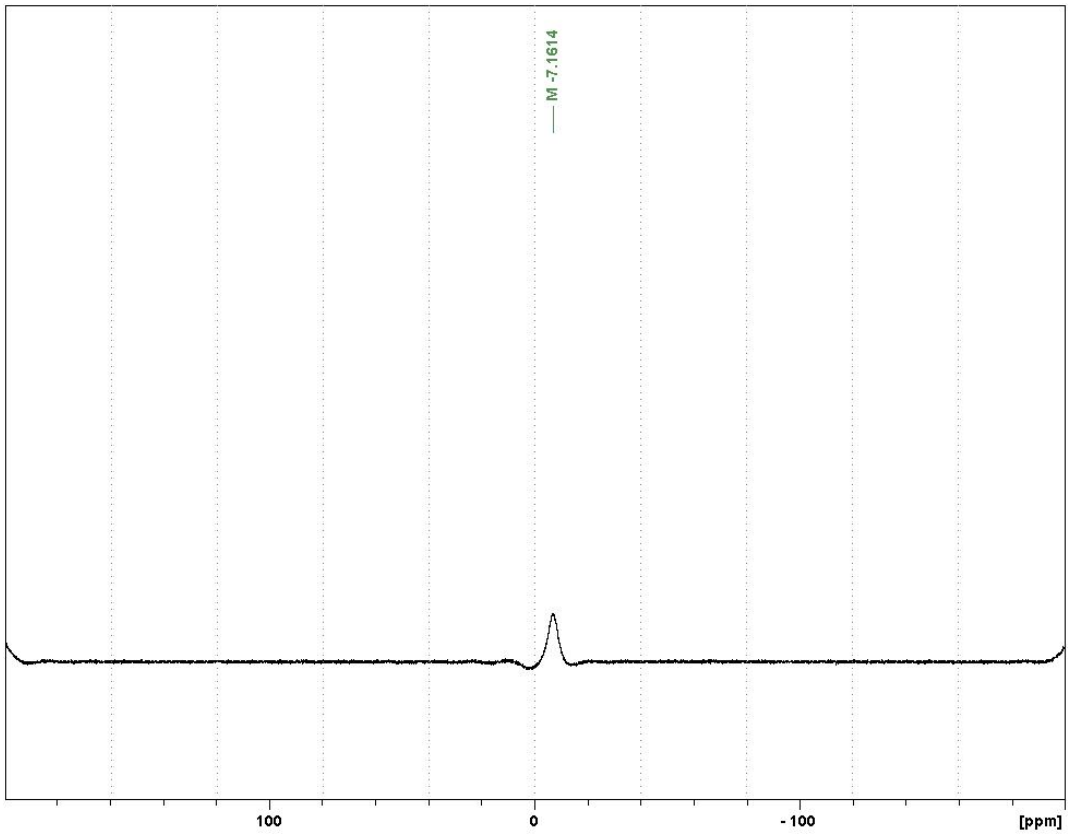



**Figure S4.** $^{11}B$ NMR spectrum ($C_6D_6$, 161 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: δ (ppm) -7.2 (br s).

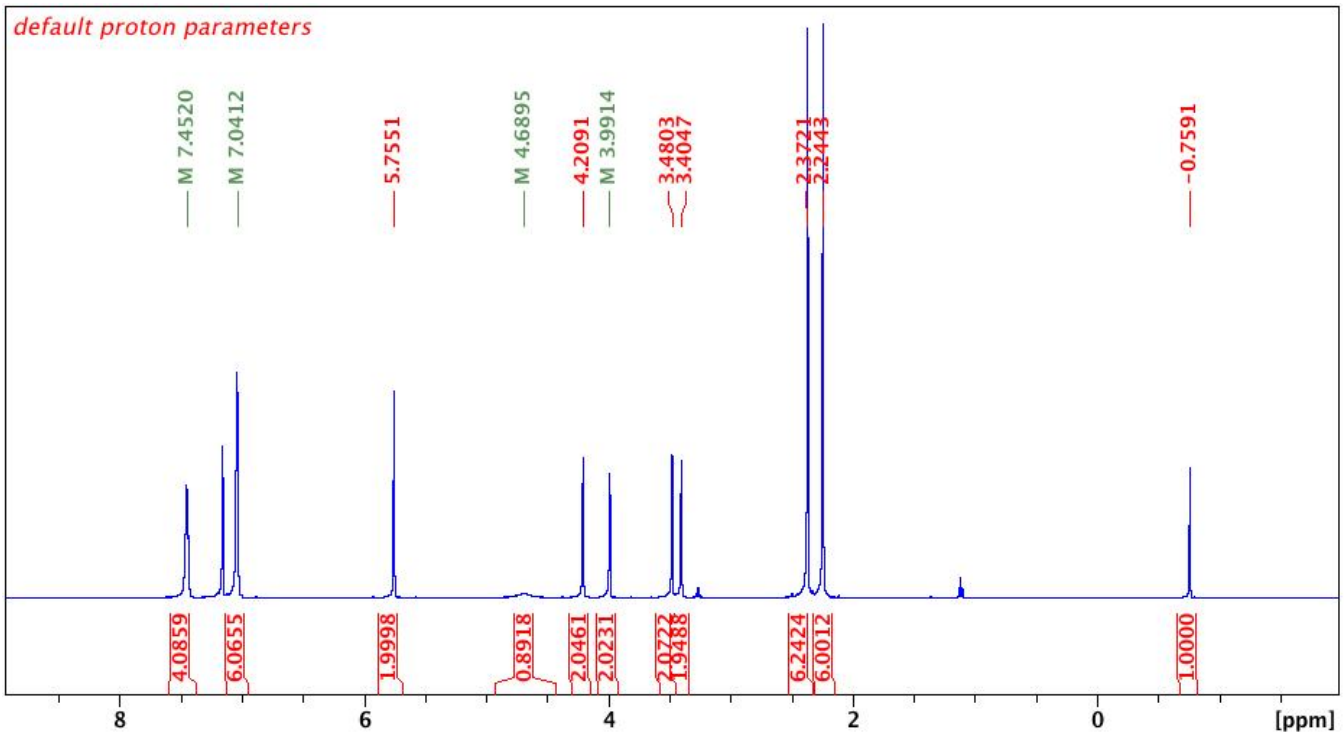



**Figure S5.** $^{1}$H NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OH)]_2$: δ (ppm) -0.76 (s, 1H, O*H*), 2.24 (s, 6H, C$H_3$), 2.37 (s, 6H, C$H_3$), 3.40 (t, 2H, Cp-*H*), 3.48 (t, 2H, Cp-*H*), 3.99 (q, 2H, Cp-*H*), 4.21 (t, 2H, Cp-*H*), 4.69 (br s, 1H, B*H*), 5.76 (s, 2H, C*H*), 7.04 (m, 6H, *m*-Ph, *p*-Ph), 7.45 (m, 4H, *o*-Ph).

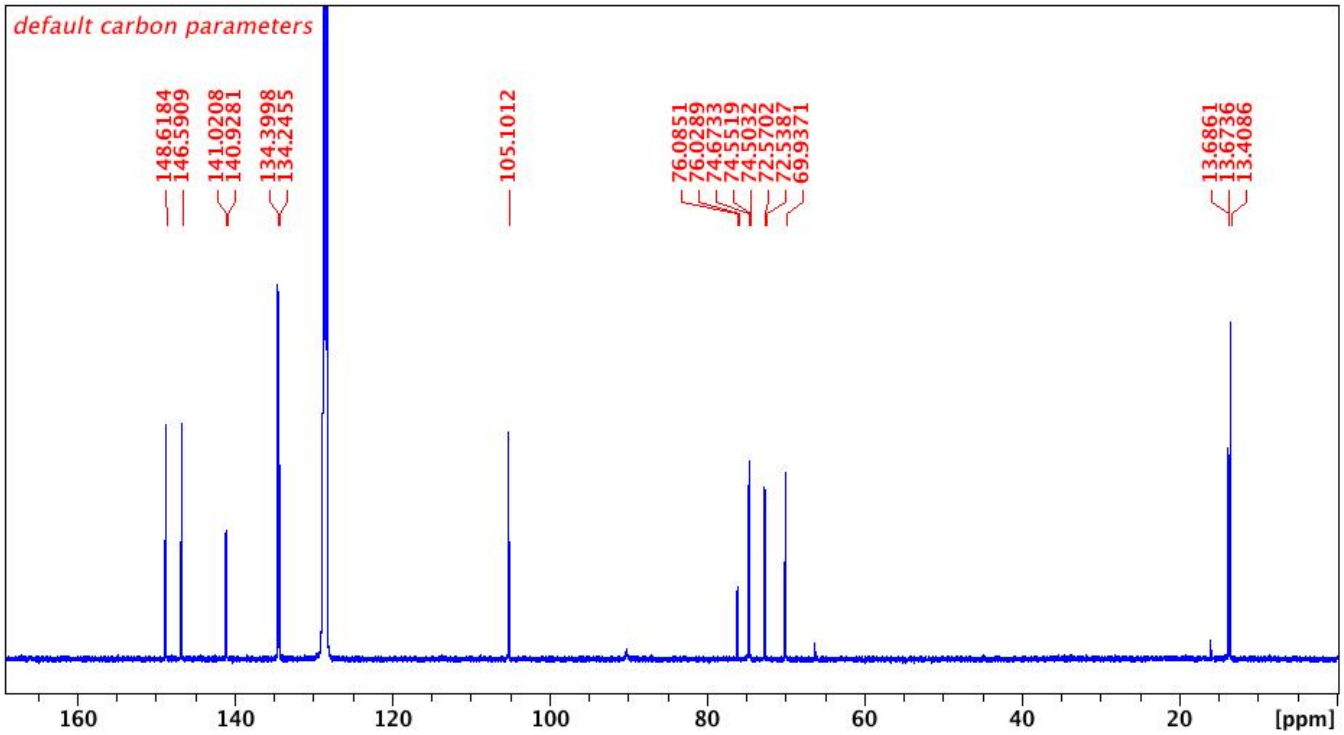



**Figure S6:** $^{13}$C NMR spectrum ($C_6D_6$, 126 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OH)]_2$: δ (ppm) 13.4 (s, *C*$H_3$), 13.7 (d, *C*$H_3$), 69.9 (s, Cp-*C*), 72.6 (d, Cp-*C*), 74.5 (s, Cp-*C*), 74.6 (d, Cp-*C*), 76.0 (d, Cp-*C*), 105.1 (s, *C*H), 134.3 (d, aromatic), 140.1 (d, aromatic), 146.6 (s, *C*$CH_3$), 148.6 (s, *C*$CH_3$).

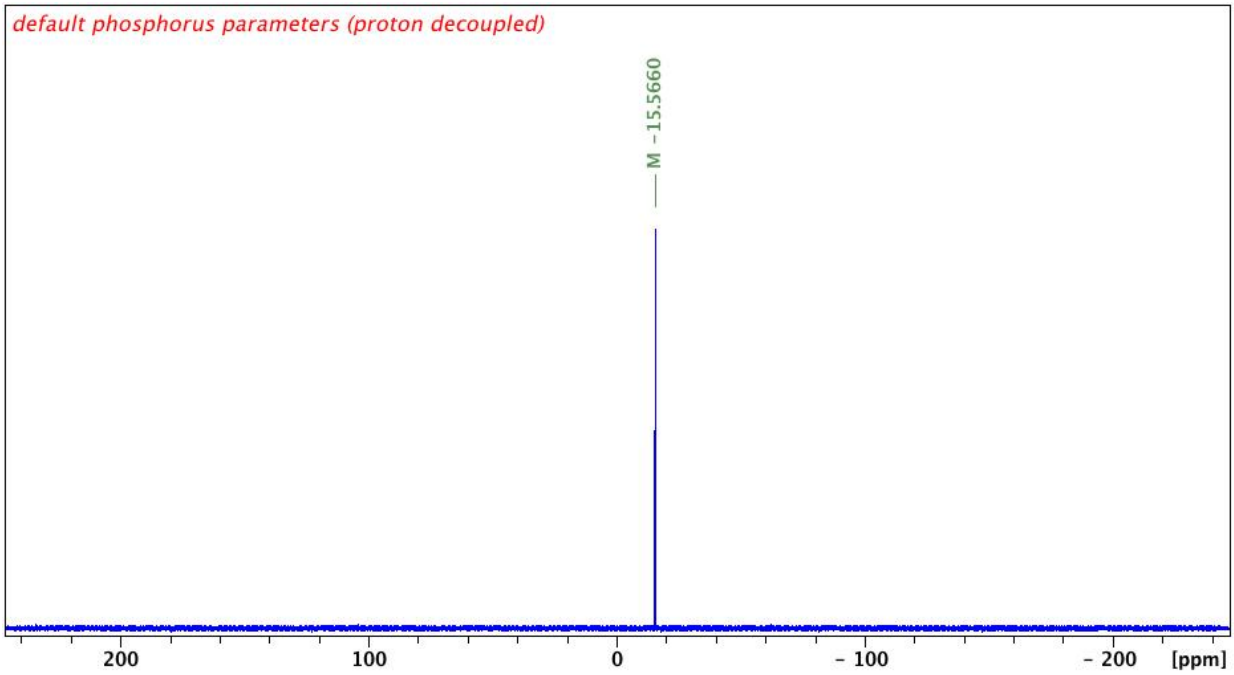



**Figure S7.** $^{31}P\{^{1}H\}$ NMR spectrum ($C_6D_6$, 203 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OH)]_2$: δ (ppm) -15.6 (s).

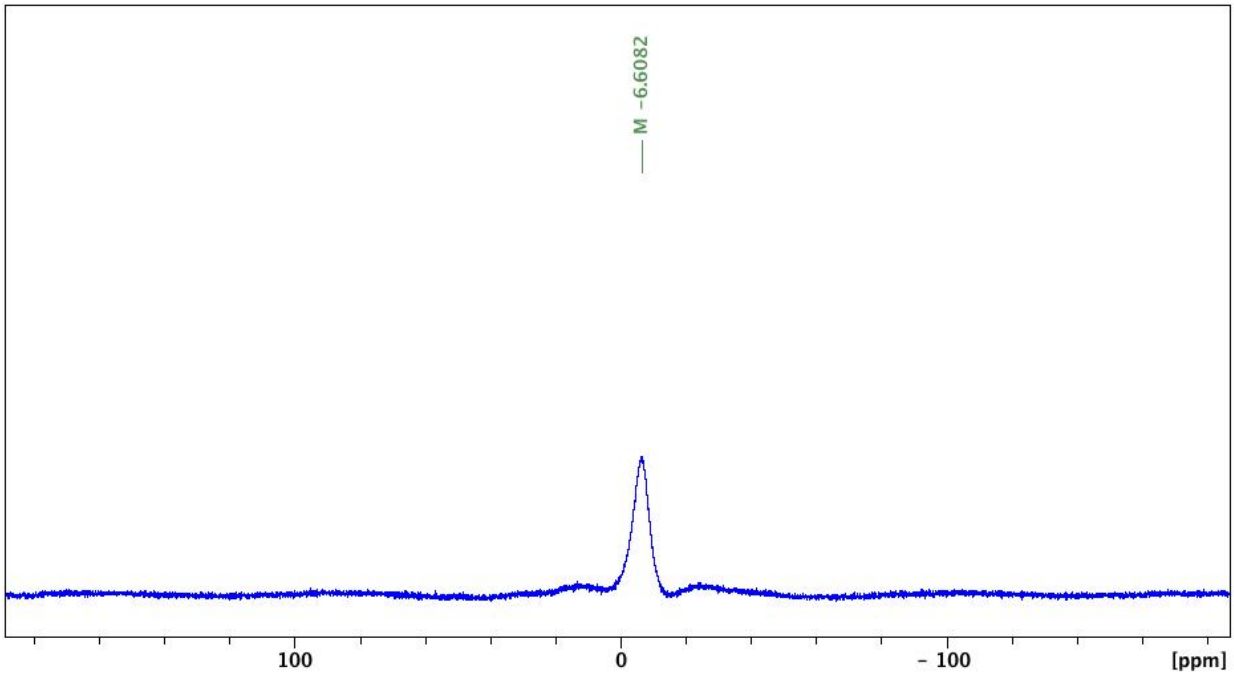



**Figure S8.** $^{11}B$ NMR spectrum ($C_6D_6$, 161 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OH)]_2$: δ (ppm) -6.6 (br s).

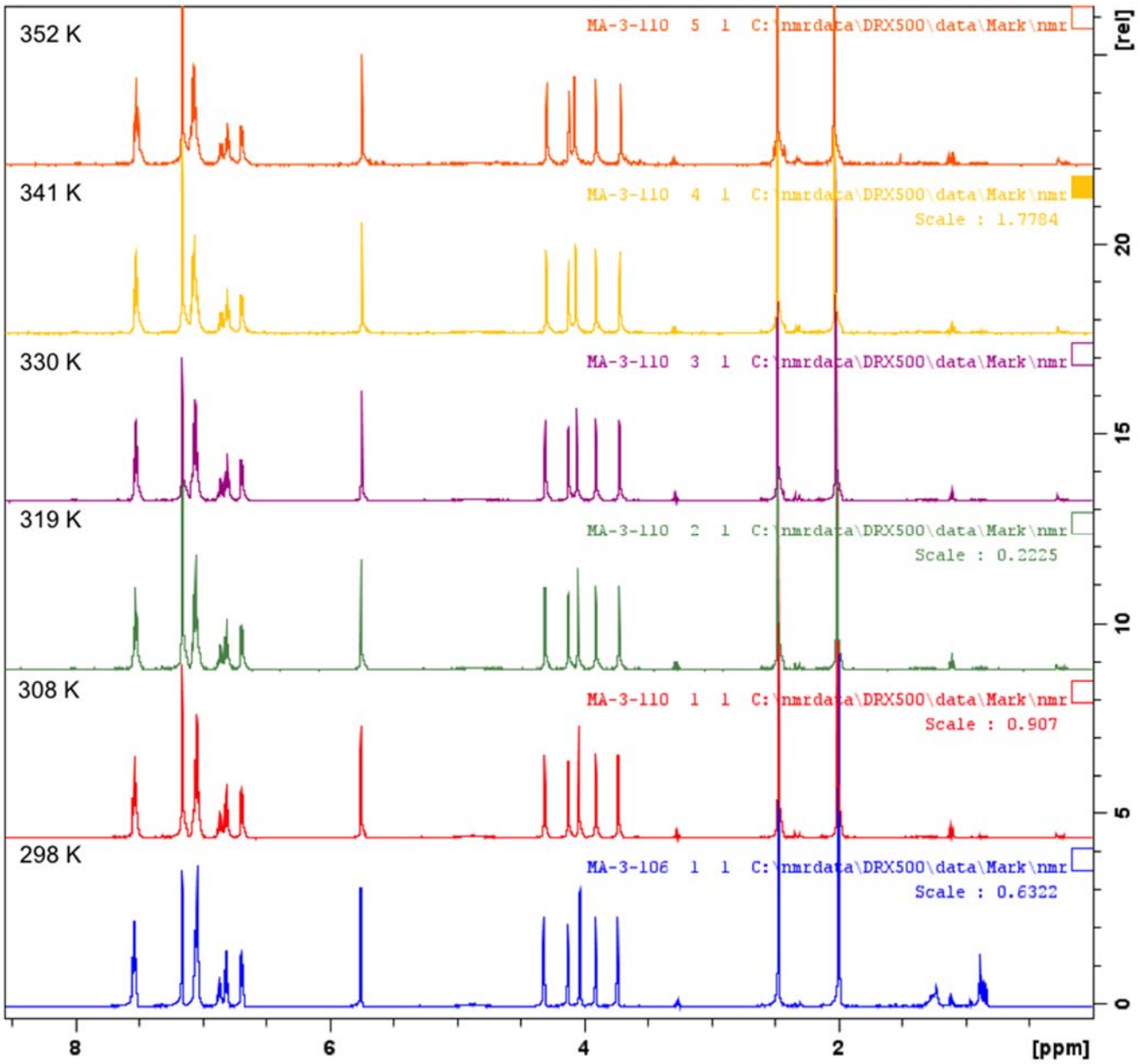



**Figure S9.** Variable temperature NMR ($C_6D_6$, 500 MHz) study of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$.

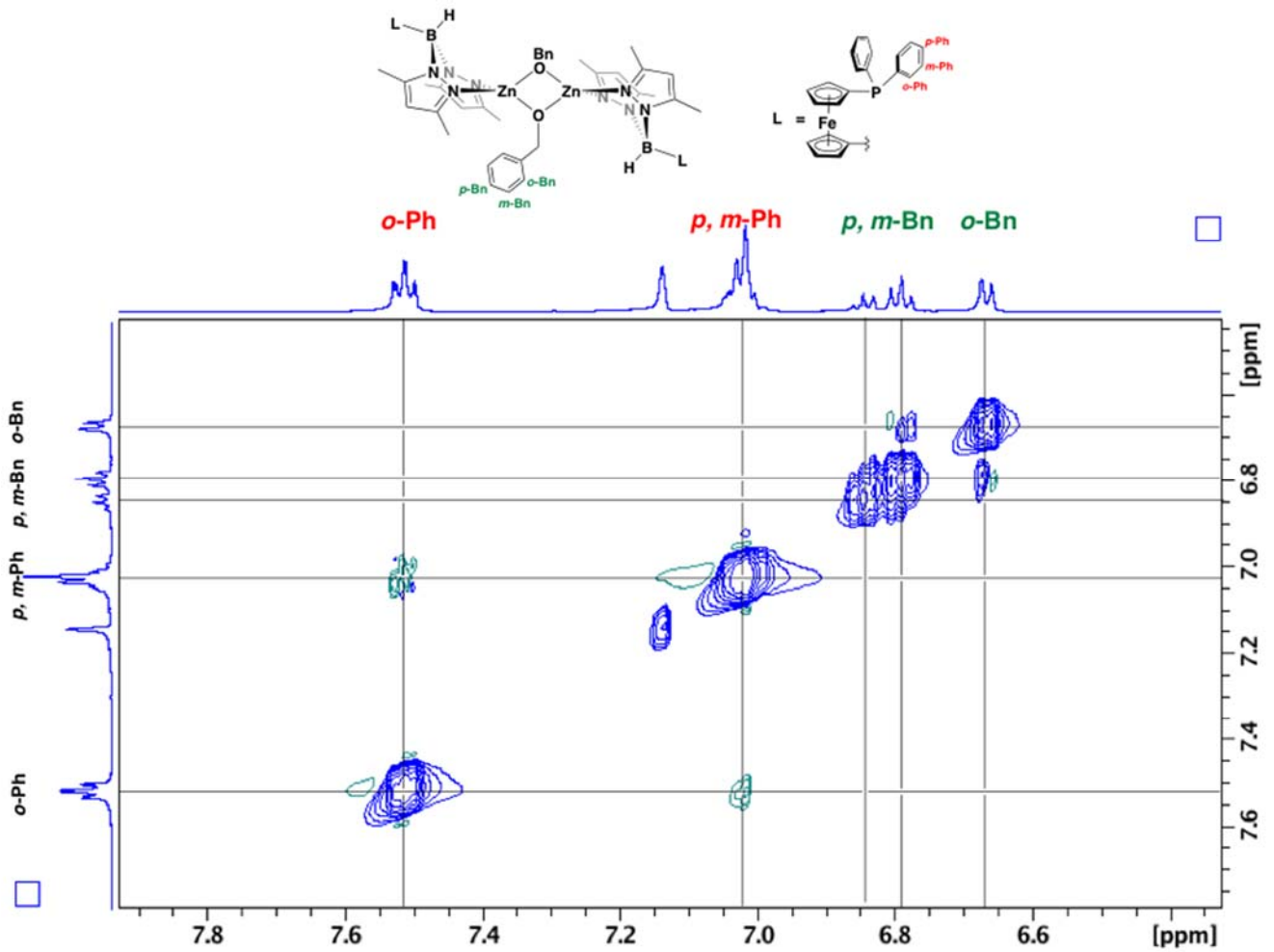



**Figure S10.** Selected region of $^{1}$H NOESY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$.

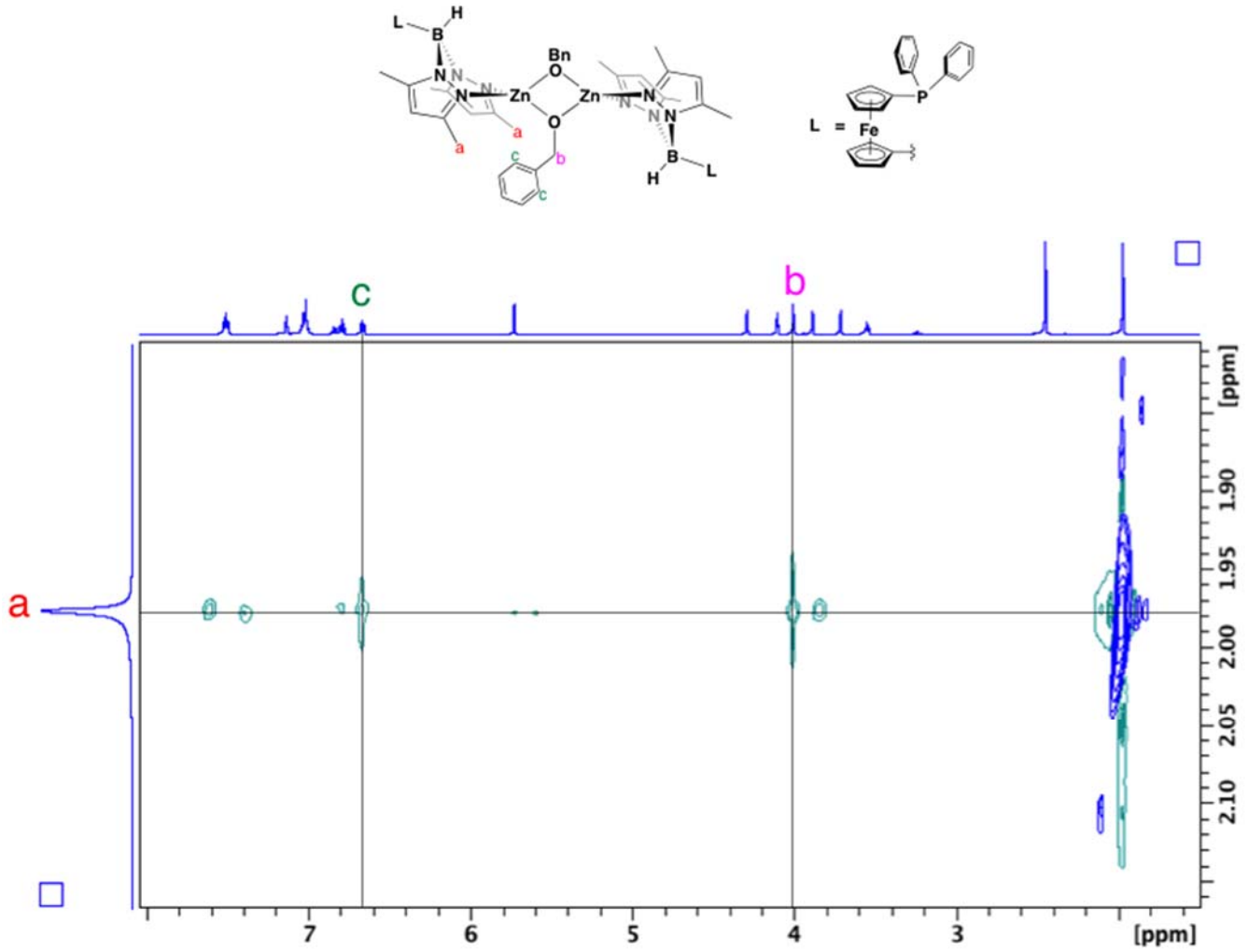



**Figure S11.** Selected region of $^{1}$H NOESY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of [($fc^{P,B}$)Zn(μ-$OCH_2Ph$)]$_2$.

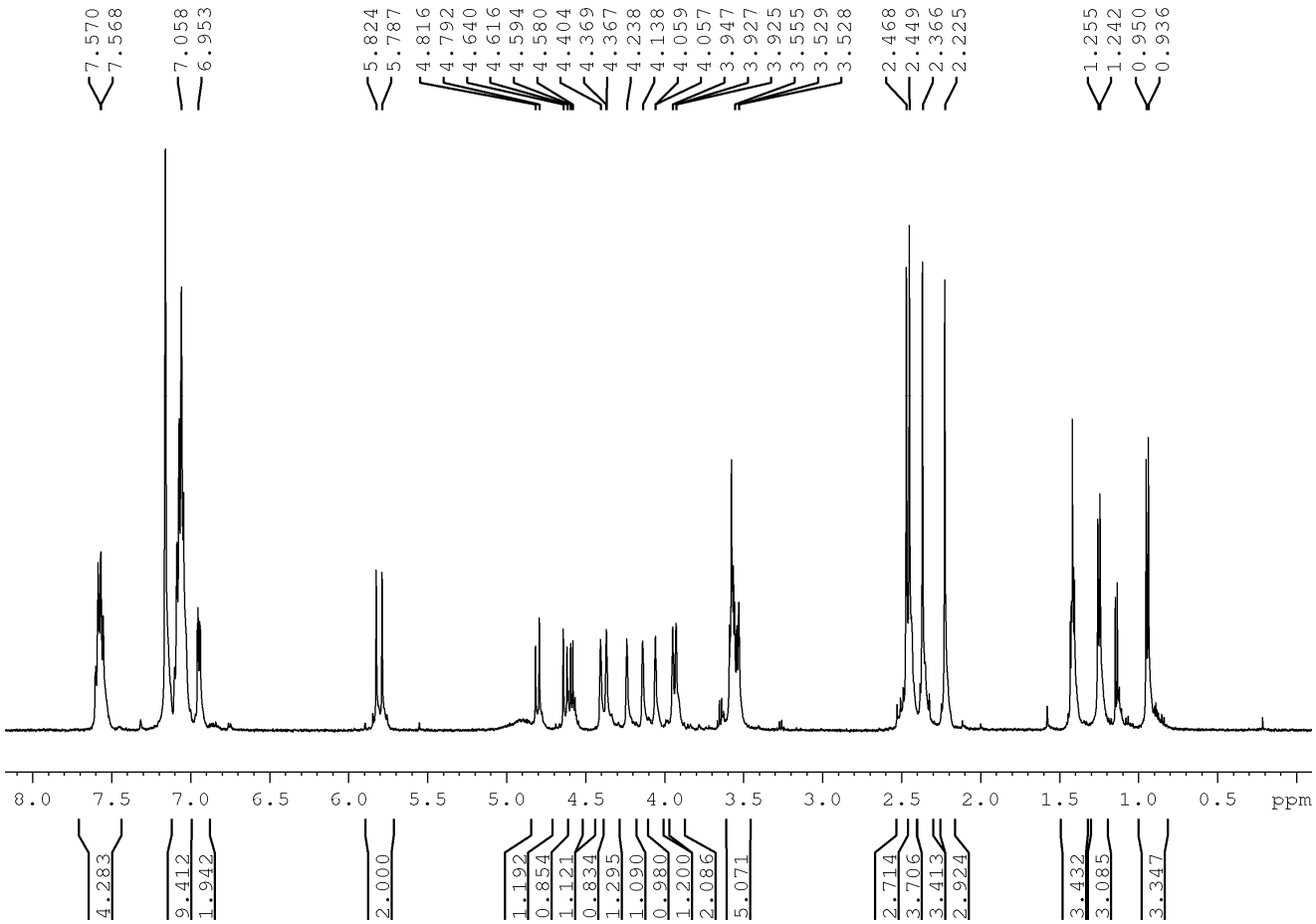
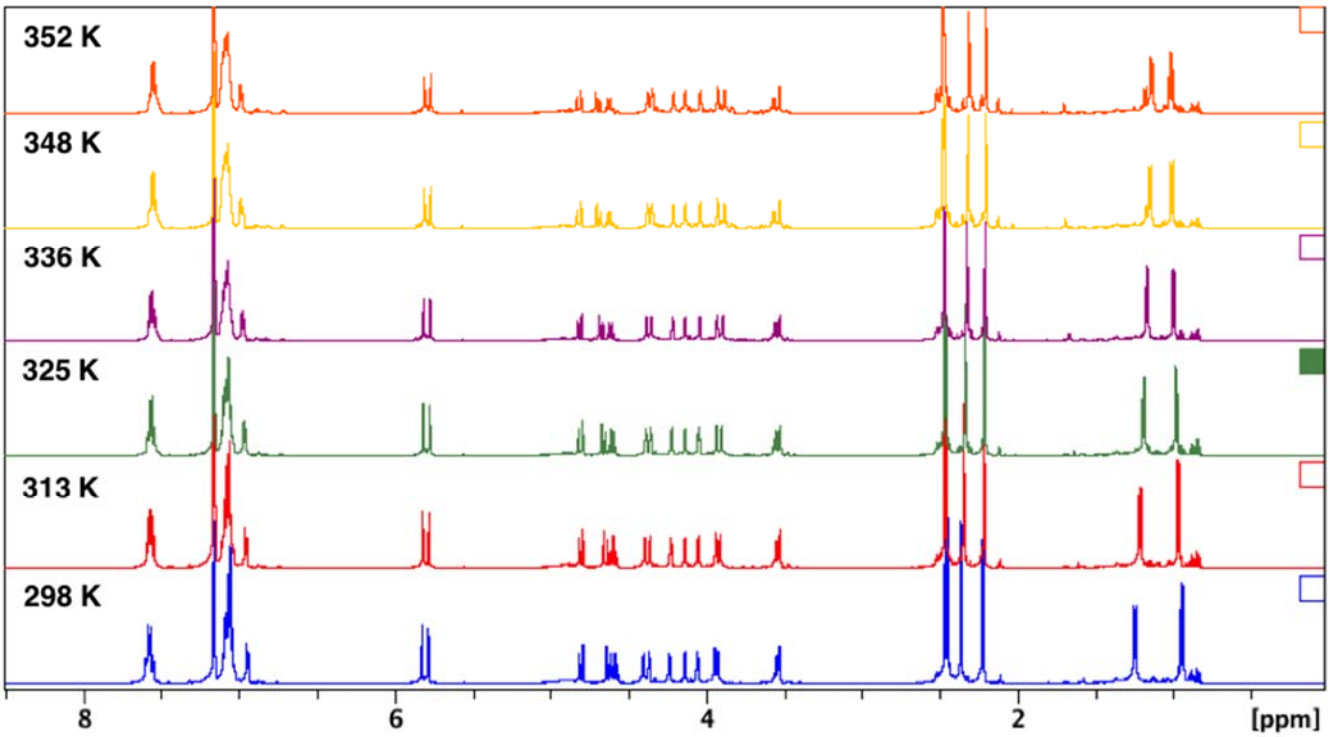



**Figure S12.** NMR scale reaction ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$ and L-lactide: δ (ppm) 0.94 (d, 3H, C*H*$_3$(LA)), 1.25 (d, 3H, C*H*$_3$(LA)), 2.22 (s, 3H, C*H*$_3$(pz)), 2.37 (s, 3H, C*H*$_3$(pz)), 2.45 (s, 3H, C*H*$_3$(pz)), 2.47 (s, 3H, C*H*$_3$(pz)), 3.53 (q, 1H, C*H*(LA)), 3.93 (s, 1H, Cp-*H*), 3.95 (s, 1H, Cp-*H*), 4.06 (s, 1H, Cp-*H*), 4.14 (s, 1H, Cp-*H*), 4.24 (s, 1H, Cp-*H*), 4.37 (s, 1H, Cp-*H*), 4.40 (s, 1H, Cp-*H*), 4.60 (q, 1H, C*H*(LA)), 4.72 (q, 2H, OC*H*$_2$Ph), 5.79 (s, 1H, C*H*(pz)), 5.82 (s, 1H, C*H*(pz)), 6.95 (m, 2H, *o*-Bn), 7.06 (m, 9H, *m*-Bn, *p*-Bn, *m*-Ph, *p*-Ph), 7.57 (m, 4H, *o*-Ph).




**Figures S13.** Variable temperature NMR ($C_6D_6$, 500 MHz) study of $[(fc^{P,B})Zn(LA)(OCH_2Ph)]_2$.

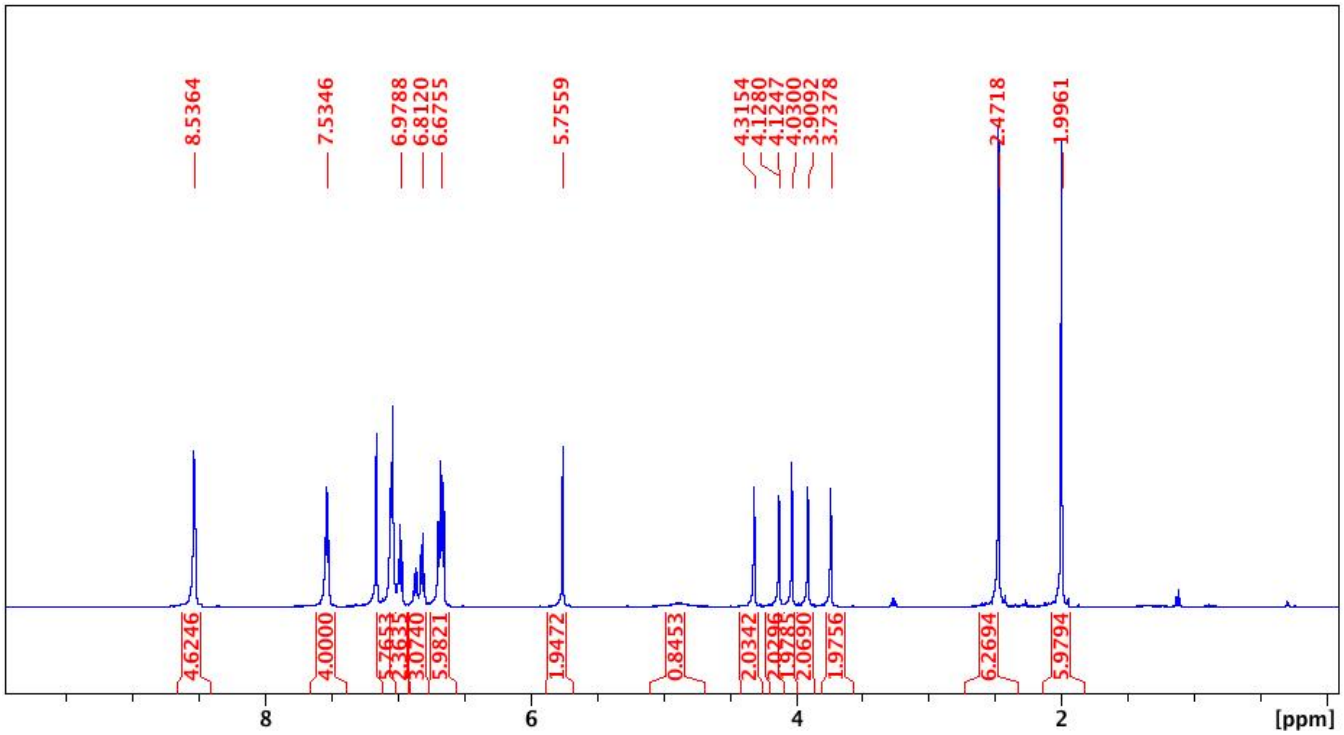



**Figure S14.** $^1H$ NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$ in the presence of 5 equivalent of pyridine. No change in the signals corresponding to $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$ is observed.

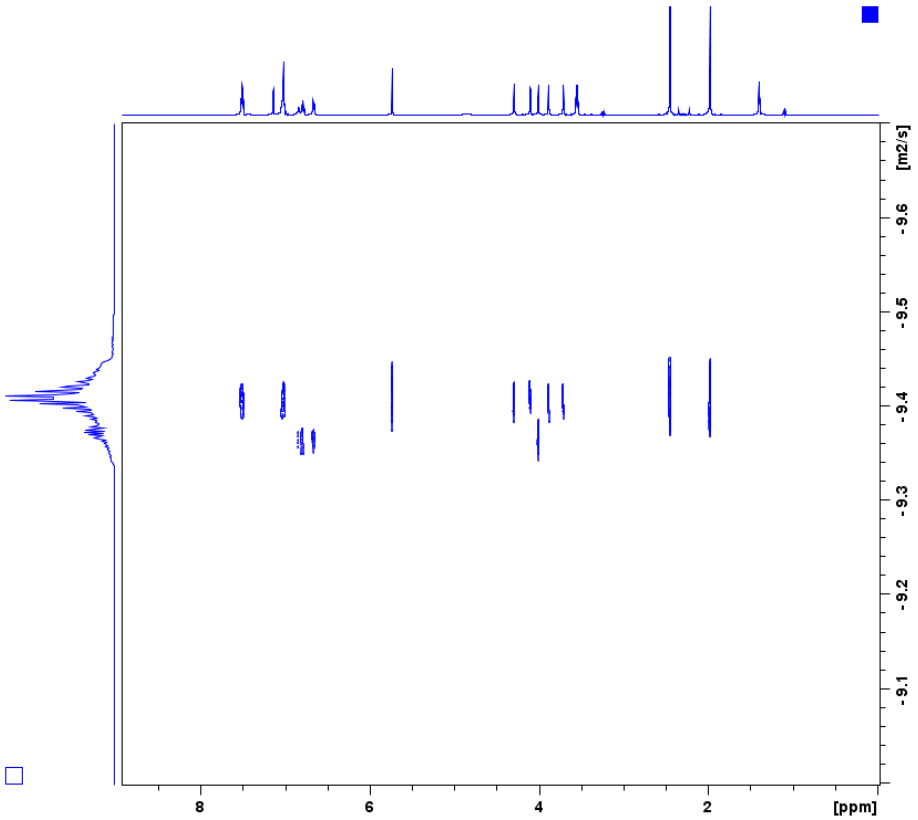



**Figure S15.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$. A minor difference in the diffusion rates of the $-OCH_2Ph$ component vs. the heteroscorpionate supporting ligand is observed. Such drifts in the signals corresponding to the same molecule can be found in various DOSY spectra in the literature.[1]

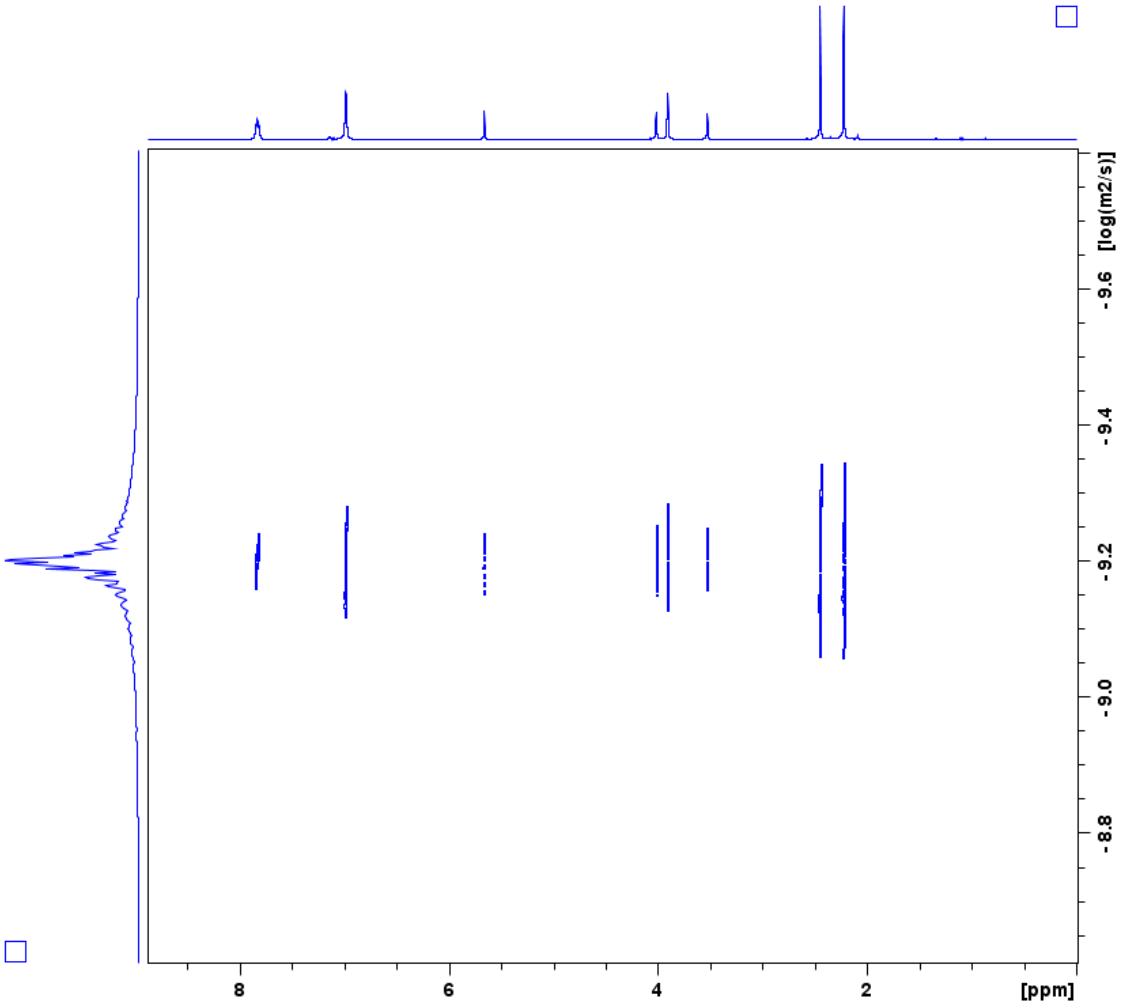



**Figure S16.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of ($fc^{P,B}$)ZnCl.

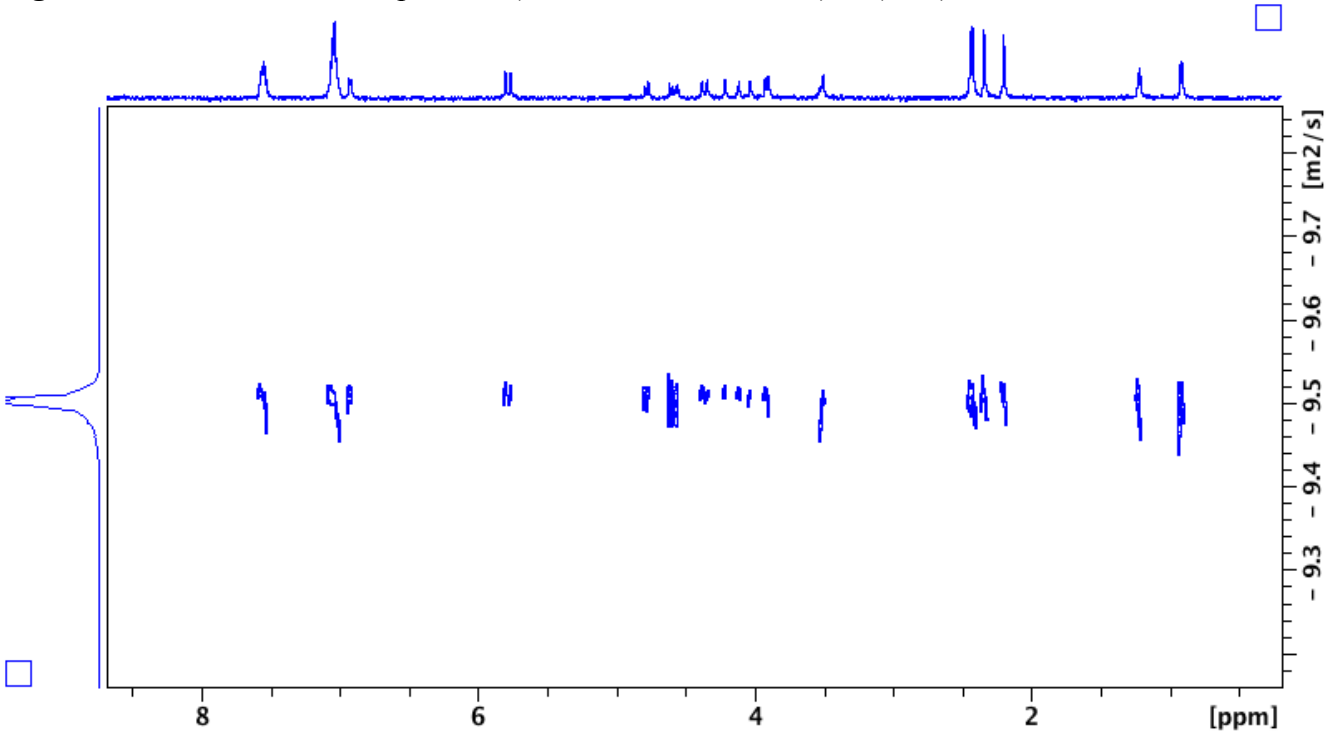



**Figure S17.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of [($fc^{P,B}$)Zn(LA)($OCH_2Ph$)]$_2$.

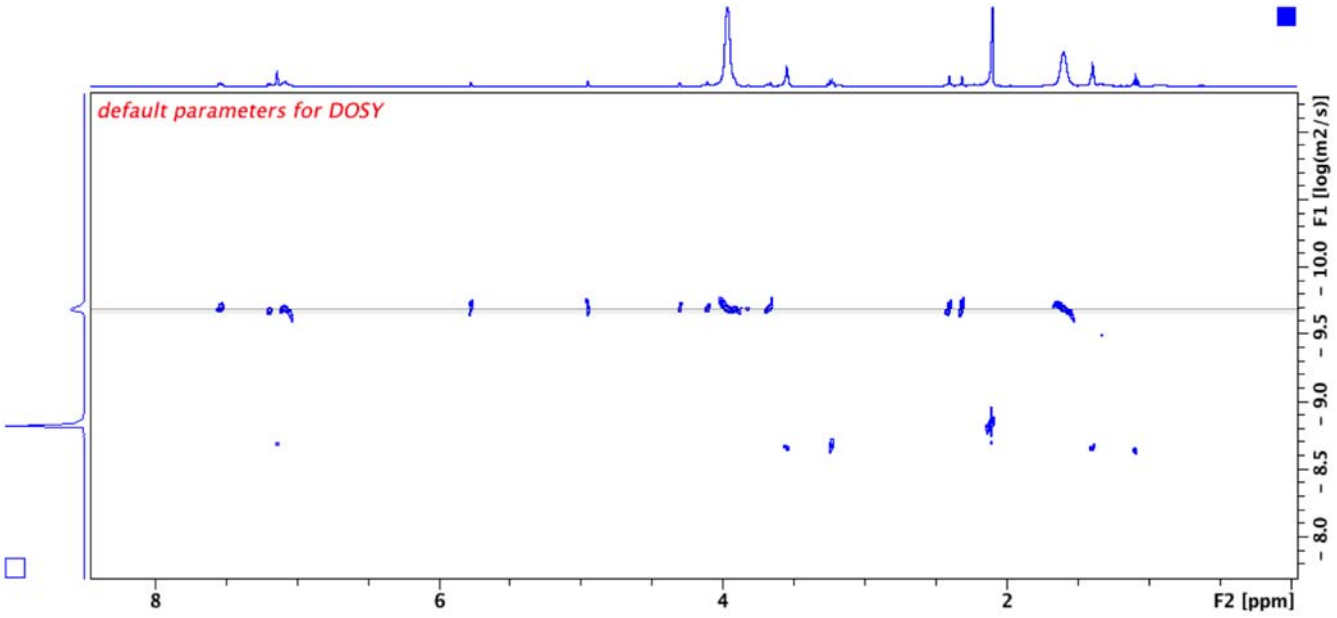



**Figure S18.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of [(fc$^{P,B}$)Zn(PTMC)$_{36}$(OCH$_2$Ph)]$_2$. Signals at 4.94 ppm, 7.07 ppm and 7.18 ppm correspond to the -OCH$_2$Ph end group. Signals not on the line are attributed to residual monomer, THF, hexamethylbenzene, and $C_6D_6$.

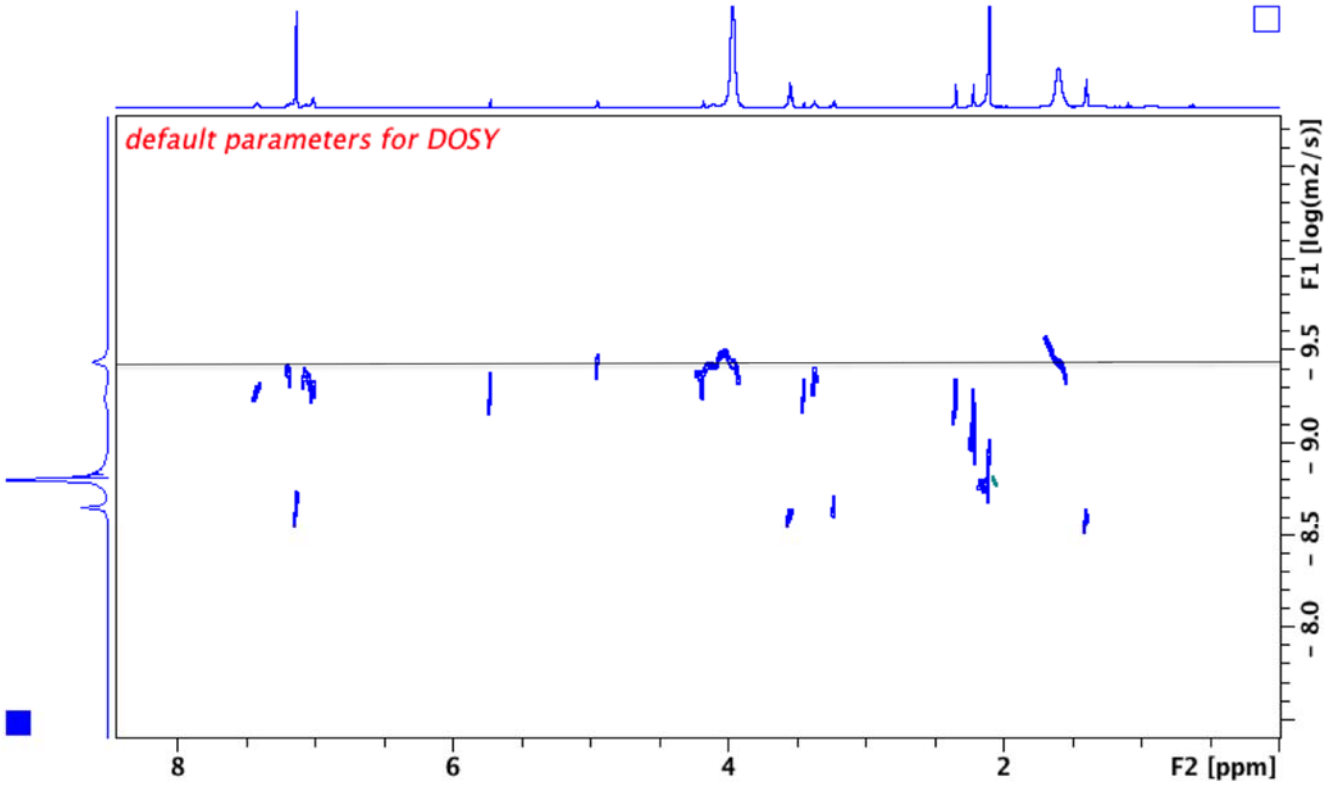



**Figure S19.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of the PhCH$_2$O(PTMC)$_{36}$H polymer. Signals at 4.94 ppm, 7.07 ppm and 7.18 ppm correspond to the -OCH$_2$Ph end group. Signals not on the line are attributed to hydrolyzed catalyst, residual monomer, THF, hexamethylbenzene, and $C_6D_6$.

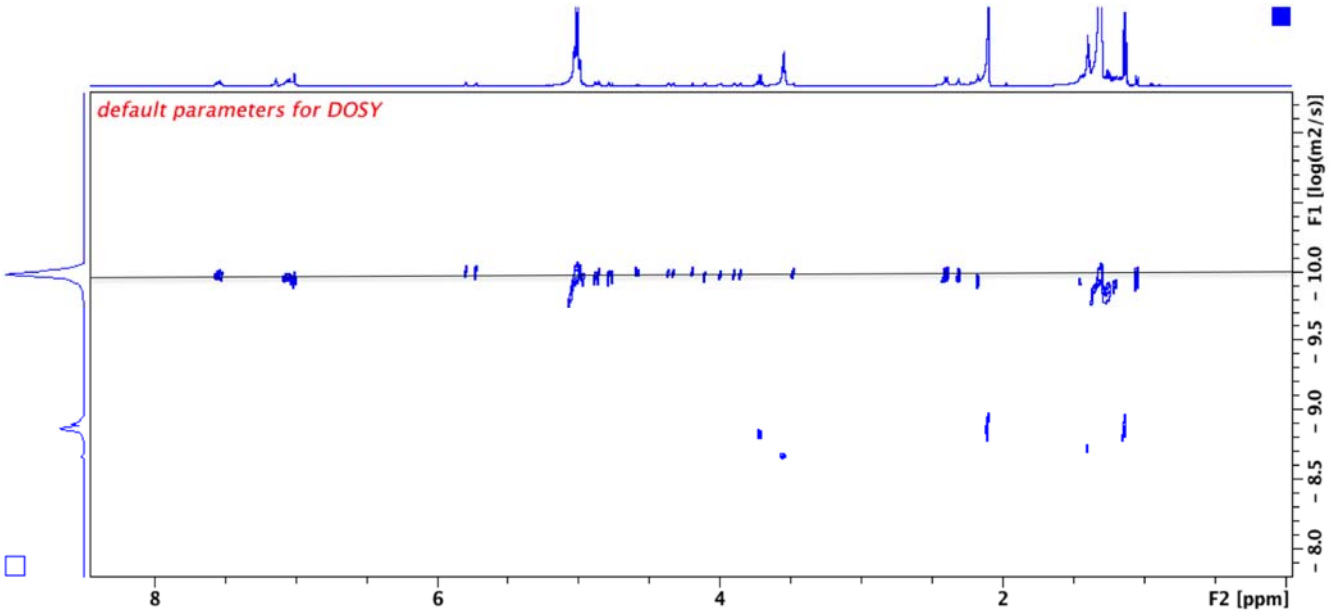



**Figure S20.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of [(fc$^{P,B}$)Zn(PLA)$_{36}$(OCH$_2$Ph)]$_2$. Signals at 4.72 ppm, 6.95 ppm and 7.06 ppm correspond to the - OCH$_2$Ph end group. Signals not on the line are attributed to residual monomer, THF, hexamethylbenzene, and $C_6D_6$.

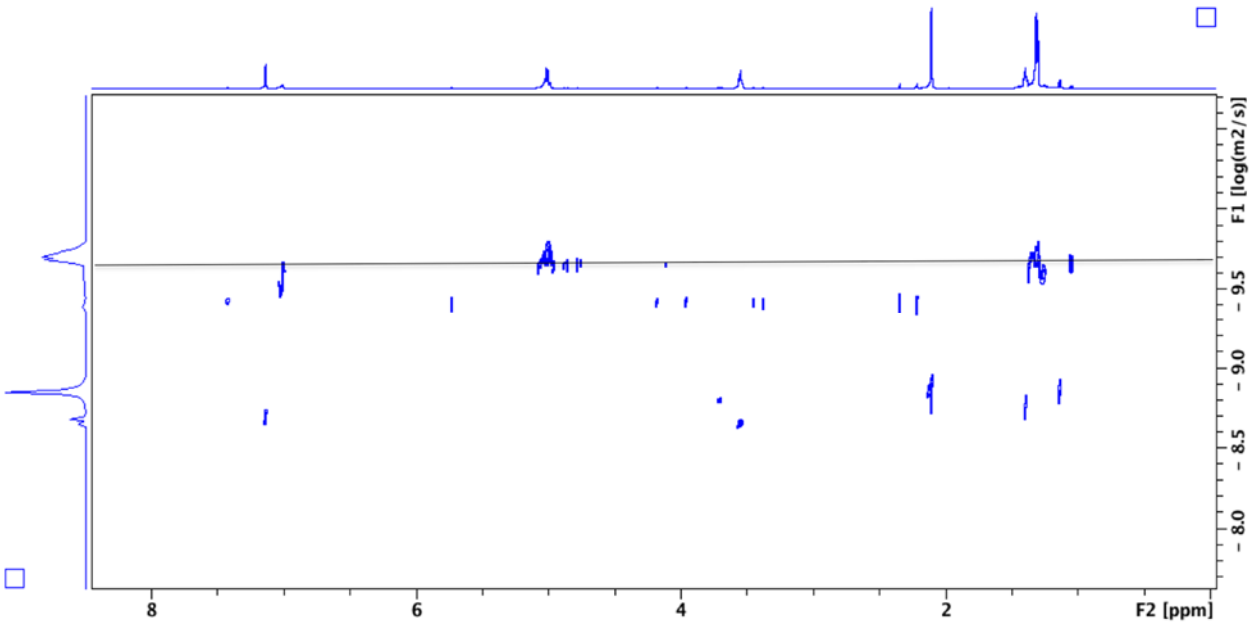



**Figure S21.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of PhCH$_2$O(PLA)$_{36}$H. Signals at 4.72 ppm, 6.95 ppm and 7.06 ppm correspond to the -OCH$_2$Ph end group. Signals not on the line are attributed to hydrolyzed catalyst, residual monomer, THF, hexamethylbenzene, and $C_6D_6$.

From the DOSY NMR spectra the following the diffusion coefficients were determined:

$D$[(fc$^{P,B}$)ZnCl] = $6.38 \times 10^{-10}$ m$^2$/s

$D$ = $3.92 \times 10^{-10}$ m$^2$/s

$D${[(fc$^{P,B}$)Zn(LA)(OCH$_2$Ph)]$_2$} = $3.16 \times 10^{-10}$ m$^2$/s

$D${[(fc$^{P,B}$)Zn(PTMC)$_{36}$(OCH$_2$Ph)]$_2$} = $2.07 \times 10^{-10}$ m$^2$/s

$D$[$PhCH_2O(PTMC)_{36}H$] = $3.80 \times 10^{-10}$ $m^2/s$

$D$[$\{[(fc^{P,B})Zn(PLA)_{36}(OCH_2Ph)]_2\}$] = $1.04 \times 10^{-10}$ $m^2/s$

$D$[$PhCH_2O(PLA)_{36}H$] = $2.00 \times 10^{-10}$ $m^2/s$

The Stokes-Einstein equation shows the relationship between the hydrodynamic radius and the diffusion coefficient:

$D = (kT)/(6\pi\eta r_H)$

By comparing the diffusion coefficients of two compounds the ratios of the hydrodynamic radii can be determined.

$D_{(ZnCl)}/D_{(ZnOBn)2} = r_{(ZnOBn)2}/r_{(ZnCl)} = 1.63$

$D_{(ZnOBn)2}/D_{[Zn(LA)OBn]2} = r_{[Zn(LA)OBn]2}/r_{(ZnOBn)2} = 1.24$

$D_{(PhCH2O(PLA)36H)}/D_{[Zn(PLA)36(OCH2Ph)]2} = r_{[Zn(PLA)36(OCH2Ph)]2}/r_{(PhCH2O(PLA)36H)} = 1.92$

$D_{(PhCH2O(PTMC)36H)}/D_{[Zn(PTMC)36(OCH2Ph)]2} = r_{[Zn(PTMC)36(OCH2Ph)]2}/r_{(PhCH2O(PTMC)36H)} = 1.84$

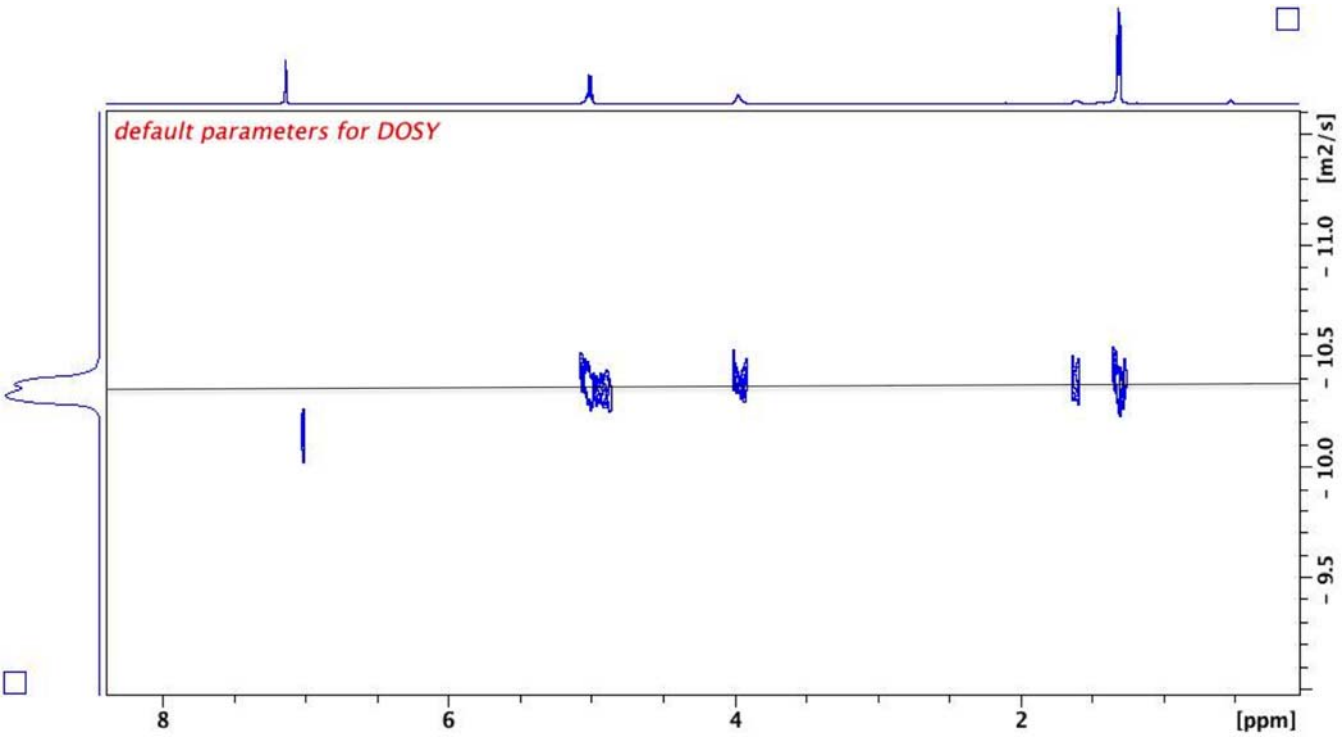



**Figure S22.** $^1$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA.

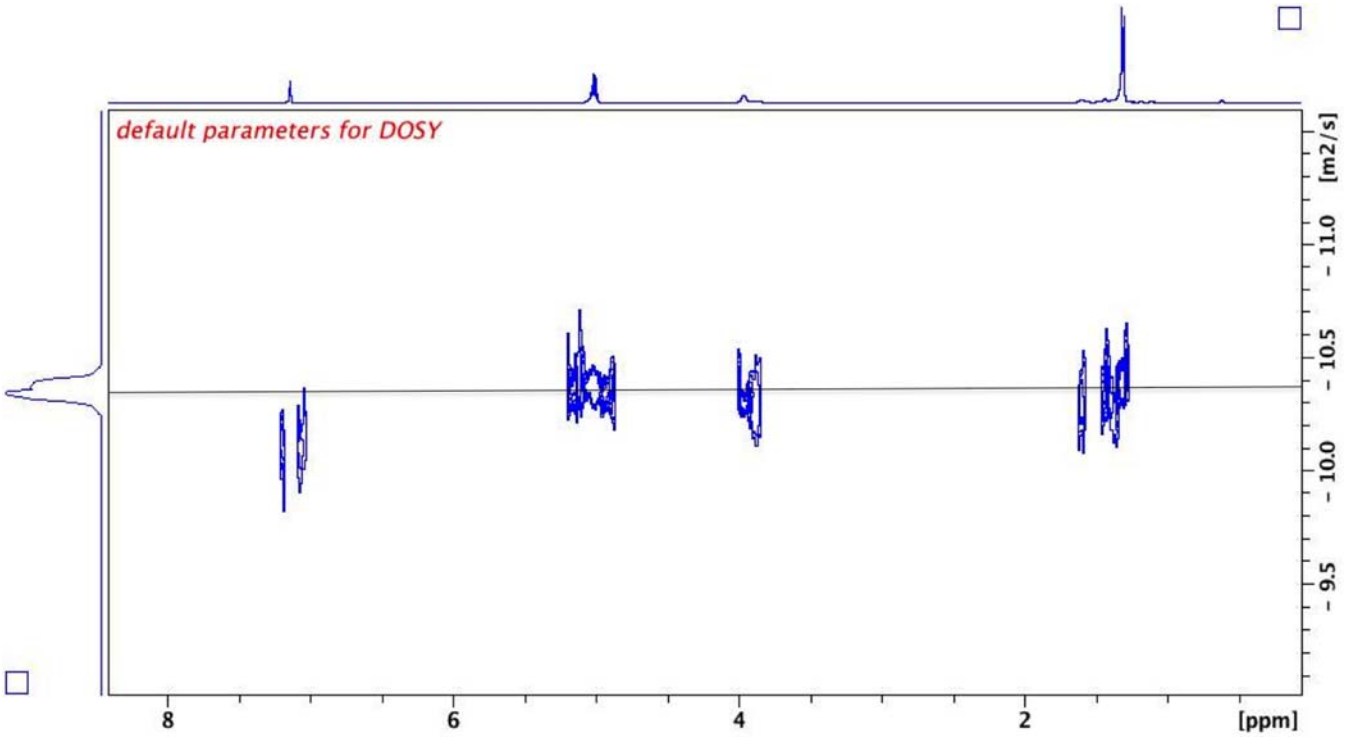



**Figure S23.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of PTMC-*b*-PLA-*b*-PTMC.

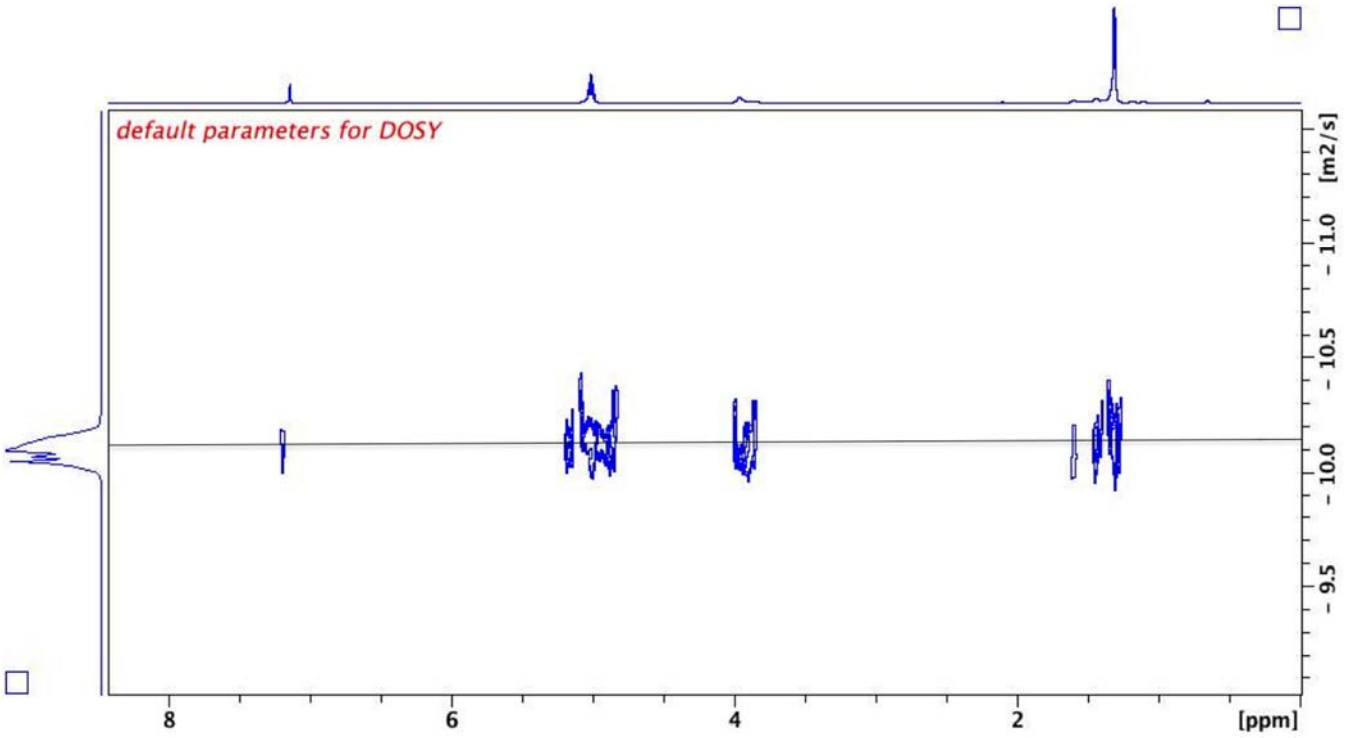



**Figure S24.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of PTMC-*b*-PLA-*b*-PTMC-*b*-PLA-*b*-PTMC.

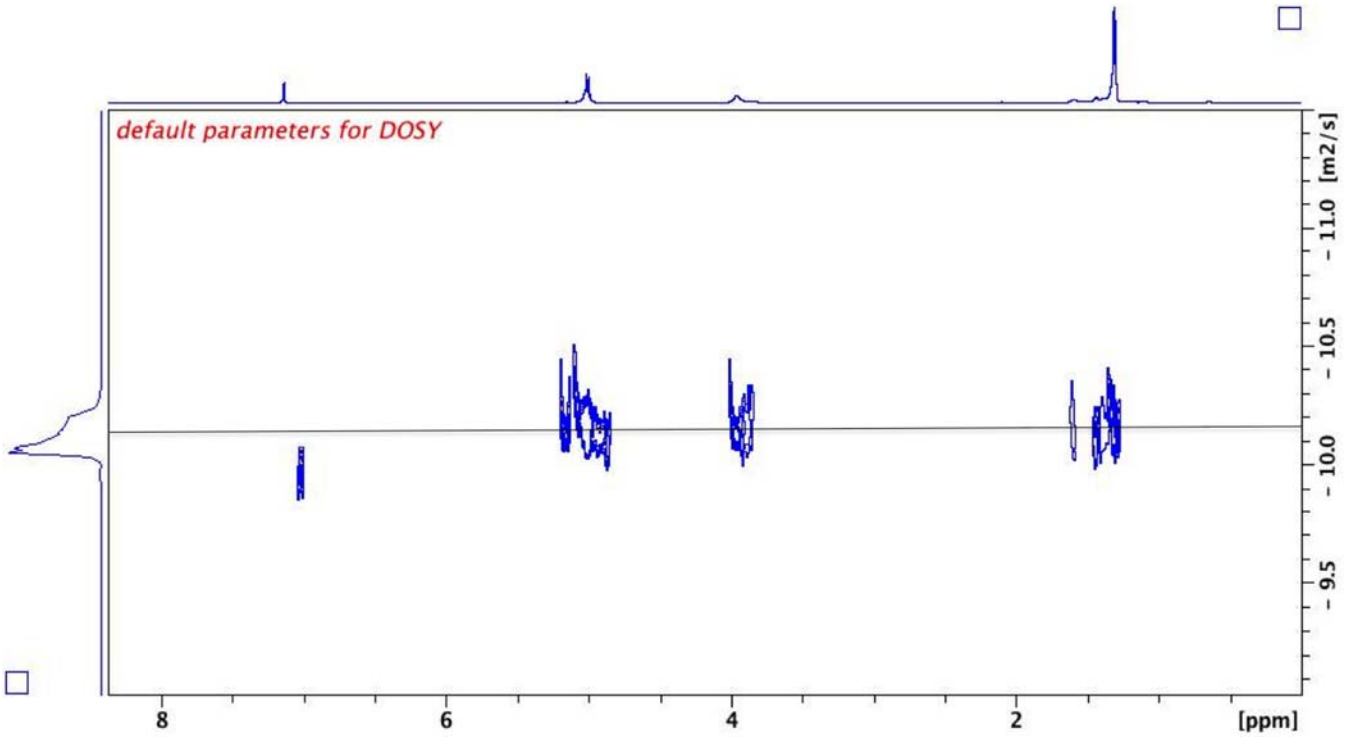



**Figure S25.** $^{1}$H DOSY NMR spectrum ($C_6D_6$, 500 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA.

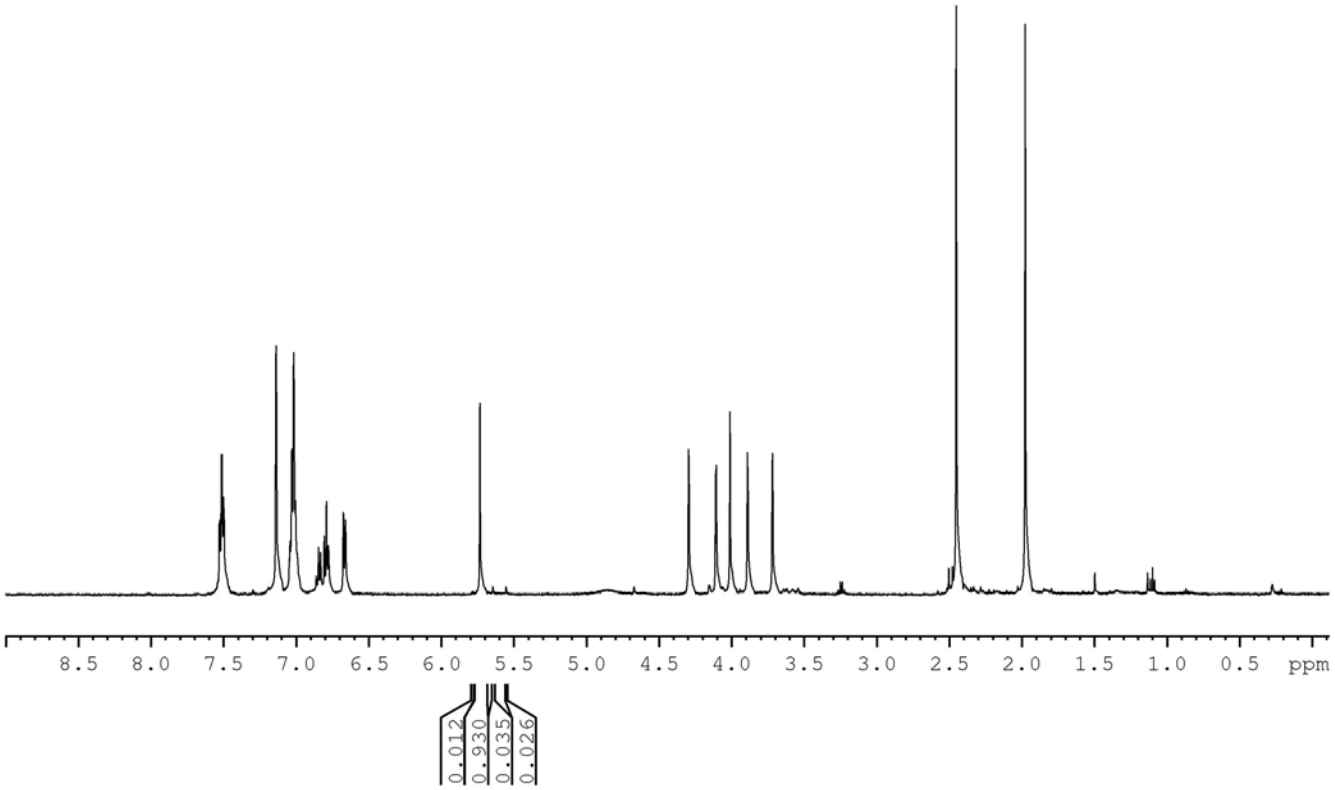



**Figure S26.** Thermal decomposition study ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$, 24 h at ambient temperature. Percent decomposition is calculated based on newly formed pyrazole signals.

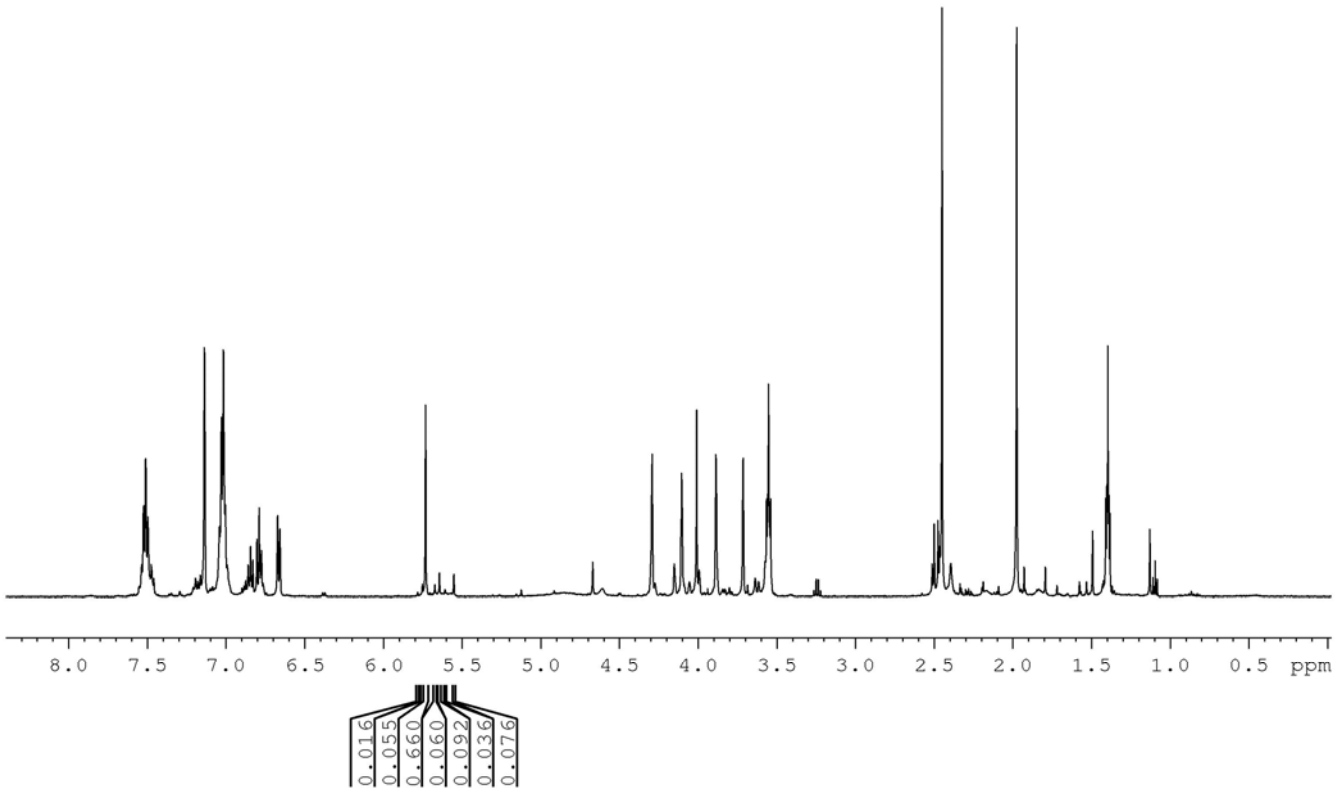



**Figure S27.** Thermal decomposition study ($C_6D_6$, 500 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$, 1.5 h at 70 °C. Percent decomposition is calculated based on newly formed pyrazole signals.

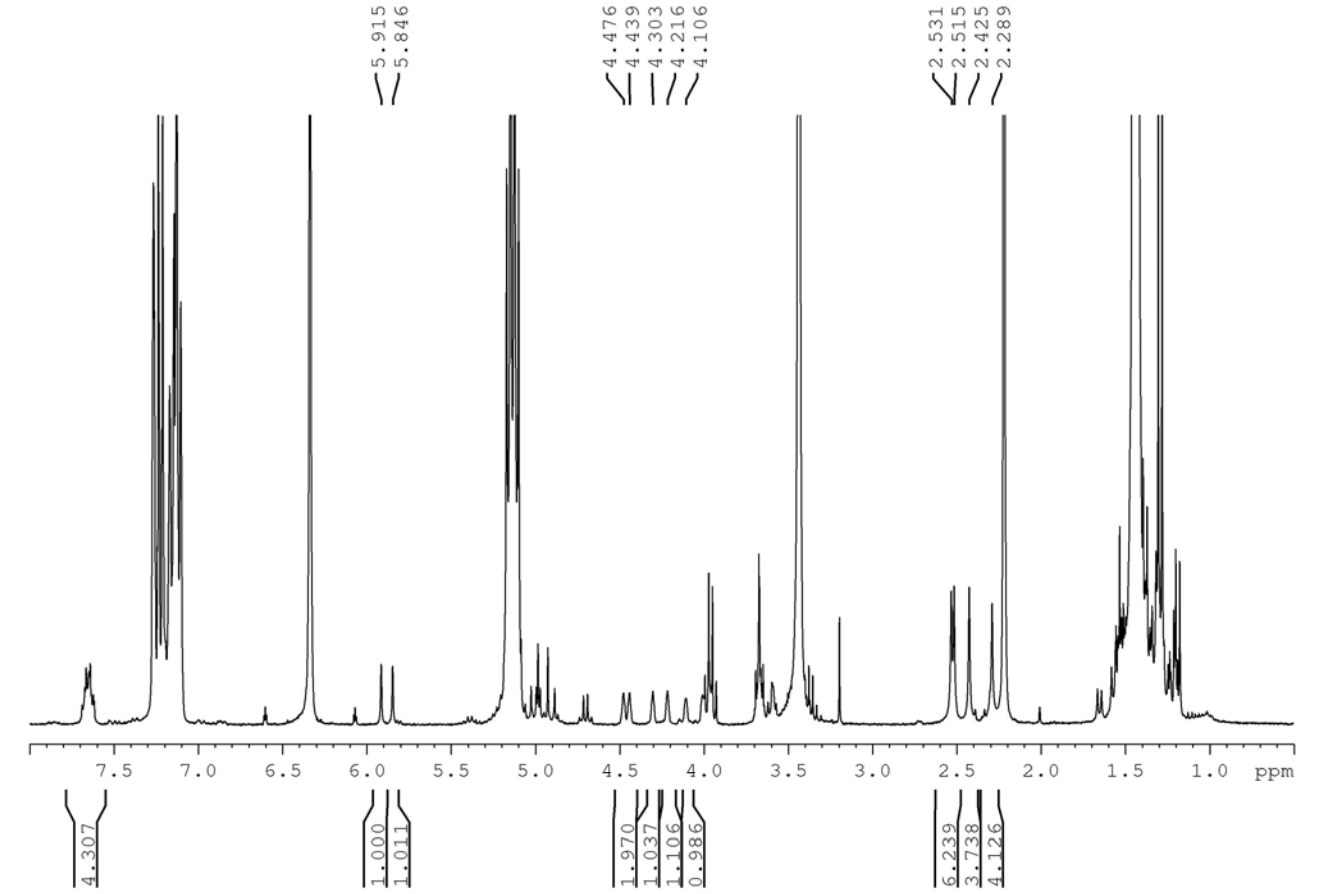



**Figure S28.** Thermal decomposition study ($C_6D_6$, 300 MHz, 298 K) of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$ in the presence of 100 equivalents of L-lactide, 3 h at 70 °C. No catalyst decomposition is observed.

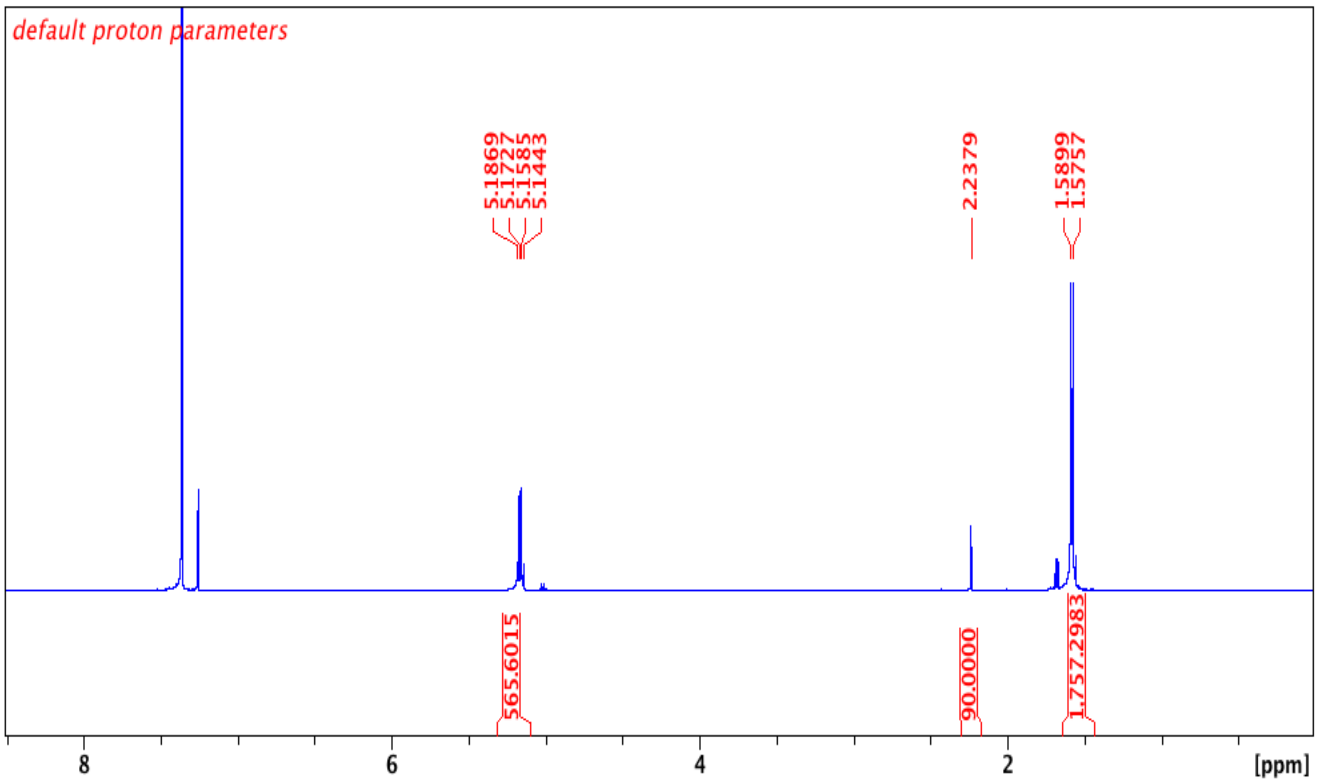



**Figure S29.** $^{1}$H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of L-LA polymerization (Table 1, entry 1). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:566. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.23 (s, 18H, C*H*$_3$ HMB), 5.16 (q, 2H, C*H*CH$_3$ PLA).

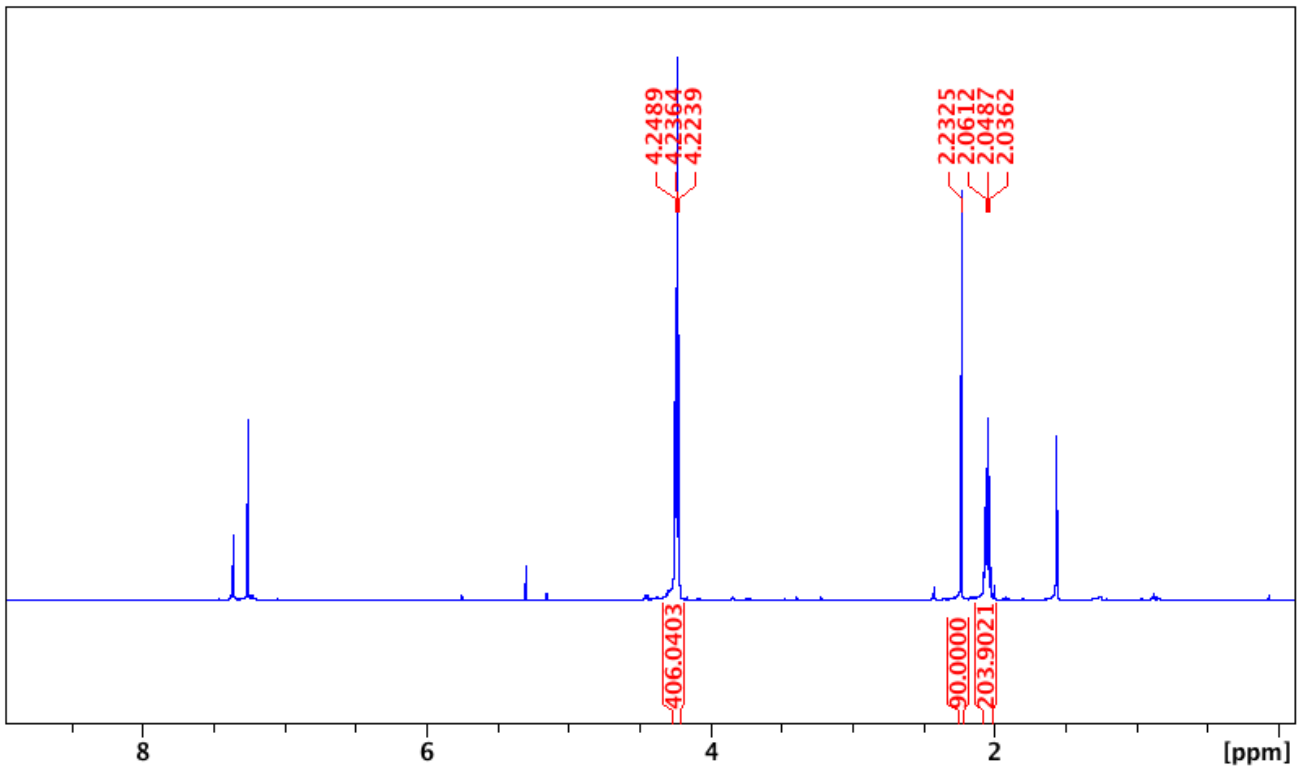



**Figure S30.** $^{1}$H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of TMC polymerization (Table 1, entry 2). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC ratio is 1:10:202. δ (ppm) 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC).

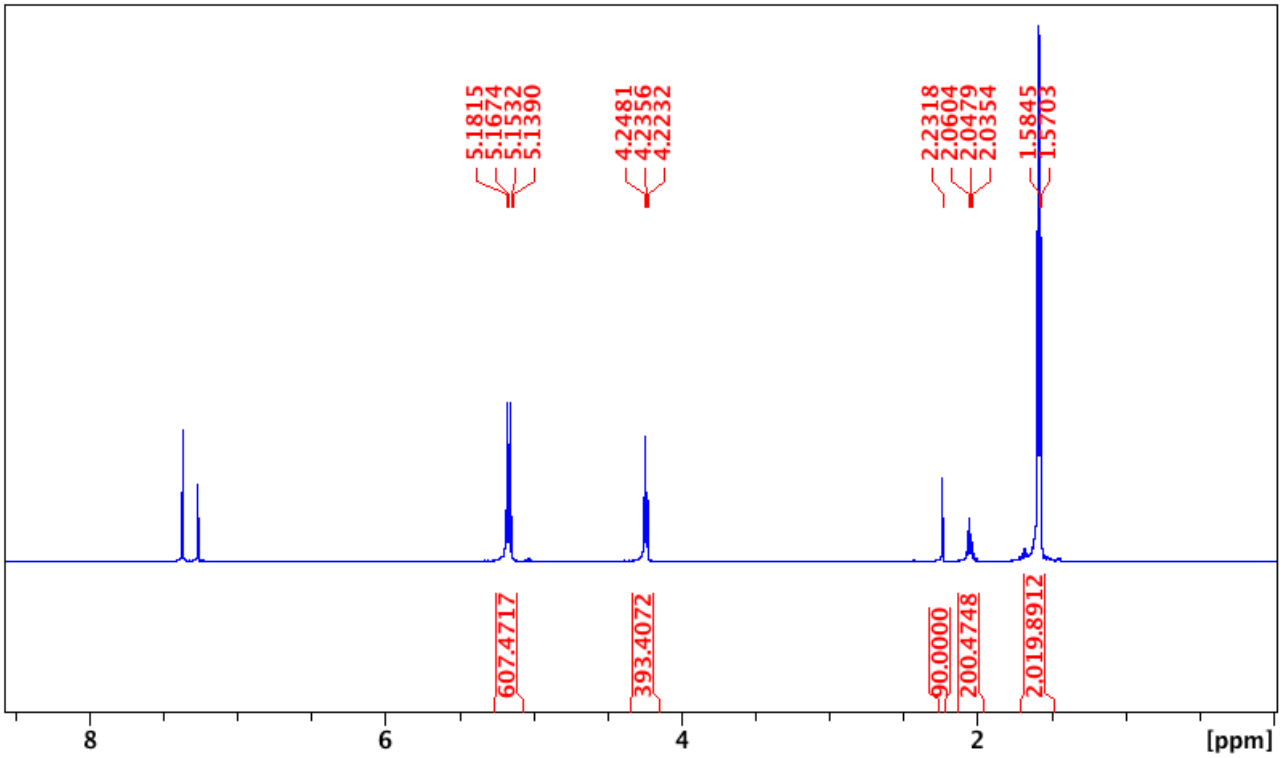



**Figure S31.** $^{1}$H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of PLA-*b*-PTMC polymerization (Table 1, entry 3). Standard is hexamethylbenzene (HMB). [(fc$^{P,B}$)Zn(μ-$OCH_2Ph$)]$_2$: HMB: TMC: LA ratio is 1:10:196:608. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

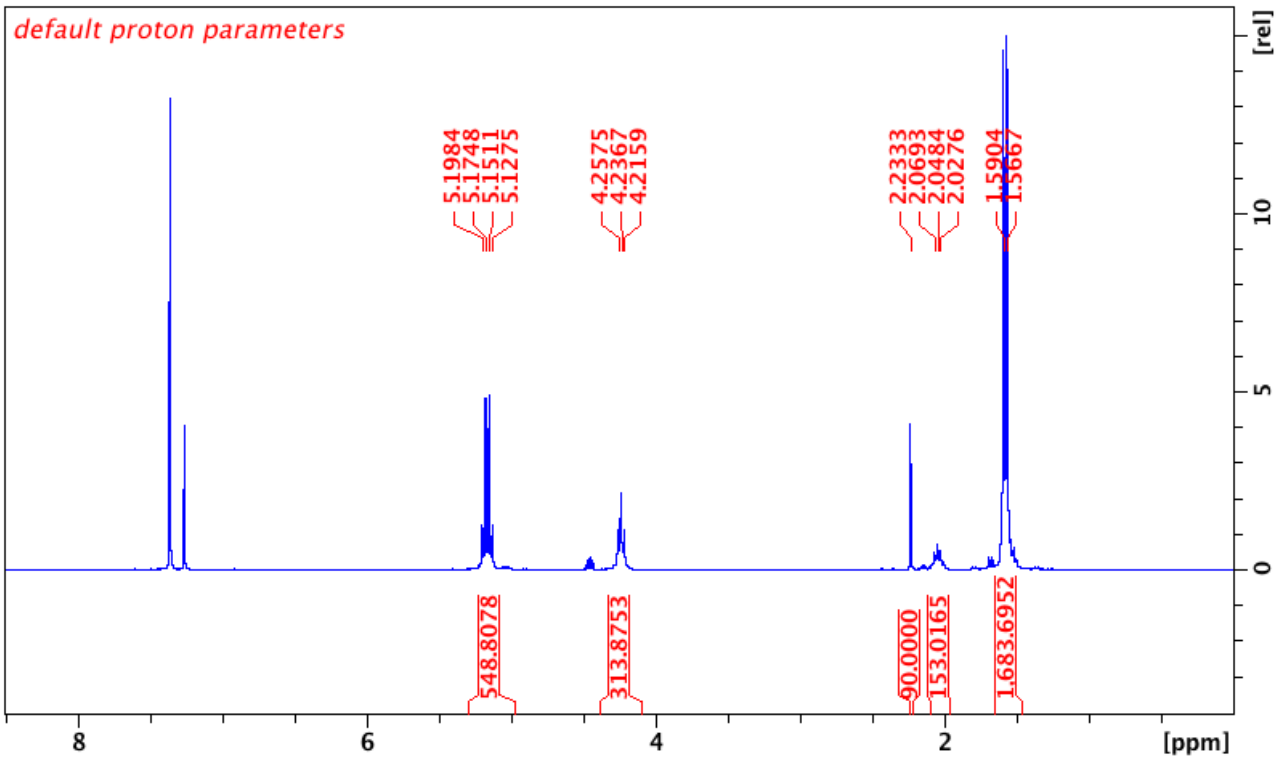



**Figure S32.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PTMC-*b*-PLA polymerization (Table 1, entry 4). Standard is hexamethylbenzene (HMB). [(fc$^{P,B}$)Zn(μ-$OCH_2Ph$)]$_2$: HMB: TMC: LA ratio is 1:10:158:550. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

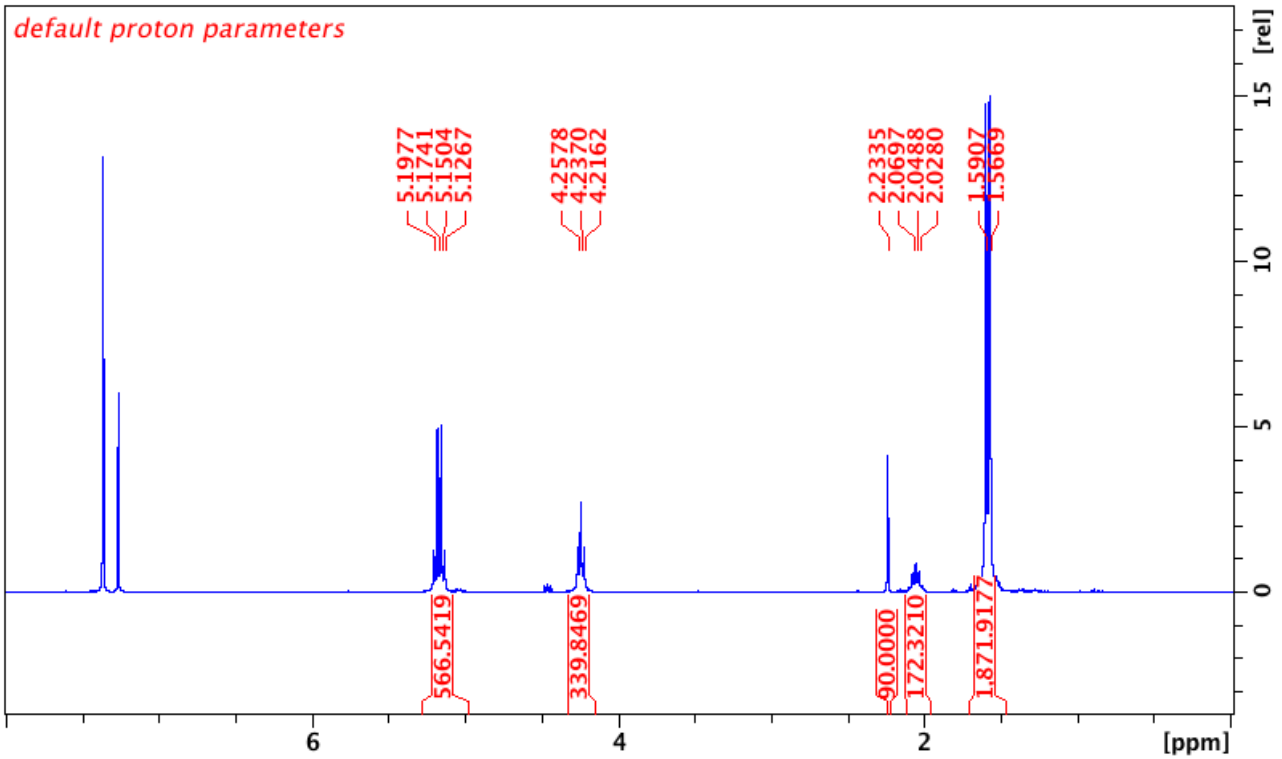



**Figure S33.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PTMC-*b*-PLA-*b*-PTMC polymerization (Table 1, entry 5). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:170:566. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

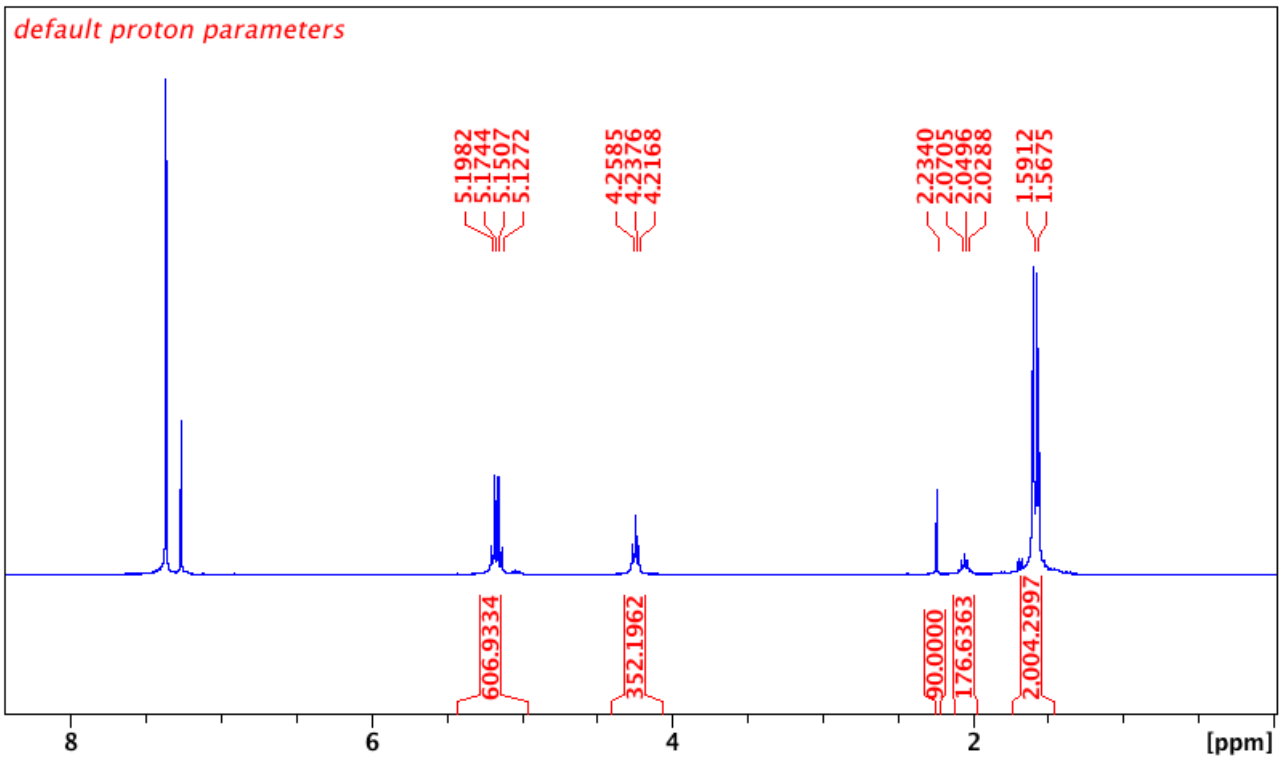



**Figure S34.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA polymerization (Table 1, entry 6). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:176:606. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

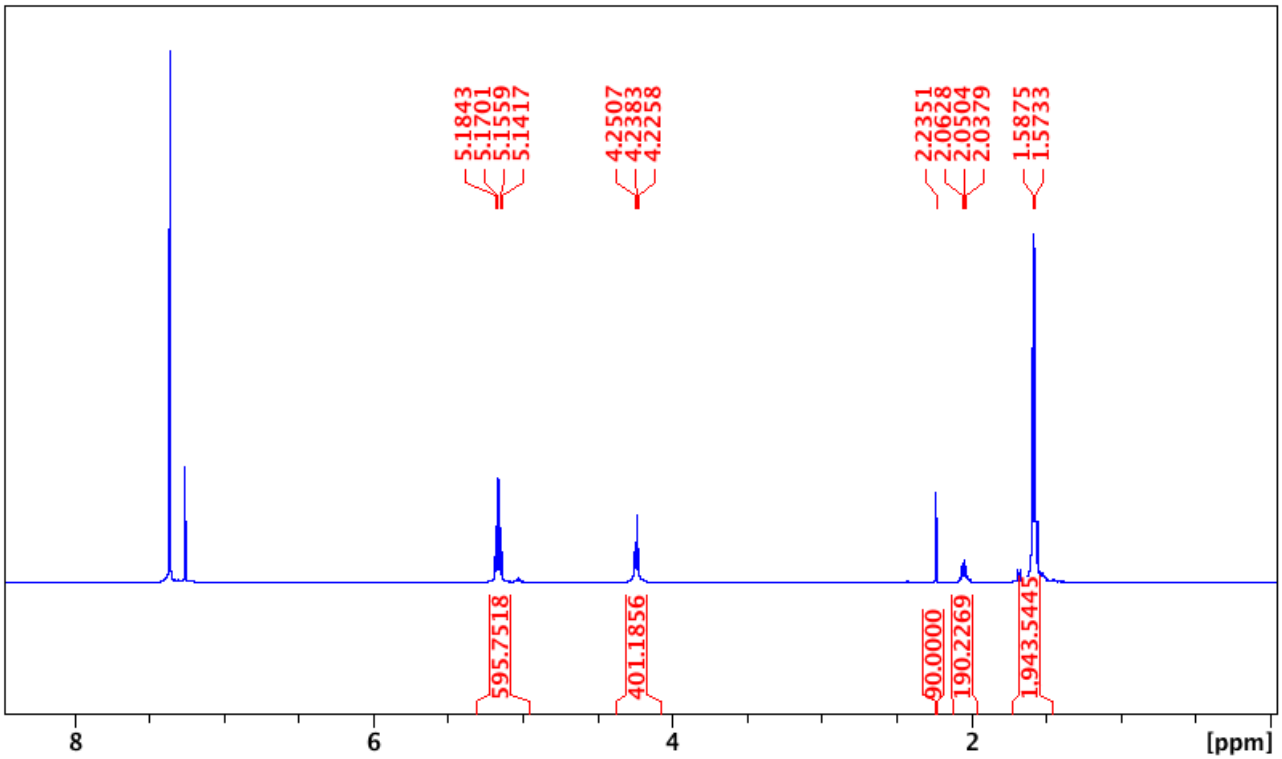



**Figure S35.** $^{1}$H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA-*b*-PTMC polymerization (Table 1, entry 7). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:200:596. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

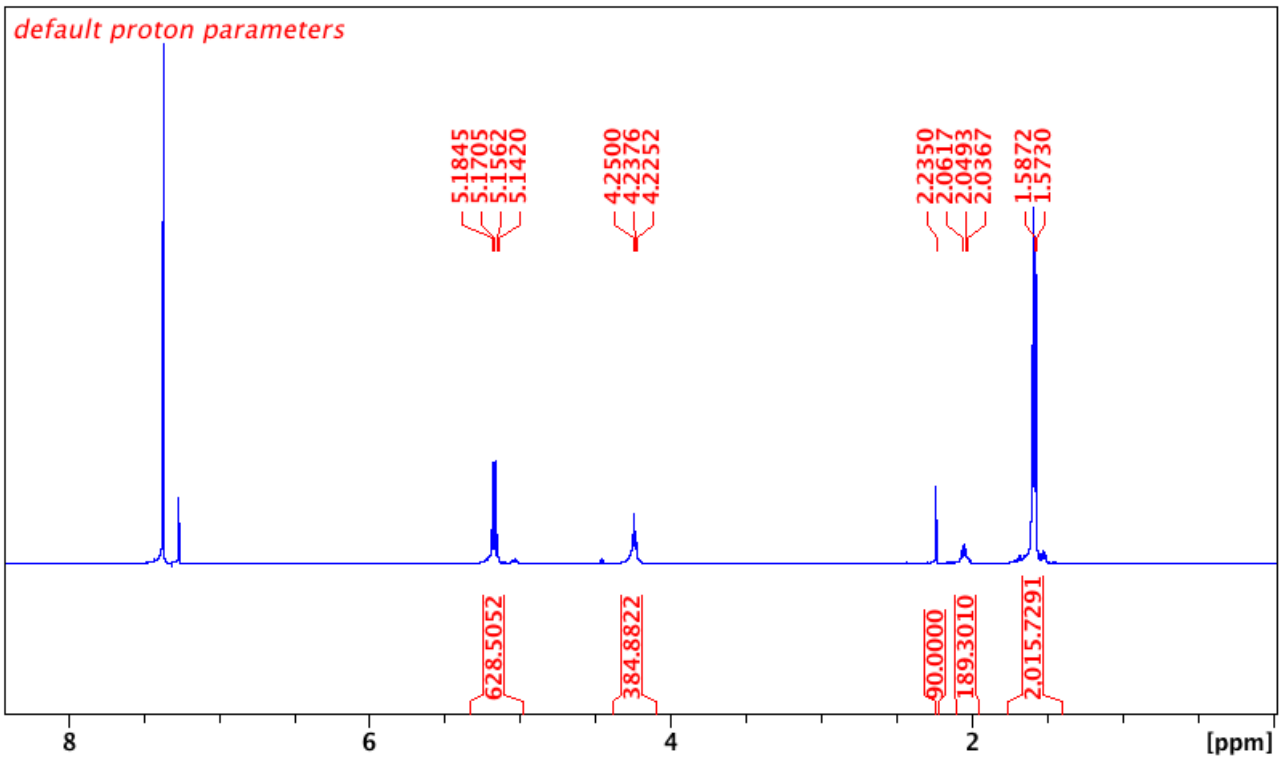



**Figure S36.** $^{1}$H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of PTMC-*b*-PLA-*b*-PTMC-*b*-PLA-*b*-PTMC polymerization (Table 1, entry 8). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:192:628. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

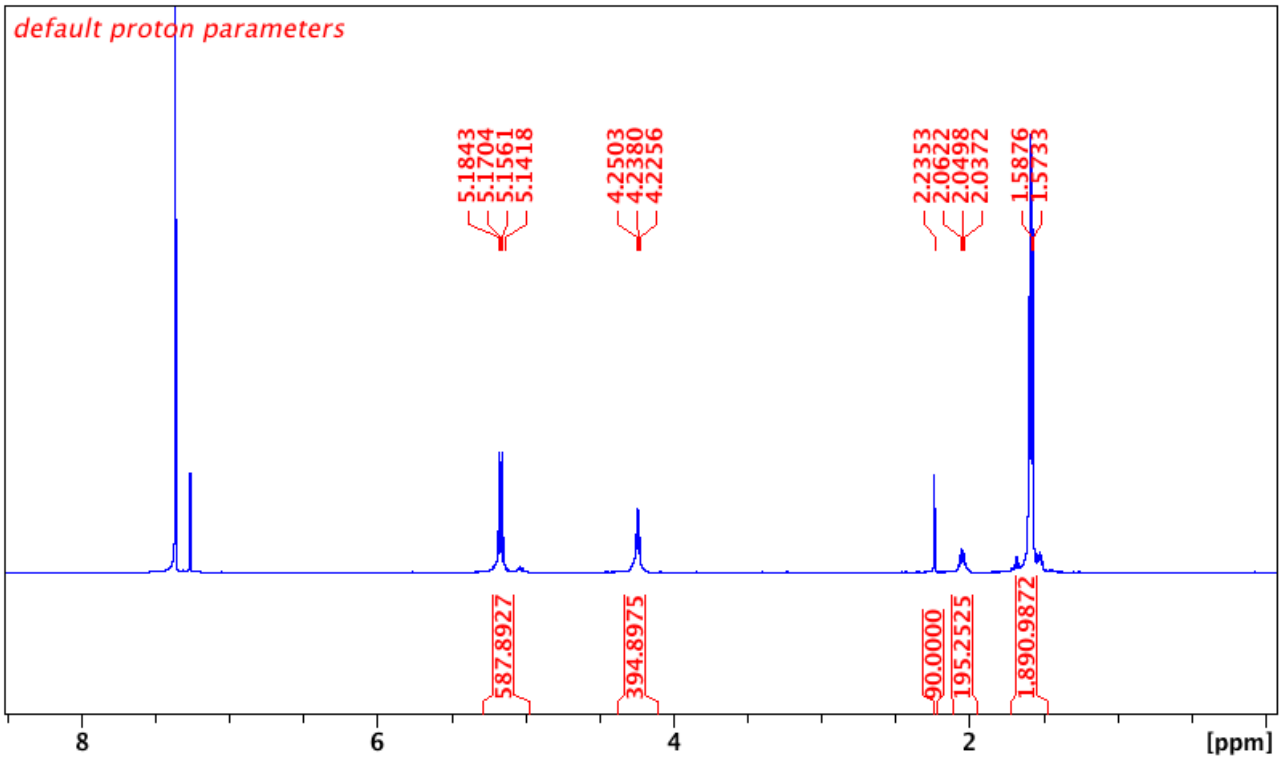



**Figure S37.** $^{1}$H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA polymerization (Table 1, entry 9). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:198:588. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

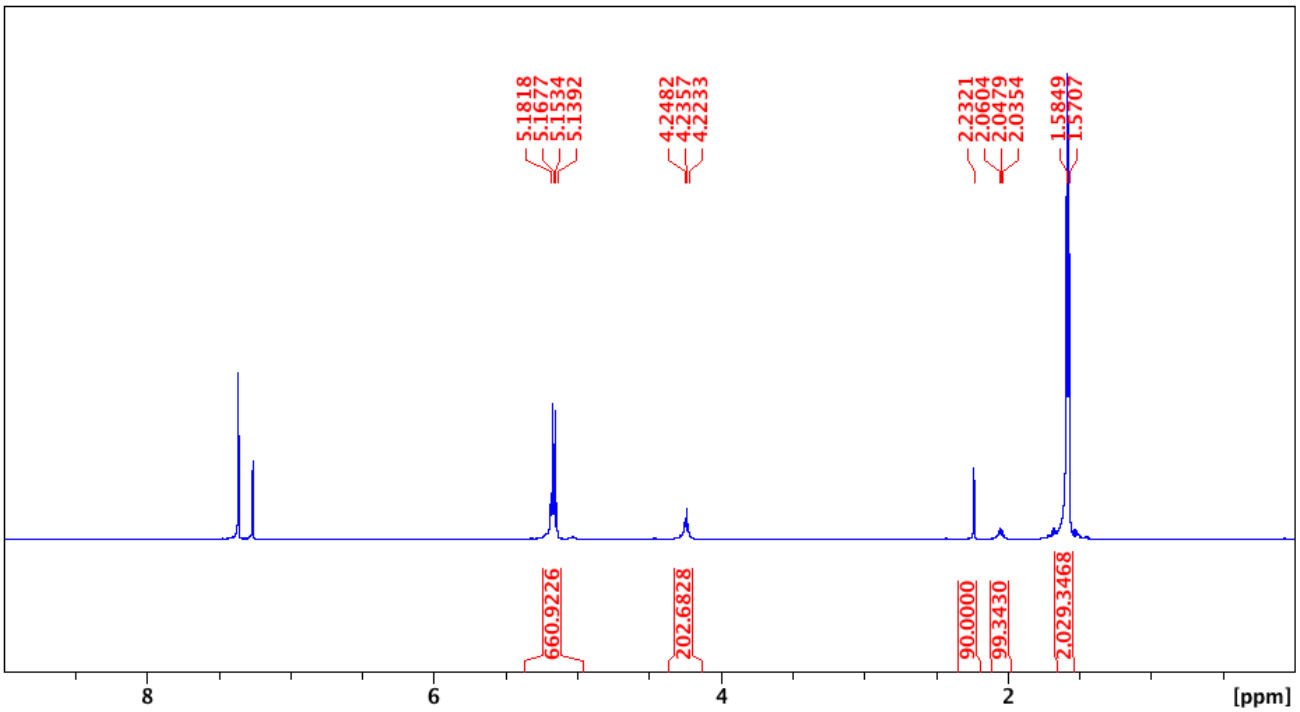



**Figure S38.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA polymerization (Table 1, entry 10). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:102:660. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

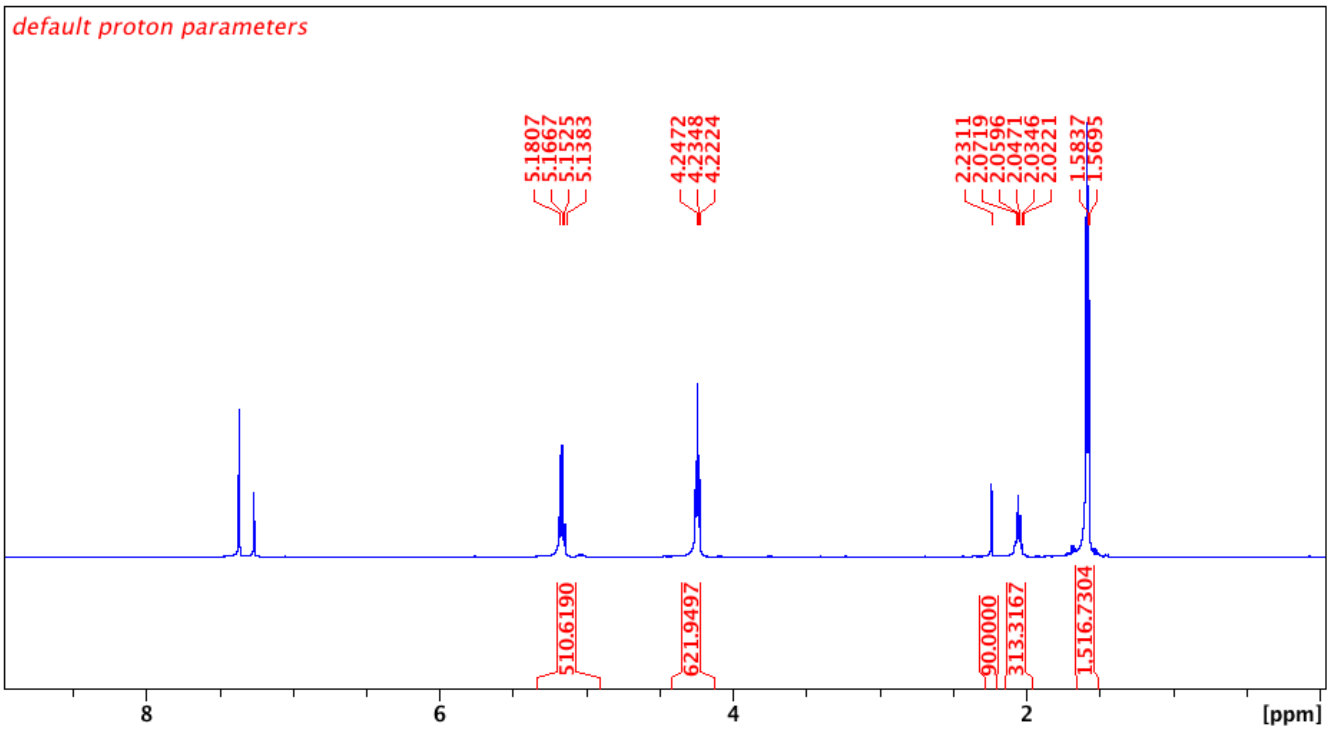



**Figure S39.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA polymerization (Table 1, entry 11). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:312:510. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

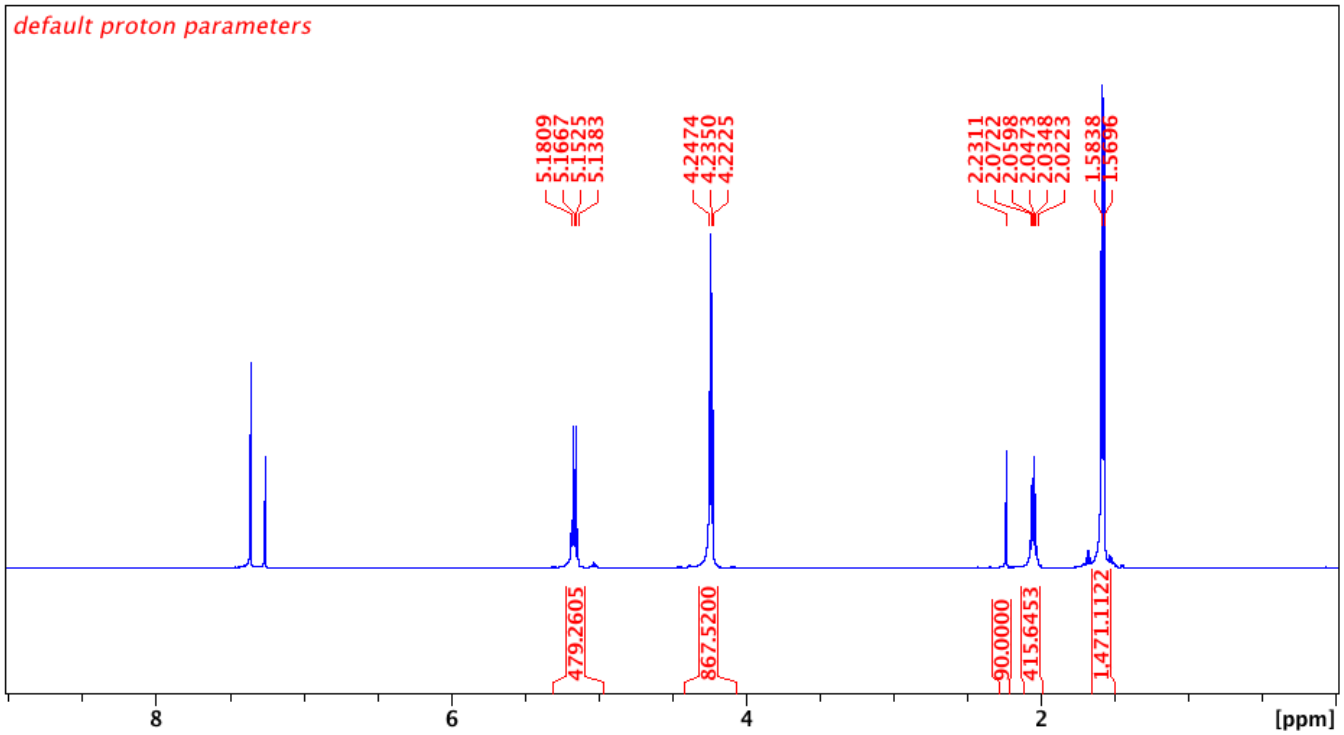



**Figure S40.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PLA-*b*-PTMC-*b*-PLA polymerization (Table 1, entry 12). Standard is hexamethylbenzene (HMB). $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$: HMB: TMC: LA ratio is 1:10:434:480. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 2.23 (s, 18H, C*H*$_3$ HMB), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

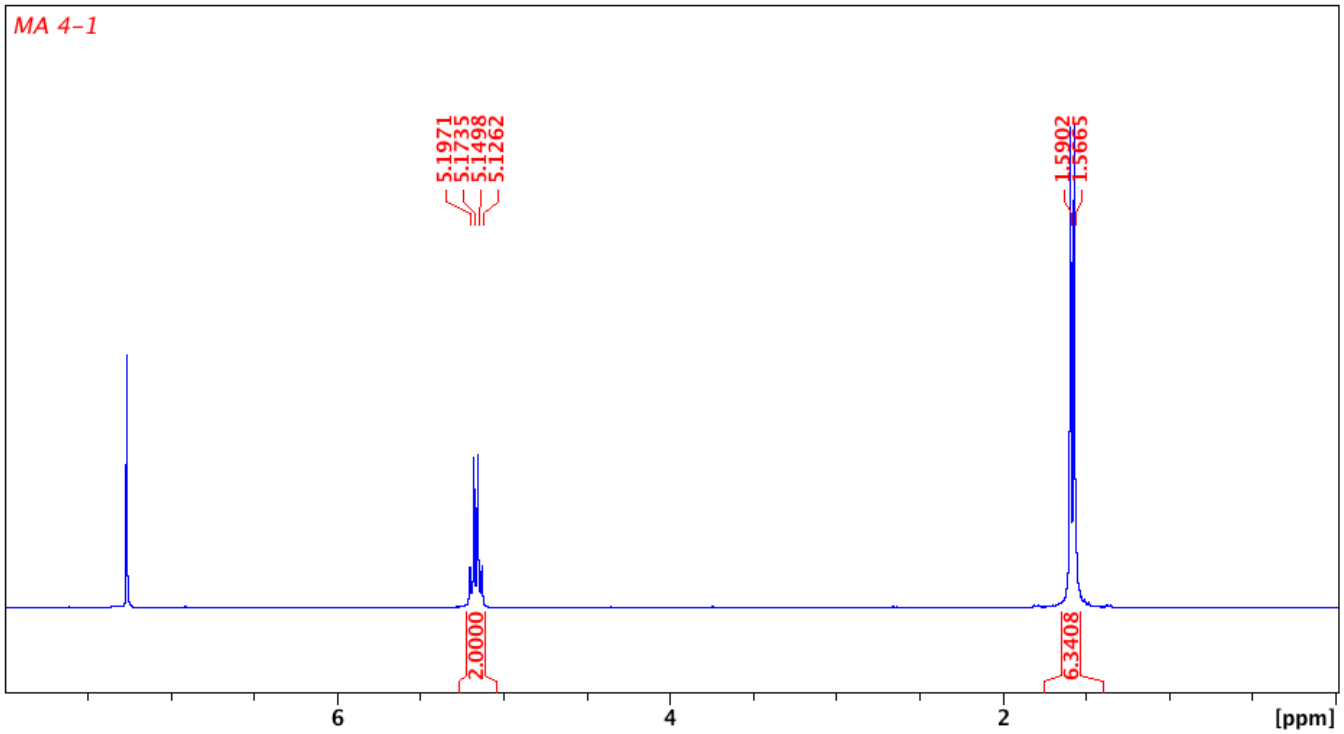



**Figure S41.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of L-LA melt polymerization. [($fc^{P,B}$)Zn(μ-$OCH_2Ph$)]$_2$: LA loading ratio is 1:600. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 5.16 (q, 2H, C*H*CH$_3$ PLA).

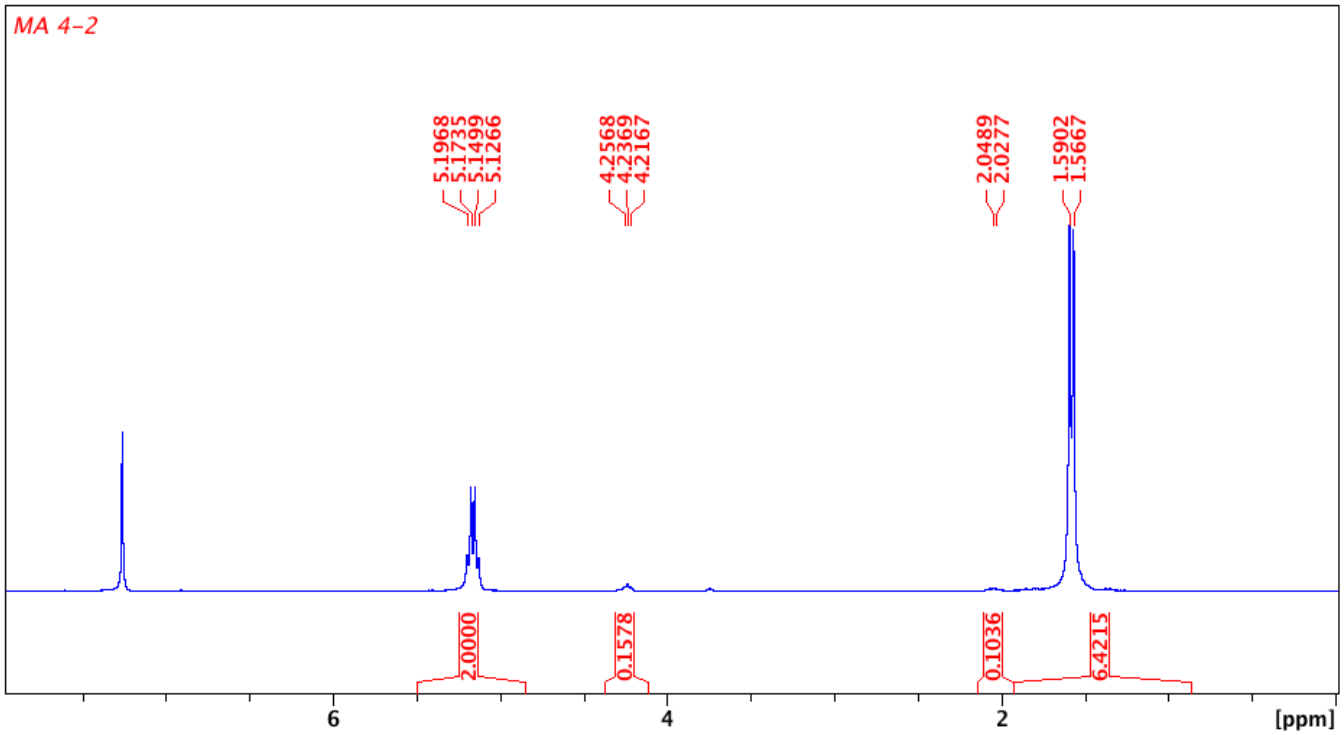



**Figure S42.** $^{1}$H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of PTMC-*b*-PLA melt polymerization. [($fc^{P,B}$)Zn(μ-$OCH_2Ph$)]$_2$:TMC:LA loading ratio is 1:600:600. δ (ppm) 1.58 (d, 6H, CHC*H*$_3$ PLA), 2.05 (t, 2H, C*H*$_2$ PTMC), 4.23 (t, 4H, C*H*$_2$ PTMC), 5.16 (q, 2H, C*H*CH$_3$ PLA).

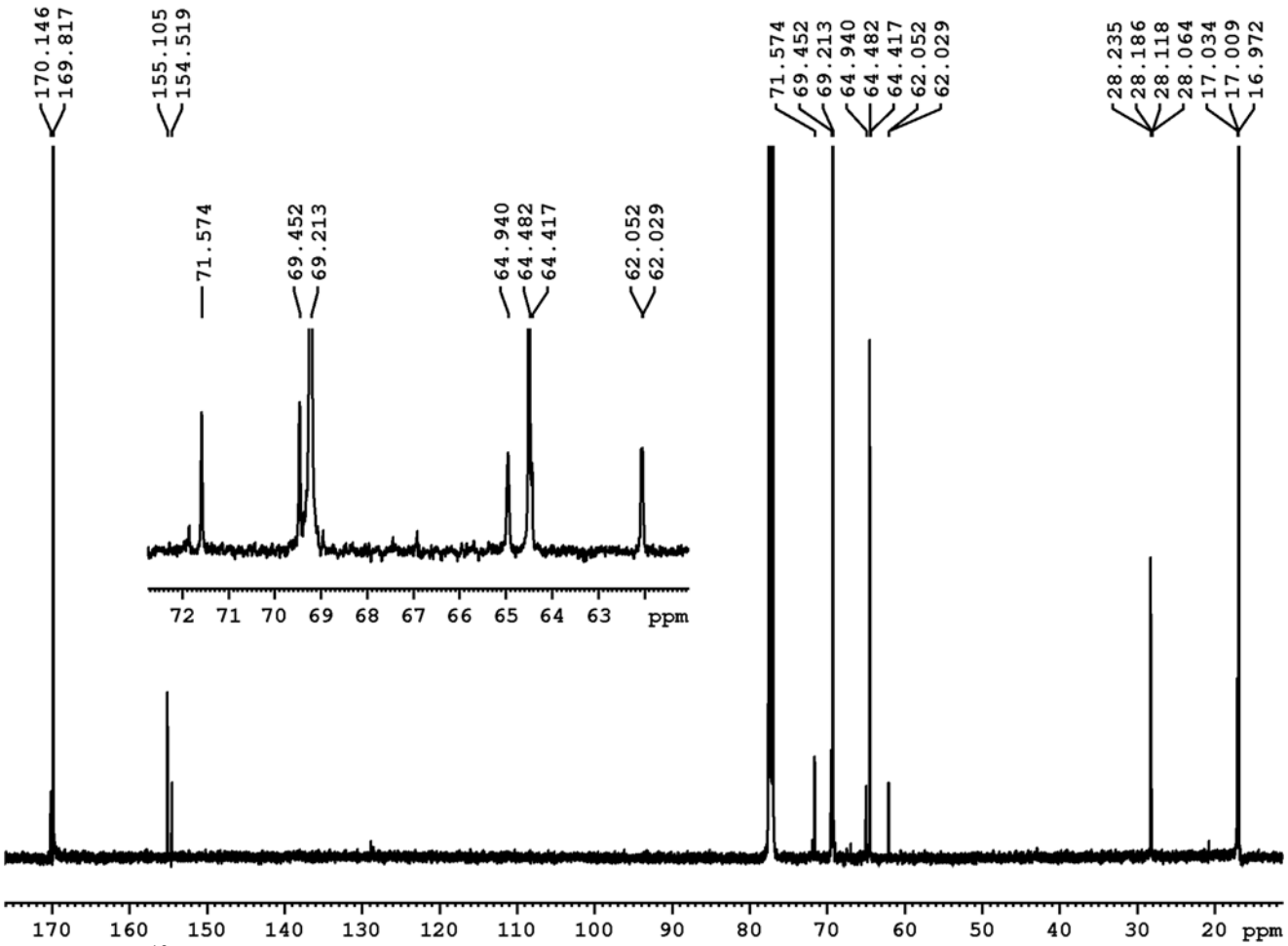



**Figure S43.** $^{13}C$ NMR spectrum ($CDCl_3$, 126 MHz, 298 K) of the PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA copolymer (Table 1, entry 9).

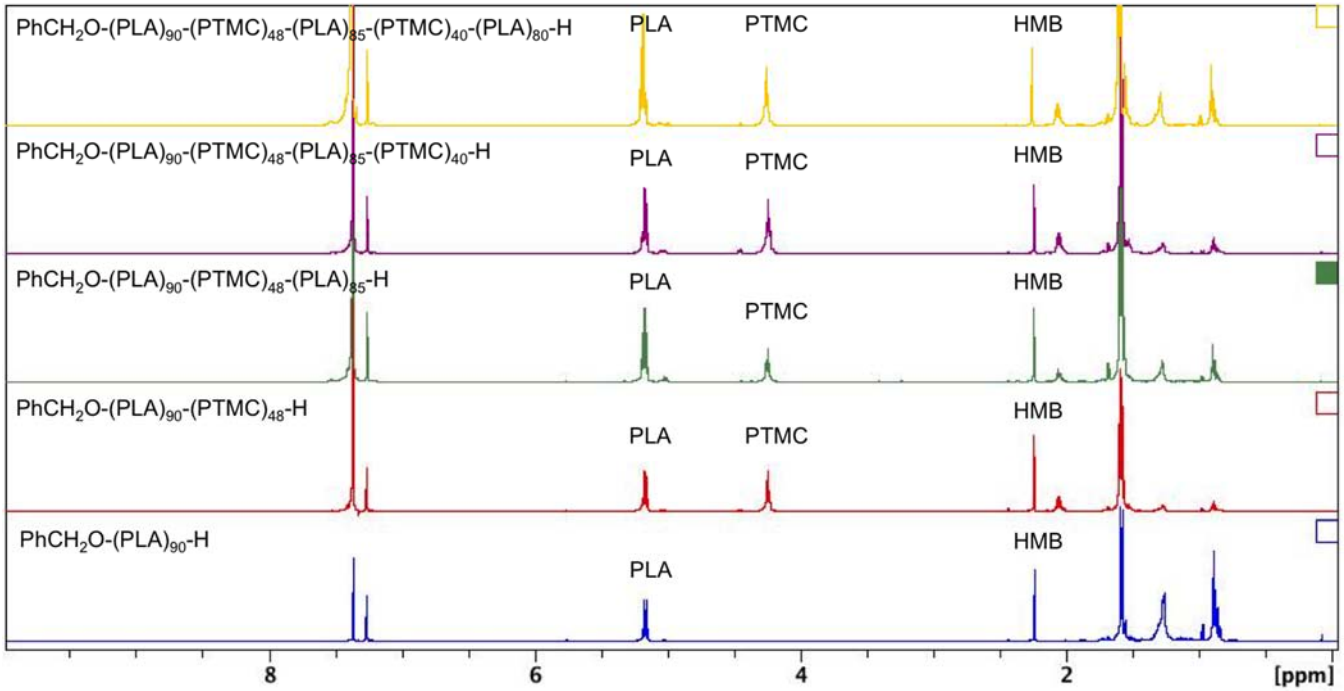



**Figure S44.** $^{1}H$ NMR spectra ($CDCl_3$, 500 MHz, 298 K) corresponding to the stepwise preparation of PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA in the presence of HMB as an internal standard.

## Conversion Studies

**Table S1.** Molar mass versus conversion study of 1,3-trimethylene carbonate.

| Time (min) | Conversion (%) | $M_n$ (NMR) | $M_n$ (SEC) | *Đ* |
|---|---|---|---|---|
| **30** | 37 | 9,400 | 10,300 | 1.04 |
| **50** | 44 | 11,200 | 12,500 | 1.09 |
| **70** | 58 | 14,800 | 14,500 | 1.14 |
| **90** | 72 | 18,400 | 17,000 | 1.17 |

Conditions: benzene as a solvent (1.5 mL) and hexamethylbenzene as an internal standard. The experiment was performed at ambient temperature.

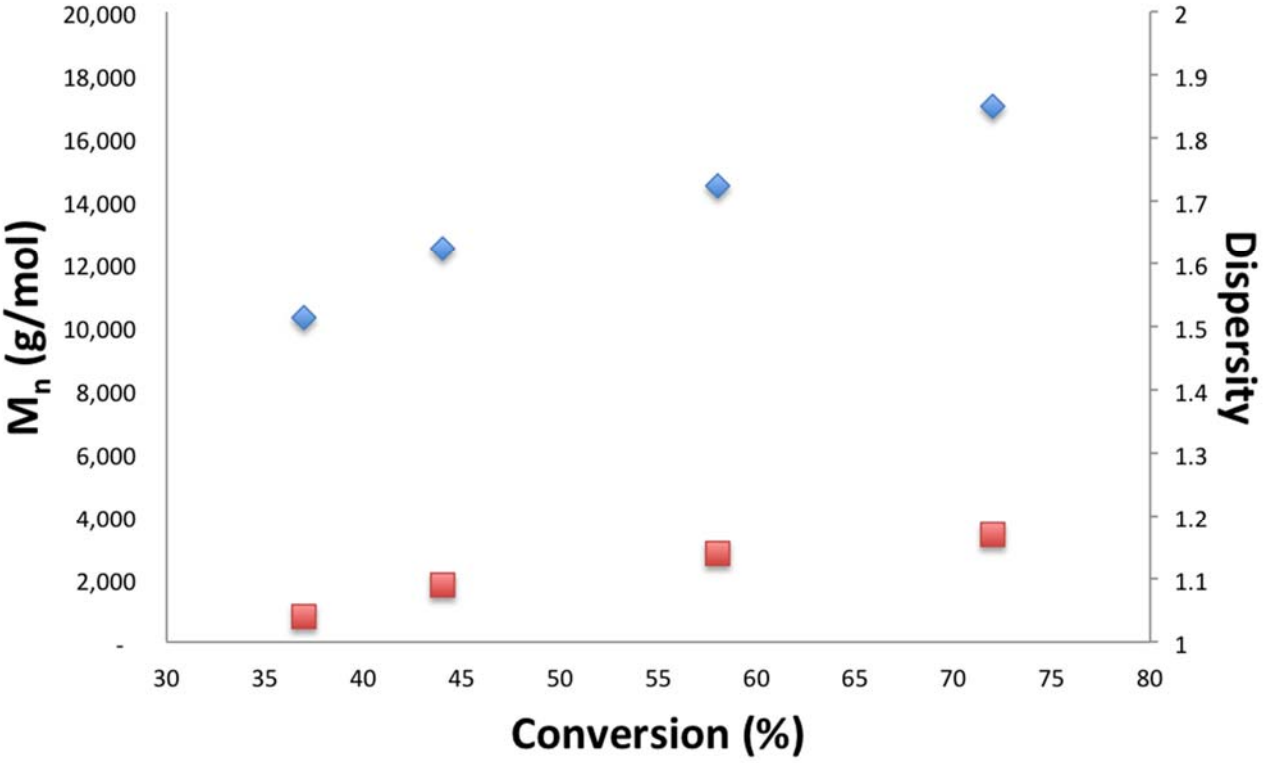



**Figure S45.** Conversion of 1,3-trimethylene carbonate versus $M_n$.

**Table S2.** Molar mass versus conversion study of L-lactide.

| Time (min) | Conversion (%) | $M_n$ (NMR) | $M_n$ (SEC) | *Đ* |
|---|---|---|---|---|
| **10** | 18 | 8,100 | 8,800 | 1.06 |
| **20** | 31 | 13,500 | 13,500 | 1.09 |
| **30** | 42 | 19,700 | 20,400 | 1.08 |
| **40** | 52 | 24,100 | 25,400 | 1.01 |
| **50** | 60 | 27,700 | 28,700 | 1.03 |
| **60** | 69 | 31,200 | 31,700 | 1.02 |

Conditions: benzene as a solvent (1.5 mL) and hexamethylbenzene as an internal standard. The experiment was performed at 70 °C.

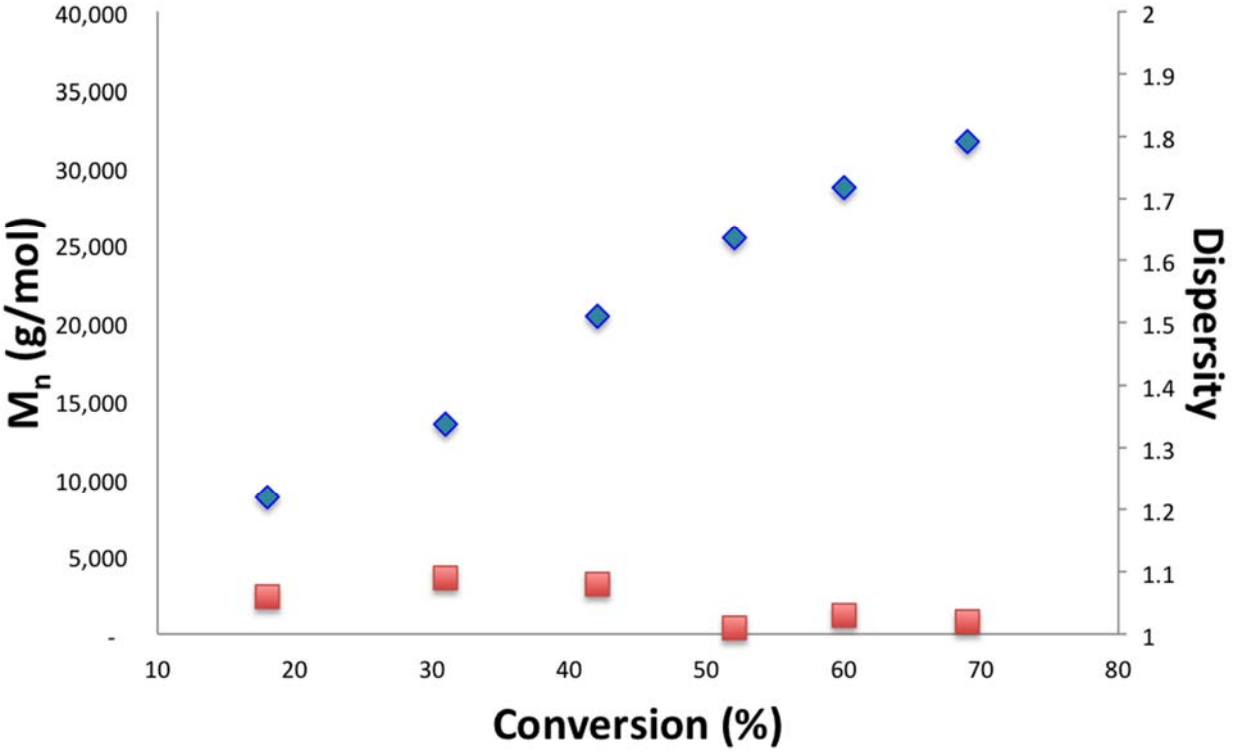



**Figure S46.** Conversion of L-lactide versus $M_n$.

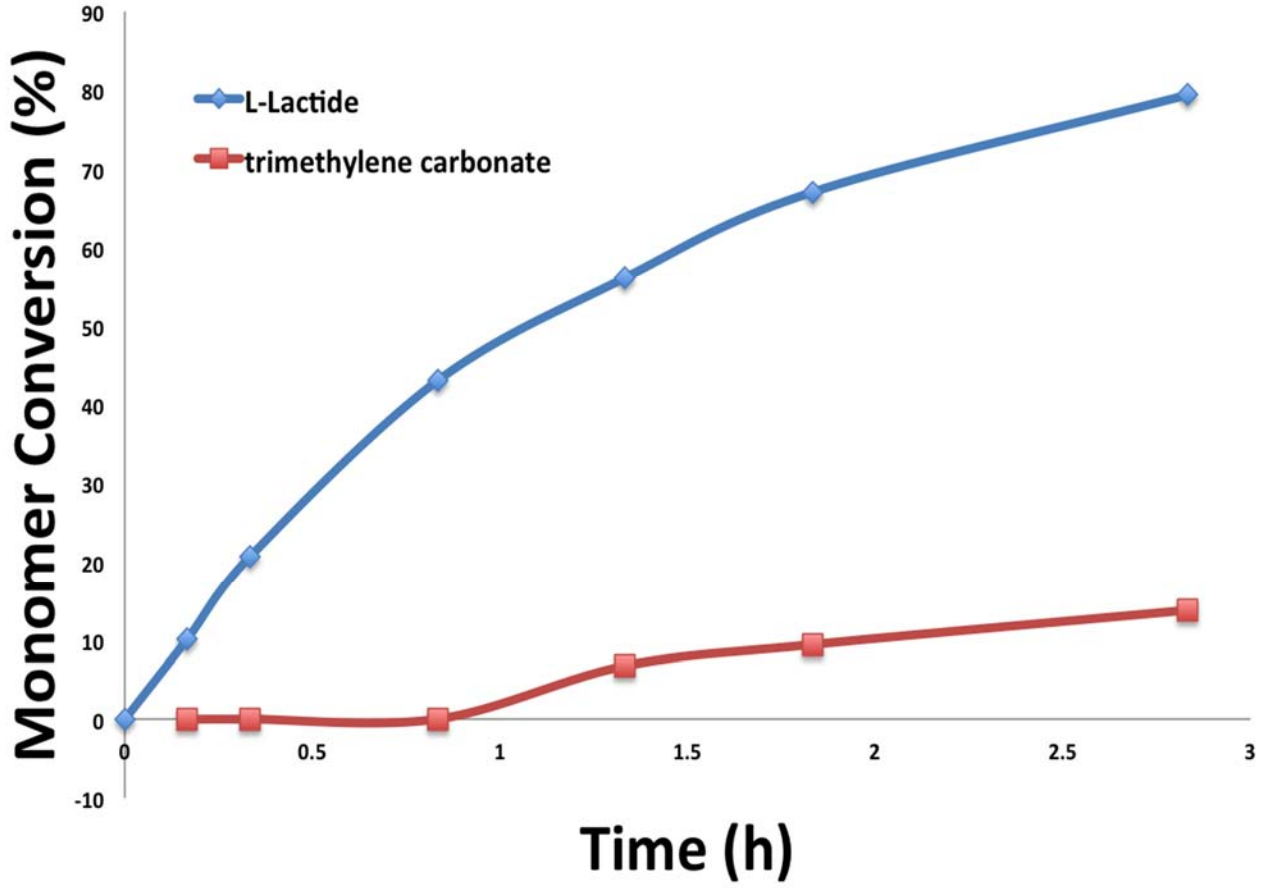



**Figure S47.** One pot polymerization of L-lactide (100 equivalents) and trimethylene carbonate (50 equivalents) in 0.5 mL of $C_6D_6$ at 50 °C.

## Size Exclusion Chromatography

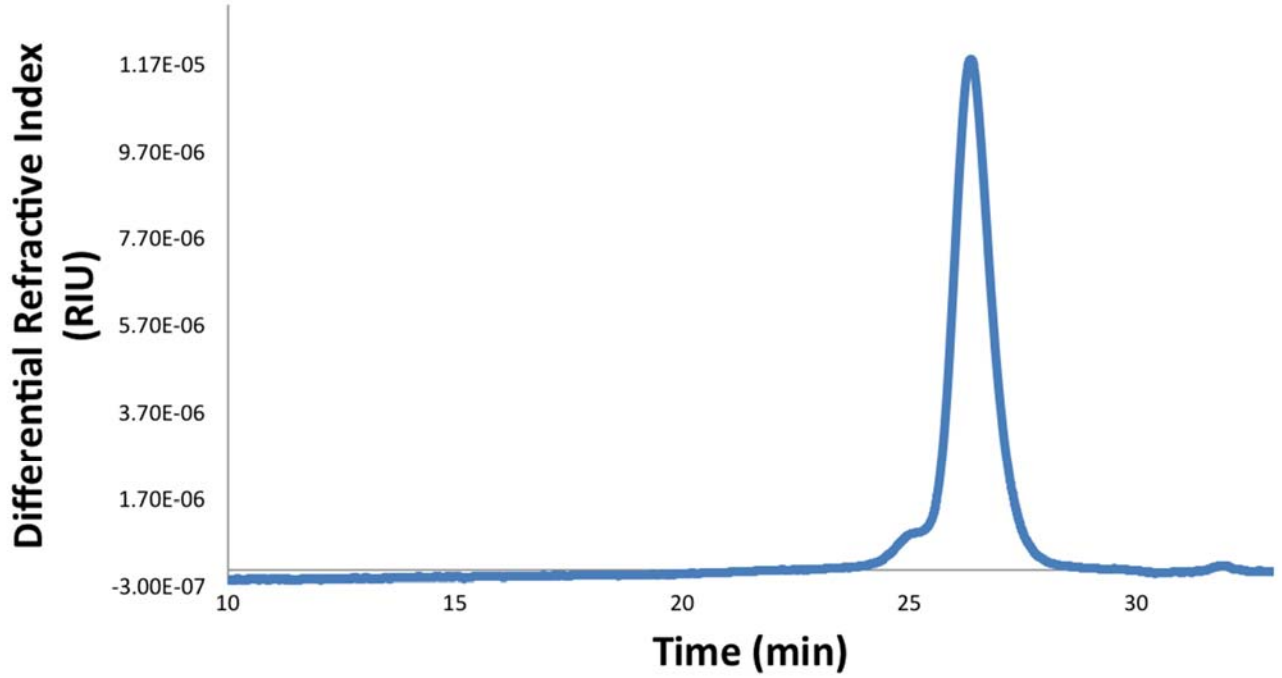



**Figure S48.** Polymerization of 101 equivalents of 1,3-trimethylene carbonate (Table 1, entry 2); $M_n$ = 9,000; $M_w$ =9,100; $Đ$ = 1.01.

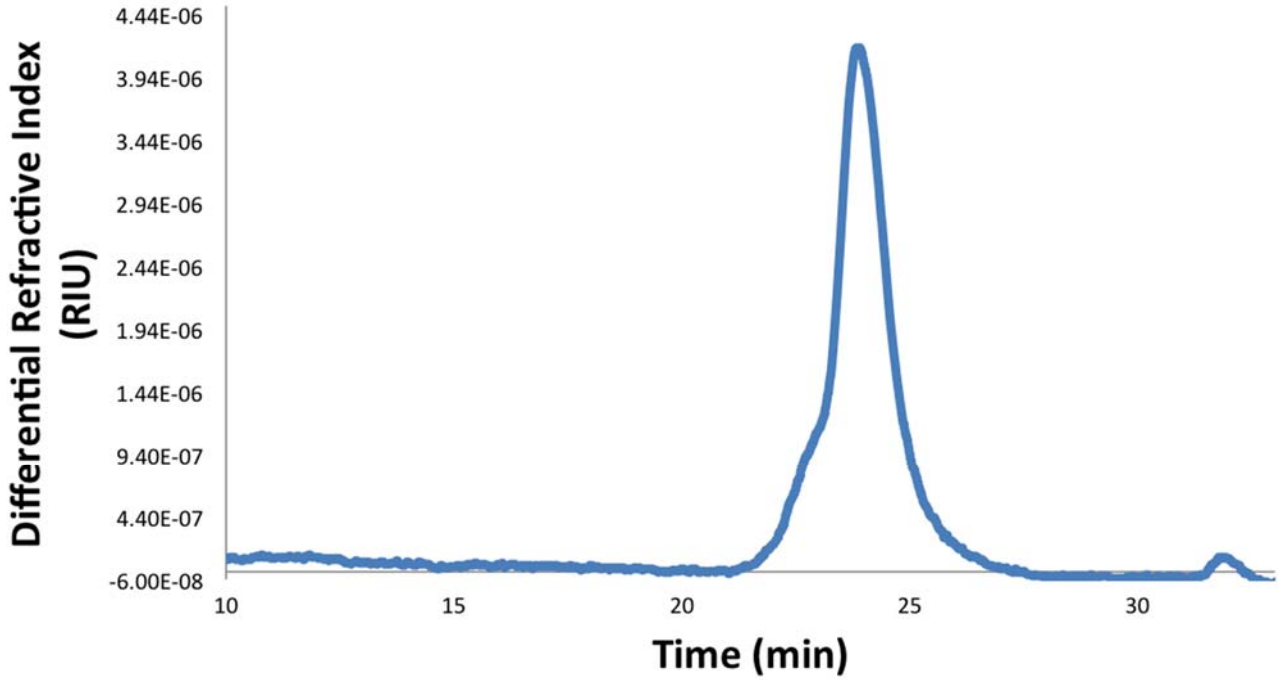



**Figure S49.** Polymerization of 283 equivalents of L-lactide (Table 1, entry 1); $M_n$ = 39,800; $M_w$ = 45,200; $Đ$ = 1.14.

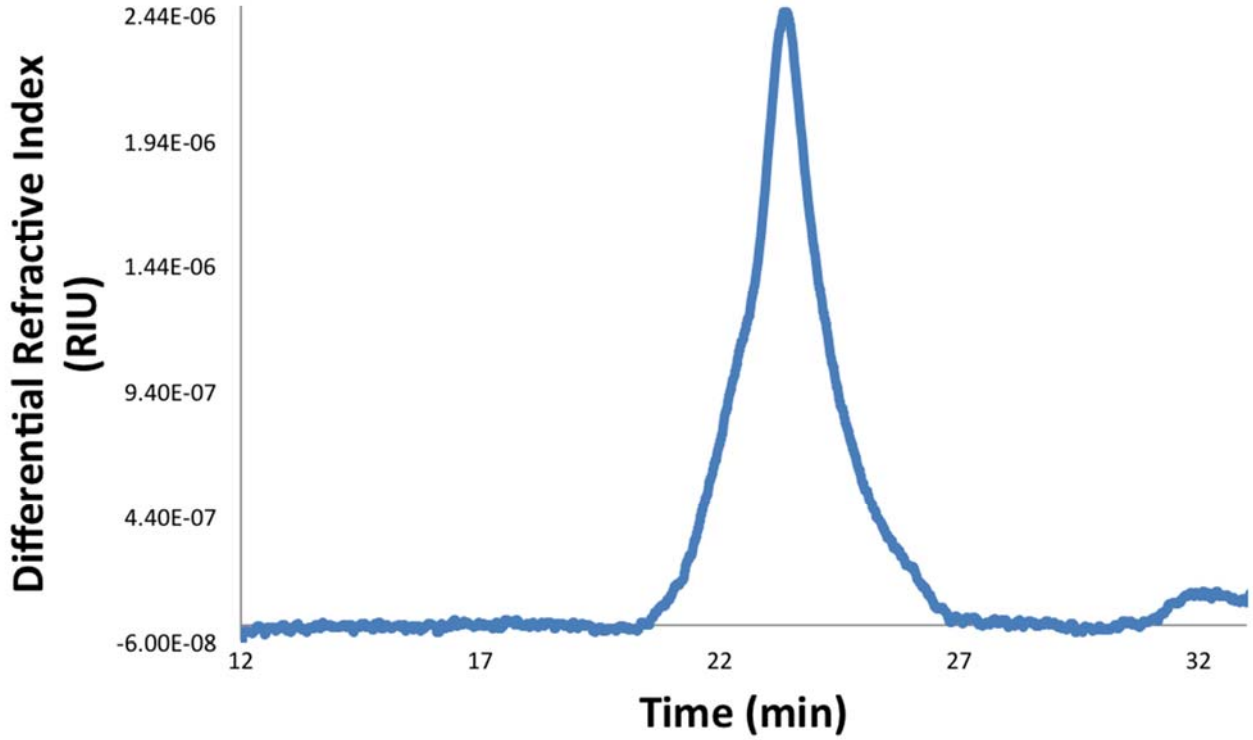



**Figure S50.** SEC trace of PLA-*b*-PTMC copolymer (Table 1, entry 3); $M_n$ = 55,500; $M_w$ = 61,800; $Đ$ = 1.12.

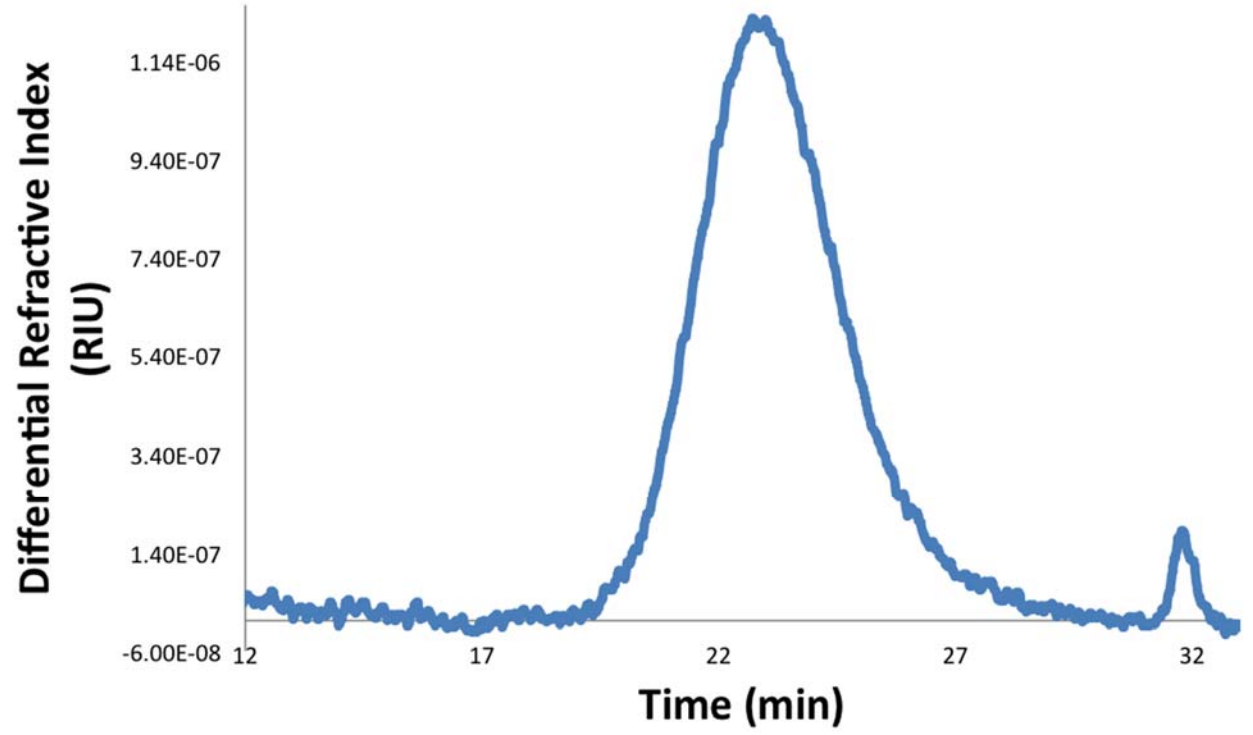



**Figure S51.** SEC trace of PTMC-*b*-PLA copolymer (Table 1, entry 4); $M_n$ = 47,000; $M_w$ = 75,000; $Đ$ = 1.60.

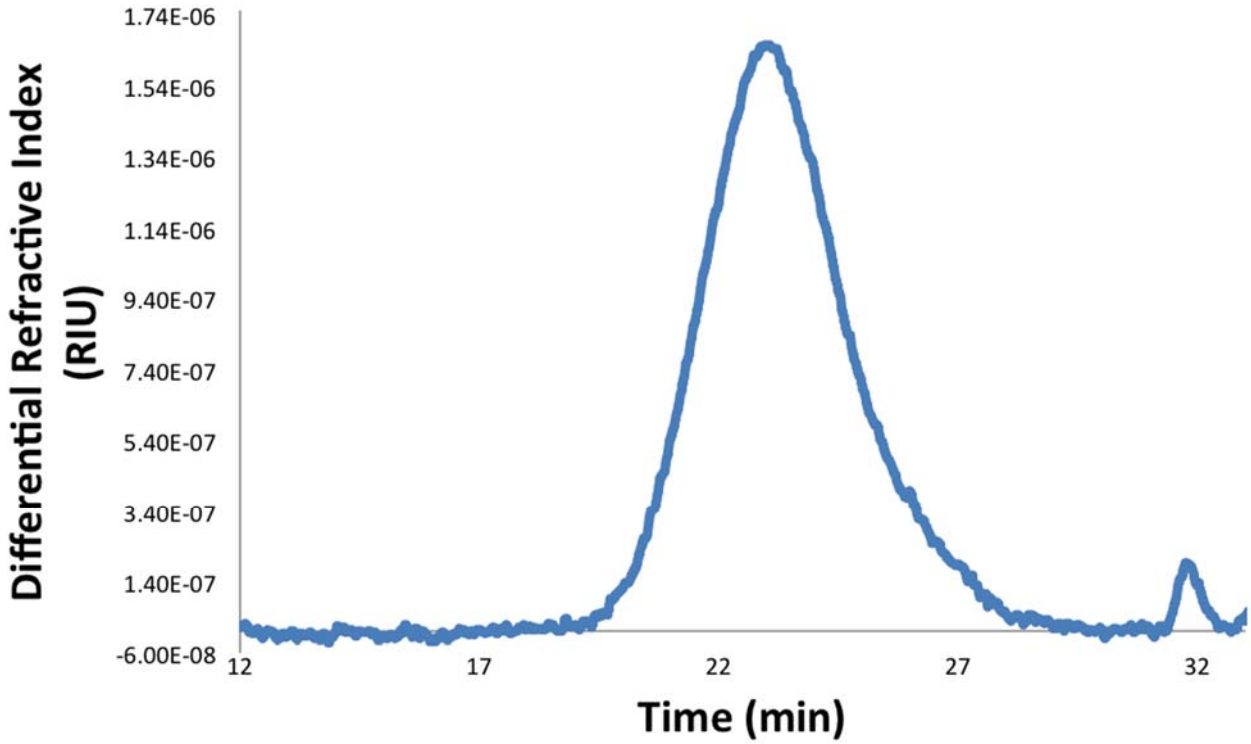



**Figure S52.** SEC trace of PTMC-*b*-PLA-*b*-PTMC copolymer (Table 1, entry 5); $M_n$ = 43,200; $M_w$ = 72,200; $Đ$ = 1.67.

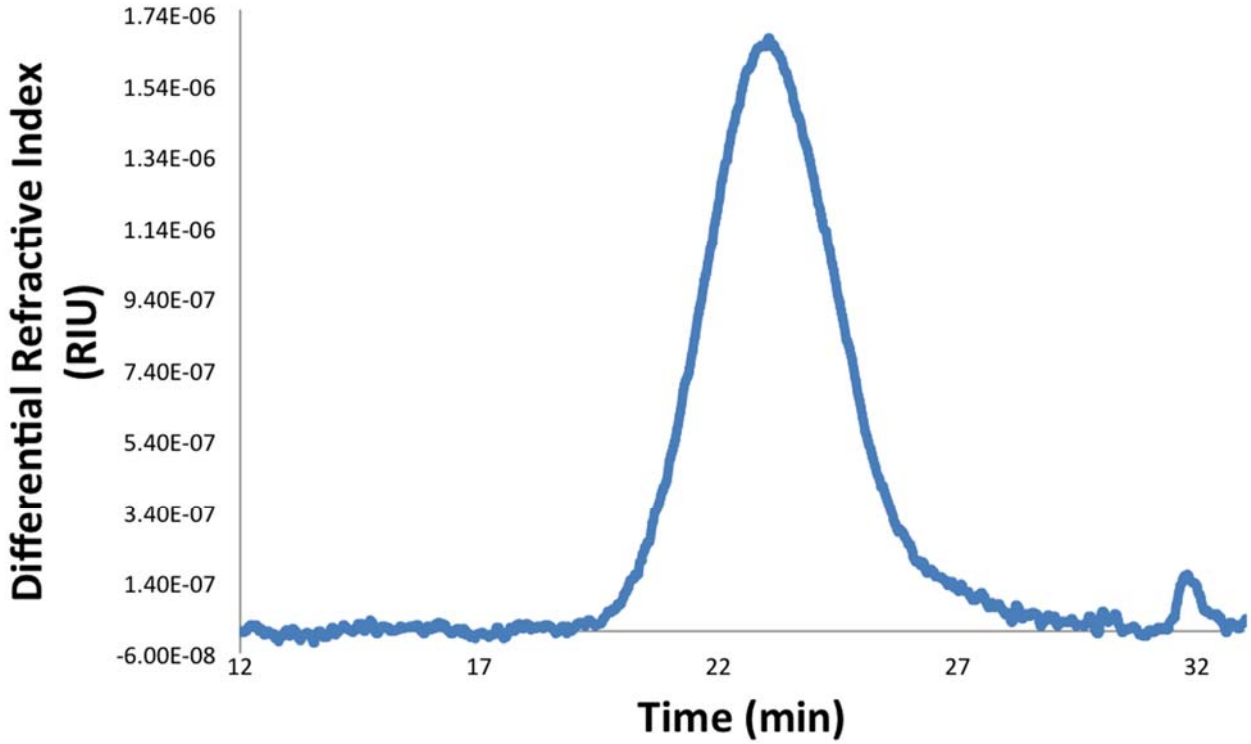



**Figure S53.** SEC trace of PLA-*b*-PTMC-*b*-PLA copolymer (Table 1, entry 6); $M_n$ = 55,600; $M_w$ = 81,400; $Đ$ = 1.46.

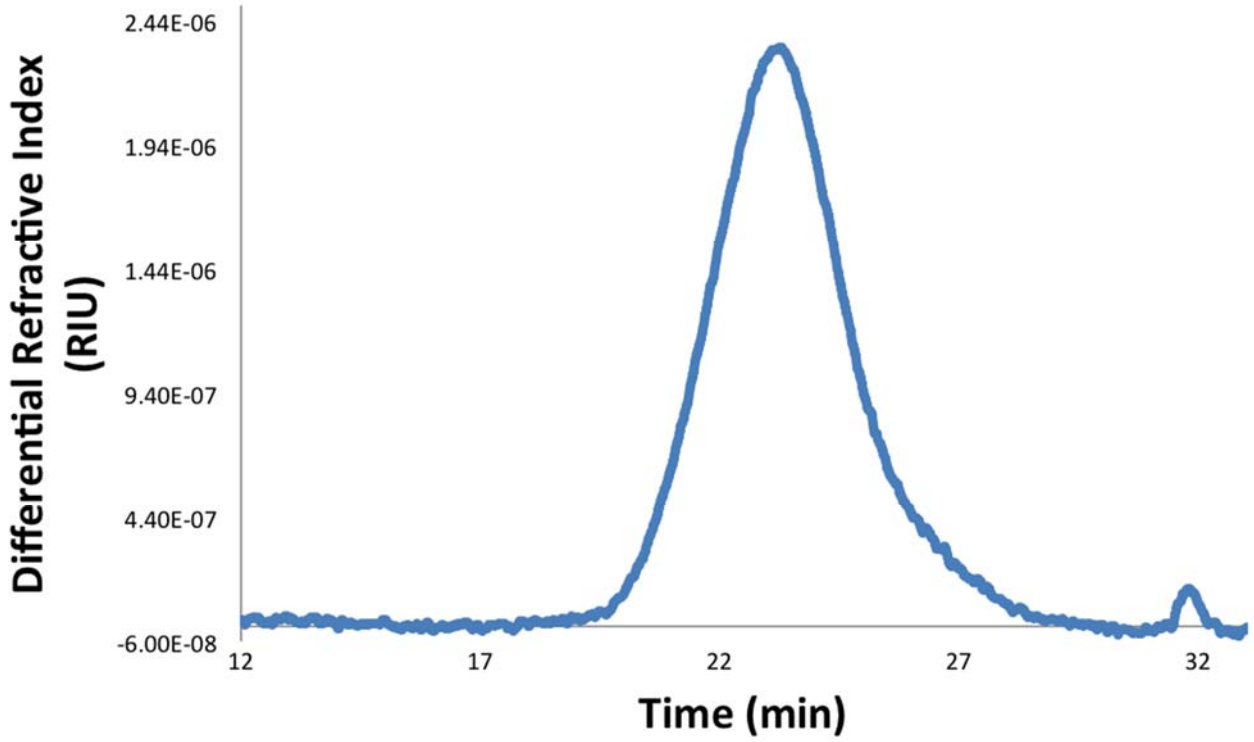



**Figure S54.** SEC trace of PLA-*b*-PTMC-*b*-PLA-*b*-PTMC copolymer (Table 1, entry 7); $M_n$ = 48,200; $M_w$ = 71,800; $Đ$ = 1.49.

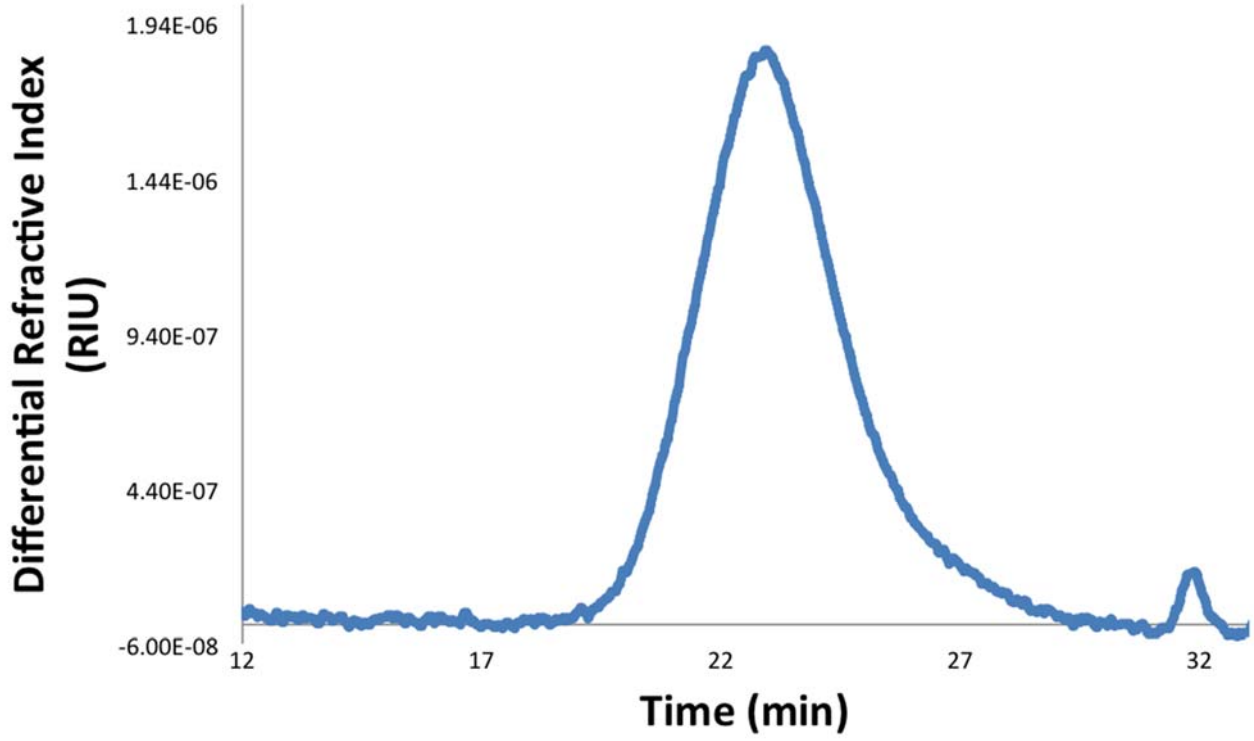



**Figure S55.** SEC trace of PTMC-*b*-PLA-*b*-PTMC-*b*-PLA-*b*-PTMC copolymer (Table 1, entry 8); $M_n$ = 58,900; $M_w$ = 87,900; $Đ$ = 1.49.

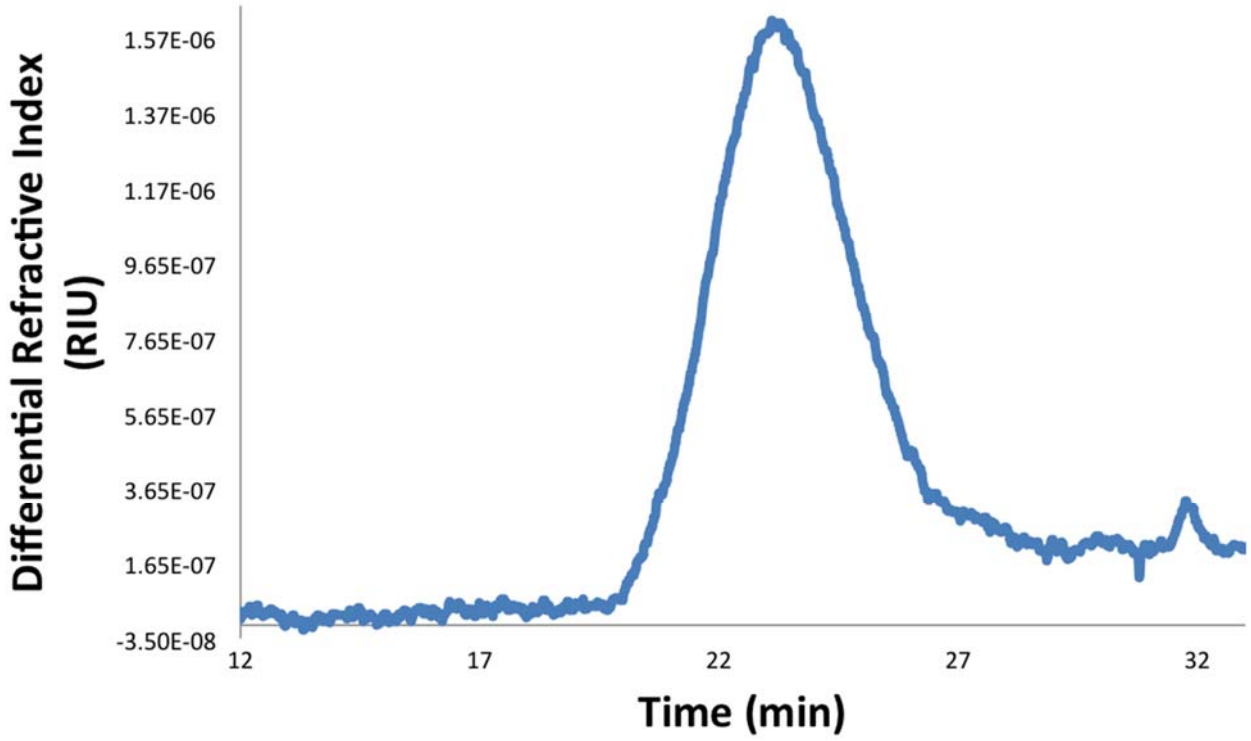



**Figure S56.** SEC trace of PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA copolymer (Table 1, entry 9); $M_n$ = 53,200; $M_w$ = 89,700; $Đ$ = 1.69.

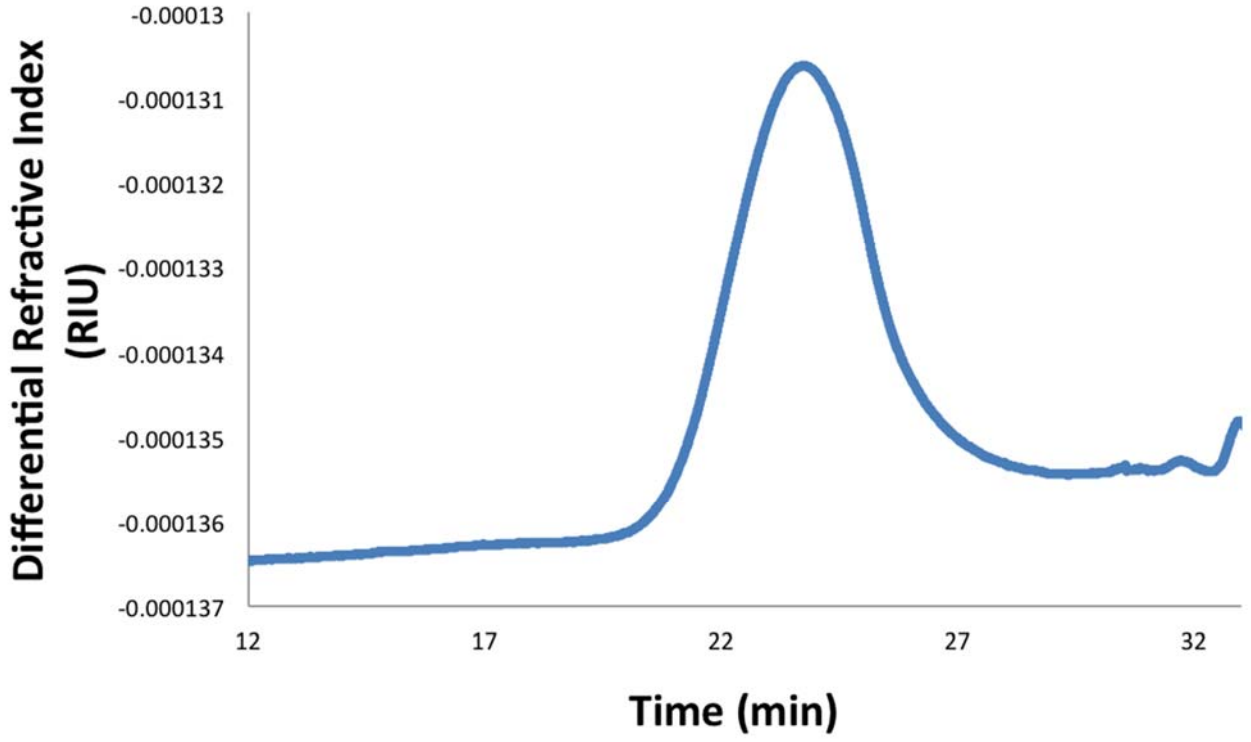



**Figure S57.** SEC trace of PLA-*b*-PTMC-*b*-PLA copolymer (Table 1, entry 10); $M_n$ = 50,800; $M_w$ = 65,800; $Đ$ = 1.29.

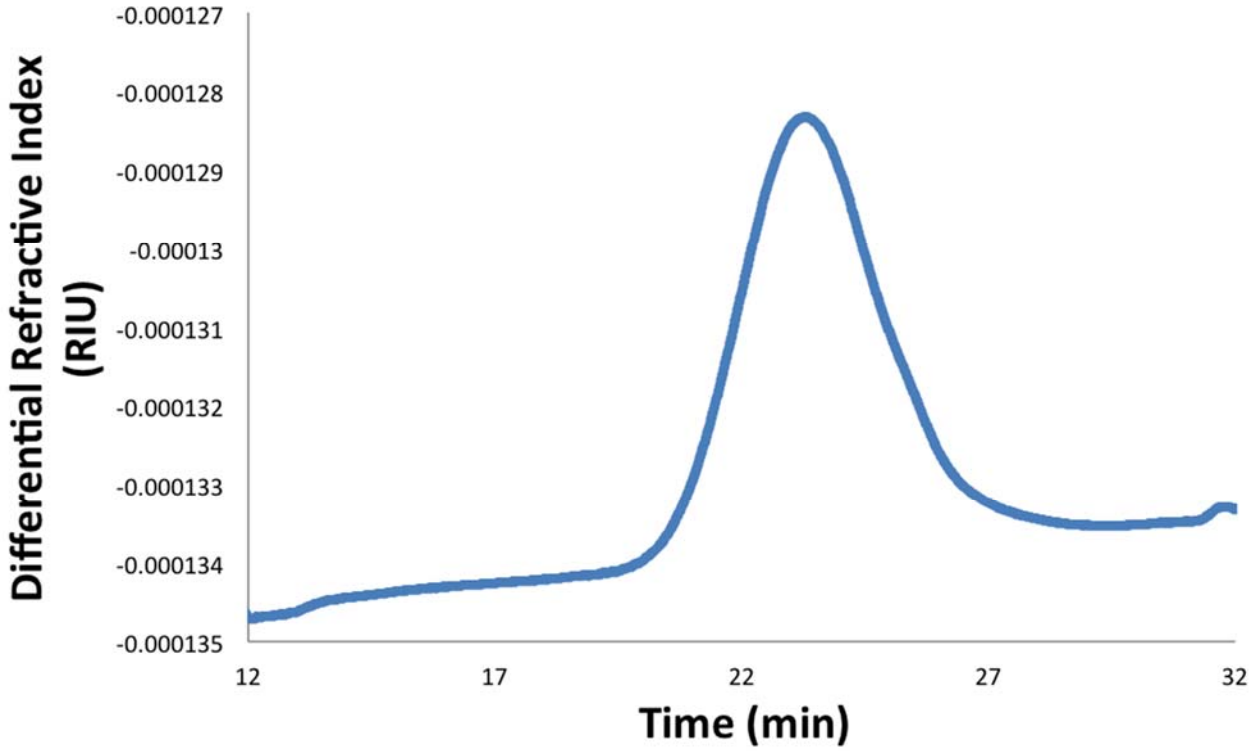



**Figure S58.** SEC trace of PLA-*b*-PTMC-*b*-PLA copolymer (Table 1, entry 11); $M_n$ = 48,900; $M_w$ = 69,400; $Đ$ = 1.42.

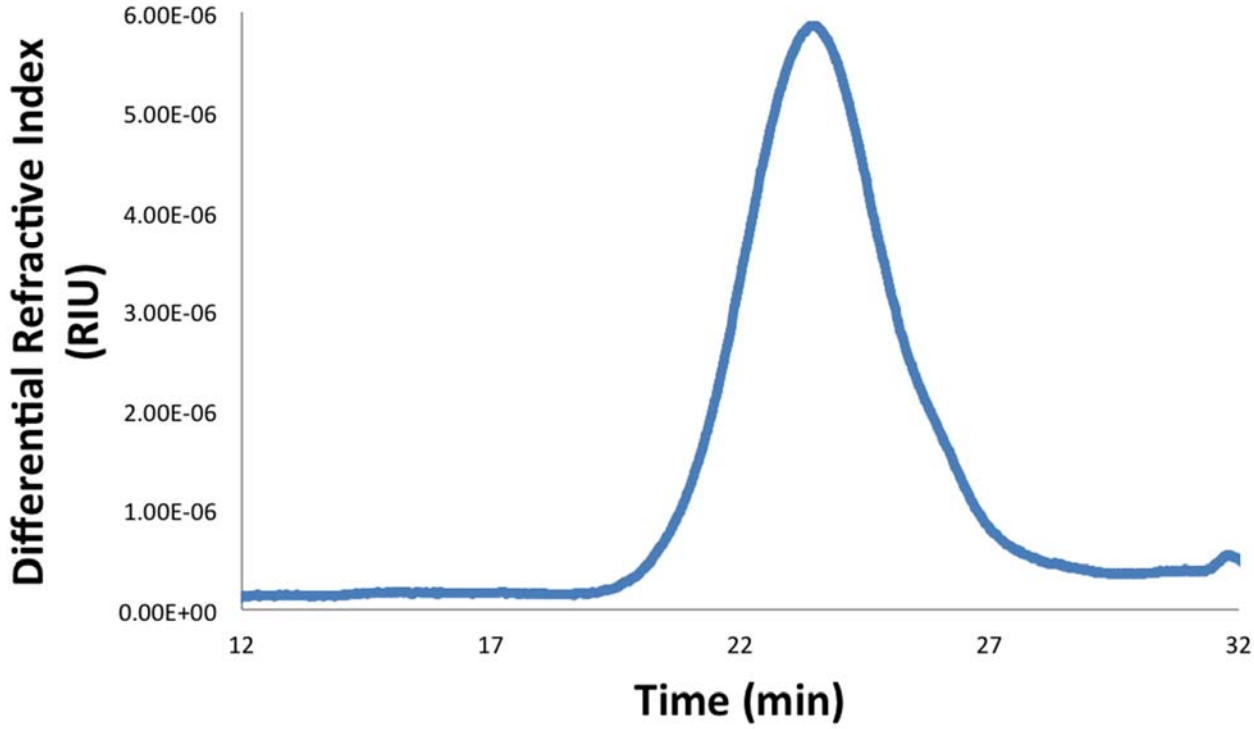



**Figure S59.** SEC trace of PLA-*b*-PTMC-*b*-PLA copolymer (Table 1, entry 12); $M_n$ = 51,200; $M_w$ = 86,000; $Đ$ = 1.68.

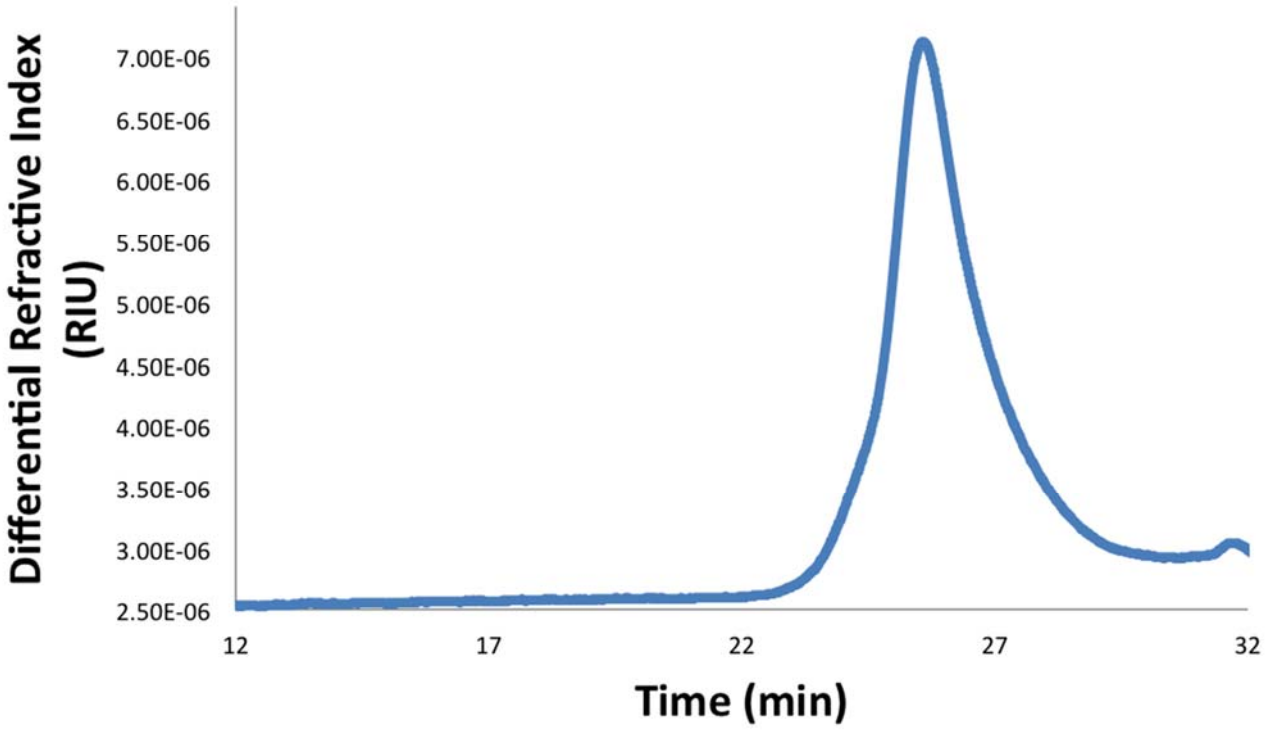



**Figure S60.** SEC trace of PLA polymer obtained by melt polymerization; $M_n$ = 25,800; $M_w$ = 29,800; $Đ$ = 1.16.

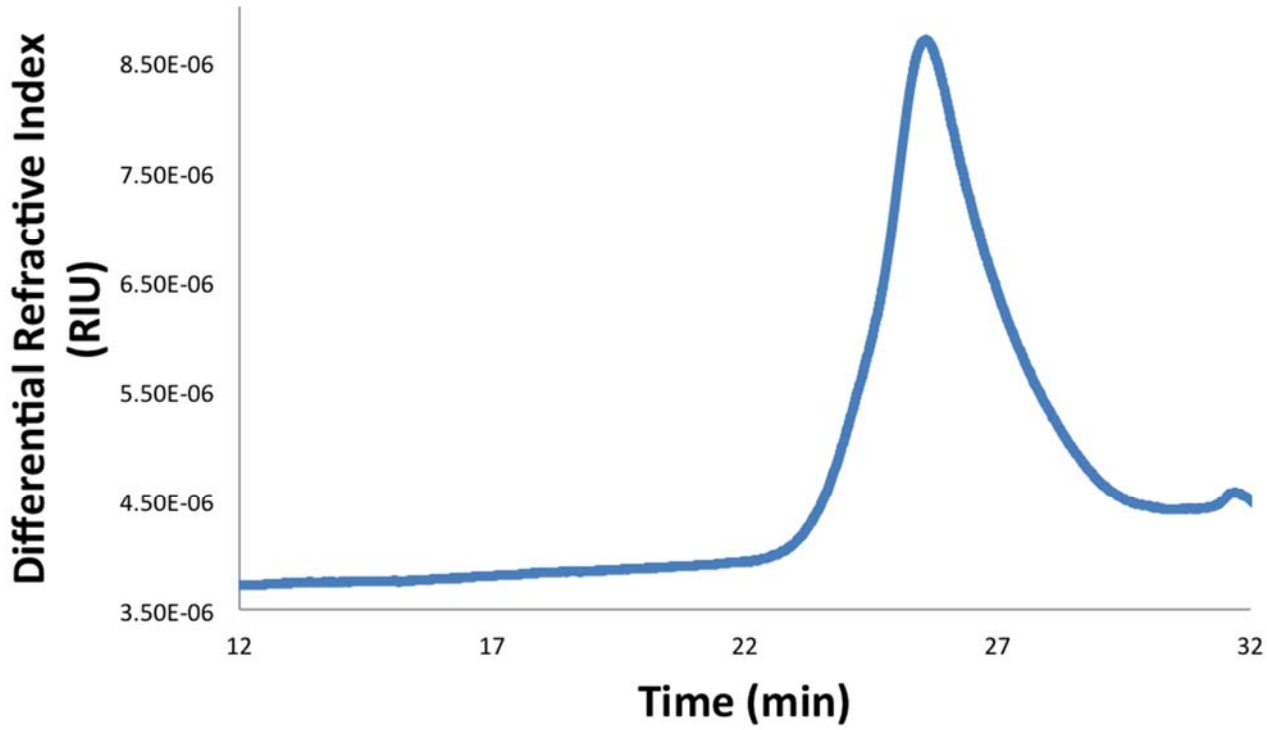



**Figure S61.** SEC trace of PTMC-*b*-PLA copolymer obtained by melt polymerization; $M_n$ = 24,800; $M_w$ = 29,000; $Đ$ = 1.17.

## Differential Scanning Calorimetry

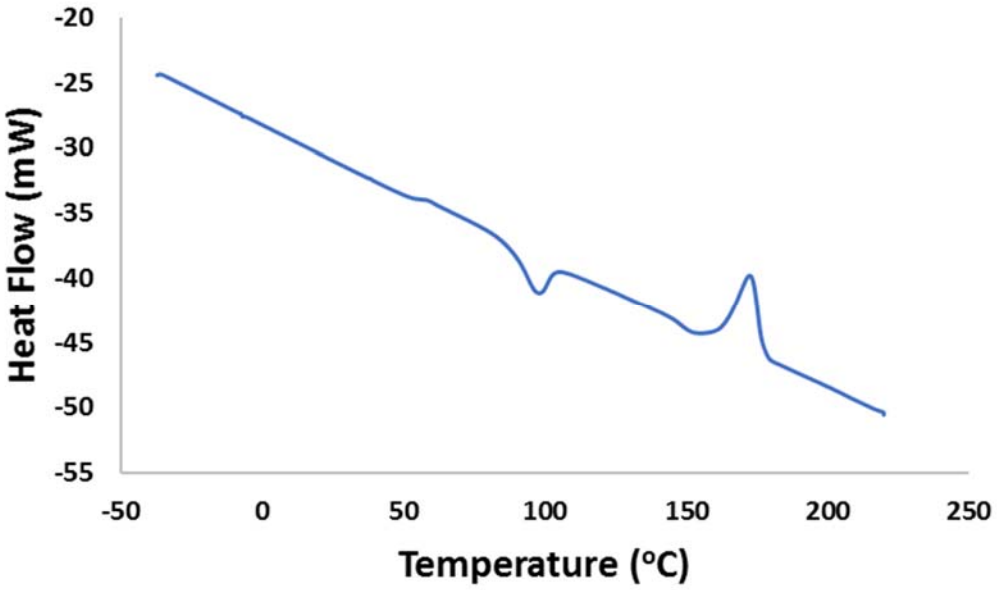



**Figure S62.** DSC curve (third heating run) of a PLA sample ($M_n$ (SEC) = 39,800; Table 1, entry 1).

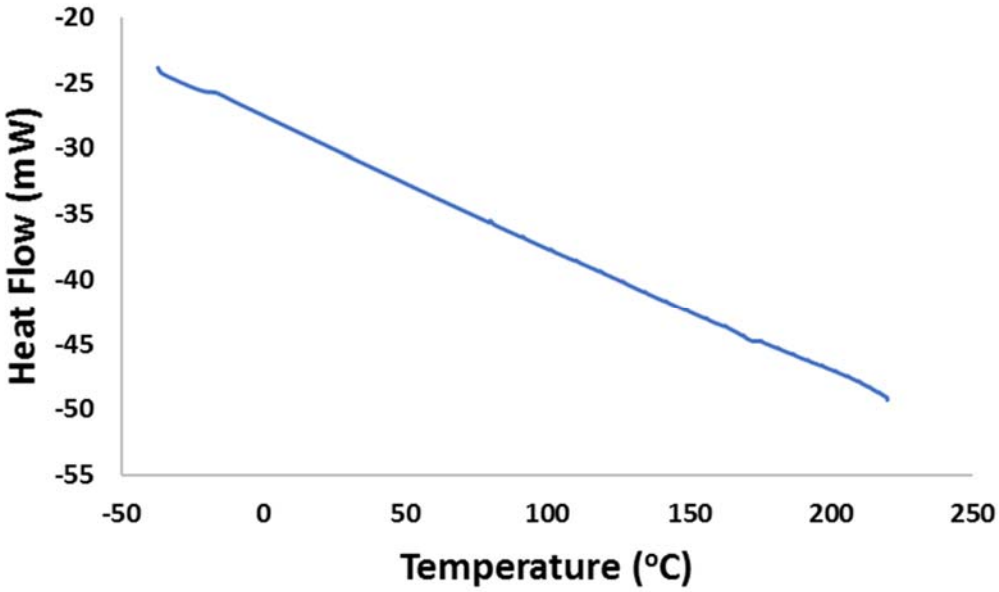



**Figure S63.** DSC curve (third heating run) of a PTMC sample ($M_n$ (SEC) = 9,000; Table 1, entry 2).

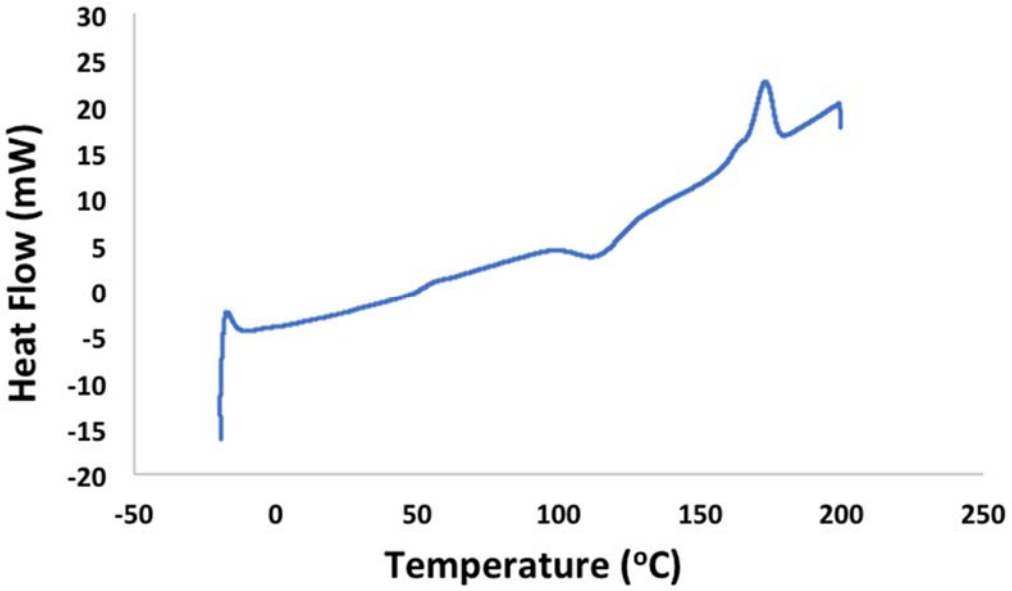



**Figure S64.** DSC curve (third heating run) of a PLA-*b*-PTMC sample ($M_n$ (SEC) = 55,500; Table 1, entry 3).

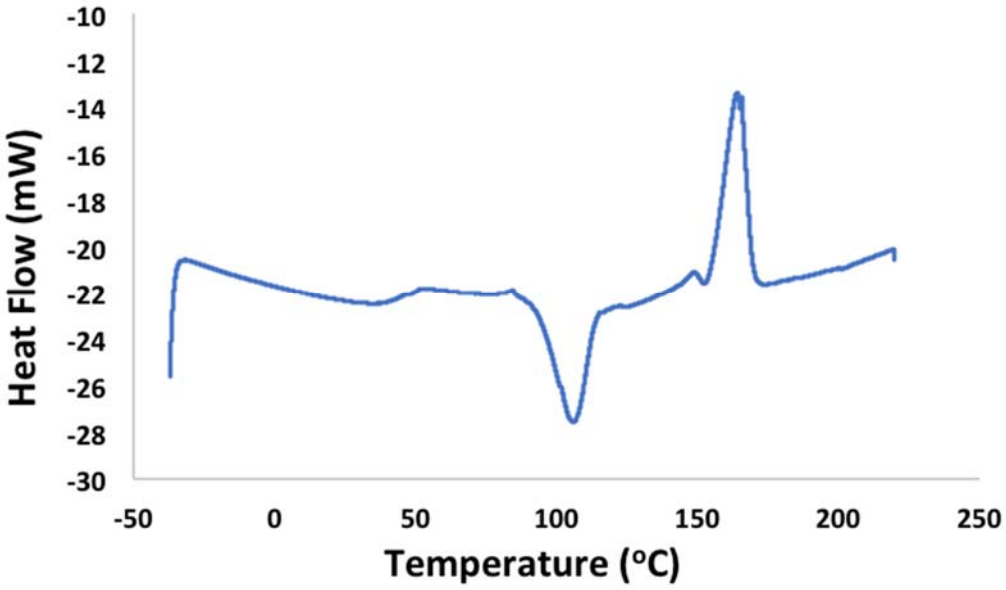



**Figure S65.** DSC curve (third heating run) of a PTMC-*b*-PLA sample ($M_n$ (SEC) = 47,000; Table 1, entry 4).

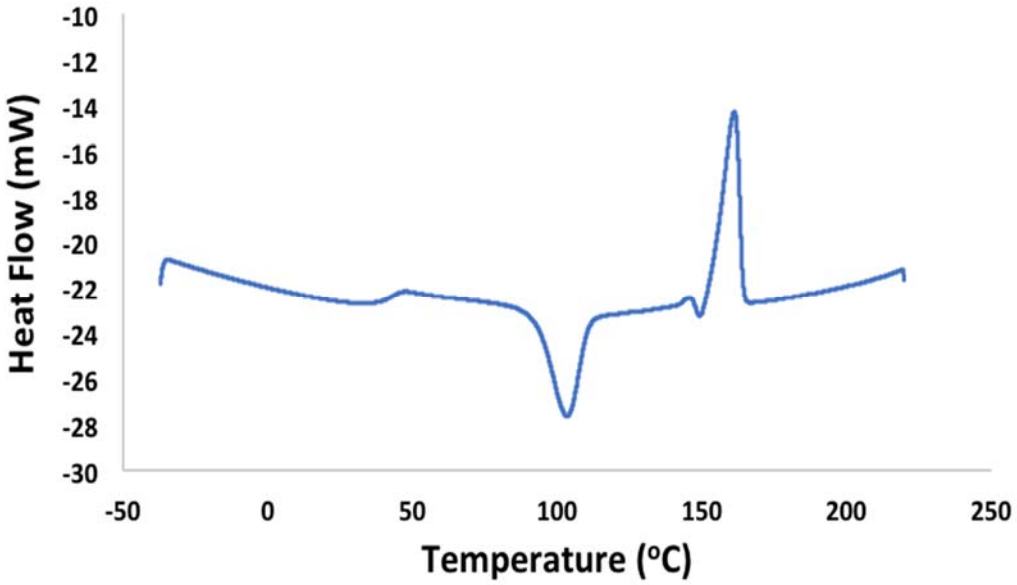



**Figure S66.** DSC curve (third heating run) of a PTMC-*b*-PLA-*b*-PTMC sample ($M_n$ (SEC) = 43,200; Table 1, entry 5).

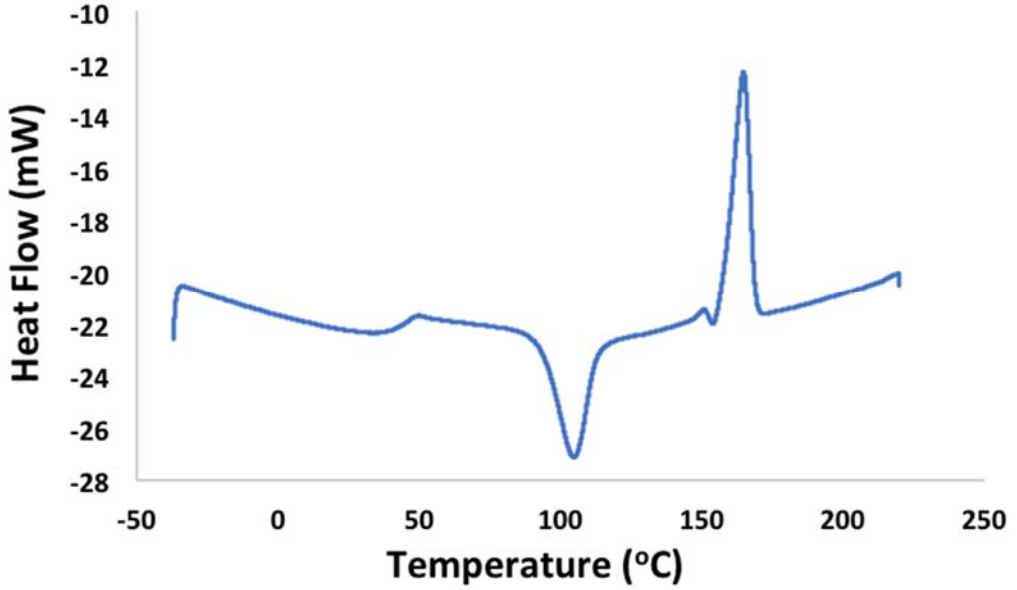



**Figure S67.** DSC curve (third heating run) of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 55,600; Table 1, entry 6).

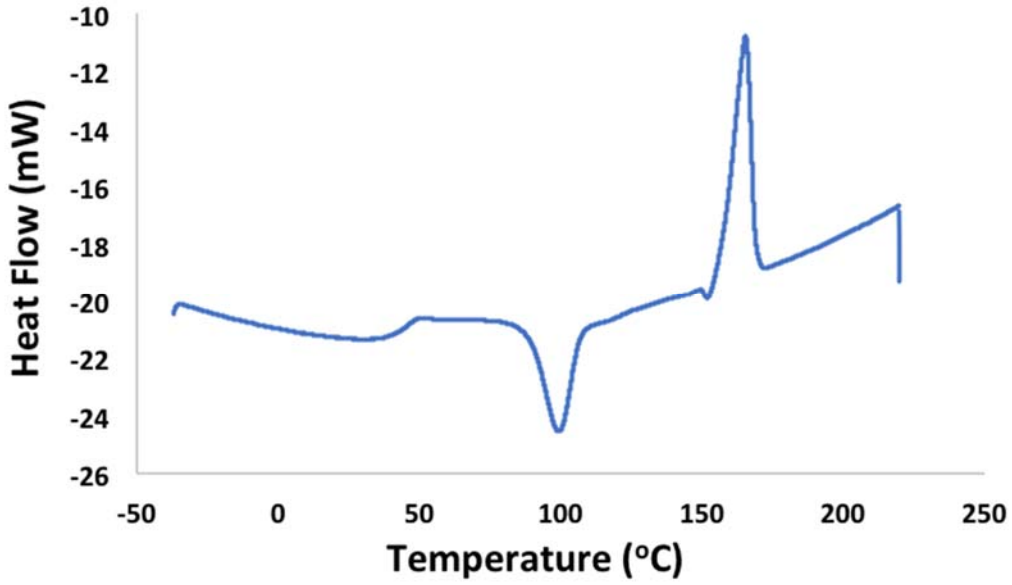



**Figure S68.** DSC curve (third heating run) of a PLA-*b*-PTMC-*b*-PLA-*b*-PTMC sample ($M_n$ (SEC) = 48,200; Table 1, entry 7).

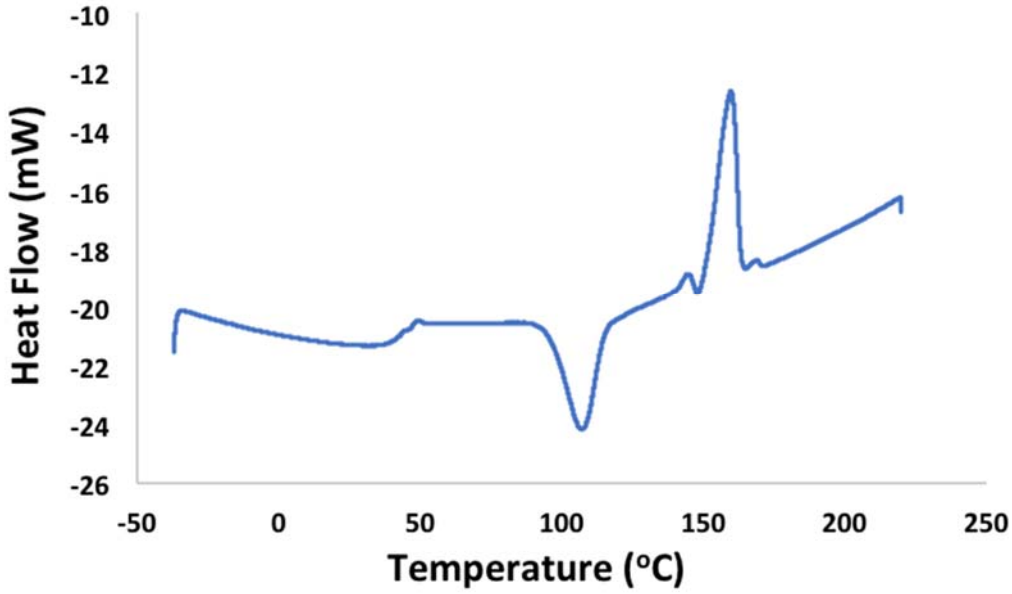



**Figure S69.** DSC curve (third heating run) of a PTMC-*b*-PLA-*b*-PTMC-*b*-PLA-*b*-PTMC sample ($M_n$ (SEC) = 58,900; Table 1, entry 8).

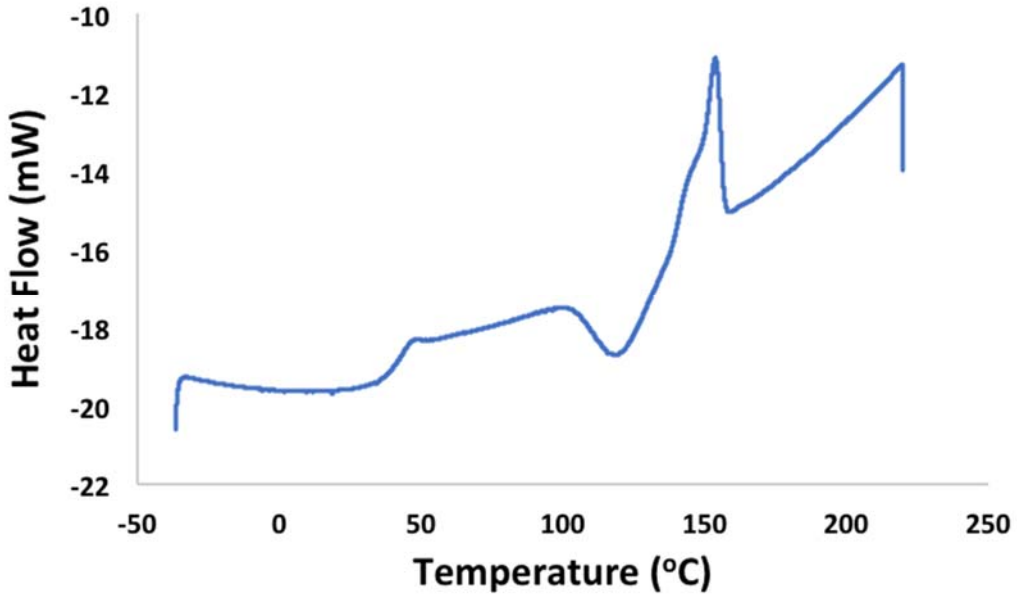



**Figure S70.** DSC curve (third heating run) of a PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 53,200; Table 1, entry 9).

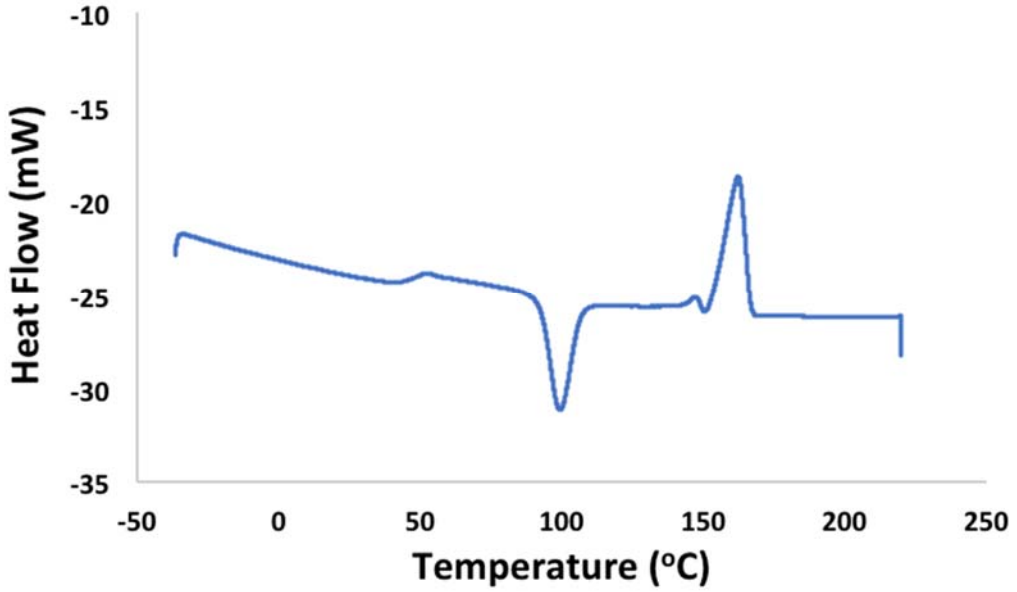



**Figure S71.** DSC curve (third heating run) of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 50,800; Table 1, entry 10).

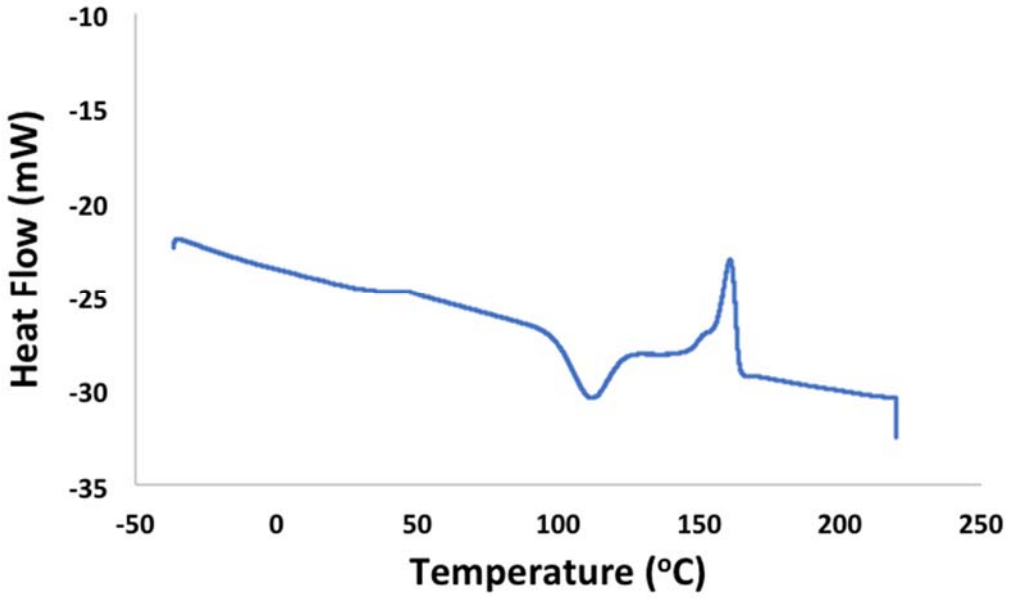



**Figure S72.** DSC curve (third heating run) of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 48,900; Table 1, entry 11).

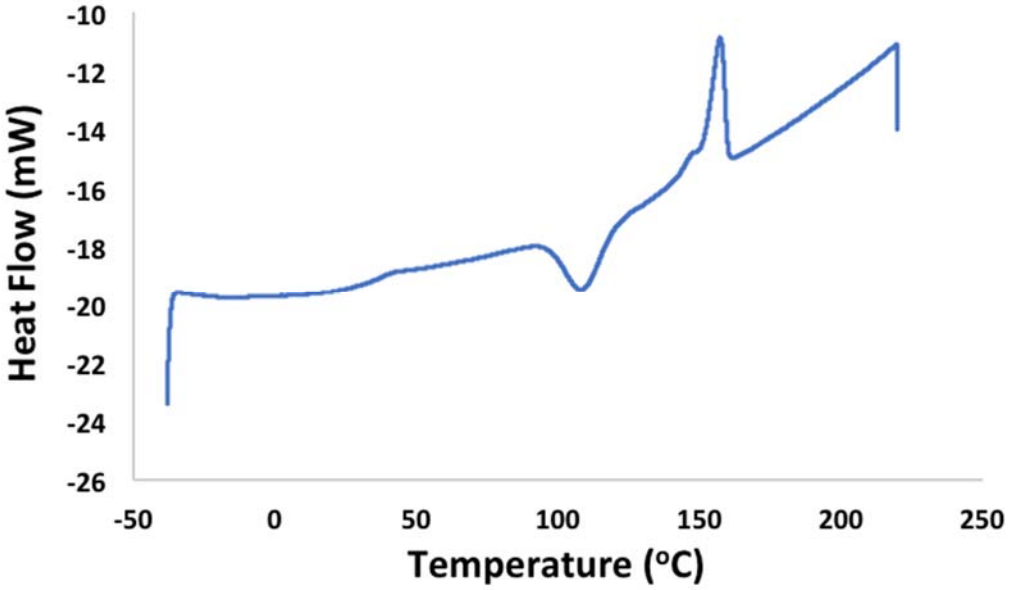



**Figure S73.** DSC curve (third heating run) of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 51,200; Table 1, entry 12).

## Dynamic Mechanical Analysis

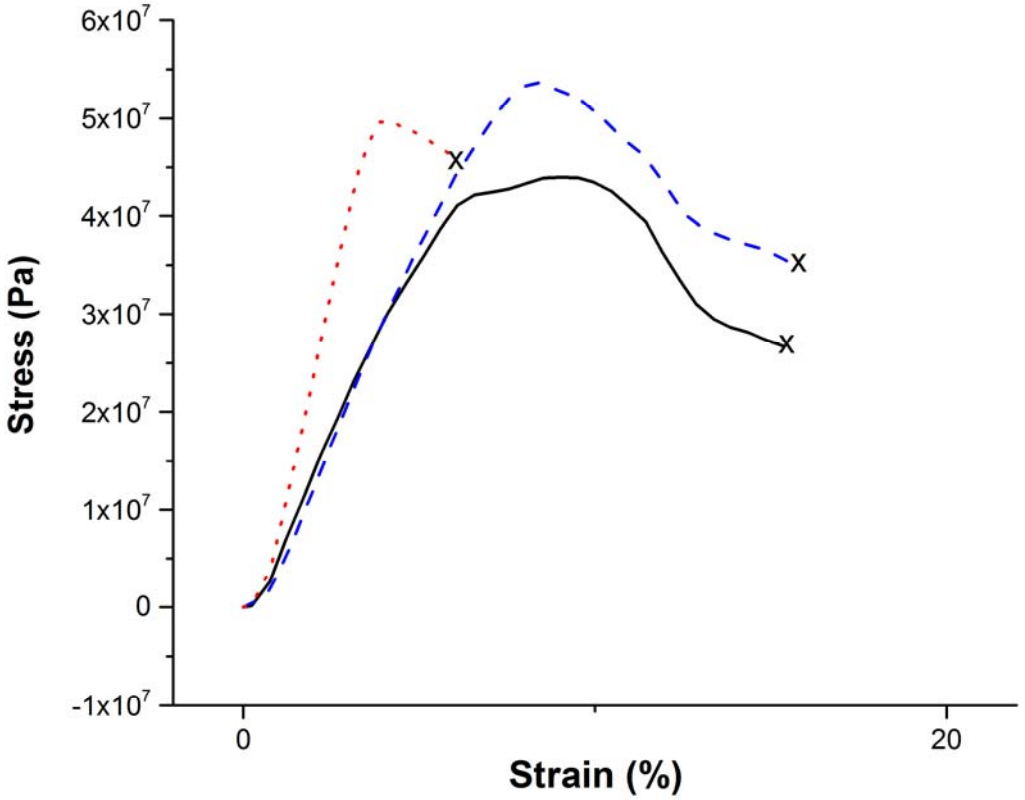



**Figure S74.** Stress vs. strain curve of a PLA sample ($M_n$ (SEC) = 39,800; Table 1, entry 2).

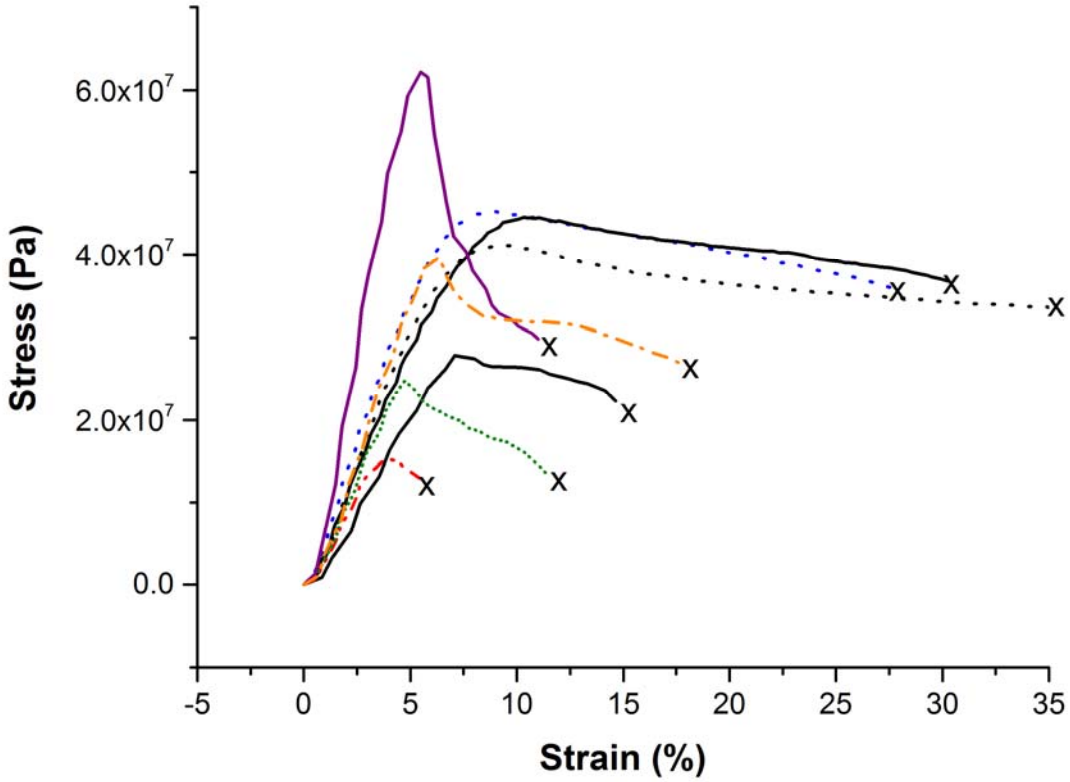



**Figure S75.** Stress vs. strain curve of a PLA-*b*-PTMC sample ($M_n$ (SEC) = 55,500; Table 1, entry 3) and PLA-*b*-PTMC sample ($M_n$ (SEC) = 53,400).

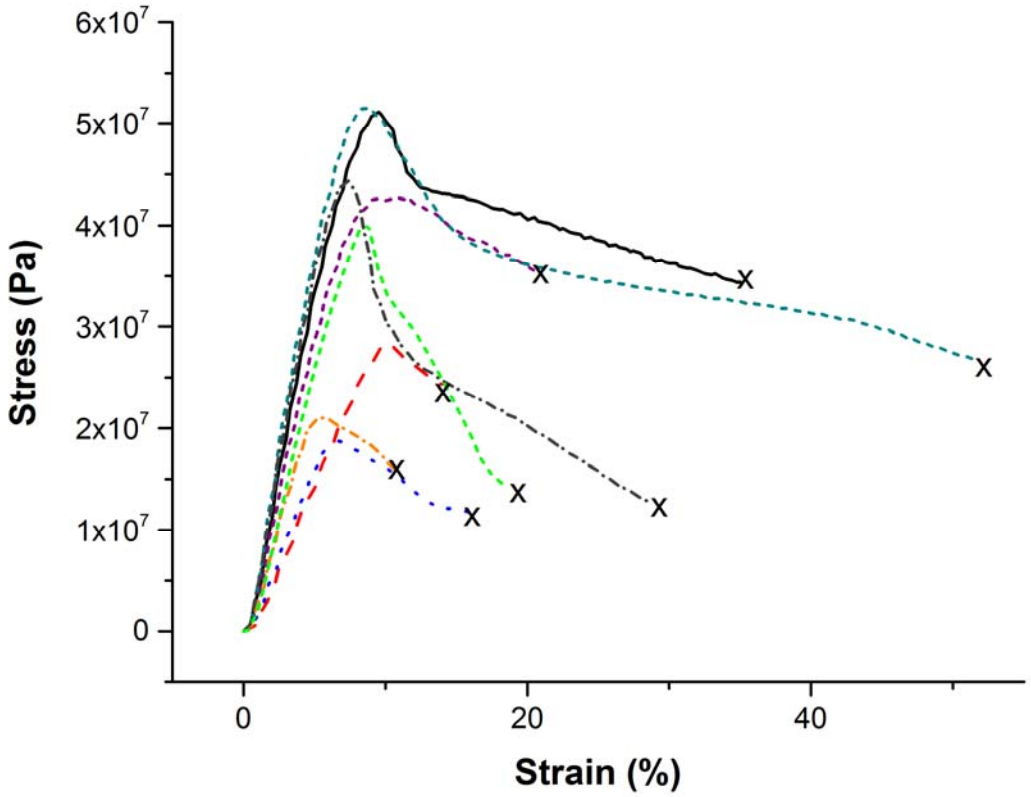



**Figure S76.** Stress vs. strain curve of a PTMC-*b*-PLA sample ($M_n$ (SEC) = 47,000; Table 1, entry 4) and PTMC-*b*-PLA sample ($M_n$ (SEC) = 59,000).

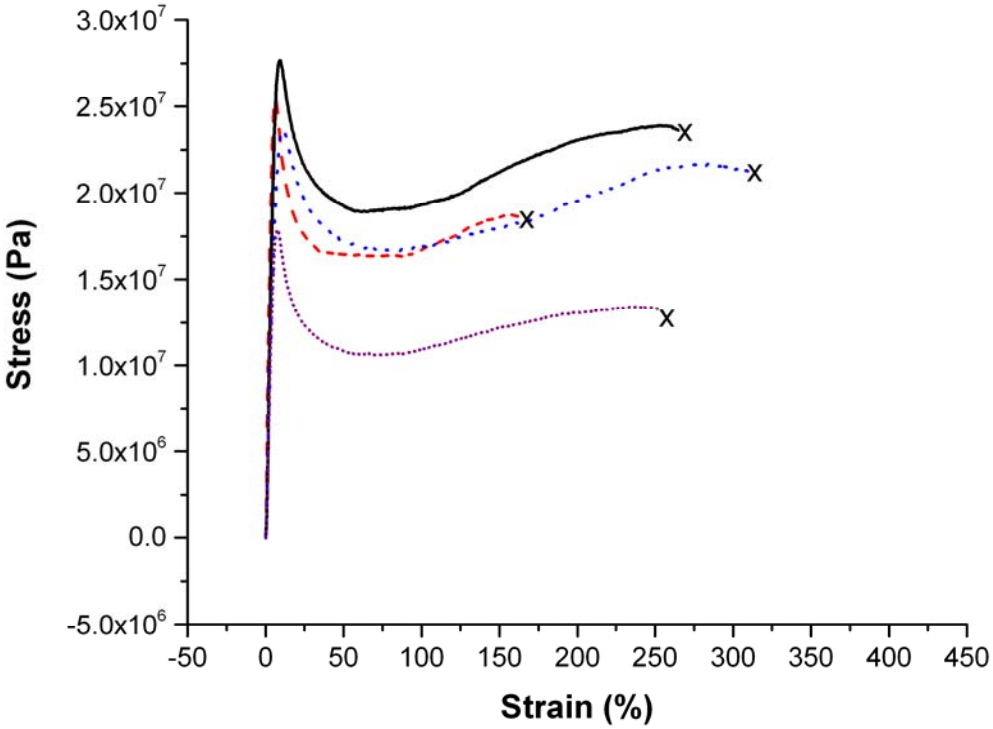



**Figure S77.** Stress vs. strain curve of a PTMC-*b*-PLA-*b*-PTMC sample ($M_n$ (SEC) = 43,200; Table 1, entry 5).

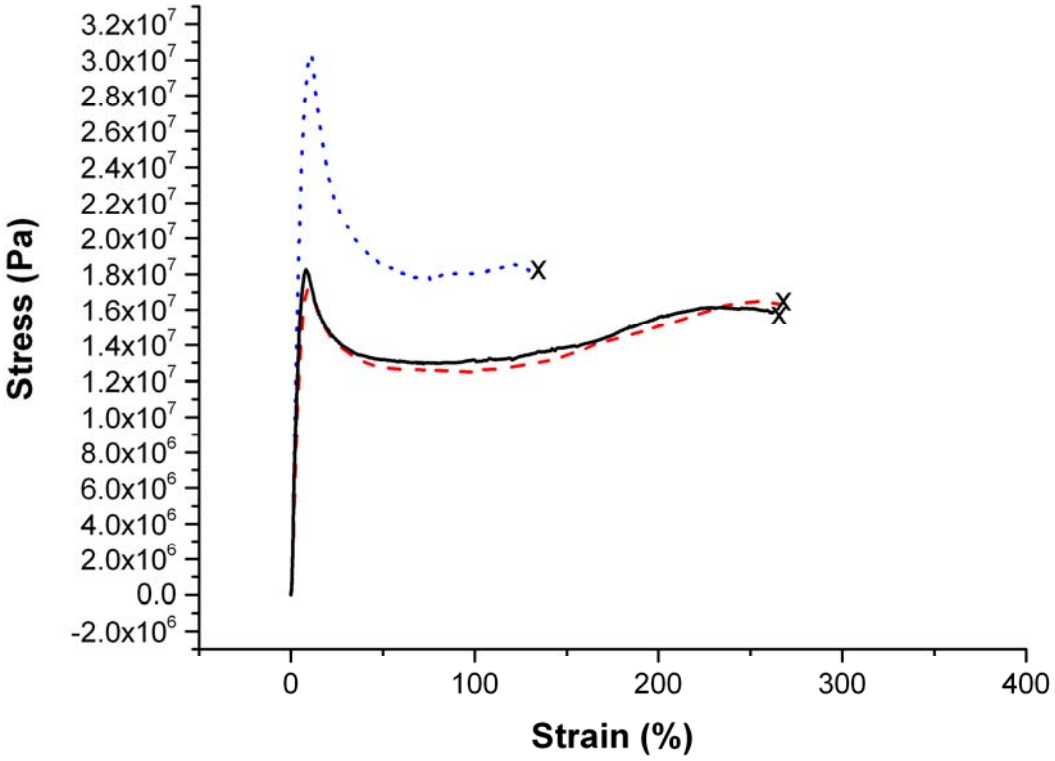



**Figure S78.** Stress vs. strain curve of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 55,600; Table 1, entry 6).

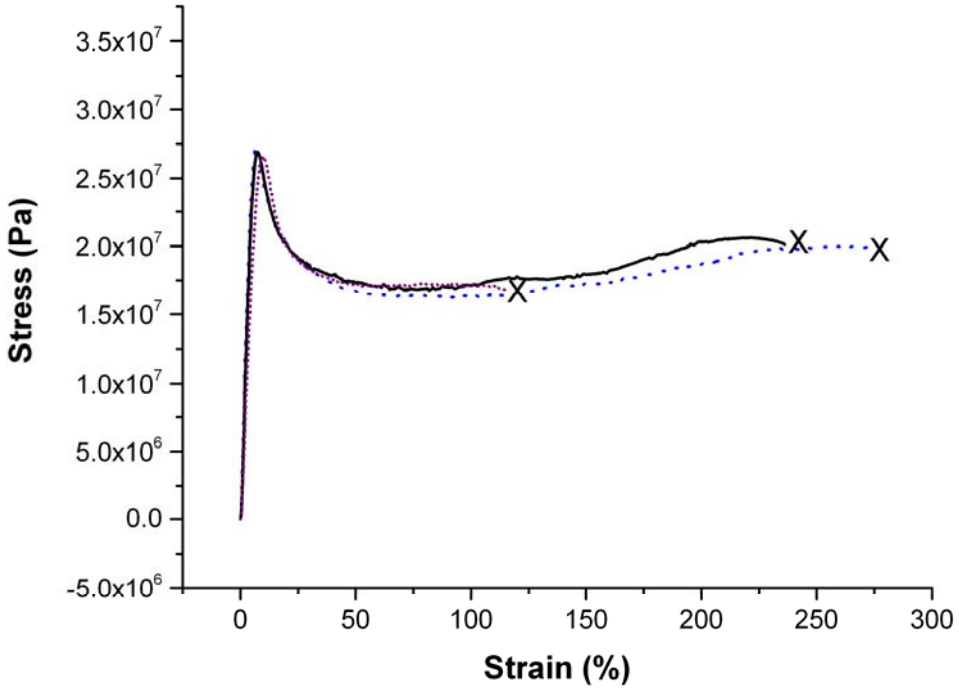



**Figure S79.** Stress vs. strain curve of a PTMC-*b*-PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 48,200; Table 1, entry 7).

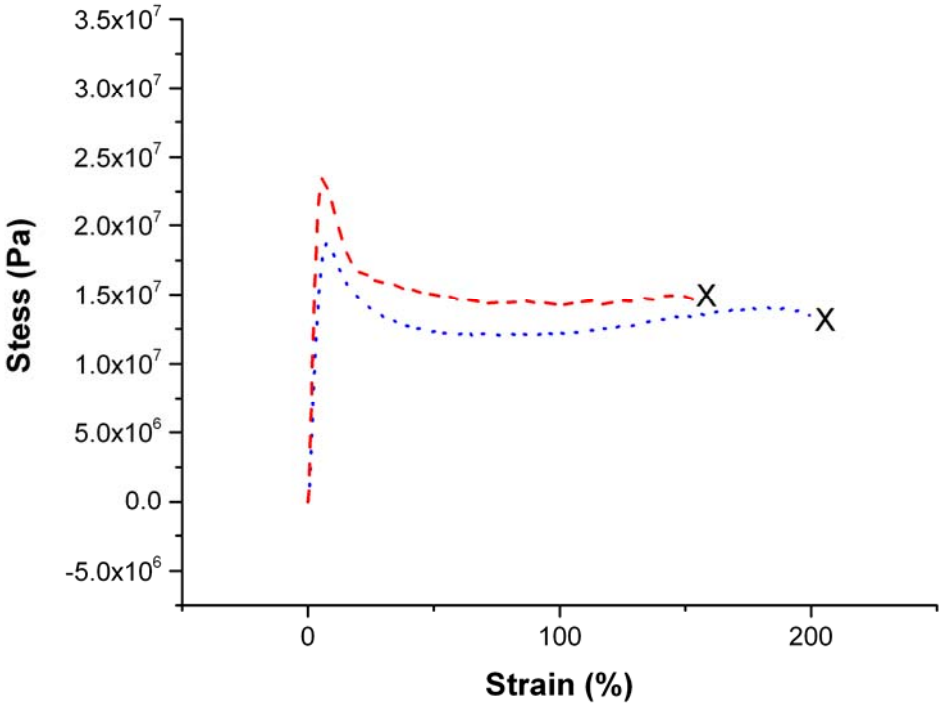



**Figure S80.** Stress vs. strain curve of a PTMC-*b*-PLA-*b*-PTMC-*b*-PLA-*b*-PTMC sample ($M_n$ (SEC) = 58,900; Table 1, entry 8).

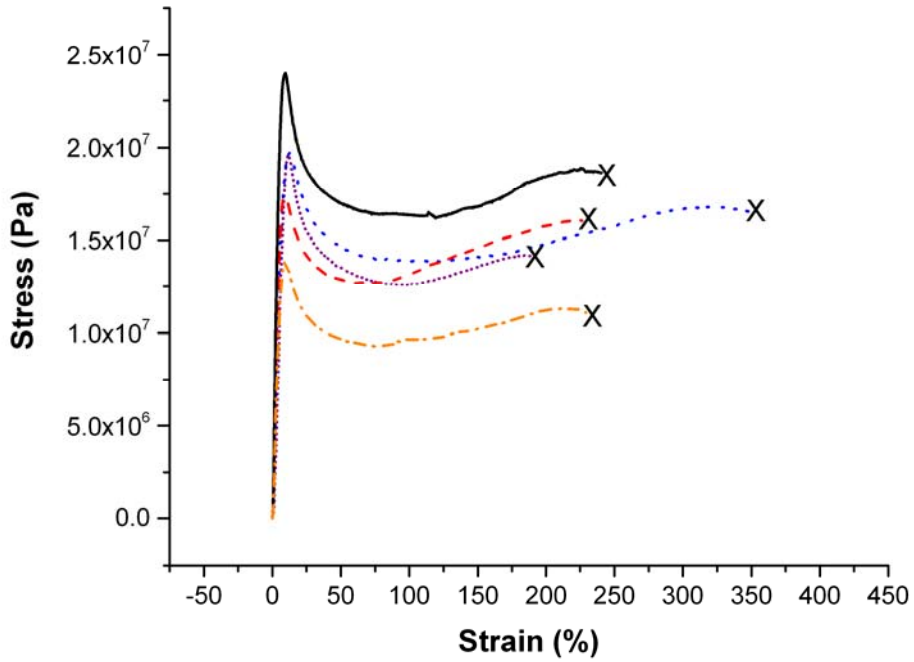



**Figure S81.** Stress vs. strain curve of a PLA-*b*-PTMC-*b*-PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 53,200; Table 1, entry 9).

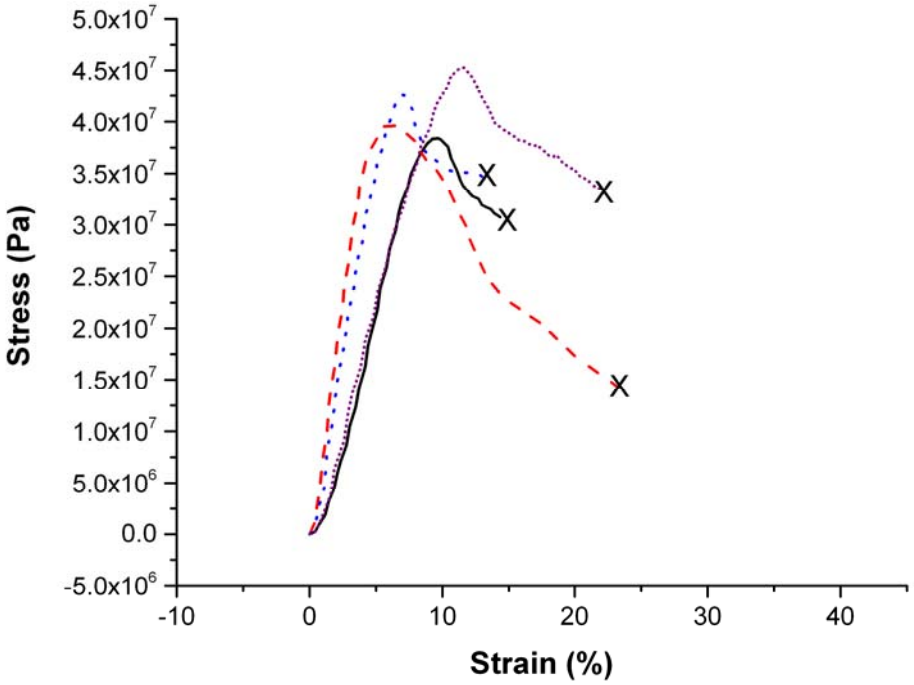



**Figure S82.** Stress vs. strain curve of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 50,800; Table 1, entry 10).

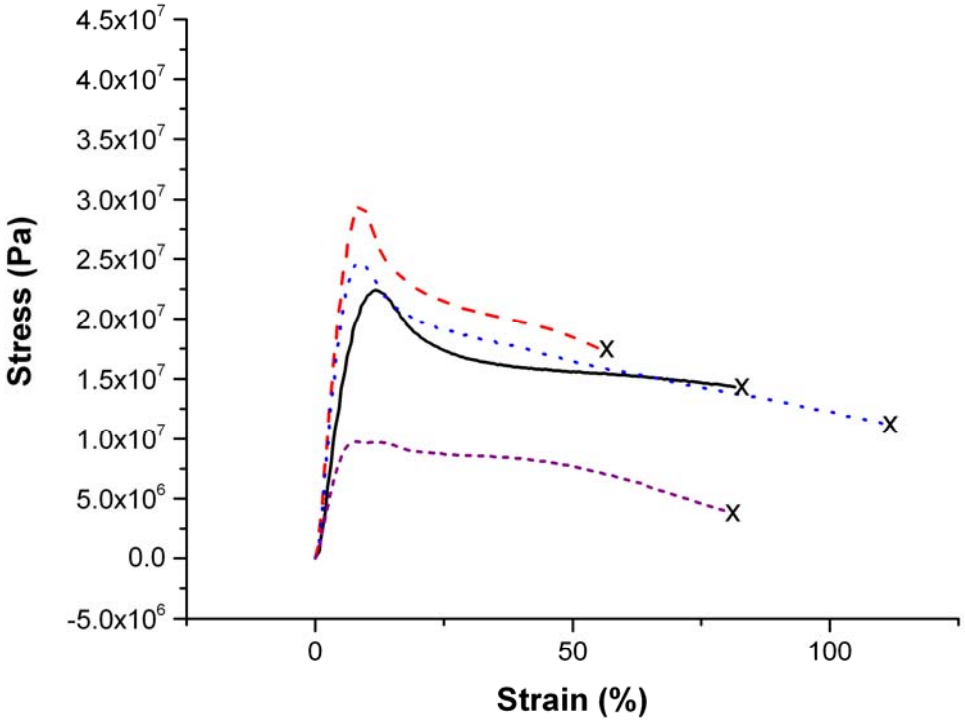



**Figure S83.** Stress vs. strain curve of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 48,900; Table 1, entry 11).

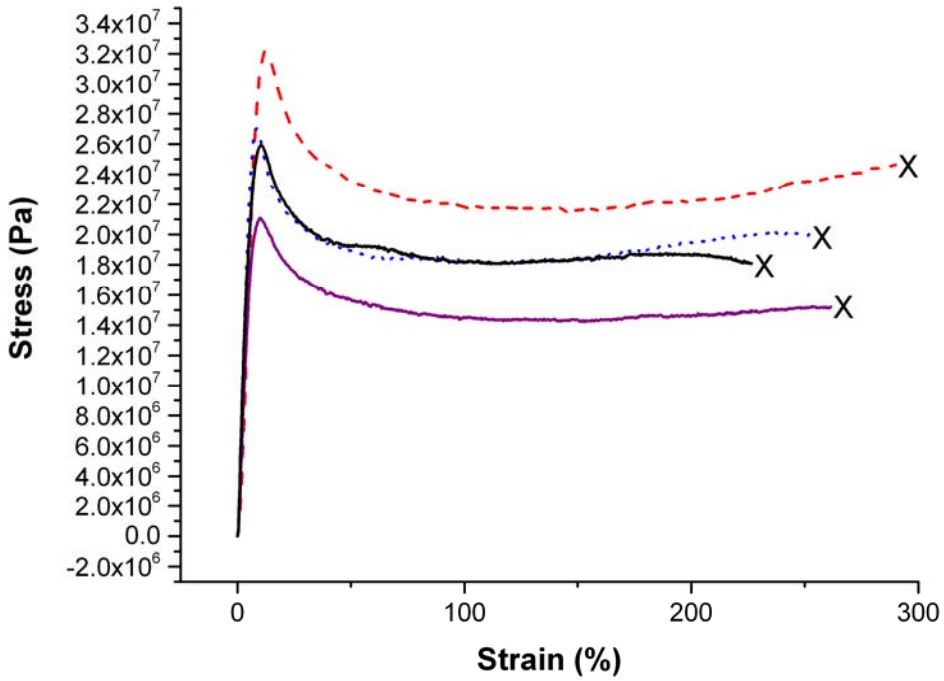



**Figure S84.** Stress vs. strain curve of a PLA-*b*-PTMC-*b*-PLA sample ($M_n$ (SEC) = 51,200; Table 1, entry 12).

## X-ray Crystallographic Data

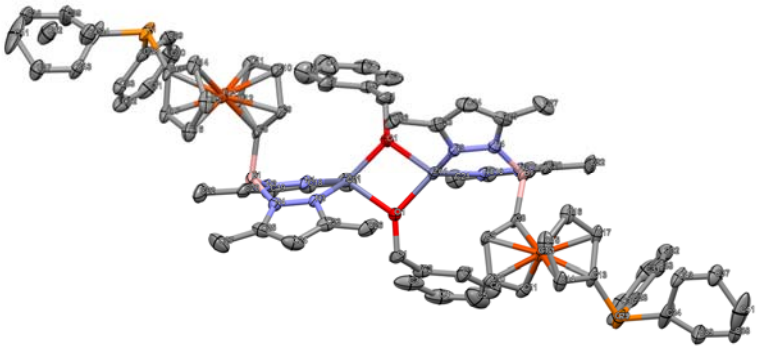


**Figure S85.** Molecular structure drawing of $[(fc^{P,B})Zn(\mu\text{-}OCH_2Ph)]_2$ with thermal ellipsoids at 50% probability; hydrogen atoms are omitted for clarity. Selected distances (Å) and angles (°): N(1)-Zn(1), 1.970(4); N(3)-Zn(1), 2.019(4); O(1)-Zn(1), 1.946(3), 1.981(4); N(1)-Zn(1)-N(3), 99.44(17); O(1)-Zn(1)-O(1) 80.26(16); N(3)-Zn(1)-O(1), 104.43(16), 131.00(17); N(1)-Zn(1)-O(1), 118.28(17), 124.18(16).

Crystal data for $C_{78}H_{78}B_2Fe_2N_8O_2P_2Zn_2$; $M_r$ = 1485.48; Monoclinic; space group P2/c; *a* = 13.855(4) Å; *b* = 9.378(2) Å; *c* = 30.742(8) Å; α = 90°; β = 101.648(3)°; γ = 90°; V = 3912.1(17) $Å^3$; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 1.058 $mm^{-1}$; $d_{calc}$ = 1.261g·$cm^{-3}$; 39551 reflections collected; 9416 unique ($R_{int}$ = 0.0667); giving $R_1$ = 0.0797, $wR_2$ = 0.2105 for 7205 data with [I>2σ(I)] and $R_1$ = 0.0983, $wR_2$ = 0.2187 for all 9416 data. Residual electron density ($e^-$·$Å^{-3}$) max/min: 1.873/-1.188.

## DFT Calculations

The full reference for the GAUSSIAN 09[2] program package can be found at the end of the document.

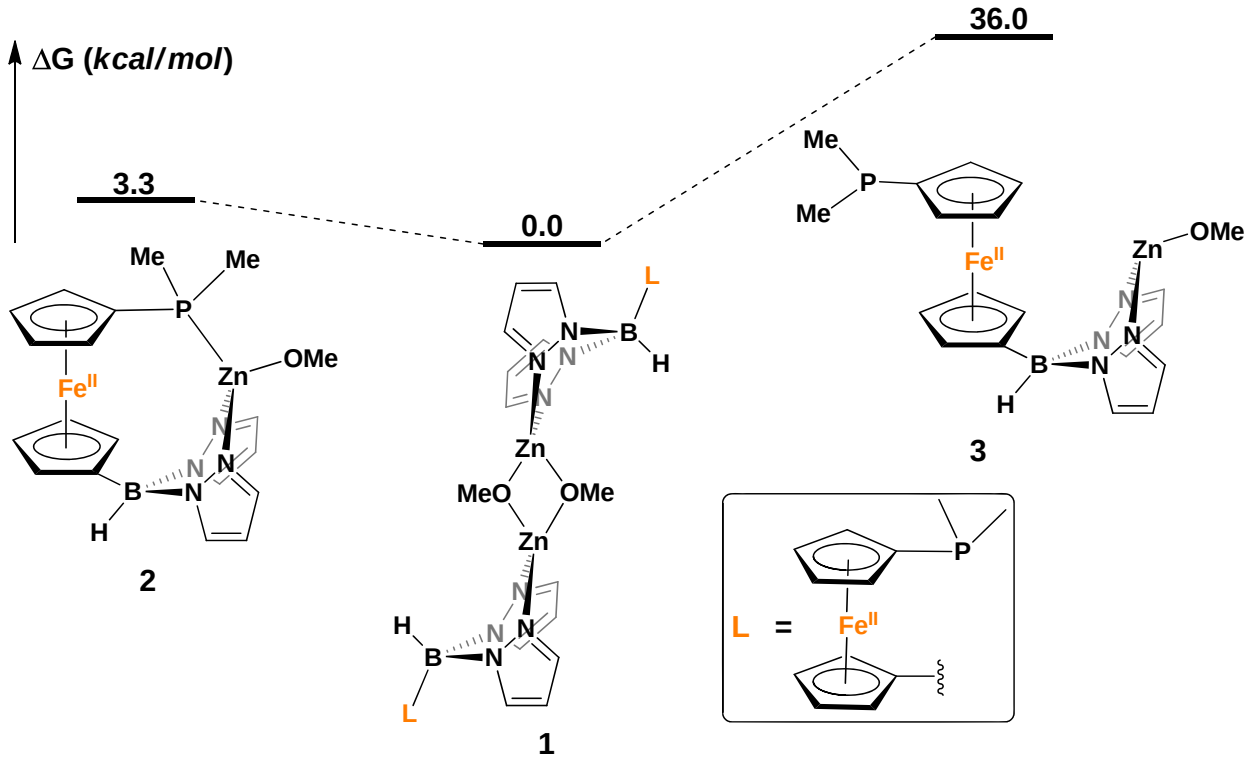



**Figure S86.** Comparison between the energies of the dimeric zinc complex and two monomeric forms.

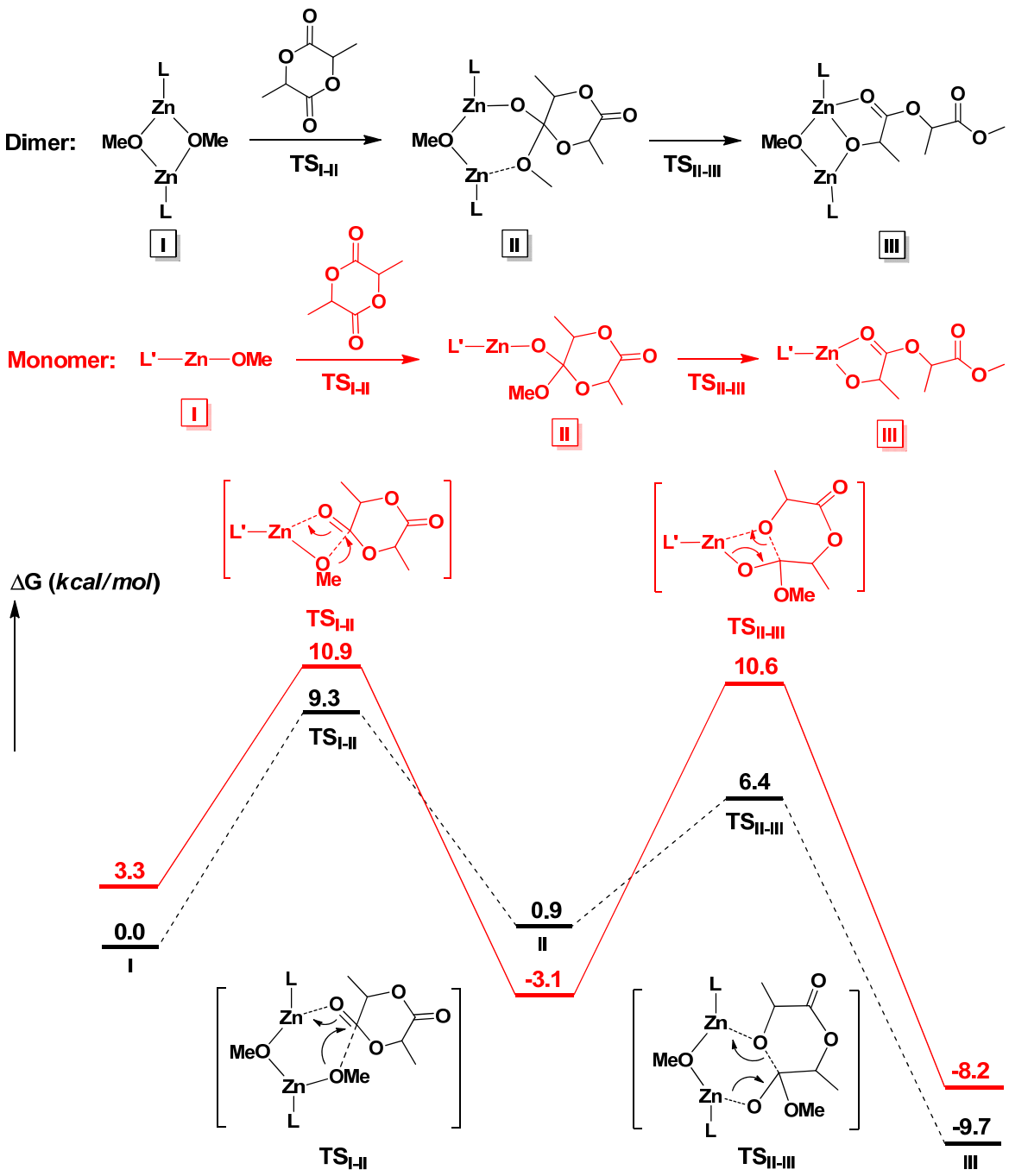



**Figure S87.** Comparison of the initiation steps of LA polymerization catalyzed by a monomeric (red) or dimeric (black) form of the zinc complex.

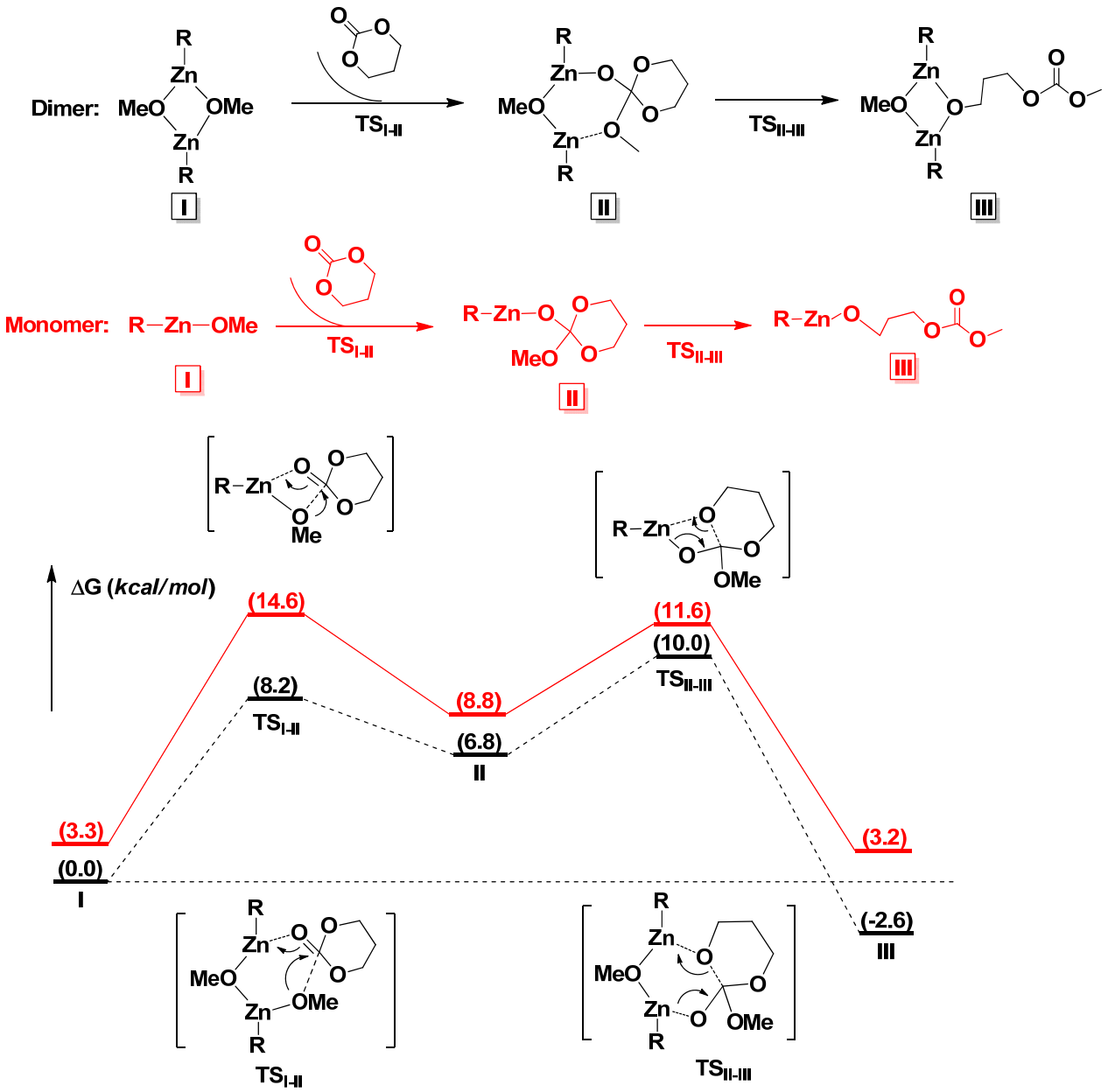


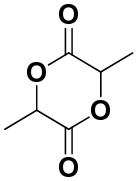

**Figure S88.** Comparison of the initiation steps of TMC polymerization catalyzed by a monomeric (red) or dimeric (black) form of the zinc complex.

**Table S3**. Energies, enthalpies, and free energies of the structures calculated at the PBE1PBE/SDD, 6-311+G(d,p) (PCM, GD3, benzene)//B3LYP/LANL2DZ, 6-31G(d) level.

| Structures | correction of H | correction of G | G | E with corrections | new G with corrections |
|---|---|---|---|---|---|
| **lactide** | 0.151554 | 0.105907 | -534.250539 | -533.935059 | -533.829152 |
| **trimethylene carbonate** | 0.111273 | 0.074079 | -381.634182 | -381.4101659 | -381.3360869 |
| **1** | 0.875728 | 0.70951 | -3175.387086 | -3497.86323 | -3497.15372 |
| **2** | 0.436398 | 0.345477 | -1587.679245 | -1748.919683 | -1748.574206 |
| **3** | 0.436644 | 0.344288 | -1587.660442 | -1748.892456 | -1748.548168 |
| **TSI-II$^{monomer}$-LA** | 0.589366 | 0.478011 | -2121.90727 | -2282.86919 | -2282.391179 |
| **II$^{monomer}$-LA** | 0.591557 | 0.481052 | -2121.921651 | -2282.894573 | -2282.413521 |
| **TSII-III$^{monomer}$-LA** | 0.58906 | 0.479528 | -2121.905148 | -2282.871218 | -2282.39169 |
| **III$^{monomer}$-LA** | 0.591123 | 0.476715 | -2121.941604 | -2282.898472 | -2282.421757 |
| **TSI-II$^{dimer}$-LA** | 1.028291 | 0.842812 | -3709.600812 | -4031.810914 | -4030.968102 |
| **II$^{dimer}$-LA** | 1.030228 | 0.846358 | -3709.610079 | -4031.827784 | -4030.981426 |
| **TSII-III$^{dimer}$-LA** | 1.029558 | 0.838501 | -3709.602191 | -4031.811084 | -4030.972583 |
| **III$^{dimer}$-LA** | 1.030265 | 0.841752 | -3709.641343 | -4031.840047 | -4030.998295 |
| **TSI-II$^{monomer}$-TMC** | 0.548666 | 0.446324 | -1969.292661 | -2130.338613 | -2129.892289 |
| **II$^{monomer}$-TMC** | 0.550803 | 0.447984 | -1969.298916 | -2130.349591 | -2129.901607 |
| **TSII-III$^{monomer}$-TMC** | 0.549183 | 0.448359 | -1969.298147 | -2130.34546 | -2129.897101 |
| **III$^{monomer}$-TMC** | 0.550702 | 0.445793 | -1969.306127 | -2130.356265 | -2129.910472 |
| **TSI-II$^{dimer}$-TMC** | 0.988222 | 0.811889 | -3556.991913 | -3879.288584 | -3878.476695 |
| **II$^{dimer}$-TMC** | 0.989541 | 0.813922 | -3556.994991 | -3879.292875 | -3878.478953 |
| **TSII-III$^{dimer}$-TMC** | 0.988158 | 0.811071 | -3556.991928 | -3879.28486 | -3878.473789 |
| **III$^{dimer}$-TMC** | 0.989914 | 0.804174 | -3557.015624 | -3879.298082 | -3878.493908 |
| **Cat$^{monomer}$-propagation** | 0.514005 | 0.413133 | -1854.818974 | -2015.915846 | -2015.502713 |
| **TSI-II$^{monomer}$-propagation-LA** | 0.666528 | 0.54449 | -2389.028178 | -2549.84817 | -2549.30368 |
| **II$^{monomer}$-propagation-LA** | 0.668844 | 0.546174 | -2389.049481 | -2549.88321 | -2549.337036 |
| **TSII-III$^{monomer}$-propagation-LA** | 0.666657 | 0.545564 | -2389.031229 | -2549.876085 | -2549.330521 |
| **III$^{monomer}$-propagation-LA** | 0.667879 | 0.537682 | -2389.06437 | -2549.876085 | -2549.338403 |

| | | | | | |
|---|---|---|---|---|---|
| **TSI-II$^{monomer}$-propagation-TMC** | 0.625781 | 0.511976 | -2236.41156 | -2397.314263 | -2396.802287 |
| **II$^{monomer}$-propagation-TMC** | 0.628223 | 0.51387 | -2236.433189 | -2397.347309 | -2396.833439 |
| **TSII-III$^{monomer}$-propagation-TMC** | 0.626479 | 0.512416 | -2236.420035 | -2397.330991 | -2396.818575 |
| **III$^{monomer}$-propagation-TMC** | 0.62831 | 0.511968 | -2236.4261 | -2397.341203 | -2396.829235 |
| **Cat$^{dimer}$-propagation** | 0.923049 | 0.750067 | -3403.230614 | -3725.575668 | -3724.825601 |
| **TSI-II$^{dimer}$-propagation-LA** | 1.076096 | 0.88247 | -3937.437068 | -4259.51908 | -4258.63661 |
| **II$^{dimer}$-propagation-LA** | 1.077715 | 0.885663 | -3937.440182 | -4259.526353 | -4258.64069 |
| **TSII-III$^{dimer}$-propagation-LA** | 1.075994 | 0.882083 | -3937.428402 | -4259.513895 | -4258.631812 |
| **III$^{dimer}$-propagation-LA** | 1.077382 | 0.883962 | -3937.432711 | -4259.521379 | -4258.637417 |
| **IV$^{dimer}$-propagation-LA** | 1.077412 | 0.87887 | -3937.459297 | -4259.52969 | -4258.65082 |
| **TSI-II$^{dimer}$-propagation-TMC** | 1.035662 | 0.849595 | -3784.822131 | -4106.984541 | -4106.134946 |
| **II$^{dimer}$-propagation-TMC** | 1.037218 | 0.850853 | -3784.826982 | -4106.991026 | -4106.140173 |
| **TSII-III$^{dimer}$-propagation-TMC** | 1.035811 | 0.848165 | -3784.826779 | -4106.991833 | -4106.143668 |
| **III$^{dimer}$-propagation-TMC** | 1.036798 | 0.847828 | -3784.829799 | -4106.99265 | -4106.144822 |
| **IV$^{dimer}$-propagation-TMC** | 1.037851 | 0.844254 | -3784.843767 | -4106.998055 | -4106.153801 |

**Cartesian coordinates for optimized structures**




**lactide**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | -0.251339 | -1.378080 | -0.499932 |
| 2 | 6 | 0 | -1.320763 | -0.564515 | -0.401020 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | -1.082296 | 0.923033 | -0.165678 |
| 4 | 8 | 0 | 0.251335 | 1.378074 | -0.499947 |
| 5 | 6 | 0 | 1.320759 | 0.564510 | -0.401039 |
| 6 | 6 | 0 | 1.082295 | -0.923036 | -0.165680 |
| 7 | 8 | 0 | -2.440962 | -1.003075 | -0.511489 |
| 8 | 6 | 0 | -1.448013 | 1.348328 | 1.258052 |
| 9 | 8 | 0 | 2.440958 | 1.003075 | -0.511486 |
| 10 | 6 | 0 | 1.448023 | -1.348318 | 1.258050 |
| 11 | 1 | 0 | 1.727506 | -1.445788 | -0.875621 |
| 12 | 1 | 0 | 1.312576 | -2.429144 | 1.358689 |
| 13 | 1 | 0 | 2.494593 | -1.098641 | 1.456161 |
| 14 | 1 | 0 | 0.821493 | -0.848560 | 2.004123 |
| 15 | 1 | 0 | -2.494581 | 1.098654 | 1.456174 |
| 16 | 1 | 0 | -0.821477 | 0.848576 | 2.004124 |
| 17 | 1 | 0 | -1.312563 | 2.429154 | 1.358681 |
| 18 | 1 | 0 | -1.727512 | 1.445780 | -0.875618 |

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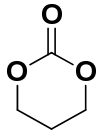

**trimethylene carbonate**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.681521 | 0.000052 | -0.395248 |
| 2 | 6 | 0 | -1.012713 | -1.221142 | 0.206605 |
| 3 | 8 | 0 | 0.415311 | -1.167911 | 0.027101 |
| 4 | 6 | 0 | 1.103441 | -0.000006 | -0.010043 |
| 5 | 8 | 0 | 0.415323 | 1.167920 | 0.026896 |
| 6 | 6 | 0 | -1.012638 | 1.221111 | 0.206784 |
| 7 | 8 | 0 | 2.299282 | -0.000024 | -0.106276 |
| 8 | 1 | 0 | -1.224172 | -1.294153 | 1.281504 |
| 9 | 1 | 0 | -1.327389 | -2.152966 | -0.269310 |
| 10 | 1 | 0 | -2.754012 | 0.000070 | -0.170748 |
| 11 | 1 | 0 | -1.561868 | 0.000156 | -1.484744 |
| 12 | 1 | 0 | -1.223874 | 1.293853 | 1.281752 |
| 13 | 1 | 0 | -1.327419 | 2.153062 | -0.268807 |

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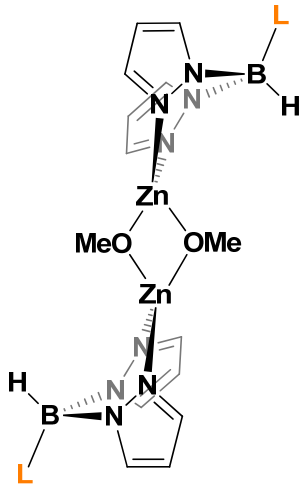


**1**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.106275 | -0.513037 | 0.699931 |
| 2 | 6 | 0 | -8.177410 | -0.416148 | -0.731992 |
| 3 | 6 | 0 | -8.487520 | 0.953686 | -1.038573 |
| 4 | 6 | 0 | -8.608985 | 1.677603 | 0.184229 |
| 5 | 6 | 0 | -8.378305 | 0.768158 | 1.260640 |
| 6 | 26 | 0 | -6.704047 | 0.854177 | 0.025945 |
| 7 | 6 | 0 | -5.082480 | 1.414357 | 1.199610 |
| 8 | 6 | 0 | -4.768410 | 0.168174 | 0.557627 |
| 9 | 6 | 0 | -4.863273 | 0.424837 | -0.853241 |
| 10 | 6 | 0 | -5.217636 | 1.792586 | -1.070879 |
| 11 | 6 | 0 | -5.352440 | 2.409650 | 0.210073 |
| 12 | 5 | 0 | -4.435514 | -1.242652 | 1.263082 |
| 13 | 7 | 0 | -3.581368 | -1.021757 | 2.567421 |
| 14 | 7 | 0 | -2.347024 | -0.447460 | 2.555770 |
| 15 | 6 | 0 | -1.947762 | -0.335524 | 3.833828 |
| 16 | 6 | 0 | -2.933399 | -0.826884 | 4.693800 |
| 17 | 6 | 0 | -3.948594 | -1.252909 | 3.841950 |
| 18 | 30 | 0 | -1.319383 | -0.322474 | 0.751435 |
| 19 | 8 | 0 | 0.653754 | -0.694750 | 0.820235 |
| 20 | 6 | 0 | 1.335878 | -1.715803 | 1.520349 |
| 21 | 15 | 0 | -7.921542 | -1.851451 | -1.841289 |
| 22 | 6 | 0 | -7.506812 | -1.009194 | -3.454119 |
| 23 | 30 | 0 | 1.267842 | 1.029411 | 0.061856 |
| 24 | 8 | 0 | -0.705452 | 1.372374 | -0.071522 |
| 25 | 6 | 0 | -1.386364 | 2.551916 | -0.448086 |
| 26 | 7 | 0 | 2.142062 | 1.398832 | -1.787589 |
| 27 | 7 | 0 | 3.384576 | 1.951384 | -1.852667 |

| | | | | | |
|---|---|---|---|---|---|
| 28 | 6 | 0 | 3.620943 | 2.358857 | -3.114032 |
| 29 | 6 | 0 | 2.509259 | 2.072025 | -3.901151 |
| 30 | 6 | 0 | 1.605430 | 1.476366 | -3.016735 |
| 31 | 5 | 0 | 4.347338 | 1.995255 | -0.614350 |
| 32 | 7 | 0 | 3.630472 | 2.788551 | 0.546946 |
| 33 | 7 | 0 | 2.450456 | 2.390468 | 1.097161 |
| 34 | 6 | 0 | 2.180923 | 3.230669 | 2.111157 |
| 35 | 6 | 0 | 3.197927 | 4.180036 | 2.236894 |
| 36 | 6 | 0 | 4.093068 | 3.858161 | 1.220469 |
| 37 | 6 | 0 | 4.724450 | 0.509935 | -0.121874 |
| 38 | 6 | 0 | 5.484448 | 0.183908 | 1.052678 |
| 39 | 6 | 0 | 5.613699 | -1.233745 | 1.162435 |
| 40 | 6 | 0 | 4.951534 | -1.817024 | 0.040546 |
| 41 | 6 | 0 | 4.408123 | -0.749407 | -0.740817 |
| 42 | 26 | 0 | 6.473860 | -0.573957 | -0.620766 |
| 43 | 6 | 0 | 8.327336 | 0.350978 | -0.832485 |
| 44 | 6 | 0 | 7.513072 | 0.598450 | -1.977130 |
| 45 | 6 | 0 | 7.189070 | -0.659769 | -2.565288 |
| 46 | 6 | 0 | 7.805878 | -1.680418 | -1.781326 |
| 47 | 6 | 0 | 8.525593 | -1.065652 | -0.701600 |
| 48 | 15 | 0 | 9.720843 | -1.892562 | 0.415605 |
| 49 | 6 | 0 | 9.434915 | -0.975019 | 2.014892 |
| 50 | 6 | 0 | 8.833711 | -3.489450 | 0.793031 |
| 51 | 7 | 0 | -2.389391 | -1.834567 | -0.178840 |
| 52 | 7 | 0 | -3.630751 | -2.161582 | 0.276381 |
| 53 | 6 | 0 | -4.044278 | -3.287662 | -0.334797 |
| 54 | 6 | 0 | -3.049609 | -3.721577 | -1.207214 |
| 55 | 6 | 0 | -2.029354 | -2.777503 | -1.065889 |
| 56 | 6 | 0 | -9.703327 | -2.300827 | -2.206233 |
| 57 | 1 | 0 | -2.913841 | -0.872067 | 5.772444 |
| 58 | 1 | 0 | -5.134706 | 1.569115 | 2.270589 |
| 59 | 1 | 0 | -5.643052 | 3.435576 | 0.397864 |
| 60 | 1 | 0 | -8.363953 | 1.018752 | 2.313407 |
| 61 | 1 | 0 | -7.840281 | -1.405805 | 1.250930 |
| 62 | 1 | 0 | -8.581376 | 1.376906 | -2.029857 |
| 63 | 1 | 0 | -8.799711 | 2.739179 | 0.277583 |
| 64 | 1 | 0 | -5.385708 | 2.267359 | -2.029317 |
| 65 | 1 | 0 | -4.713383 | -0.316173 | -1.628628 |
| 66 | 1 | 0 | -3.067211 | -4.592247 | -1.845500 |
| 67 | 1 | 0 | -5.399022 | -1.880367 | 1.610355 |
| 68 | 1 | 0 | -9.730451 | -3.095781 | -2.960535 |
| 69 | 1 | 0 | -10.173767 | -2.685535 | -1.295455 |
| 70 | 1 | 0 | -10.287175 | -1.446432 | -2.568436 |
| 71 | 1 | 0 | -7.444169 | -1.769219 | -4.240662 |
| 72 | 1 | 0 | -8.252340 | -0.263273 | -3.753683 |
| 73 | 1 | 0 | -6.531287 | -0.520695 | -3.374058 |

| | | | | | |
|---|---|---|---|---|---|
| 74 | 1 | 0 | -1.059770 | -2.727474 | -1.543672 |
| 75 | 1 | 0 | -5.023015 | -3.691528 | -0.121039 |
| 76 | 1 | 0 | -0.976793 | 0.083186 | 4.063650 |
| 77 | 1 | 0 | -4.907669 | -1.702313 | 4.054554 |
| 78 | 1 | 0 | -1.397321 | 3.291456 | 0.367709 |
| 79 | 1 | 0 | -0.898726 | 3.018961 | -1.316922 |
| 80 | 1 | 0 | -2.426450 | 2.335271 | -0.719133 |
| 81 | 1 | 0 | 2.384201 | -1.772729 | 1.204378 |
| 82 | 1 | 0 | 1.317524 | -1.544883 | 2.608430 |
| 83 | 1 | 0 | 0.871336 | -2.694297 | 1.327642 |
| 84 | 1 | 0 | 1.272709 | 3.111891 | 2.687401 |
| 85 | 1 | 0 | 3.273787 | 4.983425 | 2.954304 |
| 86 | 1 | 0 | 5.028963 | 4.314189 | 0.931984 |
| 87 | 1 | 0 | 0.602769 | 1.109194 | -3.190913 |
| 88 | 1 | 0 | 2.376913 | 2.272162 | -4.953937 |
| 89 | 1 | 0 | 4.562658 | 2.825037 | -3.364909 |
| 90 | 1 | 0 | 5.292021 | 2.677740 | -0.931800 |
| 91 | 1 | 0 | 5.906622 | 0.905245 | 1.741983 |
| 92 | 1 | 0 | 6.133756 | -1.769653 | 1.945602 |
| 93 | 1 | 0 | 4.894998 | -2.872712 | -0.192547 |
| 94 | 1 | 0 | 3.875972 | -0.870139 | -1.675903 |
| 95 | 1 | 0 | 7.727919 | -2.744636 | -1.962216 |
| 96 | 1 | 0 | 7.153488 | 1.566336 | -2.299321 |
| 97 | 1 | 0 | 6.551721 | -0.817745 | -3.425639 |
| 98 | 1 | 0 | 8.716516 | 1.107835 | -0.163858 |
| 99 | 1 | 0 | 9.385094 | -4.020724 | 1.576726 |
| 100 | 1 | 0 | 7.801240 | -3.328871 | 1.119236 |
| 101 | 1 | 0 | 8.828913 | -4.128363 | -0.096075 |
| 102 | 1 | 0 | 10.008554 | -1.466237 | 2.808763 |
| 103 | 1 | 0 | 9.810321 | 0.049411 | 1.923762 |
| 104 | 1 | 0 | 8.377870 | -0.939862 | 2.297110 |

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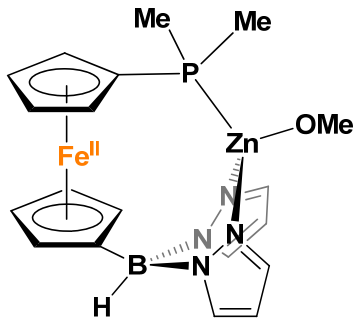


**2**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.827229 | -1.274958 | -1.833238 |
| 2 | 6 | 0 | 1.418888 | -1.250191 | -1.597444 |
| 3 | 6 | 0 | 1.121767 | -1.876085 | -0.340243 |
| 4 | 6 | 0 | 2.394767 | -2.261055 | 0.201480 |
| 5 | 6 | 0 | 3.436857 | -1.910144 | -0.710477 |
| 6 | 26 | 0 | 2.446190 | -0.206244 | -0.099199 |
| 7 | 6 | 0 | 3.027092 | 1.767541 | -0.395520 |
| 8 | 6 | 0 | 1.704067 | 1.706773 | 0.163534 |
| 9 | 6 | 0 | 1.805808 | 1.031935 | 1.431733 |
| 10 | 6 | 0 | 3.170019 | 0.690196 | 1.644059 |
| 11 | 6 | 0 | 3.921934 | 1.137148 | 0.516256 |
| 12 | 15 | 0 | 0.132646 | 2.258759 | -0.533615 |
| 13 | 6 | 0 | -0.138152 | 3.973569 | 0.107956 |
| 14 | 5 | 0 | -0.322757 | -2.341558 | 0.220645 |
| 15 | 7 | 0 | -0.782039 | -1.692158 | 1.576467 |
| 16 | 7 | 0 | -1.290874 | -0.436578 | 1.702284 |
| 17 | 6 | 0 | -1.539208 | -0.237798 | 3.008496 |
| 18 | 6 | 0 | -1.176998 | -1.366285 | 3.749525 |
| 19 | 6 | 0 | -0.709138 | -2.263674 | 2.795081 |
| 20 | 30 | 0 | -1.826235 | 0.742897 | 0.034561 |
| 21 | 8 | 0 | -3.193589 | 2.047055 | 0.066220 |
| 22 | 6 | 0 | -4.540956 | 1.818891 | 0.354689 |
| 23 | 7 | 0 | -1.962660 | -0.940686 | -1.219998 |
| 24 | 7 | 0 | -1.448660 | -2.148095 | -0.853022 |
| 25 | 6 | 0 | -1.977254 | -3.109820 | -1.635558 |
| 26 | 6 | 0 | -2.864888 | -2.529408 | -2.535140 |
| 27 | 6 | 0 | -2.824313 | -1.166880 | -2.226428 |
| 28 | 6 | 0 | 0.467555 | 2.545286 | -2.326893 |
| 29 | 1 | 0 | -1.972536 | 0.697342 | 3.338852 |
| 30 | 1 | 0 | -3.456745 | -3.023903 | -3.290854 |
| 31 | 1 | 0 | -3.372858 | -0.341778 | -2.661568 |
| 32 | 1 | 0 | -1.682416 | -4.139949 | -1.499073 |
| 33 | 1 | 0 | 2.542436 | -2.743657 | 1.160278 |
| 34 | 1 | 0 | 4.498564 | -2.058649 | -0.558428 |
| 35 | 1 | 0 | 3.560204 | 0.141478 | 2.491064 |
| 36 | 1 | 0 | 0.977708 | 0.787336 | 2.081219 |
| 37 | 1 | 0 | 3.294346 | 2.182641 | -1.358130 |
| 38 | 1 | 0 | 4.982190 | 0.986814 | 0.358858 |
| 39 | 1 | 0 | 3.342028 | -0.859754 | -2.690598 |
| 40 | 1 | 0 | 0.677297 | -0.836300 | -2.269399 |
| 41 | 1 | 0 | -1.257736 | -1.517905 | 4.815592 |
| 42 | 1 | 0 | -5.018825 | 1.078321 | -0.317278 |

| | | | | | |
|---|---|---|---|---|---|
| 43 | 1 | 0 | -4.714430 | 1.463047 | 1.389782 |
| 44 | 1 | 0 | -0.288859 | -3.531367 | 0.442109 |
| 45 | 1 | 0 | -5.121431 | 2.751394 | 0.247560 |
| 46 | 1 | 0 | -0.338183 | -3.272999 | 2.897683 |
| 47 | 1 | 0 | 0.642004 | 4.664469 | -0.229151 |
| 48 | 1 | 0 | -1.120907 | 4.318480 | -0.227377 |
| 49 | 1 | 0 | -0.144608 | 3.950007 | 1.201703 |
| 50 | 1 | 0 | 1.286506 | 3.256783 | -2.476792 |
| 51 | 1 | 0 | 0.721439 | 1.598478 | -2.810176 |
| 52 | 1 | 0 | -0.437112 | 2.947420 | -2.793605 |

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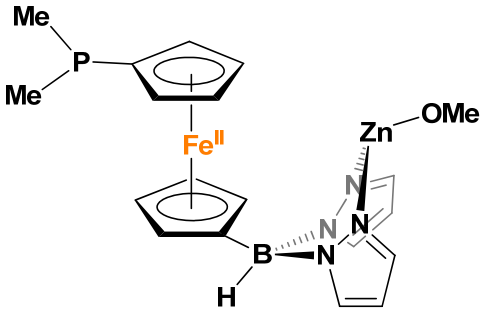


**3**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.208043 | 1.246388 | -1.476769 |
| 2 | 7 | 0 | -1.138347 | 2.119977 | -0.437135 |
| 3 | 6 | 0 | -0.848073 | 3.345818 | -0.909783 |
| 4 | 6 | 0 | -0.722276 | 3.280255 | -2.294877 |
| 5 | 6 | 0 | -0.964154 | 1.938711 | -2.602379 |
| 6 | 5 | 0 | -1.395077 | 1.664359 | 1.044100 |
| 7 | 7 | 0 | -2.839783 | 1.057191 | 1.119183 |
| 8 | 7 | 0 | -3.163167 | -0.075802 | 0.436433 |
| 9 | 6 | 0 | -4.434387 | -0.381858 | 0.747589 |
| 10 | 6 | 0 | -4.944880 | 0.554064 | 1.650841 |
| 11 | 6 | 0 | -3.895831 | 1.446789 | 1.855454 |
| 12 | 30 | 0 | -1.783937 | -0.666259 | -0.996676 |
| 13 | 8 | 0 | -1.915490 | -2.123587 | -2.151113 |
| 14 | 6 | 0 | -2.498201 | -3.363843 | -1.857214 |
| 15 | 6 | 0 | -0.318138 | 0.597739 | 1.607725 |
| 16 | 6 | 0 | 1.002549 | 0.933673 | 2.052784 |
| 17 | 6 | 0 | 1.564515 | -0.166131 | 2.769376 |
| 18 | 6 | 0 | 0.612292 | -1.226971 | 2.749693 |
| 19 | 6 | 0 | -0.529997 | -0.762671 | 2.034451 |

| | | | | | |
|---|---|---|---|---|---|
| 20 | 26 | 0 | 1.206011 | -0.740328 | 0.822281 |
| 21 | 6 | 0 | 1.097956 | -1.829247 | -0.996792 |
| 22 | 6 | 0 | 1.915135 | -2.504734 | -0.041820 |
| 23 | 6 | 0 | 2.995043 | -1.642423 | 0.306968 |
| 24 | 6 | 0 | 2.855395 | -0.410849 | -0.420691 |
| 25 | 6 | 0 | 1.669807 | -0.537936 | -1.215456 |
| 26 | 15 | 0 | 3.923562 | 1.081727 | -0.454043 |
| 27 | 6 | 0 | 5.193702 | 0.522558 | -1.712366 |
| 28 | 6 | 0 | 4.944805 | 0.854032 | 1.090938 |
| 29 | 1 | 0 | 1.491786 | 1.883557 | 1.875776 |
| 30 | 1 | 0 | -3.499470 | -3.285656 | -1.392782 |
| 31 | 1 | 0 | -0.977457 | 1.437744 | -3.561324 |
| 32 | 1 | 0 | -5.930036 | 0.582005 | 2.091808 |
| 33 | 1 | 0 | -4.907390 | -1.250117 | 0.308490 |
| 34 | 1 | 0 | -3.827991 | 2.327810 | 2.476916 |
| 35 | 1 | 0 | 2.550357 | -0.205991 | 3.214250 |
| 36 | 1 | 0 | 1.276167 | 0.231365 | -1.865558 |
| 37 | 1 | 0 | 1.732819 | -3.491312 | 0.364655 |
| 38 | 1 | 0 | 3.765325 | -1.864450 | 1.033750 |
| 39 | 1 | 0 | 0.742854 | -2.214146 | 3.174348 |
| 40 | 1 | 0 | -1.436822 | -1.335114 | 1.887322 |
| 41 | 1 | 0 | -0.490053 | 4.085969 | -2.974960 |
| 42 | 1 | 0 | -1.875713 | -3.978028 | -1.179266 |
| 43 | 1 | 0 | -1.405000 | 2.672155 | 1.709406 |
| 44 | 1 | 0 | -2.626655 | -3.943634 | -2.784249 |
| 45 | 1 | 0 | -0.751846 | 4.179852 | -0.230050 |
| 46 | 1 | 0 | 5.741894 | 1.605626 | 1.089759 |
| 47 | 1 | 0 | 4.326458 | 1.023573 | 1.977232 |
| 48 | 1 | 0 | 5.407119 | -0.137444 | 1.162065 |
| 49 | 1 | 0 | 5.989671 | 1.273215 | -1.777967 |
| 50 | 1 | 0 | 5.638341 | -0.447287 | -1.460627 |
| 51 | 1 | 0 | 4.721014 | 0.446874 | -2.696934 |
| 52 | 1 | 0 | 0.226146 | -2.235383 | -1.500688 |

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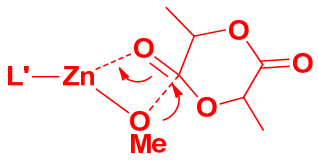


**TSI-II$^{monomer}$-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

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| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.124565 | -2.910447 | -0.442393 |
| 2 | 6 | 0 | -4.237317 | -2.829829 | 0.443867 |
| 3 | 6 | 0 | -3.838038 | -2.085691 | 1.594094 |
| 4 | 6 | 0 | -2.484895 | -1.684174 | 1.418287 |
| 5 | 6 | 0 | -2.027023 | -2.194312 | 0.151654 |
| 6 | 26 | 0 | -3.630640 | -0.923294 | -0.134036 |
| 7 | 6 | 0 | -3.213002 | 0.519402 | -1.588307 |
| 8 | 6 | 0 | -3.331082 | 1.182478 | -0.320291 |
| 9 | 6 | 0 | -4.648110 | 0.862212 | 0.153725 |
| 10 | 6 | 0 | -5.325172 | 0.047524 | -0.804265 |
| 11 | 6 | 0 | -4.426957 | -0.169766 | -1.891455 |
| 12 | 5 | 0 | -2.340618 | 2.280852 | 0.336810 |
| 13 | 7 | 0 | -1.299786 | 2.808582 | -0.700351 |
| 14 | 7 | 0 | -0.213282 | 2.102316 | -1.118147 |
| 15 | 6 | 0 | 0.405937 | 2.849099 | -2.048709 |
| 16 | 6 | 0 | -0.289415 | 4.043773 | -2.257375 |
| 17 | 6 | 0 | -1.361729 | 3.973672 | -1.375317 |
| 18 | 30 | 0 | 0.618030 | 0.443078 | -0.060979 |
| 19 | 15 | 0 | -0.377017 | -1.893158 | -0.522031 |
| 20 | 6 | 0 | 0.678279 | -3.235074 | 0.196590 |
| 21 | 8 | 0 | 2.205776 | -0.309414 | 1.396445 |
| 22 | 6 | 0 | 3.265518 | -0.270894 | 0.752455 |
| 23 | 6 | 0 | 4.201858 | 0.915083 | 0.919565 |
| 24 | 8 | 0 | 5.244787 | 0.991040 | -0.073967 |
| 25 | 6 | 0 | 5.692480 | -0.111928 | -0.691030 |
| 26 | 6 | 0 | 5.056625 | -1.464942 | -0.375450 |
| 27 | 8 | 0 | 3.798810 | -1.437510 | 0.335866 |
| 28 | 6 | 0 | 6.033251 | -2.360404 | 0.388905 |
| 29 | 8 | 0 | 6.604670 | -0.052412 | -1.481766 |
| 30 | 6 | 0 | 4.826786 | 0.923527 | 2.317747 |
| 31 | 8 | 0 | 2.385583 | 0.467405 | -1.024659 |
| 32 | 6 | 0 | 2.620860 | -0.069693 | -2.293553 |
| 33 | 7 | 0 | -0.446612 | 1.083836 | 1.669735 |
| 34 | 7 | 0 | -1.579565 | 1.837807 | 1.638823 |
| 35 | 6 | 0 | -1.966032 | 2.108816 | 2.901070 |
| 36 | 6 | 0 | -1.073218 | 1.516962 | 3.788474 |
| 37 | 6 | 0 | -0.132939 | 0.892622 | 2.963507 |
| 38 | 6 | 0 | -0.503466 | -2.391022 | -2.298777 |
| 39 | 1 | 0 | 0.753850 | 0.329257 | 3.214303 |
| 40 | 1 | 0 | -0.043700 | 4.847472 | -2.935509 |
| 41 | 1 | 0 | 1.325546 | 2.495306 | -2.491609 |
| 42 | 1 | 0 | -2.163848 | 4.670037 | -1.178718 |
| 43 | 1 | 0 | -5.063448 | 1.187265 | 1.100237 |
| 44 | 1 | 0 | -6.321234 | -0.365588 | -0.705749 |
| 45 | 1 | 0 | -4.470641 | -1.821698 | 2.431337 |
| 46 | 1 | 0 | -1.909497 | -1.073707 | 2.099963 |
| 47 | 1 | 0 | -3.123098 | -3.392462 | -1.410623 |
| 48 | 1 | 0 | -5.223427 | -3.235831 | 0.259254 |
| 49 | 1 | 0 | -4.621923 | -0.771590 | -2.770270 |
| 50 | 1 | 0 | -2.333766 | 0.547512 | -2.220084 |
| 51 | 1 | 0 | -1.093449 | 1.553005 | 4.867700 |
| 52 | 1 | 0 | 2.693918 | -1.175670 | -2.282892 |
| 53 | 1 | 0 | 1.818122 | 0.184862 | -3.007984 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 1 | 0 | -2.995972 | 3.243325 | 0.669707 |
| 55 | 1 | 0 | -2.842502 | 2.714664 | 3.079546 |
| 56 | 1 | 0 | 0.294122 | -4.227656 | -0.061332 |
| 57 | 1 | 0 | 1.705374 | -3.121787 | -0.161640 |
| 58 | 1 | 0 | 0.695482 | -3.126033 | 1.284502 |
| 59 | 1 | 0 | -0.854577 | -3.422699 | -2.406784 |
| 60 | 1 | 0 | -1.192499 | -1.722316 | -2.821666 |
| 61 | 1 | 0 | 0.484219 | -2.304813 | -2.761255 |
| 62 | 1 | 0 | 3.606397 | 1.813871 | 0.767536 |
| 63 | 1 | 0 | 3.560293 | 0.312827 | -2.726309 |
| 64 | 1 | 0 | 4.838302 | -1.916184 | -1.346797 |
| 65 | 1 | 0 | 5.487582 | 1.789613 | 2.415911 |
| 66 | 1 | 0 | 4.039243 | 0.987049 | 3.073555 |
| 67 | 1 | 0 | 5.413023 | 0.016705 | 2.501517 |
| 68 | 1 | 0 | 6.954118 | -2.469960 | -0.189568 |
| 69 | 1 | 0 | 6.279476 | -1.935028 | 1.367242 |
| 70 | 1 | 0 | 5.584515 | -3.345967 | 0.543335 |

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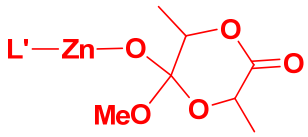


**II$^{monomer}$-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.975214 | -2.156024 | 0.514375 |
| 2 | 6 | 0 | -2.641967 | -1.457642 | 1.583197 |
| 3 | 6 | 0 | -3.993928 | -1.896628 | 1.623385 |
| 4 | 6 | 0 | -4.181941 | -2.857186 | 0.585096 |
| 5 | 6 | 0 | -2.943623 | -3.024957 | -0.098130 |
| 6 | 26 | 0 | -3.551997 | -1.041553 | -0.232050 |
| 7 | 6 | 0 | -4.608402 | 0.739323 | -0.393906 |
| 8 | 6 | 0 | -3.258968 | 1.002727 | -0.808038 |
| 9 | 6 | 0 | -3.016456 | 0.105850 | -1.902327 |
| 10 | 6 | 0 | -4.188384 | -0.665140 | -2.168683 |
| 11 | 6 | 0 | -5.184818 | -0.265880 | -1.228867 |
| 12 | 5 | 0 | -2.357994 | 2.257680 | -0.332946 |
| 13 | 7 | 0 | -1.895770 | 2.242632 | 1.168912 |
| 14 | 7 | 0 | -0.865802 | 1.499864 | 1.657732 |
| 15 | 6 | 0 | -0.788970 | 1.744237 | 2.977309 |
| 16 | 6 | 0 | -1.787955 | 2.642414 | 3.362965 |
| 17 | 6 | 0 | -2.458400 | 2.934711 | 2.179628 |
| 18 | 30 | 0 | 0.492373 | 0.515243 | 0.396250 |
| 19 | 7 | 0 | 0.023971 | 1.720633 | -1.239252 |
| 20 | 7 | 0 | -1.113977 | 2.472073 | -1.265344 |
| 21 | 6 | 0 | -1.036373 | 3.348545 | -2.286405 |
| 22 | 6 | 0 | 0.177080 | 3.178352 | -2.944203 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | 6 | 0 | 0.810445 | 2.149976 | -2.241261 |
| 24 | 15 | 0 | -0.246504 | -1.881468 | 0.075057 |
| 25 | 6 | 0 | 0.730995 | -3.075877 | 1.093846 |
| 26 | 8 | 0 | 2.250531 | 0.530330 | 1.228445 |
| 27 | 6 | 0 | 3.330602 | 0.311648 | 0.488851 |
| 28 | 8 | 0 | 3.187835 | -0.901510 | -0.274291 |
| 29 | 6 | 0 | 4.281555 | -1.175720 | -1.155871 |
| 30 | 6 | 0 | 5.660174 | -0.752817 | -0.629066 |
| 31 | 8 | 0 | 5.760643 | -0.116814 | 0.554022 |
| 32 | 6 | 0 | 4.588470 | 0.152249 | 1.368200 |
| 33 | 8 | 0 | 6.655635 | -0.974670 | -1.281135 |
| 34 | 6 | 0 | 4.280750 | -2.669350 | -1.476208 |
| 35 | 8 | 0 | 3.544778 | 1.308768 | -0.535245 |
| 36 | 6 | 0 | 3.778322 | 2.632651 | -0.073694 |
| 37 | 6 | 0 | 4.453727 | -0.925547 | 2.435617 |
| 38 | 6 | 0 | -0.056035 | -2.548078 | -1.634625 |
| 39 | 1 | 0 | -0.012214 | 1.275071 | 3.566780 |
| 40 | 1 | 0 | 0.548612 | 3.728936 | -3.795566 |
| 41 | 1 | 0 | 1.793429 | 1.716978 | -2.366896 |
| 42 | 1 | 0 | -1.851502 | 4.032133 | -2.473544 |
| 43 | 1 | 0 | -5.113660 | 1.228507 | 0.430408 |
| 44 | 1 | 0 | -6.180341 | -0.681709 | -1.137395 |
| 45 | 1 | 0 | -4.758982 | -1.526816 | 2.293196 |
| 46 | 1 | 0 | -2.199315 | -0.700508 | 2.214912 |
| 47 | 1 | 0 | -2.774829 | -3.669520 | -0.950285 |
| 48 | 1 | 0 | -5.114458 | -3.344531 | 0.331321 |
| 49 | 1 | 0 | -4.293559 | -1.433436 | -2.924364 |
| 50 | 1 | 0 | -2.084370 | 0.037629 | -2.449097 |
| 51 | 1 | 0 | -1.985258 | 3.036803 | 4.348581 |
| 52 | 1 | 0 | -3.016829 | 3.267367 | -0.443780 |
| 53 | 1 | 0 | -3.290279 | 3.595657 | 1.984856 |
| 54 | 1 | 0 | 0.443133 | -4.111698 | 0.885931 |
| 55 | 1 | 0 | 1.791988 | -2.926747 | 0.874381 |
| 56 | 1 | 0 | 0.563397 | -2.866744 | 2.154601 |
| 57 | 1 | 0 | -0.347039 | -3.602217 | -1.689362 |
| 58 | 1 | 0 | -0.668182 | -1.969253 | -2.330534 |
| 59 | 1 | 0 | 0.993864 | -2.454496 | -1.925998 |
| 60 | 1 | 0 | 4.150003 | -0.604995 | -2.083714 |
| 61 | 1 | 0 | 4.810227 | 1.109886 | 1.846459 |
| 62 | 1 | 0 | 5.102291 | -2.897102 | -2.159112 |
| 63 | 1 | 0 | 4.405011 | -3.264193 | -0.564813 |
| 64 | 1 | 0 | 3.335025 | -2.953249 | -1.949344 |
| 65 | 1 | 0 | 5.393051 | -1.019511 | 2.989633 |
| 66 | 1 | 0 | 3.652556 | -0.660016 | 3.129565 |
| 67 | 1 | 0 | 4.215494 | -1.892917 | 1.982837 |
| 68 | 1 | 0 | 3.555537 | 3.302205 | -0.908764 |
| 69 | 1 | 0 | 3.120327 | 2.881915 | 0.766779 |
| 70 | 1 | 0 | 4.826700 | 2.776986 | 0.221164 |

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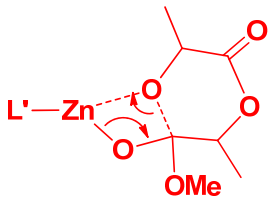


**TSII-III$^{monomer}$-LA**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.682735 | 3.477945 | -2.073251 |
| 2 | 7 | 0 | -0.749861 | 2.520221 | -1.125766 |
| 3 | 7 | 0 | 0.250783 | 1.614725 | -1.325493 |
| 4 | 6 | 0 | 0.941509 | 2.030643 | -2.403634 |
| 5 | 6 | 0 | 0.386890 | 3.205684 | -2.920763 |
| 6 | 5 | 0 | -1.908123 | 2.370032 | -0.084429 |
| 7 | 7 | 0 | -1.314519 | 2.073520 | 1.336971 |
| 8 | 7 | 0 | -0.302291 | 1.203788 | 1.614574 |
| 9 | 6 | 0 | -0.150857 | 1.188466 | 2.952421 |
| 10 | 6 | 0 | -1.076076 | 2.046006 | 3.556640 |
| 11 | 6 | 0 | -1.785574 | 2.590991 | 2.489766 |
| 12 | 30 | 0 | 0.874385 | 0.179543 | 0.145912 |
| 13 | 8 | 0 | 2.376532 | -0.068846 | 2.002512 |
| 14 | 6 | 0 | 3.488614 | 0.053225 | 1.460740 |
| 15 | 8 | 0 | 4.122509 | 1.236193 | 1.348786 |
| 16 | 6 | 0 | 3.356589 | 2.428716 | 1.576262 |
| 17 | 6 | 0 | -3.042784 | 1.337664 | -0.597347 |
| 18 | 6 | 0 | -4.382193 | 1.245738 | -0.084520 |
| 19 | 6 | 0 | -5.171706 | 0.413455 | -0.937726 |
| 20 | 6 | 0 | -4.328005 | -0.037377 | -1.998164 |
| 21 | 6 | 0 | -3.032686 | 0.526582 | -1.783518 |
| 22 | 26 | 0 | -3.591774 | -0.673490 | -0.161993 |
| 23 | 6 | 0 | -2.127854 | -2.042753 | 0.345760 |
| 24 | 6 | 0 | -3.260083 | -2.720206 | -0.234958 |
| 25 | 6 | 0 | -4.397141 | -2.460473 | 0.584268 |
| 26 | 6 | 0 | -3.988787 | -1.619755 | 1.663690 |
| 27 | 6 | 0 | -2.595705 | -1.360656 | 1.525208 |
| 28 | 15 | 0 | -0.409494 | -2.044281 | -0.216683 |
| 29 | 6 | 0 | 0.291673 | -3.569512 | 0.571456 |
| 30 | 8 | 0 | 2.756434 | -0.226691 | -0.463859 |
| 31 | 6 | 0 | 3.672414 | -0.170912 | -1.504253 |
| 32 | 6 | 0 | 5.117455 | -0.489040 | -1.055225 |
| 33 | 8 | 0 | 6.037210 | -0.388356 | -1.839561 |
| 34 | 6 | 0 | 3.308705 | -1.121953 | -2.662221 |
| 35 | 6 | 0 | -0.493754 | -2.542684 | -1.994624 |
| 36 | 6 | 0 | 4.490466 | -1.087510 | 1.302805 |
| 37 | 6 | 0 | 3.866257 | -2.472415 | 1.256794 |
| 38 | 8 | 0 | 5.412589 | -0.884836 | 0.210687 |
| 39 | 1 | 0 | 0.628011 | 0.582865 | 3.391786 |
| 40 | 1 | 0 | 0.718404 | 3.778600 | -3.774575 |

| | | | | | |
|---|---|---|---|---|---|
| 41 | 1 | 0 | 1.804594 | 1.476436 | -2.741909 |
| 42 | 1 | 0 | -1.403551 | 4.283056 | -2.080931 |
| 43 | 1 | 0 | -4.738704 | 1.722412 | 0.821288 |
| 44 | 1 | 0 | -6.209066 | 0.141423 | -0.786513 |
| 45 | 1 | 0 | -4.633946 | -1.211011 | 2.430570 |
| 46 | 1 | 0 | -1.997868 | -0.737467 | 2.175364 |
| 47 | 1 | 0 | -3.257896 | -3.307680 | -1.143618 |
| 48 | 1 | 0 | -5.407301 | -2.796236 | 0.386881 |
| 49 | 1 | 0 | -4.612120 | -0.708563 | -2.799315 |
| 50 | 1 | 0 | -2.172271 | 0.374974 | -2.423774 |
| 51 | 1 | 0 | -1.199332 | 2.256379 | 4.609303 |
| 52 | 1 | 0 | -2.405478 | 3.470694 | 0.006310 |
| 53 | 1 | 0 | -2.583682 | 3.319617 | 2.470551 |
| 54 | 1 | 0 | -0.352752 | -4.433176 | 0.373732 |
| 55 | 1 | 0 | 1.293719 | -3.769892 | 0.181273 |
| 56 | 1 | 0 | 0.365876 | -3.423298 | 1.653287 |
| 57 | 1 | 0 | -1.002040 | -3.505001 | -2.118859 |
| 58 | 1 | 0 | -1.026199 | -1.780783 | -2.569679 |
| 59 | 1 | 0 | 0.523326 | -2.630081 | -2.389060 |
| 60 | 1 | 0 | 4.085772 | 3.239476 | 1.594990 |
| 61 | 1 | 0 | 2.648816 | 2.587065 | 0.755967 |
| 62 | 1 | 0 | 2.817738 | 2.369835 | 2.524583 |
| 63 | 1 | 0 | 3.760773 | 0.850281 | -1.917414 |
| 64 | 1 | 0 | 4.048308 | -1.063220 | -3.466246 |
| 65 | 1 | 0 | 3.259954 | -2.157389 | -2.303533 |
| 66 | 1 | 0 | 2.325100 | -0.851949 | -3.063664 |
| 67 | 1 | 0 | 5.151465 | -1.025324 | 2.177875 |
| 68 | 1 | 0 | 3.258632 | -2.640108 | 2.151432 |
| 69 | 1 | 0 | 3.230850 | -2.572343 | 0.375307 |
| 70 | 1 | 0 | 4.659672 | -3.225793 | 1.221270 |

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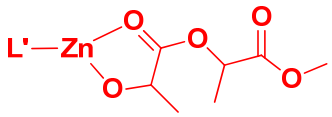


**III$^{monomer}$-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.196687 | 0.999243 | -1.896885 |
| 2 | 6 | 0 | 3.136149 | 1.533222 | -0.945330 |
| 3 | 6 | 0 | 4.448960 | 1.288233 | -1.435147 |
| 4 | 6 | 0 | 4.340462 | 0.600040 | -2.681014 |
| 5 | 6 | 0 | 2.957688 | 0.423036 | -2.973130 |
| 6 | 26 | 0 | 3.412932 | -0.507791 | -1.173034 |
| 7 | 6 | 0 | 4.303107 | -1.544234 | 0.390483 |
| 8 | 6 | 0 | 2.886952 | -1.542546 | 0.627082 |
| 9 | 6 | 0 | 2.310063 | -2.169212 | -0.527421 |
| 10 | 6 | 0 | 3.340264 | -2.562490 | -1.435461 |
| 11 | 6 | 0 | 4.587115 | -2.175411 | -0.859246 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 5 | 0 | 2.168041 | -1.164057 | 2.026771 |
| 13 | 7 | 0 | 0.701486 | -1.718648 | 2.099379 |
| 14 | 6 | 0 | 0.327996 | -2.847805 | 2.733971 |
| 15 | 6 | 0 | -1.021942 | -3.079194 | 2.498231 |
| 16 | 6 | 0 | -1.418295 | -2.012016 | 1.686945 |
| 17 | 7 | 0 | -0.375212 | -1.200116 | 1.440112 |
| 18 | 30 | 0 | -0.430733 | 0.799391 | 0.765299 |
| 19 | 8 | 0 | -2.567599 | 0.362285 | -0.404730 |
| 20 | 6 | 0 | -3.355088 | 1.162482 | 0.091727 |
| 21 | 8 | 0 | -4.668534 | 1.139851 | -0.193125 |
| 22 | 6 | 0 | -5.127242 | 0.125420 | -1.099158 |
| 23 | 6 | 0 | -6.590470 | 0.435882 | -1.406442 |
| 24 | 15 | 0 | 0.405686 | 1.024122 | -1.664435 |
| 25 | 6 | 0 | -0.149346 | 2.589640 | -2.493154 |
| 26 | 6 | 0 | -0.241129 | -0.265463 | -2.818824 |
| 27 | 7 | 0 | 2.170157 | 0.353266 | 2.414137 |
| 28 | 7 | 0 | 1.294559 | 1.268243 | 1.923300 |
| 29 | 6 | 0 | 1.586432 | 2.446512 | 2.496545 |
| 30 | 6 | 0 | 2.680629 | 2.308996 | 3.358418 |
| 31 | 6 | 0 | 3.009037 | 0.959888 | 3.279201 |
| 32 | 8 | 0 | -1.614185 | 2.196265 | 1.386435 |
| 33 | 6 | 0 | -2.943223 | 2.267227 | 1.073089 |
| 34 | 6 | 0 | -3.329988 | 3.642765 | 0.479548 |
| 35 | 6 | 0 | -4.972833 | -1.257759 | -0.461702 |
| 36 | 8 | 0 | -4.827398 | -1.475605 | 0.719136 |
| 37 | 8 | 0 | -5.066591 | -2.206752 | -1.410295 |
| 38 | 6 | 0 | -4.972986 | -3.565084 | -0.940242 |
| 39 | 1 | 0 | 2.553663 | -0.088426 | -3.836538 |
| 40 | 1 | 0 | -6.989076 | -0.301253 | -2.109030 |
| 41 | 1 | 0 | 0.975403 | 3.311215 | 2.275408 |
| 42 | 1 | 0 | -1.628602 | -3.889875 | 2.873717 |
| 43 | 1 | 0 | -2.396179 | -1.776956 | 1.289547 |
| 44 | 1 | 0 | 1.051954 | -3.407700 | 3.307633 |
| 45 | 1 | 0 | 5.045191 | -1.124721 | 1.059392 |
| 46 | 1 | 0 | 5.564920 | -2.299090 | -1.307900 |
| 47 | 1 | 0 | 5.369986 | 1.534014 | -0.923077 |
| 48 | 1 | 0 | 2.882444 | 1.997322 | -0.002814 |
| 49 | 1 | 0 | 5.164878 | 0.237729 | -3.281569 |
| 50 | 1 | 0 | 3.201612 | -3.038853 | -2.398025 |
| 51 | 1 | 0 | 1.248841 | -2.326569 | -0.675333 |
| 52 | 1 | 0 | 3.149349 | 3.067533 | 3.967781 |
| 53 | 1 | 0 | 2.763805 | -1.720448 | 2.923076 |
| 54 | 1 | 0 | 3.770657 | 0.386533 | 3.787492 |
| 55 | 1 | 0 | 0.193540 | 2.634908 | -3.532351 |
| 56 | 1 | 0 | -1.242534 | 2.647883 | -2.469761 |
| 57 | 1 | 0 | 0.250518 | 3.450740 | -1.949582 |
| 58 | 1 | 0 | 0.013739 | -0.046908 | -3.861426 |
| 59 | 1 | 0 | 0.173975 | -1.238604 | -2.545235 |
| 60 | 1 | 0 | -1.328417 | -0.307668 | -2.711905 |
| 61 | 1 | 0 | -3.593374 | 2.103733 | 1.958020 |
| 62 | 1 | 0 | -4.403232 | 3.723569 | 0.276215 |
| 63 | 1 | 0 | -3.043475 | 4.413945 | 1.200085 |
| 64 | 1 | 0 | -2.773052 | 3.825781 | -0.447421 |
| 65 | 1 | 0 | -4.522179 | 0.149951 | -2.009941 |

| | | | | | |
|---|---|---|---|---|---|
| 66 | 1 | 0 | -7.185670 | 0.413093 | -0.488489 |
| 67 | 1 | 0 | -6.673440 | 1.431575 | -1.851414 |
| 68 | 1 | 0 | -5.106416 | -4.188663 | -1.824134 |
| 69 | 1 | 0 | -3.993286 | -3.741592 | -0.489055 |
| 70 | 1 | 0 | -5.751729 | -3.768670 | -0.201103 |

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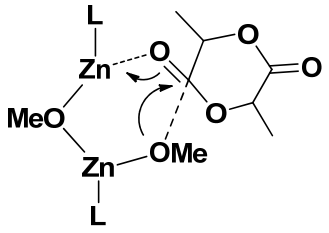


**TSI-II$^{dimer}$-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.323833 | 4.177595 | -1.181677 |
| 2 | 6 | 0 | 0.537592 | 3.374464 | -0.165993 |
| 3 | 8 | 0 | 0.999589 | 3.314073 | 1.083857 |
| 4 | 6 | 0 | 2.429641 | 3.337239 | 1.333824 |
| 5 | 6 | 0 | 3.308044 | 3.810396 | 0.179660 |
| 6 | 8 | 0 | 2.749703 | 4.137162 | -1.000033 |
| 7 | 8 | 0 | -0.680353 | 3.220890 | -0.356524 |
| 8 | 30 | 0 | -1.846708 | 1.546551 | -0.138297 |
| 9 | 7 | 0 | -3.685295 | 2.318624 | 0.427225 |
| 10 | 6 | 0 | -4.016996 | 3.303907 | 1.279041 |
| 11 | 6 | 0 | -5.366325 | 3.634133 | 1.134981 |
| 12 | 6 | 0 | -5.821952 | 2.787998 | 0.127455 |
| 13 | 7 | 0 | -4.803295 | 2.012299 | -0.289230 |
| 14 | 5 | 0 | -4.874243 | 0.821313 | -1.312347 |
| 15 | 6 | 0 | -4.745322 | -0.588667 | -0.541103 |
| 16 | 6 | 0 | -4.298734 | -1.840581 | -1.084831 |
| 17 | 6 | 0 | -4.365294 | -2.852877 | -0.077300 |
| 18 | 6 | 0 | -4.867575 | -2.243990 | 1.112519 |
| 19 | 6 | 0 | -5.101583 | -0.864104 | 0.822627 |
| 20 | 26 | 0 | -6.254776 | -2.074508 | -0.415400 |
| 21 | 6 | 0 | -7.501222 | -3.659108 | -0.935031 |
| 22 | 6 | 0 | -8.030555 | -2.966915 | 0.194164 |
| 23 | 6 | 0 | -8.271940 | -1.599349 | -0.177900 |
| 24 | 6 | 0 | -7.875638 | -1.469172 | -1.553256 |
| 25 | 6 | 0 | -7.410940 | -2.733168 | -2.018309 |
| 26 | 15 | 0 | -8.955092 | -0.206813 | 0.796619 |
| 27 | 6 | 0 | -10.785183 | -0.584030 | 0.663538 |
| 28 | 6 | 0 | 2.661928 | 4.177826 | 2.585200 |
| 29 | 8 | 0 | 4.505564 | 3.870636 | 0.323010 |
| 30 | 6 | 0 | 0.858974 | 5.638337 | -1.164753 |
| 31 | 8 | 0 | -0.902029 | 0.313007 | 1.054265 |
| 32 | 6 | 0 | -1.607130 | -0.503285 | 1.983554 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 7 | 0 | -2.405273 | 1.021553 | -2.062529 |
| 34 | 7 | 0 | -3.728476 | 0.972939 | -2.380887 |
| 35 | 6 | 0 | -3.856322 | 0.921003 | -3.720595 |
| 36 | 6 | 0 | -2.591398 | 0.940519 | -4.301263 |
| 37 | 6 | 0 | -1.715325 | 1.011780 | -3.215096 |
| 38 | 30 | 0 | 1.012361 | -0.046757 | 0.581499 |
| 39 | 8 | 0 | 1.272533 | 1.378683 | -0.744198 |
| 40 | 6 | 0 | 1.998537 | 1.105360 | -1.924657 |
| 41 | 7 | 0 | 2.033046 | -0.239162 | 2.406121 |
| 42 | 7 | 0 | 2.923425 | -1.255358 | 2.572781 |
| 43 | 6 | 0 | 3.215213 | -1.378833 | 3.881203 |
| 44 | 6 | 0 | 2.499361 | -0.425427 | 4.600216 |
| 45 | 6 | 0 | 1.765817 | 0.258153 | 3.626835 |
| 46 | 5 | 0 | 3.529150 | -2.063763 | 1.365939 |
| 47 | 7 | 0 | 2.347414 | -2.738035 | 0.572142 |
| 48 | 7 | 0 | 1.332434 | -2.029251 | 0.005050 |
| 49 | 6 | 0 | 0.552653 | -2.905920 | -0.650348 |
| 50 | 6 | 0 | 1.068025 | -4.199054 | -0.526397 |
| 51 | 6 | 0 | 2.204878 | -4.040423 | 0.260618 |
| 52 | 6 | 0 | 4.377657 | -1.092629 | 0.403030 |
| 53 | 6 | 0 | 4.761961 | -1.355506 | -0.955587 |
| 54 | 6 | 0 | 5.500197 | -0.243857 | -1.466631 |
| 55 | 6 | 0 | 5.603640 | 0.726268 | -0.425169 |
| 56 | 6 | 0 | 4.920160 | 0.201668 | 0.714668 |
| 57 | 26 | 0 | 6.487606 | -1.054044 | 0.176250 |
| 58 | 6 | 0 | 8.450823 | -1.629914 | -0.343555 |
| 59 | 6 | 0 | 7.686481 | -2.755988 | 0.115181 |
| 60 | 6 | 0 | 7.249146 | -2.503345 | 1.449347 |
| 61 | 6 | 0 | 7.729084 | -1.216075 | 1.831450 |
| 62 | 6 | 0 | 8.461432 | -0.677675 | 0.731119 |
| 63 | 15 | 0 | 9.480012 | -1.560048 | -1.858656 |
| 64 | 6 | 0 | 9.302834 | 0.229948 | -2.353194 |
| 65 | 6 | 0 | -8.671532 | -0.795449 | 2.544589 |
| 66 | 6 | 0 | 8.356709 | -2.363153 | -3.113439 |
| 67 | 1 | 0 | -0.335566 | -2.563130 | -1.165059 |
| 68 | 1 | 0 | 3.912065 | -2.135828 | 4.210402 |
| 69 | 1 | 0 | 1.141839 | 3.740341 | -2.163493 |
| 70 | 1 | 0 | -5.065379 | -2.744426 | 2.052020 |
| 71 | 1 | 0 | 2.506959 | -0.260679 | 5.667381 |
| 72 | 1 | 0 | -7.599126 | -0.805303 | 2.760501 |
| 73 | 1 | 0 | -4.838604 | 0.869468 | -4.167109 |
| 74 | 1 | 0 | -0.635332 | 1.061125 | -3.195925 |
| 75 | 1 | 0 | -2.347348 | 0.912333 | -5.352741 |
| 76 | 1 | 0 | -3.987771 | -1.999269 | -2.110386 |
| 77 | 1 | 0 | -4.117492 | -3.899230 | -0.203988 |
| 78 | 1 | 0 | -7.014874 | -2.942776 | -3.003406 |
| 79 | 1 | 0 | -7.883045 | -0.546351 | -2.118621 |
| 80 | 1 | 0 | -8.187706 | -3.394913 | 1.175349 |
| 81 | 1 | 0 | -7.185010 | -4.694347 | -0.954715 |
| 82 | 1 | 0 | -5.505698 | -0.136955 | 1.515971 |
| 83 | 1 | 0 | -5.931695 | 4.377796 | 1.676375 |
| 84 | 1 | 0 | -5.903164 | 0.972206 | -1.924323 |
| 85 | 1 | 0 | -11.346819 | 0.111837 | 1.297525 |
| 86 | 1 | 0 | -11.112120 | -0.435351 | -0.370792 |

| | | | | | |
|---|---|---|---|---|---|
| 87 | 1 | 0 | -11.024652 | -1.611122 | 0.962846 |
| 88 | 1 | 0 | -9.151439 | -0.091308 | 3.233165 |
| 89 | 1 | 0 | -9.079500 | -1.795219 | 2.734719 |
| 90 | 1 | 0 | -3.268342 | 3.724191 | 1.937754 |
| 91 | 1 | 0 | -6.804278 | 2.670952 | -0.306310 |
| 92 | 1 | 0 | -2.447500 | 0.048226 | 2.425062 |
| 93 | 1 | 0 | -2.011644 | -1.404041 | 1.504720 |
| 94 | 1 | 0 | -0.938710 | -0.810540 | 2.799168 |
| 95 | 1 | 0 | 3.066389 | 1.340233 | -1.822980 |
| 96 | 1 | 0 | 1.922377 | 0.045431 | -2.212258 |
| 97 | 1 | 0 | 1.605554 | 1.694231 | -2.772294 |
| 98 | 1 | 0 | 0.674039 | -5.115152 | -0.940517 |
| 99 | 1 | 0 | 2.923283 | -4.763129 | 0.619411 |
| 100 | 1 | 0 | 1.055331 | 1.067135 | 3.735546 |
| 101 | 1 | 0 | 4.149182 | -2.977391 | 1.855439 |
| 102 | 1 | 0 | 4.535663 | -2.262239 | -1.503689 |
| 103 | 1 | 0 | 5.915630 | -0.157401 | -2.461767 |
| 104 | 1 | 0 | 6.109849 | 1.680612 | -0.477368 |
| 105 | 1 | 0 | 4.855540 | 0.690692 | 1.678863 |
| 106 | 1 | 0 | 8.930513 | 0.297399 | 0.705955 |
| 107 | 1 | 0 | 6.613270 | -3.149240 | 2.039945 |
| 108 | 1 | 0 | 7.535643 | -0.714350 | 2.770738 |
| 109 | 1 | 0 | 7.462532 | -3.643642 | -0.462079 |
| 110 | 1 | 0 | 9.769380 | 0.370148 | -3.334706 |
| 111 | 1 | 0 | 8.259094 | 0.556643 | -2.395896 |
| 112 | 1 | 0 | 9.841212 | 0.863308 | -1.640613 |
| 113 | 1 | 0 | 8.808471 | -2.258243 | -4.106179 |
| 114 | 1 | 0 | 8.274814 | -3.434207 | -2.901342 |
| 115 | 1 | 0 | 7.352707 | -1.927388 | -3.122159 |
| 116 | 1 | 0 | 1.443894 | 6.208625 | -1.891673 |
| 117 | 1 | 0 | -0.200377 | 5.698021 | -1.427365 |
| 118 | 1 | 0 | 1.002988 | 6.084010 | -0.174562 |
| 119 | 1 | 0 | 2.719450 | 2.298888 | 1.517723 |
| 120 | 1 | 0 | 2.088522 | 3.766012 | 3.420458 |
| 121 | 1 | 0 | 3.724592 | 4.161943 | 2.836030 |
| 122 | 1 | 0 | 2.351070 | 5.215588 | 2.425524 |

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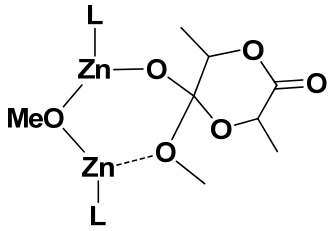


**II$^{dimer}$-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 6.649038 | -0.641174 | 0.553489 |

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| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 6.040091 | 0.473905 | -1.099749 |
| 3 | 6 | 0 | 5.581397 | 1.085155 | 0.104922 |
| 4 | 6 | 0 | 4.738698 | 0.141900 | 0.768500 |
| 5 | 6 | 0 | 4.652946 | -1.063924 | -0.008646 |
| 6 | 6 | 0 | 5.483442 | -0.841259 | -1.160873 |
| 7 | 6 | 0 | 8.159909 | -2.075531 | 0.572036 |
| 8 | 6 | 0 | 7.296624 | -2.246791 | 1.694636 |
| 9 | 6 | 0 | 7.337995 | -1.048297 | 2.466651 |
| 10 | 6 | 0 | 8.227468 | -0.140677 | 1.817649 |
| 11 | 6 | 0 | 8.754812 | -0.770050 | 0.639651 |
| 12 | 15 | 0 | 10.147841 | -0.160447 | -0.383840 |
| 13 | 1 | 0 | 3.663160 | -3.550329 | 2.914096 |
| 14 | 7 | 0 | 2.966697 | -2.805598 | -0.969277 |
| 15 | 7 | 0 | 1.998471 | -2.003769 | -1.493818 |
| 16 | 6 | 0 | 1.547947 | -2.603502 | -2.610753 |
| 17 | 6 | 0 | 2.237928 | -3.797365 | -2.830878 |
| 18 | 6 | 0 | 3.125021 | -3.882340 | -1.760726 |
| 19 | 7 | 0 | 2.838001 | -2.213936 | 1.513057 |
| 20 | 6 | 0 | 1.868494 | -2.333355 | 3.520639 |
| 21 | 7 | 0 | 1.794909 | -1.336192 | 1.505241 |
| 22 | 30 | 0 | 1.134241 | -0.532318 | -0.294006 |
| 23 | 8 | 0 | -0.820524 | -0.578158 | -0.543101 |
| 24 | 6 | 0 | -5.076597 | -1.012602 | 0.668280 |
| 25 | 6 | 0 | -5.120275 | -0.433833 | -0.645355 |
| 26 | 6 | 0 | -5.196166 | -1.543307 | -1.554619 |
| 27 | 6 | 0 | -5.185300 | -2.769635 | -0.817961 |
| 28 | 1 | 0 | -5.116367 | -3.138677 | 1.394258 |
| 29 | 6 | 0 | -5.112390 | -2.438023 | 0.568875 |
| 30 | 1 | 0 | -8.548184 | -1.631701 | -2.519811 |
| 31 | 6 | 0 | -8.520286 | -2.805220 | -0.609589 |
| 32 | 6 | 0 | -8.553089 | -1.642431 | -1.437554 |
| 33 | 6 | 0 | -8.527677 | -0.499096 | -0.587746 |
| 34 | 6 | 0 | -8.491074 | -0.939845 | 0.779700 |
| 35 | 6 | 0 | -8.483760 | -2.377376 | 0.750488 |
| 36 | 1 | 0 | -8.424995 | -3.029534 | 1.611641 |
| 37 | 15 | 0 | -8.478217 | 0.216961 | 2.199916 |
| 38 | 5 | 0 | -5.144627 | 1.137555 | -1.006507 |
| 39 | 7 | 0 | -4.482723 | 1.971896 | 0.148802 |
| 40 | 7 | 0 | -3.154233 | 1.921548 | 0.447581 |
| 41 | 6 | 0 | -2.967586 | 2.657333 | 1.556272 |
| 42 | 6 | 0 | -5.116415 | 2.716076 | 1.075372 |
| 43 | 6 | 0 | -4.184959 | 3.178171 | 2.001338 |
| 44 | 6 | 0 | -4.945019 | 1.780820 | -3.532230 |
| 45 | 7 | 0 | -4.392009 | 1.422081 | -2.357466 |
| 46 | 6 | 0 | -3.953446 | 1.829639 | -4.507482 |
| 47 | 1 | 0 | -6.005866 | 1.975445 | -3.592126 |
| 48 | 30 | 0 | -1.779730 | 1.133538 | -0.891800 |
| 49 | 8 | 0 | -0.226285 | 2.307007 | -1.315043 |
| 50 | 6 | 0 | 0.819146 | 2.416627 | -0.551517 |
| 51 | 6 | 0 | 1.493794 | 3.794705 | -0.646215 |
| 52 | 8 | 0 | 2.687053 | 3.863584 | 0.170920 |
| 53 | 6 | 0 | 2.749997 | 3.197141 | 1.338200 |
| 54 | 6 | 0 | 1.599439 | 2.279267 | 1.764318 |
| 55 | 1 | 0 | 0.230977 | 2.047130 | 3.419397 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 6 | 0 | 0.541848 | 4.930425 | -0.287279 |
| 57 | 8 | 0 | 1.862544 | 1.335153 | -0.864000 |
| 58 | 6 | 0 | 2.531321 | 1.444828 | -2.133562 |
| 59 | 8 | 0 | 0.529008 | 2.109911 | 0.809199 |
| 60 | 6 | 0 | -2.784639 | 1.482578 | -3.824851 |
| 61 | 7 | 0 | -3.056152 | 1.228165 | -2.534086 |
| 62 | 6 | 0 | 2.895573 | -2.816940 | 2.714566 |
| 63 | 6 | 0 | 1.201477 | -1.412574 | 2.710777 |
| 64 | 6 | 0 | 0.992668 | 2.757645 | 3.082852 |
| 65 | 8 | 0 | 3.722630 | 3.305639 | 2.049414 |
| 66 | 26 | 0 | -6.828667 | -1.639466 | -0.270463 |
| 67 | 6 | 0 | -10.293960 | 0.188009 | 2.659560 |
| 68 | 6 | 0 | -7.822787 | -0.873954 | 3.564918 |
| 69 | 6 | 0 | -1.504147 | -1.811251 | -0.320865 |
| 70 | 5 | 0 | 3.819354 | -2.403507 | 0.296323 |
| 71 | 6 | 0 | 9.744152 | 1.655289 | -0.525167 |
| 72 | 6 | 0 | 9.645277 | -0.743396 | -2.083891 |
| 73 | 1 | 0 | 0.751333 | -2.149826 | -3.185732 |
| 74 | 1 | 0 | 1.856162 | 3.938453 | -1.665762 |
| 75 | 1 | 0 | 1.639613 | -2.613922 | 4.537785 |
| 76 | 1 | 0 | -6.775371 | -1.120991 | 3.368110 |
| 77 | 1 | 0 | -1.766547 | 1.416487 | -4.184912 |
| 78 | 1 | 0 | -4.064814 | 2.087233 | -5.550170 |
| 79 | 1 | 0 | -5.278089 | -1.462726 | -2.631935 |
| 80 | 1 | 0 | -5.256941 | -3.766692 | -1.233973 |
| 81 | 1 | 0 | -8.489024 | 0.532617 | -0.911448 |
| 82 | 1 | 0 | -8.485050 | -3.830937 | -0.954110 |
| 83 | 1 | 0 | -5.044393 | -0.447412 | 1.591464 |
| 84 | 1 | 0 | -4.367773 | 3.802506 | 2.863164 |
| 85 | 1 | 0 | -6.250408 | 1.597405 | -1.156212 |
| 86 | 1 | 0 | -10.442983 | 0.751257 | 3.588113 |
| 87 | 1 | 0 | -10.875132 | 0.678542 | 1.871869 |
| 88 | 1 | 0 | -10.676542 | -0.830340 | 2.795232 |
| 89 | 1 | 0 | -7.871243 | -0.320868 | 4.509378 |
| 90 | 1 | 0 | -8.389982 | -1.804985 | 3.681150 |
| 91 | 1 | 0 | -1.969782 | 2.776771 | 1.955126 |
| 92 | 1 | 0 | -6.187534 | 2.847134 | 1.024262 |
| 93 | 1 | 0 | -2.449280 | -1.831872 | -0.872534 |
| 94 | 1 | 0 | -0.892379 | -2.657806 | -0.662588 |
| 95 | 1 | 0 | -1.730399 | -1.957719 | 0.744197 |
| 96 | 1 | 0 | 3.298831 | 2.221096 | -2.079832 |
| 97 | 1 | 0 | 3.016244 | 0.486642 | -2.322217 |
| 98 | 1 | 0 | 1.804974 | 1.665887 | -2.922768 |
| 99 | 1 | 0 | 2.111450 | -4.499566 | -3.641295 |
| 100 | 1 | 0 | 3.860502 | -4.632983 | -1.510262 |
| 101 | 1 | 0 | 0.328489 | -0.809405 | 2.923095 |
| 102 | 1 | 0 | 4.487506 | -3.375733 | 0.553945 |
| 103 | 1 | 0 | 5.670599 | -1.565501 | -1.944933 |
| 104 | 1 | 0 | 6.708305 | 0.917489 | -1.826245 |
| 105 | 1 | 0 | 5.829587 | 2.073385 | 0.468472 |
| 106 | 1 | 0 | 4.272683 | 0.304227 | 1.731498 |
| 107 | 1 | 0 | 8.449400 | 0.864942 | 2.150303 |
| 108 | 1 | 0 | 6.680458 | -3.114008 | 1.891069 |
| 109 | 1 | 0 | 6.761827 | -0.841285 | 3.359099 |

| | | | | | |
|---|---|---|---|---|---|
| 110 | 1 | 0 | 8.326613 | -2.805642 | -0.209515 |
| 111 | 1 | 0 | 10.435998 | 2.113439 | -1.240764 |
| 112 | 1 | 0 | 8.713881 | 1.835611 | -0.847908 |
| 113 | 1 | 0 | 9.901044 | 2.144013 | 0.441872 |
| 114 | 1 | 0 | 10.339835 | -0.321359 | -2.818781 |
| 115 | 1 | 0 | 9.730565 | -1.833577 | -2.138997 |
| 116 | 1 | 0 | 8.621442 | -0.455644 | -2.342973 |
| 117 | 1 | 0 | 1.076560 | 5.883886 | -0.331883 |
| 118 | 1 | 0 | -0.291035 | 4.951657 | -0.994037 |
| 119 | 1 | 0 | 0.134754 | 4.802996 | 0.720435 |
| 120 | 1 | 0 | 2.070359 | 1.303751 | 1.923657 |
| 121 | 1 | 0 | 1.775976 | 2.826069 | 3.841546 |
| 122 | 1 | 0 | 0.524506 | 3.741012 | 2.969223 |

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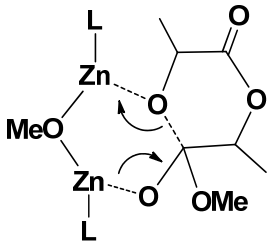


**TSII-III$^{dimer}$-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.248474 | -1.784240 | -3.281377 |
| 2 | 7 | 0 | -1.785186 | -1.457371 | -2.092121 |
| 3 | 7 | 0 | -2.676934 | -2.435784 | -1.772091 |
| 4 | 6 | 0 | -2.700676 | -3.352099 | -2.758860 |
| 5 | 6 | 0 | -1.801830 | -2.977102 | -3.753075 |
| 6 | 30 | 0 | -1.151312 | -0.090033 | -0.638005 |
| 7 | 8 | 0 | 0.836714 | -0.191452 | -0.411055 |
| 8 | 30 | 0 | 1.912889 | 1.329646 | 0.220184 |
| 9 | 7 | 0 | 2.767658 | 1.351567 | 2.112825 |
| 10 | 7 | 0 | 4.122559 | 1.412350 | 2.238515 |
| 11 | 6 | 0 | 4.432872 | 1.700153 | 3.516716 |
| 12 | 6 | 0 | 3.259472 | 1.838091 | 4.252926 |
| 13 | 6 | 0 | 2.242424 | 1.618464 | 3.320984 |
| 14 | 5 | 0 | 5.129177 | 1.075078 | 1.073172 |
| 15 | 6 | 0 | 5.038656 | -0.480605 | 0.662865 |
| 16 | 6 | 0 | 4.827963 | -1.603429 | 1.532914 |
| 17 | 6 | 0 | 4.859756 | -2.813415 | 0.772403 |
| 18 | 6 | 0 | 5.103530 | -2.460700 | -0.589480 |
| 19 | 6 | 0 | 5.215425 | -1.036353 | -0.650640 |
| 20 | 26 | 0 | 6.674757 | -1.833171 | 0.604460 |
| 21 | 6 | 0 | 8.114333 | -2.053561 | 2.092278 |
| 22 | 6 | 0 | 8.362095 | -0.875673 | 1.329647 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | 6 | 0 | 8.571228 | -1.248226 | -0.042581 |
| 24 | 6 | 0 | 8.436725 | -2.678211 | -0.107310 |
| 25 | 6 | 0 | 8.155719 | -3.169078 | 1.201934 |
| 26 | 15 | 0 | 8.950518 | -0.029929 | -1.356893 |
| 27 | 6 | 0 | 8.509575 | -0.985605 | -2.897523 |
| 28 | 5 | 0 | -3.623887 | -2.380620 | -0.511417 |
| 29 | 6 | 0 | -4.657770 | -1.152596 | -0.633695 |
| 30 | 6 | 0 | -5.396722 | -0.768658 | -1.805105 |
| 31 | 6 | 0 | -6.208111 | 0.370027 | -1.510274 |
| 32 | 6 | 0 | -5.993719 | 0.707991 | -0.140949 |
| 33 | 6 | 0 | -5.053721 | -0.228312 | 0.393761 |
| 34 | 26 | 0 | -6.751607 | -1.224244 | -0.294574 |
| 35 | 6 | 0 | -7.908915 | -2.793979 | -0.996732 |
| 36 | 6 | 0 | -8.748279 | -1.689448 | -0.659138 |
| 37 | 6 | 0 | -8.587661 | -1.394322 | 0.736961 |
| 38 | 6 | 0 | -7.623634 | -2.329931 | 1.244150 |
| 39 | 6 | 0 | -7.212381 | -3.189902 | 0.182464 |
| 40 | 15 | 0 | -9.637310 | -0.271086 | 1.735486 |
| 41 | 6 | 0 | -9.841051 | 1.177265 | 0.578319 |
| 42 | 7 | 0 | -1.876655 | -1.215838 | 0.981949 |
| 43 | 6 | 0 | -1.357505 | -1.368959 | 2.211730 |
| 44 | 6 | 0 | -1.904611 | -2.494839 | 2.833712 |
| 45 | 6 | 0 | -2.777694 | -3.018208 | 1.884601 |
| 46 | 7 | 0 | -2.746213 | -2.243925 | 0.782791 |
| 47 | 8 | 0 | -1.650812 | 1.802754 | -0.906094 |
| 48 | 6 | 0 | -2.825660 | 2.185938 | -1.584895 |
| 49 | 6 | 0 | -3.417784 | 3.495097 | -1.056018 |
| 50 | 8 | 0 | -4.524102 | 3.866497 | -1.363817 |
| 51 | 6 | 0 | -2.646321 | 2.248975 | -3.110776 |
| 52 | 6 | 0 | -8.394627 | 0.432687 | 2.937349 |
| 53 | 6 | 0 | 1.402087 | -1.504335 | -0.372292 |
| 54 | 8 | 0 | 0.584850 | 2.842882 | -0.058245 |
| 55 | 6 | 0 | -0.593030 | 2.987480 | 0.336848 |
| 56 | 6 | 0 | -1.302998 | 4.292355 | -0.043047 |
| 57 | 8 | 0 | -2.734247 | 4.221221 | -0.113960 |
| 58 | 7 | 0 | 3.588975 | 2.038937 | -0.759968 |
| 59 | 6 | 0 | 3.706030 | 2.822986 | -1.844906 |
| 60 | 6 | 0 | 5.021930 | 3.272527 | -1.976034 |
| 61 | 6 | 0 | 5.686846 | 2.715378 | -0.886881 |
| 62 | 7 | 0 | 4.814124 | 1.985969 | -0.166001 |
| 63 | 8 | 0 | -0.895458 | 2.353431 | 1.493809 |
| 64 | 6 | 0 | -2.210869 | 2.420755 | 2.075581 |
| 65 | 6 | 0 | 10.813940 | -0.202560 | -1.435617 |
| 66 | 6 | 0 | -0.702693 | 4.930762 | -1.291974 |
| 67 | 1 | 0 | -5.360543 | -1.278832 | -2.760261 |
| 68 | 1 | 0 | 9.006190 | -1.961180 | -2.957162 |
| 69 | 1 | 0 | 5.214420 | -3.149338 | -1.417398 |
| 70 | 1 | 0 | 3.162819 | 2.071520 | 5.302768 |
| 71 | 1 | 0 | -1.138752 | 4.970514 | 0.806284 |
| 72 | 1 | 0 | -2.393570 | 1.251920 | -3.485129 |
| 73 | 1 | 0 | -0.612906 | -0.671848 | 2.572583 |
| 74 | 1 | 0 | -3.358168 | -4.206219 | -2.686090 |
| 75 | 1 | 0 | -1.581071 | -3.495954 | -4.673952 |
| 76 | 1 | 0 | 7.427075 | -1.137581 | -2.940183 |

| | | | | | |
|---|---|---|---|---|---|
| 77 | 1 | 0 | 5.467841 | 1.786822 | 3.813778 |
| 78 | 1 | 0 | 1.168313 | 1.657932 | 3.443542 |
| 79 | 1 | 0 | 4.693857 | -1.544138 | 2.606333 |
| 80 | 1 | 0 | 4.755625 | -3.817723 | 1.163301 |
| 81 | 1 | 0 | 7.885741 | -2.091224 | 3.149481 |
| 82 | 1 | 0 | 8.345450 | 0.139732 | 1.703734 |
| 83 | 1 | 0 | 8.500189 | -3.282380 | -1.002542 |
| 84 | 1 | 0 | 7.963860 | -4.201489 | 1.465342 |
| 85 | 1 | 0 | 5.424045 | -0.461287 | -1.544375 |
| 86 | 1 | 0 | 5.434436 | 3.909735 | -2.743872 |
| 87 | 1 | 0 | 6.210504 | 1.424488 | 1.478391 |
| 88 | 1 | 0 | 11.198060 | 0.393028 | -2.271909 |
| 89 | 1 | 0 | 11.253271 | 0.190992 | -0.513156 |
| 90 | 1 | 0 | 11.136364 | -1.242751 | -1.561405 |
| 91 | 1 | 0 | 8.804962 | -0.394746 | -3.771578 |
| 92 | 1 | 0 | 2.838921 | 3.025971 | -2.459237 |
| 93 | 1 | 0 | 6.723579 | 2.769440 | -0.588438 |
| 94 | 1 | 0 | 2.465319 | -1.476426 | -0.630980 |
| 95 | 1 | 0 | 1.302619 | -1.955550 | 0.624538 |
| 96 | 1 | 0 | 0.894393 | -2.156396 | -1.095098 |
| 97 | 1 | 0 | -1.693071 | -2.880205 | 3.819987 |
| 98 | 1 | 0 | -3.419367 | -3.886603 | 1.917607 |
| 99 | 1 | 0 | -0.491119 | -1.151711 | -3.725910 |
| 100 | 1 | 0 | -4.136246 | -3.473044 | -0.455246 |
| 101 | 1 | 0 | -4.712445 | -0.257823 | 1.421159 |
| 102 | 1 | 0 | -6.460355 | 1.525003 | 0.391815 |
| 103 | 1 | 0 | -6.880367 | 0.872230 | -2.193492 |
| 104 | 1 | 0 | -9.387107 | -1.151574 | -1.347550 |
| 105 | 1 | 0 | -6.461667 | -3.966110 | 0.247432 |
| 106 | 1 | 0 | -7.788828 | -3.222217 | -1.983406 |
| 107 | 1 | 0 | -7.256739 | -2.367497 | 2.261818 |
| 108 | 1 | 0 | -10.326437 | 1.995287 | 1.122191 |
| 109 | 1 | 0 | -8.889760 | 1.528618 | 0.166659 |
| 110 | 1 | 0 | -10.501517 | 0.896235 | -0.248632 |
| 111 | 1 | 0 | -8.878354 | 1.225951 | 3.518356 |
| 112 | 1 | 0 | -8.082777 | -0.346393 | 3.640889 |
| 113 | 1 | 0 | -7.506323 | 0.835420 | 2.440411 |
| 114 | 1 | 0 | -1.287346 | 5.818211 | -1.552922 |
| 115 | 1 | 0 | 0.331936 | 5.227080 | -1.104494 |
| 116 | 1 | 0 | -0.706740 | 4.233058 | -2.132801 |
| 117 | 1 | 0 | -3.576167 | 2.575075 | -3.586654 |
| 118 | 1 | 0 | -1.842990 | 2.936735 | -3.394527 |
| 119 | 1 | 0 | -3.629581 | 1.462535 | -1.387210 |
| 120 | 1 | 0 | -2.129377 | 1.881954 | 3.020433 |
| 121 | 1 | 0 | -2.514835 | 3.453450 | 2.259836 |
| 122 | 1 | 0 | -2.936125 | 1.927089 | 1.426689 |

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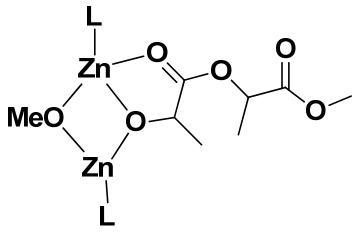


**III$^{dimer}$-LA**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 6.570533 | -0.914018 | 0.833703 |
| 2 | 6 | 0 | 7.732491 | -1.914410 | -0.585517 |
| 3 | 6 | 0 | 8.061101 | -0.515586 | -0.550070 |
| 4 | 6 | 0 | 8.518576 | -0.185586 | 0.758286 |
| 5 | 6 | 0 | 8.468988 | -1.371297 | 1.552787 |
| 6 | 1 | 0 | 8.710963 | -1.442701 | 2.605650 |
| 7 | 6 | 0 | 7.987876 | -2.432933 | 0.731162 |
| 8 | 15 | 0 | 7.148261 | -2.762536 | -2.099202 |
| 9 | 6 | 0 | 5.375316 | 0.604603 | 1.597268 |
| 10 | 6 | 0 | 5.386473 | -0.519986 | 2.480086 |
| 11 | 6 | 0 | 4.864923 | -1.637647 | 1.759727 |
| 12 | 6 | 0 | 4.537185 | -1.183381 | 0.443927 |
| 13 | 1 | 0 | 5.739432 | 1.594990 | 1.842884 |
| 14 | 5 | 0 | 4.663312 | 1.139515 | -0.987409 |
| 15 | 7 | 0 | 4.126564 | 2.566828 | -0.612964 |
| 16 | 7 | 0 | 2.880035 | 2.813502 | -0.123201 |
| 17 | 6 | 0 | 2.870614 | -0.840273 | -3.624019 |
| 18 | 7 | 0 | 2.345877 | 0.322470 | -1.771480 |
| 19 | 7 | 0 | 3.680263 | 0.460425 | -2.003757 |
| 20 | 6 | 0 | 4.013341 | -0.234412 | -3.109060 |
| 21 | 6 | 0 | 2.819401 | 4.126416 | 0.158335 |
| 22 | 6 | 0 | 4.038944 | 4.743882 | -0.133803 |
| 23 | 6 | 0 | 4.834089 | 3.713779 | -0.624627 |
| 24 | 6 | 0 | 1.850817 | -0.455914 | -2.748780 |
| 25 | 1 | 0 | -4.544949 | -1.427597 | -2.883041 |
| 26 | 6 | 0 | -4.880631 | -0.251896 | 0.240262 |
| 27 | 6 | 0 | -3.868110 | -2.009848 | -0.822686 |
| 28 | 6 | 0 | -5.137643 | -0.116555 | -1.159602 |
| 29 | 6 | 0 | -8.001694 | -2.012246 | -0.791812 |
| 30 | 1 | 0 | -7.330916 | -3.223022 | -2.560944 |
| 31 | 6 | 0 | -7.686932 | -2.174806 | 0.600041 |
| 32 | 6 | 0 | -6.618697 | -3.869478 | -0.542122 |
| 33 | 1 | 0 | -5.988717 | -4.718598 | -0.773469 |
| 34 | 15 | 0 | -9.271857 | -0.891044 | -1.491054 |
| 35 | 1 | 0 | -8.555082 | -1.333123 | -3.803168 |
| 36 | 1 | 0 | -7.877609 | 0.976443 | -0.586156 |
| 37 | 6 | 0 | -8.932987 | 0.687644 | -0.556009 |
| 38 | 6 | 0 | -8.520993 | -0.459869 | -3.143659 |
| 39 | 5 | 0 | -3.554302 | -1.965525 | 1.895635 |
| 40 | 7 | 0 | -3.187849 | -0.757015 | 2.832787 |

| | | | | | |
|---|---|---|---|---|---|
| 41 | 7 | 0 | -2.222789 | 0.143012 | 2.505682 |
| 42 | 6 | 0 | -2.177556 | 1.055224 | 3.490497 |
| 43 | 1 | 0 | -3.351312 | 1.303643 | 5.374186 |
| 44 | 6 | 0 | -3.137756 | 0.763029 | 4.464060 |
| 45 | 6 | 0 | -3.750402 | -0.399169 | 4.002487 |
| 46 | 7 | 0 | -2.273941 | -2.860916 | 1.708449 |
| 47 | 6 | 0 | -0.262477 | -3.425476 | 1.088109 |
| 48 | 7 | 0 | -1.106396 | -2.385337 | 1.190953 |
| 49 | 6 | 0 | -0.883419 | -4.597220 | 1.529716 |
| 50 | 6 | 0 | -2.156049 | -4.186595 | 1.914829 |
| 51 | 30 | 0 | -0.823422 | -0.333780 | 1.036656 |
| 52 | 30 | 0 | 1.330179 | 1.378835 | -0.269730 |
| 53 | 8 | 0 | -0.614141 | 0.547359 | -0.745987 |
| 54 | 6 | 0 | -1.556020 | 1.391312 | -1.332931 |
| 55 | 6 | 0 | -1.130507 | 2.837009 | -1.089501 |
| 56 | 8 | 0 | -0.026584 | 3.141779 | -0.641576 |
| 57 | 1 | 0 | -0.728187 | 1.283785 | -3.347356 |
| 58 | 6 | 0 | -1.692787 | 1.144051 | -2.847150 |
| 59 | 1 | 0 | -2.430613 | 1.816354 | -3.297026 |
| 60 | 6 | 0 | -2.102992 | 4.990790 | 2.482326 |
| 61 | 8 | 0 | -2.212480 | 4.698278 | 1.076088 |
| 62 | 6 | 0 | -1.472899 | 5.473017 | 0.267353 |
| 63 | 6 | 0 | -1.678992 | 5.137454 | -1.210886 |
| 64 | 8 | 0 | -2.043055 | 3.749660 | -1.415404 |
| 65 | 6 | 0 | -2.802455 | 5.976863 | -1.809877 |
| 66 | 8 | 0 | 0.890412 | 0.542827 | 1.493971 |
| 67 | 6 | 0 | 4.839285 | 0.214850 | 0.324128 |
| 68 | 6 | 0 | -4.512129 | -1.216436 | -1.821774 |
| 69 | 6 | 0 | -4.078933 | -1.422005 | 0.471228 |
| 70 | 6 | 0 | -7.323595 | -3.068079 | -1.489785 |
| 71 | 6 | 0 | -6.844478 | -3.315635 | 0.752068 |
| 72 | 6 | 0 | 6.264039 | -4.243403 | -1.386609 |
| 73 | 6 | 0 | 8.733576 | -3.609061 | -2.629998 |
| 74 | 26 | 0 | -5.916273 | -1.919453 | -0.468637 |
| 75 | 8 | 0 | -0.766519 | 6.384840 | 0.634547 |
| 76 | 1 | 0 | 8.528264 | -4.261952 | -3.486333 |
| 77 | 1 | 0 | -3.324847 | -2.928072 | -1.008765 |
| 78 | 1 | 0 | 5.359102 | -3.914681 | -0.867594 |
| 79 | 1 | 0 | 6.883214 | -4.818347 | -0.688145 |
| 80 | 1 | 0 | 4.301934 | 5.784831 | -0.017836 |
| 81 | 1 | 0 | 5.758182 | -0.532050 | 3.497052 |
| 82 | 1 | 0 | 8.804644 | 0.799984 | 1.102319 |
| 83 | 1 | 0 | 7.927749 | 0.177753 | -1.370060 |
| 84 | 1 | 0 | 7.815150 | -3.449711 | 1.058187 |
| 85 | 1 | 0 | 4.767873 | -2.649462 | 2.133140 |
| 86 | 1 | 0 | 4.142993 | -1.800239 | -0.354177 |
| 87 | 1 | 0 | 2.795901 | -1.464129 | -4.502306 |
| 88 | 1 | 0 | 5.692043 | 1.333271 | -1.590519 |
| 89 | 1 | 0 | 9.458571 | -2.853343 | -2.949677 |
| 90 | 1 | 0 | 9.180962 | -4.206010 | -1.826475 |
| 91 | 1 | 0 | 5.966455 | -4.903830 | -2.208650 |
| 92 | 1 | 0 | 0.795153 | -0.687030 | -2.757353 |
| 93 | 1 | 0 | 5.041780 | -0.272918 | -3.437193 |
| 94 | 1 | 0 | 1.900482 | 4.560644 | 0.527271 |

| | | | | | |
|---|---|---|---|---|---|
| 95 | 1 | 0 | 5.852640 | 3.715208 | -0.984530 |
| 96 | 1 | 0 | -2.553578 | 1.276344 | -0.881303 |
| 97 | 1 | 0 | -1.448798 | 1.853594 | 3.448856 |
| 98 | 1 | 0 | -4.545836 | -0.995485 | 4.425407 |
| 99 | 1 | 0 | 0.739819 | -3.273546 | 0.709604 |
| 100 | 1 | 0 | -0.470841 | -5.594207 | 1.569757 |
| 101 | 1 | 0 | -2.986694 | -4.746157 | 2.319836 |
| 102 | 1 | 0 | -4.342567 | -2.636735 | 2.517302 |
| 103 | 1 | 0 | -5.246992 | 0.414883 | 1.011429 |
| 104 | 1 | 0 | -5.718005 | 0.666316 | -1.629645 |
| 105 | 1 | 0 | -6.406666 | -3.660115 | 1.679201 |
| 106 | 1 | 0 | -8.020321 | -1.529277 | 1.402402 |
| 107 | 1 | 0 | -9.125792 | 0.326587 | -3.608680 |
| 108 | 1 | 0 | -7.483754 | -0.119994 | -3.060188 |
| 109 | 1 | 0 | -9.543514 | 1.488694 | -0.987553 |
| 110 | 1 | 0 | -9.237178 | 0.569511 | 0.489094 |
| 111 | 1 | 0 | -2.019498 | 0.111950 | -2.998064 |
| 112 | 1 | 0 | -0.727423 | 5.331504 | -1.710518 |
| 113 | 1 | 0 | -2.567407 | 7.038689 | -1.692501 |
| 114 | 1 | 0 | -2.909151 | 5.754435 | -2.875440 |
| 115 | 1 | 0 | -3.751096 | 5.763584 | -1.308152 |
| 116 | 1 | 0 | -2.730698 | 4.252123 | 2.980246 |
| 117 | 1 | 0 | -1.063620 | 4.902532 | 2.808477 |
| 118 | 1 | 0 | -2.457632 | 6.004124 | 2.687250 |
| 119 | 6 | 0 | 1.702140 | 0.431390 | 2.647140 |
| 120 | 1 | 0 | 1.079246 | 0.340533 | 3.550144 |
| 121 | 1 | 0 | 2.366107 | -0.441038 | 2.595434 |
| 122 | 1 | 0 | 2.334372 | 1.322001 | 2.759243 |

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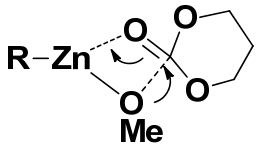


**TSI-II$^{monomer}$-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 4.114057 | 0.800200 | -0.556480 |
| 2 | 6 | 0 | 3.604932 | -0.483333 | -0.571586 |
| 3 | 8 | 0 | 4.526644 | -1.502732 | -0.573369 |
| 4 | 6 | 0 | 5.736956 | -1.345572 | 0.186456 |
| 5 | 6 | 0 | 6.331800 | 0.045350 | 0.011584 |
| 6 | 6 | 0 | 5.232469 | 1.058749 | 0.299349 |
| 7 | 8 | 0 | 2.607327 | -0.643371 | -1.334416 |
| 8 | 30 | 0 | 1.098428 | 0.049861 | 0.016515 |
| 9 | 15 | 0 | -0.284820 | -1.981883 | -0.658759 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 6 | 0 | -0.479007 | -2.016744 | -2.493418 |
| 11 | 7 | 0 | 0.529626 | 1.678909 | -1.179463 |
| 12 | 6 | 0 | 1.191216 | 2.154394 | -2.247165 |
| 13 | 6 | 0 | 0.679196 | 3.403110 | -2.614051 |
| 14 | 6 | 0 | -0.325091 | 3.650065 | -1.684500 |
| 15 | 7 | 0 | -0.400710 | 2.609360 | -0.829851 |
| 16 | 5 | 0 | -1.471678 | 2.417252 | 0.293707 |
| 17 | 6 | 0 | -2.714418 | 1.505980 | -0.196441 |
| 18 | 6 | 0 | -2.915080 | 0.925299 | -1.493165 |
| 19 | 6 | 0 | -4.263115 | 0.472512 | -1.621458 |
| 20 | 6 | 0 | -4.926903 | 0.754460 | -0.390084 |
| 21 | 6 | 0 | -3.974078 | 1.370033 | 0.478572 |
| 22 | 26 | 0 | -3.356864 | -0.539816 | -0.056808 |
| 23 | 6 | 0 | -2.273476 | -1.605348 | 1.354463 |
| 24 | 6 | 0 | -1.951526 | -2.063598 | 0.027479 |
| 25 | 6 | 0 | -3.168566 | -2.548166 | -0.564113 |
| 26 | 6 | 0 | -4.217022 | -2.388755 | 0.386930 |
| 27 | 6 | 0 | -3.664005 | -1.812834 | 1.570298 |
| 28 | 8 | 0 | 2.867153 | -0.502078 | 1.058026 |
| 29 | 6 | 0 | 2.872939 | -1.732302 | 1.753474 |
| 30 | 7 | 0 | 0.157218 | 0.968353 | 1.715892 |
| 31 | 7 | 0 | -0.770537 | 1.959494 | 1.619831 |
| 32 | 6 | 0 | -1.005475 | 2.470127 | 2.845542 |
| 33 | 6 | 0 | -0.219843 | 1.800016 | 3.776420 |
| 34 | 6 | 0 | 0.499229 | 0.876246 | 3.012148 |
| 35 | 6 | 0 | 0.456392 | -3.649980 | -0.335414 |
| 36 | 1 | 0 | -3.278587 | -2.933981 | -1.568815 |
| 37 | 1 | 0 | 1.258086 | 0.170586 | 3.319173 |
| 38 | 1 | 0 | 0.998475 | 4.041473 | -3.424518 |
| 39 | 1 | 0 | 2.004642 | 1.575501 | -2.661345 |
| 40 | 1 | 0 | -0.993296 | 4.491382 | -1.571150 |
| 41 | 1 | 0 | -4.172332 | 1.684573 | 1.496457 |
| 42 | 1 | 0 | -5.951176 | 0.503847 | -0.143708 |
| 43 | 1 | 0 | -4.215852 | -1.532927 | 2.458060 |
| 44 | 1 | 0 | -1.581320 | -1.144807 | 2.046105 |
| 45 | 1 | 0 | -5.261064 | -2.622406 | 0.222288 |
| 46 | 1 | 0 | -4.694704 | -0.023750 | -2.481736 |
| 47 | 1 | 0 | -2.154501 | 0.853812 | -2.260349 |
| 48 | 1 | 0 | -0.163922 | 1.972929 | 4.840965 |
| 49 | 1 | 0 | -1.893352 | 3.528787 | 0.530434 |
| 50 | 1 | 0 | -1.706626 | 3.282888 | 2.967131 |
| 51 | 1 | 0 | -0.144162 | -4.445322 | -0.789723 |
| 52 | 1 | 0 | 1.467720 | -3.670839 | -0.753486 |
| 53 | 1 | 0 | 0.518904 | -3.826374 | 0.742126 |
| 54 | 1 | 0 | -0.997771 | -2.920431 | -2.830924 |
| 55 | 1 | 0 | -1.036891 | -1.137488 | -2.822746 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 1 | 0 | 0.520329 | -1.985637 | -2.937516 |
| 57 | 1 | 0 | 5.539707 | 2.083266 | 0.075853 |
| 58 | 1 | 0 | 4.903150 | 1.003507 | 1.344110 |
| 59 | 1 | 0 | 7.178332 | 0.180136 | 0.695720 |
| 60 | 1 | 0 | 6.695368 | 0.175773 | -1.014126 |
| 61 | 1 | 0 | 6.402933 | -2.131910 | -0.178234 |
| 62 | 1 | 0 | 5.525155 | -1.537068 | 1.246141 |
| 63 | 1 | 0 | 3.645671 | -1.741216 | 2.538281 |
| 64 | 1 | 0 | 1.904361 | -1.901259 | 2.247390 |
| 65 | 1 | 0 | 3.063255 | -2.578879 | 1.079681 |

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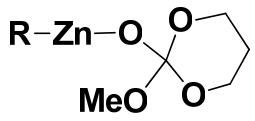


**II$^{monomer}$-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.199588 | 3.955288 | -1.203369 |
| 2 | 7 | 0 | -1.006441 | 2.793818 | -0.545561 |
| 3 | 7 | 0 | 0.004251 | 2.104978 | -1.142851 |
| 4 | 6 | 0 | 0.446846 | 2.854790 | -2.165171 |
| 5 | 6 | 0 | -0.293134 | 4.038201 | -2.254619 |
| 6 | 5 | 0 | -1.860213 | 2.249124 | 0.646750 |
| 7 | 7 | 0 | -0.909694 | 1.797258 | 1.813306 |
| 8 | 7 | 0 | 0.204313 | 1.027248 | 1.668318 |
| 9 | 6 | 0 | 0.736548 | 0.861036 | 2.891118 |
| 10 | 6 | 0 | -0.042696 | 1.511865 | 3.851116 |
| 11 | 6 | 0 | -1.069650 | 2.096674 | 3.117753 |
| 12 | 30 | 0 | 1.006558 | 0.505566 | -0.194386 |
| 13 | 15 | 0 | 0.010698 | -1.630623 | -1.152781 |
| 14 | 6 | 0 | -0.461924 | -1.452777 | -2.928409 |
| 15 | 8 | 0 | 2.997009 | -0.503599 | 0.983636 |
| 16 | 6 | 0 | 3.672248 | -0.018841 | -0.219825 |
| 17 | 8 | 0 | 4.219745 | -1.141767 | -0.904489 |
| 18 | 6 | 0 | 5.266784 | -1.822153 | -0.197247 |
| 19 | 6 | 0 | 4.985313 | -1.882121 | 1.314128 |
| 20 | 6 | 0 | 3.483661 | -1.734943 | 1.535755 |
| 21 | 8 | 0 | 2.799611 | 0.607988 | -0.972683 |
| 22 | 8 | 0 | 4.721959 | 0.794838 | 0.279318 |
| 23 | 6 | 0 | 5.333172 | 1.610418 | -0.713710 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 6 | 0 | 1.130710 | -3.105906 | -1.192969 |
| 25 | 6 | 0 | -1.479173 | -2.165845 | -0.287562 |
| 26 | 6 | 0 | -2.656594 | -2.820161 | -0.789070 |
| 27 | 6 | 0 | -3.557878 | -3.002294 | 0.298769 |
| 28 | 6 | 0 | -2.951088 | -2.472075 | 1.476923 |
| 29 | 6 | 0 | -1.676136 | -1.950752 | 1.123219 |
| 30 | 26 | 0 | -3.148445 | -0.972978 | 0.036477 |
| 31 | 6 | 0 | -4.977000 | -0.020078 | 0.093157 |
| 32 | 6 | 0 | -4.051627 | 0.663365 | 0.940531 |
| 33 | 6 | 0 | -2.953551 | 1.161952 | 0.161858 |
| 34 | 6 | 0 | -3.217292 | 0.732980 | -1.181778 |
| 35 | 6 | 0 | -4.452871 | 0.019576 | -1.233218 |
| 36 | 1 | 0 | -3.404397 | -2.425273 | 2.458312 |
| 37 | 1 | 0 | -2.843308 | -3.098661 | -1.817733 |
| 38 | 1 | 0 | 1.662063 | 0.313192 | 2.994382 |
| 39 | 1 | 0 | -0.179545 | 4.843037 | -2.965588 |
| 40 | 1 | 0 | 1.283651 | 2.509362 | -2.757386 |
| 41 | 1 | 0 | -1.968415 | 4.640334 | -0.877007 |
| 42 | 1 | 0 | -4.161256 | 0.783171 | 2.011898 |
| 43 | 1 | 0 | -5.885236 | -0.519243 | 0.407166 |
| 44 | 1 | 0 | -0.989010 | -1.439172 | 1.783627 |
| 45 | 1 | 0 | -4.550286 | -3.429338 | 0.232636 |
| 46 | 1 | 0 | -4.894190 | -0.438283 | -2.109746 |
| 47 | 1 | 0 | -2.578686 | 0.941956 | -2.030416 |
| 48 | 1 | 0 | 0.124204 | 1.570768 | 4.916355 |
| 49 | 1 | 0 | -2.453293 | 3.210819 | 1.084117 |
| 50 | 1 | 0 | -1.896727 | 2.716726 | 3.431565 |
| 51 | 1 | 0 | 0.727655 | -3.899438 | -1.831258 |
| 52 | 1 | 0 | 2.116140 | -2.793877 | -1.553789 |
| 53 | 1 | 0 | 1.242660 | -3.496742 | -0.177353 |
| 54 | 1 | 0 | -0.904922 | -2.372935 | -3.323795 |
| 55 | 1 | 0 | -1.174348 | -0.632824 | -3.041093 |
| 56 | 1 | 0 | 0.438071 | -1.218608 | -3.505914 |
| 57 | 1 | 0 | 5.332179 | -2.832656 | 1.737616 |
| 58 | 1 | 0 | 5.500256 | -1.068731 | 1.831134 |
| 59 | 1 | 0 | 3.236827 | -1.716538 | 2.602570 |
| 60 | 1 | 0 | 2.950165 | -2.580597 | 1.079748 |
| 61 | 1 | 0 | 5.285051 | -2.826741 | -0.633171 |
| 62 | 1 | 0 | 6.234590 | -1.345379 | -0.396713 |
| 63 | 1 | 0 | 6.141913 | 2.147205 | -0.210487 |
| 64 | 1 | 0 | 5.750298 | 1.005583 | -1.530282 |
| 65 | 1 | 0 | 4.617259 | 2.325085 | -1.131308 |

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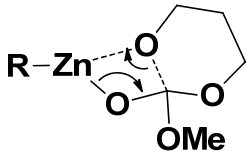


**TSII-III$^{monomer}$-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.563560 | 1.901949 | -1.172259 |
| 2 | 7 | 0 | -0.481521 | 2.735011 | -0.911911 |
| 3 | 6 | 0 | -0.384629 | 3.829764 | -1.691881 |
| 4 | 6 | 0 | 0.753236 | 3.723043 | -2.484012 |
| 5 | 6 | 0 | 1.316275 | 2.498725 | -2.112068 |
| 6 | 5 | 0 | -1.657946 | 2.389583 | 0.058555 |
| 7 | 7 | 0 | -1.057445 | 2.012433 | 1.459371 |
| 8 | 7 | 0 | 0.010682 | 1.192902 | 1.649985 |
| 9 | 6 | 0 | 0.224860 | 1.119659 | 2.974677 |
| 10 | 6 | 0 | -0.721710 | 1.887396 | 3.661882 |
| 11 | 6 | 0 | -1.507654 | 2.440525 | 2.656145 |
| 12 | 30 | 0 | 1.165606 | 0.285927 | 0.090335 |
| 13 | 8 | 0 | 2.679995 | -0.168656 | 1.560552 |
| 14 | 6 | 0 | 3.697623 | -0.458940 | 0.889100 |
| 15 | 8 | 0 | 4.828728 | 0.282993 | 0.925615 |
| 16 | 6 | 0 | 4.641720 | 1.675661 | 1.194688 |
| 17 | 6 | 0 | -2.667556 | 1.313902 | -0.606975 |
| 18 | 6 | 0 | -2.458753 | 0.483667 | -1.760074 |
| 19 | 6 | 0 | -3.686915 | -0.140774 | -2.138110 |
| 20 | 6 | 0 | -4.686722 | 0.287468 | -1.214259 |
| 21 | 6 | 0 | -4.057986 | 1.166038 | -0.280149 |
| 22 | 26 | 0 | -3.183880 | -0.714466 | -0.212670 |
| 23 | 6 | 0 | -3.671945 | -1.601634 | 1.616285 |
| 24 | 6 | 0 | -2.274569 | -1.344876 | 1.540497 |
| 25 | 6 | 0 | -1.747739 | -2.061117 | 0.408124 |
| 26 | 6 | 0 | -2.847572 | -2.759510 | -0.203635 |
| 27 | 6 | 0 | -4.027175 | -2.468499 | 0.540100 |
| 28 | 15 | 0 | -0.019706 | -2.000187 | -0.126182 |
| 29 | 6 | 0 | 0.822834 | -3.307507 | 0.879532 |
| 30 | 8 | 0 | 2.972412 | 0.053958 | -0.847544 |
| 31 | 6 | 0 | 3.661224 | -0.409881 | -1.972397 |
| 32 | 6 | 0 | 4.132250 | -1.862550 | -1.787665 |
| 33 | 6 | 0 | 4.858148 | -2.058134 | -0.459967 |
| 34 | 8 | 0 | 3.972633 | -1.765426 | 0.644616 |
| 35 | 6 | 0 | -0.048300 | -2.740614 | -1.820263 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 1 | 0 | 1.055730 | 0.535420 | 3.344462 |
| 37 | 1 | 0 | 1.121433 | 4.433381 | -3.209400 |
| 38 | 1 | 0 | 2.226135 | 2.021114 | -2.444428 |
| 39 | 1 | 0 | -1.132934 | 4.606305 | -1.628436 |
| 40 | 1 | 0 | -4.552658 | 1.643641 | 0.557230 |
| 41 | 1 | 0 | -5.721899 | -0.029779 | -1.200273 |
| 42 | 1 | 0 | -4.353862 | -1.172309 | 2.338428 |
| 43 | 1 | 0 | -1.711889 | -0.699632 | 2.199815 |
| 44 | 1 | 0 | -2.799154 | -3.370480 | -1.094810 |
| 45 | 1 | 0 | -5.025398 | -2.812096 | 0.301641 |
| 46 | 1 | 0 | -3.828493 | -0.836651 | -2.955776 |
| 47 | 1 | 0 | -1.509382 | 0.357887 | -2.265899 |
| 48 | 1 | 0 | -0.810869 | 2.038777 | 4.727558 |
| 49 | 1 | 0 | -2.255525 | 3.427436 | 0.239490 |
| 50 | 1 | 0 | -2.346053 | 3.119985 | 2.707574 |
| 51 | 1 | 0 | 0.385417 | -4.295188 | 0.698596 |
| 52 | 1 | 0 | 1.891783 | -3.313156 | 0.650132 |
| 53 | 1 | 0 | 0.713578 | -3.057147 | 1.938814 |
| 54 | 1 | 0 | -0.468423 | -3.751913 | -1.814243 |
| 55 | 1 | 0 | -0.643120 | -2.109875 | -2.486582 |
| 56 | 1 | 0 | 0.974120 | -2.789159 | -2.206544 |
| 57 | 1 | 0 | 5.643962 | 2.105893 | 1.230403 |
| 58 | 1 | 0 | 4.061036 | 2.132792 | 0.388092 |
| 59 | 1 | 0 | 4.130246 | 1.819700 | 2.149498 |
| 60 | 1 | 0 | 4.550359 | 0.221393 | -2.157791 |
| 61 | 1 | 0 | 3.033844 | -0.341024 | -2.877567 |
| 62 | 1 | 0 | 5.752052 | -1.431005 | -0.391359 |
| 63 | 1 | 0 | 5.149499 | -3.100945 | -0.310029 |
| 64 | 1 | 0 | 3.272220 | -2.544278 | -1.820335 |
| 65 | 1 | 0 | 4.805504 | -2.145752 | -2.608613 |

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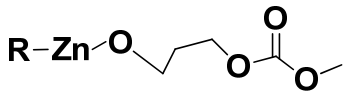


**III$^{monomer}$-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.000231 | 2.090315 | -1.234561 |
| 2 | 7 | 0 | -0.946637 | 2.811143 | -0.570541 |
| 3 | 6 | 0 | -1.132172 | 3.988467 | -1.200268 |
| 4 | 6 | 0 | -0.285784 | 4.054885 | -2.301255 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | 0.408415 | 2.842401 | -2.271444 |
| 6 | 5 | 0 | -1.812705 | 2.258499 | 0.611191 |
| 7 | 7 | 0 | -0.885529 | 1.755060 | 1.774151 |
| 8 | 7 | 0 | 0.193612 | 0.940703 | 1.618699 |
| 9 | 6 | 0 | 0.660339 | 0.651723 | 2.846199 |
| 10 | 6 | 0 | -0.127413 | 1.275865 | 3.818418 |
| 11 | 6 | 0 | -1.089325 | 1.967644 | 3.089625 |
| 12 | 30 | 0 | 1.067192 | 0.545281 | -0.239338 |
| 13 | 15 | 0 | 0.102809 | -1.709881 | -1.004362 |
| 14 | 6 | 0 | 1.171554 | -3.198757 | -0.761283 |
| 15 | 6 | 0 | -2.908268 | 1.195520 | 0.079235 |
| 16 | 6 | 0 | -3.084180 | 0.712200 | -1.261505 |
| 17 | 6 | 0 | -4.323502 | 0.011006 | -1.366790 |
| 18 | 6 | 0 | -4.939009 | 0.035738 | -0.079788 |
| 19 | 6 | 0 | -4.066640 | 0.747805 | 0.799080 |
| 20 | 26 | 0 | -3.118325 | -0.932611 | 0.030209 |
| 21 | 6 | 0 | -2.991579 | -2.367044 | 1.543836 |
| 22 | 6 | 0 | -1.699270 | -1.864985 | 1.227214 |
| 23 | 6 | 0 | -1.440862 | -2.135319 | -0.162683 |
| 24 | 6 | 0 | -2.597604 | -2.810024 | -0.688735 |
| 25 | 6 | 0 | -3.547899 | -2.945201 | 0.363802 |
| 26 | 8 | 0 | 2.953471 | 0.826223 | -0.368685 |
| 27 | 6 | 0 | 3.794005 | 1.051132 | -1.450050 |
| 28 | 6 | 0 | 4.285672 | -0.244002 | -2.126211 |
| 29 | 6 | 0 | 5.041886 | -1.195312 | -1.201711 |
| 30 | 8 | 0 | 4.158291 | -1.793613 | -0.220070 |
| 31 | 6 | 0 | 3.912668 | -1.169761 | 0.940220 |
| 32 | 8 | 0 | 2.913938 | -1.407720 | 1.592999 |
| 33 | 8 | 0 | 4.934749 | -0.400302 | 1.342236 |
| 34 | 6 | 0 | 4.664779 | 0.438714 | 2.472874 |
| 35 | 6 | 0 | -0.306536 | -1.788113 | -2.806444 |
| 36 | 1 | 0 | 1.527323 | 0.012157 | 2.944083 |
| 37 | 1 | 0 | -0.183622 | 4.864475 | -3.008458 |
| 38 | 1 | 0 | 1.187132 | 2.479265 | -2.928876 |
| 39 | 1 | 0 | -1.859372 | 4.693245 | -0.824598 |
| 40 | 1 | 0 | -4.249027 | 0.917960 | 1.853567 |
| 41 | 1 | 0 | -5.874879 | -0.437155 | 0.190567 |
| 42 | 1 | 0 | -3.485246 | -2.280702 | 2.502853 |
| 43 | 1 | 0 | -1.036908 | -1.339641 | 1.899959 |
| 44 | 1 | 0 | -2.740672 | -3.129120 | -1.712327 |
| 45 | 1 | 0 | -4.537571 | -3.373484 | 0.270370 |
| 46 | 1 | 0 | -4.711261 | -0.479045 | -2.251109 |
| 47 | 1 | 0 | -2.377847 | 0.861226 | -2.068256 |
| 48 | 1 | 0 | -0.010734 | 1.242936 | 4.891537 |
| 49 | 1 | 0 | -2.389664 | 3.221654 | 1.065784 |
| 50 | 1 | 0 | -1.901928 | 2.601032 | 3.414515 |

| | | | | | |
|---|---|---|---|---|---|
| 51 | 1 | 0 | 0.645213 | -4.109613 | -1.065102 |
| 52 | 1 | 0 | 2.096232 | -3.088441 | -1.333697 |
| 53 | 1 | 0 | 1.452005 | -3.259652 | 0.292922 |
| 54 | 1 | 0 | -0.722254 | -2.761455 | -3.087115 |
| 55 | 1 | 0 | -1.027091 | -1.005017 | -3.056556 |
| 56 | 1 | 0 | 0.607532 | -1.620907 | -3.385473 |
| 57 | 1 | 0 | 5.600711 | 0.960349 | 2.677790 |
| 58 | 1 | 0 | 3.878107 | 1.150600 | 2.213123 |
| 59 | 1 | 0 | 4.366345 | -0.161637 | 3.336175 |
| 60 | 1 | 0 | 4.688051 | 1.610872 | -1.114678 |
| 61 | 1 | 0 | 3.331523 | 1.681789 | -2.236813 |
| 62 | 1 | 0 | 5.869753 | -0.692682 | -0.697096 |
| 63 | 1 | 0 | 5.436573 | -2.050120 | -1.758346 |
| 64 | 1 | 0 | 3.432722 | -0.783094 | -2.563585 |
| 65 | 1 | 0 | 4.959964 | 0.014647 | -2.957082 |

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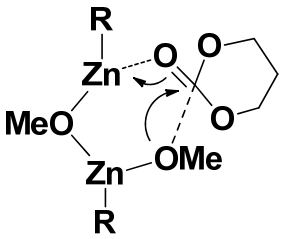


**TSI-II$^{dimer}$-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.565372 | 1.478202 | 2.667863 |
| 2 | 7 | 0 | -2.877315 | 1.484887 | 1.360321 |
| 3 | 7 | 0 | -4.232080 | 1.590289 | 1.269432 |
| 4 | 6 | 0 | -4.757163 | 1.628277 | 2.508964 |
| 5 | 6 | 0 | -3.725766 | 1.557360 | 3.441527 |
| 6 | 30 | 0 | -1.687940 | 1.652613 | -0.336775 |
| 7 | 8 | 0 | -0.251367 | 3.058993 | -0.084637 |
| 8 | 6 | 0 | 0.785782 | 2.954158 | 0.601533 |
| 9 | 8 | 0 | 1.567884 | 4.038987 | 0.683830 |
| 10 | 6 | 0 | 2.828216 | 3.928205 | 1.379906 |
| 11 | 6 | 0 | 2.628950 | 3.216053 | 2.707563 |
| 12 | 6 | 0 | 1.971715 | 1.876245 | 2.422870 |
| 13 | 8 | 0 | 0.767946 | 2.062838 | 1.628033 |
| 14 | 5 | 0 | -5.021666 | 1.534759 | -0.090003 |
| 15 | 6 | 0 | -4.961834 | 0.050892 | -0.717549 |
| 16 | 6 | 0 | -5.107874 | -0.318686 | -2.097914 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 6 | 0 | -5.035981 | -1.741466 | -2.224144 |
| 18 | 6 | 0 | -4.852489 | -2.281178 | -0.915283 |
| 19 | 6 | 0 | -4.812560 | -1.184229 | 0.000203 |
| 20 | 26 | 0 | -6.631870 | -1.225898 | -1.012972 |
| 21 | 6 | 0 | -8.351220 | -0.203683 | -0.478757 |
| 22 | 6 | 0 | -8.445802 | -0.621014 | -1.837902 |
| 23 | 6 | 0 | -8.344513 | -2.044928 | -1.867444 |
| 24 | 6 | 0 | -8.196643 | -2.504896 | -0.525631 |
| 25 | 6 | 0 | -8.201745 | -1.366378 | 0.352874 |
| 26 | 15 | 0 | -8.071465 | -1.276230 | 2.177609 |
| 27 | 6 | 0 | -7.291885 | -2.923361 | 2.580756 |
| 28 | 8 | 0 | -0.660181 | 0.108602 | -1.009424 |
| 29 | 6 | 0 | -1.346575 | -1.077865 | -1.408192 |
| 30 | 30 | 0 | 1.300888 | -0.026490 | -0.591961 |
| 31 | 8 | 0 | 2.031657 | 1.793116 | -0.549352 |
| 32 | 6 | 0 | 2.342402 | 2.431615 | -1.765512 |
| 33 | 7 | 0 | 2.306635 | -1.348305 | -1.884102 |
| 34 | 7 | 0 | 3.127368 | -2.304466 | -1.365779 |
| 35 | 6 | 0 | 3.508450 | -3.141465 | -2.350286 |
| 36 | 6 | 0 | 2.927483 | -2.733606 | -3.546631 |
| 37 | 6 | 0 | 2.178639 | -1.606294 | -3.196566 |
| 38 | 5 | 0 | 3.601069 | -2.317099 | 0.133561 |
| 39 | 7 | 0 | 2.330895 | -2.322732 | 1.062725 |
| 40 | 7 | 0 | 1.411144 | -1.320835 | 1.054439 |
| 41 | 6 | 0 | 0.506370 | -1.604695 | 2.006602 |
| 42 | 6 | 0 | 0.846321 | -2.793512 | 2.659004 |
| 43 | 6 | 0 | 2.010039 | -3.213130 | 2.021056 |
| 44 | 6 | 0 | 4.527277 | -1.042873 | 0.472442 |
| 45 | 6 | 0 | 5.005373 | -0.680359 | 1.779032 |
| 46 | 6 | 0 | 5.787762 | 0.512858 | 1.690581 |
| 47 | 6 | 0 | 5.813981 | 0.906325 | 0.317987 |
| 48 | 6 | 0 | 5.051003 | -0.049133 | -0.421038 |
| 49 | 26 | 0 | 6.645094 | -0.987733 | 0.543569 |
| 50 | 6 | 0 | 7.718247 | -2.560598 | 1.365293 |
| 51 | 6 | 0 | 7.294519 | -2.892249 | 0.045299 |
| 52 | 6 | 0 | 7.866170 | -1.940416 | -0.851125 |
| 53 | 6 | 0 | 8.659037 | -1.010824 | -0.096761 |
| 54 | 6 | 0 | 8.550556 | -1.404147 | 1.279951 |
| 55 | 15 | 0 | 9.828727 | 0.223571 | -0.781764 |
| 56 | 6 | 0 | 8.844450 | 0.925865 | -2.202316 |
| 57 | 6 | 0 | 9.666359 | 1.615343 | 0.450320 |
| 58 | 7 | 0 | -3.122453 | 2.602209 | -1.488029 |
| 59 | 7 | 0 | -4.424817 | 2.592093 | -1.088495 |
| 60 | 6 | 0 | -5.100857 | 3.536693 | -1.770324 |
| 61 | 6 | 0 | -4.227367 | 4.189372 | -2.635078 |
| 62 | 6 | 0 | -2.995326 | 3.569698 | -2.411161 |

| | | | | | |
|---|---|---|---|---|---|
| 63 | 6 | 0 | -9.838932 | -1.677871 | 2.651379 |
| 64 | 1 | 0 | 4.824178 | -1.242723 | 2.687481 |
| 65 | 1 | 0 | 8.754808 | 0.175676 | -2.994741 |
| 66 | 1 | 0 | 7.428211 | -3.069378 | 2.275424 |
| 67 | 1 | 0 | -1.621512 | -1.697111 | -0.543391 |
| 68 | 1 | 0 | 1.627770 | 1.371991 | 3.327721 |
| 69 | 1 | 0 | 1.553049 | -0.974706 | -3.813850 |
| 70 | 1 | 0 | 2.631775 | -4.081886 | 2.181886 |
| 71 | 1 | 0 | -4.786748 | -3.331699 | -0.661550 |
| 72 | 1 | 0 | 0.322910 | -3.283021 | 3.466805 |
| 73 | 1 | 0 | -6.261552 | -2.944185 | 2.213780 |
| 74 | 1 | 0 | -6.157315 | 3.676964 | -1.593954 |
| 75 | 1 | 0 | -2.027239 | 3.774777 | -2.848383 |
| 76 | 1 | 0 | -4.452321 | 4.996861 | -3.315677 |
| 77 | 1 | 0 | -5.274082 | 0.373553 | -2.914545 |
| 78 | 1 | 0 | -5.138911 | -2.308388 | -3.140824 |
| 79 | 1 | 0 | -8.527875 | 0.028834 | -2.699464 |
| 80 | 1 | 0 | -8.340455 | 0.819368 | -0.126381 |
| 81 | 1 | 0 | -8.065575 | -3.536820 | -0.227703 |
| 82 | 1 | 0 | -8.337015 | -2.664112 | -2.755600 |
| 83 | 1 | 0 | -4.708790 | -1.266423 | 1.075003 |
| 84 | 1 | 0 | -3.809543 | 1.570586 | 4.517969 |
| 85 | 1 | 0 | -6.135052 | 1.925549 | 0.163060 |
| 86 | 1 | 0 | -9.910047 | -1.776258 | 3.740820 |
| 87 | 1 | 0 | -10.492761 | -0.854996 | 2.344515 |
| 88 | 1 | 0 | -10.197378 | -2.603326 | 2.185749 |
| 89 | 1 | 0 | -7.268588 | -3.042512 | 3.669607 |
| 90 | 1 | 0 | -7.837188 | -3.772711 | 2.152561 |
| 91 | 1 | 0 | -1.527458 | 1.441081 | 2.970034 |
| 92 | 1 | 0 | -5.827859 | 1.685450 | 2.641179 |
| 93 | 1 | 0 | -2.265150 | -0.832283 | -1.952360 |
| 94 | 1 | 0 | -0.709333 | -1.679883 | -2.070060 |
| 95 | 1 | 0 | 2.845964 | 1.740538 | -2.459220 |
| 96 | 1 | 0 | 1.443273 | 2.826513 | -2.266706 |
| 97 | 1 | 0 | 3.023663 | 3.279596 | -1.596895 |
| 98 | 1 | 0 | 3.028699 | -3.190232 | -4.519856 |
| 99 | 1 | 0 | 4.166804 | -3.969480 | -2.131369 |
| 100 | 1 | 0 | -0.340246 | -0.949015 | 2.161541 |
| 101 | 1 | 0 | 4.133657 | -3.387304 | 0.311116 |
| 102 | 1 | 0 | 4.903726 | -0.034895 | -1.493264 |
| 103 | 1 | 0 | 6.334712 | 1.761380 | -0.091791 |
| 104 | 1 | 0 | 6.302870 | 1.002170 | 2.508119 |
| 105 | 1 | 0 | 9.011348 | -0.898632 | 2.119001 |
| 106 | 1 | 0 | 6.610812 | -3.686690 | -0.221119 |
| 107 | 1 | 0 | 7.713504 | -1.915437 | -1.922223 |
| 108 | 1 | 0 | 10.222712 | 2.482144 | 0.076503 |

| | | | | | |
|---|---|---|---|---|---|
| 109 | 1 | 0 | 8.624469 | 1.900010 | 0.628677 |
| 110 | 1 | 0 | 10.119991 | 1.319372 | 1.401885 |
| 111 | 1 | 0 | 9.391303 | 1.779284 | -2.618548 |
| 112 | 1 | 0 | 7.840949 | 1.246608 | -1.905253 |
| 113 | 1 | 0 | 3.522469 | 3.376903 | 0.739366 |
| 114 | 1 | 0 | 3.169173 | 4.958253 | 1.499694 |
| 115 | 1 | 0 | 3.594925 | 3.054642 | 3.199047 |
| 116 | 1 | 0 | 2.001740 | 3.821978 | 3.371900 |
| 117 | 1 | 0 | 2.643988 | 1.214206 | 1.873875 |

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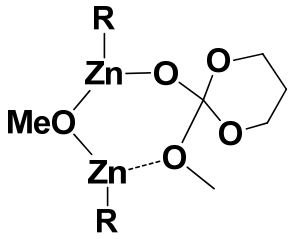


**II$^{dimer}$-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.711342 | -2.163021 | -1.870140 |
| 2 | 6 | 0 | -1.184750 | -3.412456 | -2.278430 |
| 3 | 6 | 0 | -2.333294 | -3.609310 | -1.516823 |
| 4 | 7 | 0 | -2.521711 | -2.541407 | -0.718671 |
| 5 | 7 | 0 | -1.526861 | -1.638420 | -0.938700 |
| 6 | 5 | 0 | -3.731042 | -2.264741 | 0.250039 |
| 7 | 7 | 0 | -3.169262 | -2.006222 | 1.694669 |
| 8 | 7 | 0 | -2.269177 | -1.023633 | 1.977670 |
| 9 | 6 | 0 | -2.070809 | -1.040280 | 3.307280 |
| 10 | 6 | 0 | -2.857196 | -2.029645 | 3.903838 |
| 11 | 6 | 0 | -3.533041 | -2.616869 | 2.838661 |
| 12 | 30 | 0 | -1.179339 | -0.110095 | 0.427666 |
| 13 | 8 | 0 | -1.955423 | 1.812147 | 0.280387 |
| 14 | 6 | 0 | -2.396844 | 2.537230 | 1.435532 |
| 15 | 8 | 0 | 0.723404 | 0.043800 | 0.935631 |
| 16 | 6 | 0 | 1.398020 | -1.102841 | 1.447104 |
| 17 | 30 | 0 | 1.687216 | 1.665294 | 0.280927 |
| 18 | 7 | 0 | 3.075008 | 2.596754 | 1.518009 |
| 19 | 7 | 0 | 4.394146 | 2.612501 | 1.179820 |
| 20 | 6 | 0 | 5.026151 | 3.547882 | 1.914801 |
| 21 | 6 | 0 | 4.105640 | 4.168253 | 2.754052 |
| 22 | 6 | 0 | 2.893573 | 3.539299 | 2.457371 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | 5 | 0 | 5.049529 | 1.599128 | 0.171517 |
| 24 | 7 | 0 | 4.312260 | 1.689217 | -1.212550 |
| 25 | 7 | 0 | 2.963910 | 1.561064 | -1.353930 |
| 26 | 6 | 0 | 2.694893 | 1.602683 | -2.669163 |
| 27 | 6 | 0 | 3.878323 | 1.736991 | -3.399916 |
| 28 | 6 | 0 | 4.877002 | 1.789151 | -2.431312 |
| 29 | 6 | 0 | 4.994413 | 0.093243 | 0.746089 |
| 30 | 6 | 0 | 4.844486 | -1.116155 | -0.013551 |
| 31 | 6 | 0 | 4.889240 | -2.244812 | 0.862852 |
| 32 | 6 | 0 | 5.075303 | -1.750633 | 2.189492 |
| 33 | 6 | 0 | 5.145401 | -0.324056 | 2.112169 |
| 34 | 26 | 0 | 6.666979 | -1.193304 | 0.993908 |
| 35 | 6 | 0 | 8.234144 | -2.463984 | 0.492285 |
| 36 | 6 | 0 | 8.383701 | -2.014461 | 1.837454 |
| 37 | 6 | 0 | 8.481115 | -0.589971 | 1.819144 |
| 38 | 6 | 0 | 8.382767 | -0.162071 | 0.463669 |
| 39 | 6 | 0 | 8.234677 | -1.318442 | -0.376908 |
| 40 | 15 | 0 | 8.104942 | -1.213794 | -2.200798 |
| 41 | 6 | 0 | 7.300794 | -2.846349 | -2.615418 |
| 42 | 6 | 0 | 9.866041 | -1.639342 | -2.677842 |
| 43 | 8 | 0 | 0.128098 | 2.874096 | 0.088574 |
| 44 | 6 | 0 | -0.928700 | 2.583839 | -0.582800 |
| 45 | 8 | 0 | -1.562892 | 3.718426 | -1.062184 |
| 46 | 6 | 0 | -2.672501 | 3.521937 | -1.948698 |
| 47 | 6 | 0 | -2.238452 | 2.659040 | -3.124829 |
| 48 | 6 | 0 | -1.705991 | 1.345346 | -2.572594 |
| 49 | 8 | 0 | -0.674717 | 1.582321 | -1.581934 |
| 50 | 6 | 0 | -4.590620 | -1.003855 | -0.268104 |
| 51 | 6 | 0 | -4.968197 | -0.724994 | -1.626683 |
| 52 | 6 | 0 | -5.732181 | 0.482752 | -1.674924 |
| 53 | 6 | 0 | -5.848273 | 0.970142 | -0.338109 |
| 54 | 6 | 0 | -5.160310 | 0.054746 | 0.516960 |
| 55 | 26 | 0 | -6.700025 | -0.922954 | -0.495218 |
| 56 | 6 | 0 | -8.744412 | -0.880591 | 0.042001 |
| 57 | 6 | 0 | -8.012455 | -1.801130 | 0.865756 |
| 58 | 6 | 0 | -7.419354 | -2.795124 | 0.031995 |
| 59 | 6 | 0 | -7.768034 | -2.499421 | -1.317985 |
| 60 | 6 | 0 | -8.575436 | -1.322360 | -1.313642 |
| 61 | 15 | 0 | -9.918460 | 0.398667 | 0.630388 |
| 62 | 6 | 0 | -8.969500 | 1.148593 | 2.050639 |
| 63 | 6 | 0 | -9.696767 | 1.731976 | -0.655621 |
| 64 | 1 | 0 | -3.030241 | -4.434294 | -1.488721 |
| 65 | 1 | 0 | 4.825370 | -3.286110 | 0.572848 |
| 66 | 1 | 0 | 8.563123 | 0.053264 | 2.685635 |
| 67 | 1 | 0 | 8.105076 | -3.493778 | 0.186099 |
| 68 | 1 | 0 | 6.087360 | 3.706263 | 1.789557 |

| | | | | | |
|---|---|---|---|---|---|
| 69 | 1 | 0 | -1.371342 | -0.349108 | 3.759186 |
| 70 | 1 | 0 | -0.756195 | -4.079489 | -3.011446 |
| 71 | 1 | 0 | 6.270445 | -2.853561 | -2.248082 |
| 72 | 1 | 0 | 1.903293 | 3.722668 | 2.852496 |
| 73 | 1 | 0 | 4.288442 | 4.961890 | 3.463051 |
| 74 | 1 | 0 | 5.313771 | 0.339650 | 2.951731 |
| 75 | 1 | 0 | 5.181998 | -2.348975 | 3.085595 |
| 76 | 1 | 0 | 8.368125 | 0.863652 | 0.119469 |
| 77 | 1 | 0 | 8.379695 | -2.640807 | 2.720612 |
| 78 | 1 | 0 | 4.739300 | -1.159422 | -1.090426 |
| 79 | 1 | 0 | 3.997389 | 1.796977 | -4.471469 |
| 80 | 1 | 0 | 6.165848 | 2.016888 | -0.020115 |
| 81 | 1 | 0 | 9.935325 | -1.731521 | -3.767963 |
| 82 | 1 | 0 | 10.532371 | -0.828486 | -2.365864 |
| 83 | 1 | 0 | 10.210858 | -2.573178 | -2.218610 |
| 84 | 1 | 0 | 7.275524 | -2.957546 | -3.705103 |
| 85 | 1 | 0 | 7.832985 | -3.706993 | -2.193218 |
| 86 | 1 | 0 | 1.667017 | 1.555780 | -3.001720 |
| 87 | 1 | 0 | 5.949818 | 1.873603 | -2.525618 |
| 88 | 1 | 0 | 2.318179 | -0.808889 | 1.962670 |
| 89 | 1 | 0 | 0.759542 | -1.636133 | 2.165592 |
| 90 | 1 | 0 | 1.671588 | -1.802797 | 0.645638 |
| 91 | 1 | 0 | -2.986486 | 3.403411 | 1.123122 |
| 92 | 1 | 0 | -3.018246 | 1.857292 | 2.020716 |
| 93 | 1 | 0 | -1.536612 | 2.874757 | 2.021921 |
| 94 | 1 | 0 | -2.921831 | -2.288046 | 4.950224 |
| 95 | 1 | 0 | -4.247956 | -3.426401 | 2.815359 |
| 96 | 1 | 0 | 0.167566 | -1.618210 | -2.188694 |
| 97 | 1 | 0 | -4.338818 | -3.306803 | 0.309563 |
| 98 | 1 | 0 | -5.093785 | 0.134404 | 1.594966 |
| 99 | 1 | 0 | -6.380489 | 1.859096 | -0.026699 |
| 100 | 1 | 0 | -6.175937 | 0.924670 | -2.558285 |
| 101 | 1 | 0 | -4.731469 | -1.348311 | -2.480824 |
| 102 | 1 | 0 | -8.982019 | -0.836120 | -2.191071 |
| 103 | 1 | 0 | -6.768443 | -3.594196 | 0.360487 |
| 104 | 1 | 0 | -7.445241 | -3.045517 | -2.194926 |
| 105 | 1 | 0 | -7.914312 | -1.743581 | 1.942029 |
| 106 | 1 | 0 | -10.252651 | 2.621075 | -0.337810 |
| 107 | 1 | 0 | -8.646398 | 1.997076 | -0.813673 |
| 108 | 1 | 0 | -10.124676 | 1.400086 | -1.607255 |
| 109 | 1 | 0 | -9.511880 | 2.030561 | 2.409151 |
| 110 | 1 | 0 | -8.921024 | 0.434111 | 2.878825 |
| 111 | 1 | 0 | -7.950543 | 1.435350 | 1.772185 |
| 112 | 1 | 0 | -1.225707 | 0.734577 | -3.341253 |
| 113 | 1 | 0 | -2.518893 | 0.761823 | -2.126812 |
| 114 | 1 | 0 | -3.085169 | 2.461117 | -3.793110 |

| | | | | | |
|---|---|---|---|---|---|
| 115 | 1 | 0 | -1.461262 | 3.179199 | -3.696741 |
| 116 | 1 | 0 | -3.508112 | 3.053111 | -1.412205 |
| 117 | 1 | 0 | -2.970366 | 4.526741 | -2.258277 |

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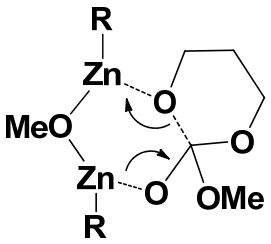


**TSII-III$^{dimer}$-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -4.578219 | 1.830268 | 0.889064 |
| 2 | 7 | 0 | -3.319366 | 1.723395 | 1.398276 |
| 3 | 6 | 0 | -3.386634 | 2.062944 | 2.696405 |
| 4 | 6 | 0 | -4.701840 | 2.375972 | 3.048124 |
| 5 | 6 | 0 | -5.420992 | 2.214520 | 1.866925 |
| 6 | 30 | 0 | -1.680314 | 1.457224 | 0.146959 |
| 7 | 8 | 0 | -0.324341 | 2.803957 | 0.772554 |
| 8 | 6 | 0 | 0.811620 | 2.966036 | 0.238458 |
| 9 | 8 | 0 | 0.904495 | 2.670814 | -1.086706 |
| 10 | 6 | 0 | 2.167408 | 2.896969 | -1.732899 |
| 11 | 5 | 0 | -4.961941 | 1.410137 | -0.576058 |
| 12 | 6 | 0 | -4.861889 | -0.190124 | -0.745281 |
| 13 | 6 | 0 | -4.660111 | -0.934342 | -1.956991 |
| 14 | 6 | 0 | -4.685707 | -2.335673 | -1.669537 |
| 15 | 6 | 0 | -4.915016 | -2.483392 | -0.267836 |
| 16 | 6 | 0 | -5.025601 | -1.172229 | 0.289343 |
| 17 | 26 | 0 | -6.497383 | -1.482316 | -1.154290 |
| 18 | 6 | 0 | -7.985875 | -2.531717 | -2.163432 |
| 19 | 6 | 0 | -7.944949 | -1.179380 | -2.619902 |
| 20 | 6 | 0 | -8.184660 | -0.331823 | -1.499689 |
| 21 | 6 | 0 | -8.389035 | -1.150321 | -0.336178 |
| 22 | 6 | 0 | -8.258982 | -2.516969 | -0.763768 |
| 23 | 15 | 0 | -8.757795 | -0.456681 | 1.318444 |
| 24 | 6 | 0 | -10.621356 | -0.645310 | 1.344708 |
| 25 | 8 | 0 | -0.639568 | -0.228947 | 0.192388 |
| 26 | 6 | 0 | -1.307036 | -1.476187 | -0.001350 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 30 | 0 | 1.317248 | -0.256442 | 0.564068 |
| 28 | 8 | 0 | 1.864061 | 1.608728 | 0.915573 |
| 29 | 6 | 0 | 2.704940 | 2.047759 | 1.974459 |
| 30 | 6 | 0 | 1.962298 | 3.078570 | 2.832194 |
| 31 | 6 | 0 | 1.614136 | 4.322939 | 2.000879 |
| 32 | 8 | 0 | 1.585565 | 4.023393 | 0.585238 |
| 33 | 7 | 0 | 1.885939 | -1.567715 | 2.089323 |
| 34 | 6 | 0 | 1.293583 | -1.899294 | 3.249425 |
| 35 | 6 | 0 | 1.911906 | -3.021325 | 3.806564 |
| 36 | 6 | 0 | 2.913021 | -3.346117 | 2.895691 |
| 37 | 7 | 0 | 2.884238 | -2.468130 | 1.875137 |
| 38 | 5 | 0 | 3.909878 | -2.370114 | 0.678227 |
| 39 | 7 | 0 | 3.113461 | -2.347543 | -0.673131 |
| 40 | 7 | 0 | 2.167645 | -1.410809 | -0.962424 |
| 41 | 6 | 0 | 1.754045 | -1.639492 | -2.220334 |
| 42 | 6 | 0 | 2.443003 | -2.725454 | -2.767493 |
| 43 | 6 | 0 | 3.290670 | -3.142437 | -1.745747 |
| 44 | 7 | 0 | -2.664559 | 2.068501 | -1.575159 |
| 45 | 7 | 0 | -4.024053 | 2.149624 | -1.597892 |
| 46 | 6 | 0 | -4.403632 | 2.866601 | -2.673019 |
| 47 | 6 | 0 | -3.272045 | 3.273210 | -3.373688 |
| 48 | 6 | 0 | -2.205386 | 2.753739 | -2.635659 |
| 49 | 6 | 0 | -8.311786 | -1.885402 | 2.432972 |
| 50 | 6 | 0 | 4.841823 | -1.067075 | 0.831646 |
| 51 | 6 | 0 | 5.708928 | -0.785106 | 1.942220 |
| 52 | 6 | 0 | 6.384362 | 0.454078 | 1.723041 |
| 53 | 6 | 0 | 5.950496 | 0.961851 | 0.461884 |
| 54 | 6 | 0 | 5.015113 | 0.028009 | -0.082573 |
| 55 | 26 | 0 | 6.859832 | -0.893670 | 0.214427 |
| 56 | 6 | 0 | 7.378458 | -2.733218 | -0.587679 |
| 57 | 6 | 0 | 8.227212 | -2.422007 | 0.514541 |
| 58 | 6 | 0 | 8.919258 | -1.212361 | 0.205562 |
| 59 | 6 | 0 | 8.512361 | -0.764130 | -1.096500 |
| 60 | 6 | 0 | 7.548170 | -1.715297 | -1.573460 |
| 61 | 15 | 0 | 9.298650 | 0.568121 | -2.079663 |
| 62 | 6 | 0 | 7.826539 | 1.304127 | -2.959013 |
| 63 | 6 | 0 | 9.582724 | 1.870648 | -0.774020 |
| 64 | 1 | 0 | 5.853232 | -1.430750 | 2.800344 |
| 65 | 1 | 0 | -8.810616 | -2.820968 | 2.153951 |
| 66 | 1 | 0 | -5.017220 | -3.418817 | 0.267447 |
| 67 | 1 | 0 | -3.231930 | 3.865776 | -4.275511 |
| 68 | 1 | 0 | 0.978339 | -1.022182 | -2.653793 |
| 69 | 1 | 0 | 3.644551 | -4.140969 | 2.903576 |
| 70 | 1 | 0 | 1.667385 | -3.528067 | 4.728149 |
| 71 | 1 | 0 | -7.229395 | -2.043154 | 2.414367 |
| 72 | 1 | 0 | -5.453099 | 3.037234 | -2.863823 |

| | | | | | |
|---|---|---|---|---|---|
| 73 | 1 | 0 | -1.139312 | 2.850466 | -2.787367 |
| 74 | 1 | 0 | -4.537533 | -0.500839 | -2.942312 |
| 75 | 1 | 0 | -4.587401 | -3.138388 | -2.389586 |
| 76 | 1 | 0 | -7.720640 | -0.855089 | -3.627833 |
| 77 | 1 | 0 | -8.163930 | 0.750165 | -1.503452 |
| 78 | 1 | 0 | -8.320009 | -3.389666 | -0.127058 |
| 79 | 1 | 0 | -7.798009 | -3.412331 | -2.764442 |
| 80 | 1 | 0 | -5.221615 | -0.945859 | 1.330112 |
| 81 | 1 | 0 | -5.079222 | 2.680660 | 4.012827 |
| 82 | 1 | 0 | -6.064325 | 1.861710 | -0.768226 |
| 83 | 1 | 0 | -11.000031 | -0.369649 | 2.335799 |
| 84 | 1 | 0 | -11.064928 | 0.038226 | 0.613368 |
| 85 | 1 | 0 | -10.944383 | -1.666589 | 1.111178 |
| 86 | 1 | 0 | -8.601761 | -1.632927 | 3.458883 |
| 87 | 1 | 0 | -2.487008 | 2.075924 | 3.297408 |
| 88 | 1 | 0 | -6.475603 | 2.324629 | 1.659564 |
| 89 | 1 | 0 | -0.588642 | -2.256044 | -0.287401 |
| 90 | 1 | 0 | -1.819445 | -1.800153 | 0.914567 |
| 91 | 1 | 0 | -2.056710 | -1.400617 | -0.796754 |
| 92 | 1 | 0 | 2.336924 | -3.153199 | -3.753253 |
| 93 | 1 | 0 | 4.008122 | -3.949096 | -1.708445 |
| 94 | 1 | 0 | 0.452937 | -1.322483 | 3.612488 |
| 95 | 1 | 0 | 4.519355 | -3.413081 | 0.702306 |
| 96 | 1 | 0 | 4.532132 | 0.115226 | -1.047369 |
| 97 | 1 | 0 | 6.284186 | 1.879177 | -0.005014 |
| 98 | 1 | 0 | 7.117933 | 0.908100 | 2.377263 |
| 99 | 1 | 0 | 9.623821 | -0.708033 | 0.854174 |
| 100 | 1 | 0 | 6.681052 | -3.558562 | -0.637769 |
| 101 | 1 | 0 | 8.299618 | -2.976673 | 1.440973 |
| 102 | 1 | 0 | 7.021963 | -1.661421 | -2.517741 |
| 103 | 1 | 0 | 9.915786 | 2.792555 | -1.263612 |
| 104 | 1 | 0 | 8.684239 | 2.075499 | -0.182888 |
| 105 | 1 | 0 | 10.383599 | 1.548964 | -0.100233 |
| 106 | 1 | 0 | 8.150715 | 2.204506 | -3.492819 |
| 107 | 1 | 0 | 7.452480 | 0.595824 | -3.705467 |
| 108 | 1 | 0 | 7.010924 | 1.559106 | -2.274892 |
| 109 | 1 | 0 | 2.064201 | 2.470992 | -2.732487 |
| 110 | 1 | 0 | 2.378712 | 3.967081 | -1.800959 |
| 111 | 1 | 0 | 2.963808 | 2.388576 | -1.185055 |
| 112 | 1 | 0 | 2.391959 | 5.086350 | 2.076721 |
| 113 | 1 | 0 | 0.655853 | 4.761415 | 2.294298 |
| 114 | 1 | 0 | 2.580670 | 3.371922 | 3.689627 |
| 115 | 1 | 0 | 1.050451 | 2.615539 | 3.222766 |
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| 117 | 1 | 0 | 3.003855 | 1.187042 | 2.584622 |

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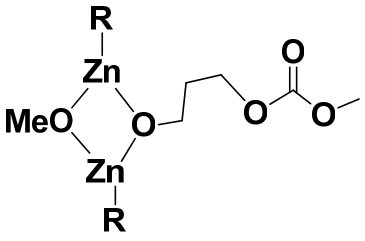


**III$^{dimer}$-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 7.014163 | -1.106044 | 0.498989 |
| 2 | 6 | 0 | 8.879169 | -1.869307 | 1.025413 |
| 3 | 6 | 0 | 8.499933 | -0.835055 | 1.933750 |
| 4 | 6 | 0 | 8.307531 | 0.359380 | 1.181154 |
| 5 | 6 | 0 | 5.313481 | -0.784169 | -0.658260 |
| 6 | 6 | 0 | 5.648071 | -2.654134 | 0.646466 |
| 7 | 7 | 0 | 3.897731 | 1.867422 | 0.053430 |
| 8 | 6 | 0 | 5.247019 | -1.572297 | 1.490516 |
| 9 | 6 | 0 | 5.026298 | -0.396097 | 0.695453 |
| 10 | 6 | 0 | 2.477640 | 2.313718 | -1.537085 |
| 11 | 7 | 0 | 2.722217 | 1.476022 | -0.514100 |
| 12 | 30 | 0 | 1.571010 | 0.027190 | 0.429466 |
| 13 | 7 | 0 | 2.379433 | 0.334327 | 2.315038 |
| 14 | 7 | 0 | 3.591076 | 0.944375 | 2.423087 |
| 15 | 5 | 0 | 4.591433 | 1.066725 | 1.214905 |
| 16 | 6 | 0 | 3.793702 | 1.299146 | 3.706092 |
| 17 | 6 | 0 | 2.689158 | 0.919673 | 4.463801 |
| 18 | 6 | 0 | 1.826513 | 0.323993 | 3.539683 |
| 19 | 30 | 0 | -0.900085 | -1.469670 | -0.397938 |
| 20 | 7 | 0 | -1.809437 | -1.721221 | -2.251157 |
| 21 | 7 | 0 | -2.998931 | -2.380719 | -2.322887 |
| 22 | 5 | 0 | -3.905292 | -2.636694 | -1.063811 |
| 23 | 6 | 0 | -4.385442 | -1.238622 | -0.421162 |
| 24 | 26 | 0 | -6.375428 | -0.504038 | -0.377109 |
| 25 | 6 | 0 | -4.981923 | 1.011376 | -0.149808 |
| 26 | 6 | 0 | -8.184329 | 0.328066 | -0.993516 |
| 27 | 6 | 0 | -8.415256 | -0.469701 | 0.177728 |
| 28 | 6 | 0 | -7.989350 | -1.802467 | -0.145277 |
| 29 | 15 | 0 | -9.359246 | 0.032015 | 1.666647 |
| 30 | 7 | 0 | -1.917070 | -3.022320 | 0.528491 |
| 31 | 7 | 0 | -3.083916 | -3.469232 | -0.011018 |
| 32 | 6 | 0 | -3.418878 | -4.638003 | 0.567494 |

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| 33 | 8 | 0 | -0.430160 | 0.267399 | 0.441625 |
| 34 | 6 | 0 | -1.215708 | 1.329351 | 0.946866 |
| 35 | 8 | 0 | 1.086753 | -1.721127 | -0.363300 |
| 36 | 6 | 0 | 1.865612 | -2.791486 | -0.859785 |
| 37 | 6 | 0 | 3.506194 | 3.251786 | -1.650924 |
| 38 | 6 | 0 | 4.383549 | 2.927285 | -0.619903 |
| 39 | 6 | 0 | 5.692119 | -2.162038 | -0.693586 |
| 40 | 6 | 0 | 8.928889 | -1.308967 | -0.285053 |
| 41 | 6 | 0 | 8.577201 | 0.082808 | -0.203058 |
| 42 | 6 | 0 | -2.449294 | -4.975136 | 1.507796 |
| 43 | 6 | 0 | -1.524134 | -3.930085 | 1.437855 |
| 44 | 6 | 0 | -3.271538 | -2.660020 | -3.611424 |
| 45 | 6 | 0 | -2.238477 | -2.179316 | -4.410946 |
| 46 | 6 | 0 | -1.342249 | -1.604986 | -3.505694 |
| 47 | 6 | 0 | -4.494228 | 0.036877 | -1.075706 |
| 48 | 6 | 0 | -5.183554 | 0.352057 | 1.100958 |
| 49 | 6 | 0 | -4.829144 | -1.021525 | 0.927999 |
| 50 | 6 | 0 | -7.520828 | -1.823672 | -1.492321 |
| 51 | 6 | 0 | -7.641716 | -0.503922 | -2.018931 |
| 52 | 15 | 0 | 8.462561 | 1.356472 | -1.515046 |
| 53 | 6 | 0 | 10.269108 | 1.825763 | -1.674626 |
| 54 | 6 | 0 | -8.406265 | -0.827640 | 3.020834 |
| 55 | 6 | 0 | -8.770537 | 1.785197 | 1.908287 |
| 56 | 6 | 0 | 8.307256 | 0.300990 | -3.046156 |
| 57 | 1 | 0 | -8.007692 | -2.650697 | 0.526906 |
| 58 | 1 | 0 | 9.056639 | -2.906470 | 1.279938 |
| 59 | 1 | 0 | 5.150697 | -1.622963 | 2.568346 |
| 60 | 1 | 0 | -5.192551 | 2.050772 | -0.366928 |
| 61 | 1 | 0 | -8.370990 | 1.390682 | -1.079169 |
| 62 | 1 | 0 | -7.332257 | -0.177767 | -3.003487 |
| 63 | 1 | 0 | -9.189351 | 2.425926 | 1.125469 |
| 64 | 1 | 0 | -7.331620 | -0.625398 | 2.974153 |
| 65 | 1 | 0 | -2.419878 | -5.848740 | 2.141693 |
| 66 | 1 | 0 | 10.391446 | 2.517394 | -2.516249 |
| 67 | 1 | 0 | -4.273298 | 0.223003 | -2.119607 |
| 68 | 1 | 0 | 7.342238 | -0.214377 | -3.042256 |
| 69 | 1 | 0 | 9.106129 | -0.444283 | -3.136588 |
| 70 | 1 | 0 | 2.535875 | 1.059620 | 5.523433 |
| 71 | 1 | 0 | 5.909536 | -3.654042 | 0.968843 |
| 72 | 1 | 0 | 8.339891 | -0.949691 | 2.998018 |
| 73 | 1 | 0 | 7.964279 | 1.308470 | 1.571578 |
| 74 | 1 | 0 | 9.158192 | -1.853766 | -1.191223 |
| 75 | 1 | 0 | 5.985974 | -2.724328 | -1.570853 |
| 76 | 1 | 0 | 5.274788 | -0.121720 | -1.514168 |
| 77 | 1 | 0 | 3.601597 | 4.050116 | -2.371478 |
| 78 | 1 | 0 | 5.494578 | 1.762625 | 1.609763 |

| | | | | | |
|---|---|---|---|---|---|
| 79 | 1 | 0 | 10.590451 | 2.343521 | -0.764955 |
| 80 | 1 | 0 | 10.918250 | 0.956256 | -1.831070 |
| 81 | 1 | 0 | 8.342184 | 0.952613 | -3.926120 |
| 82 | 1 | 0 | 1.577594 | 2.201391 | -2.126955 |
| 83 | 1 | 0 | 5.327665 | 3.365438 | -0.331040 |
| 84 | 1 | 0 | 0.843044 | -0.103046 | 3.685175 |
| 85 | 1 | 0 | 4.710395 | 1.794490 | 3.991296 |
| 86 | 1 | 0 | -0.600104 | -3.785802 | 1.982010 |
| 87 | 1 | 0 | -4.324617 | -5.147146 | 0.271714 |
| 88 | 1 | 0 | -0.390529 | -1.123196 | -3.687130 |
| 89 | 1 | 0 | -2.150858 | -2.242255 | -5.485274 |
| 90 | 1 | 0 | -4.182405 | -3.179633 | -3.870952 |
| 91 | 1 | 0 | -4.792823 | -3.366493 | -1.434883 |
| 92 | 1 | 0 | -4.902420 | -1.787495 | 1.690316 |
| 93 | 1 | 0 | -5.555737 | 0.806378 | 2.009645 |
| 94 | 1 | 0 | -7.088248 | -2.676970 | -1.997332 |
| 95 | 1 | 0 | -9.147872 | 2.152178 | 2.869168 |
| 96 | 1 | 0 | -7.679539 | 1.871905 | 1.889453 |
| 97 | 1 | 0 | -8.798153 | -0.498563 | 3.989735 |
| 98 | 1 | 0 | -8.564884 | -1.908835 | 2.952067 |
| 99 | 1 | 0 | 1.375729 | -3.754681 | -0.653080 |
| 100 | 1 | 0 | 2.010901 | -2.715100 | -1.948501 |
| 101 | 1 | 0 | 2.855836 | -2.807609 | -0.389790 |
| 102 | 6 | 0 | -1.340191 | 2.470571 | -0.068307 |
| 103 | 1 | 0 | -2.216391 | 0.958569 | 1.208146 |
| 104 | 1 | 0 | -0.760604 | 1.711101 | 1.875452 |
| 105 | 6 | 0 | -2.165131 | 3.628511 | 0.470319 |
| 106 | 1 | 0 | -0.338550 | 2.829597 | -0.336211 |
| 107 | 1 | 0 | -1.809317 | 2.085717 | -0.981913 |
| 108 | 8 | 0 | -2.228265 | 4.633541 | -0.566911 |
| 109 | 1 | 0 | -3.182147 | 3.316914 | 0.727106 |
| 110 | 1 | 0 | -1.714557 | 4.073229 | 1.364845 |
| 111 | 6 | 0 | -2.981045 | 5.702547 | -0.276235 |
| 112 | 8 | 0 | -2.930724 | 6.540440 | -1.325185 |
| 113 | 6 | 0 | -3.697713 | 7.741740 | -1.163761 |
| 114 | 1 | 0 | -3.551412 | 8.303693 | -2.086762 |
| 115 | 1 | 0 | -4.756606 | 7.508923 | -1.021221 |
| 116 | 1 | 0 | -3.340697 | 8.316566 | -0.304820 |
| 117 | 8 | 0 | -3.601343 | 5.887161 | 0.749234 |

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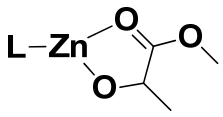

**Cat$^{monomer}$- propagation**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.500633 | 1.259161 | -0.657368 |
| 2 | 6 | 0 | -2.303585 | 0.482252 | -1.847928 |
| 3 | 6 | 0 | -3.523680 | -0.161665 | -2.217586 |
| 4 | 6 | 0 | -4.506809 | 0.199215 | -1.248142 |
| 5 | 6 | 0 | -3.874480 | 1.054802 | -0.294667 |
| 6 | 26 | 0 | -2.954847 | -0.806431 | -0.332337 |
| 7 | 6 | 0 | -2.079444 | -1.486379 | 1.420681 |
| 8 | 6 | 0 | -3.462943 | -1.816816 | 1.424989 |
| 9 | 6 | 0 | -3.729294 | -2.642043 | 0.291303 |
| 10 | 6 | 0 | -2.508441 | -2.833282 | -0.416993 |
| 11 | 6 | 0 | -1.471999 | -2.116225 | 0.276958 |
| 12 | 15 | 0 | 0.273559 | -1.941923 | -0.153032 |
| 13 | 30 | 0 | 1.334808 | 0.340823 | 0.421472 |
| 14 | 8 | 0 | 3.177396 | -0.353507 | -1.017295 |
| 15 | 6 | 0 | 4.169063 | -0.362434 | -0.290240 |
| 16 | 8 | 0 | 5.394846 | -0.616845 | -0.760283 |
| 17 | 6 | 0 | 5.508160 | -0.877077 | -2.170351 |
| 18 | 5 | 0 | -1.505259 | 2.358595 | -0.010828 |
| 19 | 7 | 0 | -1.036148 | 2.087331 | 1.455685 |
| 20 | 7 | 0 | -0.027746 | 1.240874 | 1.789330 |
| 21 | 6 | 0 | 0.103219 | 1.283121 | 3.124605 |
| 22 | 6 | 0 | -0.845052 | 2.151694 | 3.677355 |
| 23 | 6 | 0 | -1.537830 | 2.645257 | 2.577098 |
| 24 | 7 | 0 | -0.254220 | 2.603201 | -0.928547 |
| 25 | 7 | 0 | 0.796475 | 1.745616 | -1.070030 |
| 26 | 6 | 0 | 1.567888 | 2.228186 | -2.059076 |
| 27 | 6 | 0 | 1.017571 | 3.402592 | -2.579807 |
| 28 | 6 | 0 | -0.135998 | 3.599305 | -1.829119 |
| 29 | 6 | 0 | 0.381974 | -2.413367 | -1.935957 |
| 30 | 6 | 0 | 1.100401 | -3.383507 | 0.673059 |
| 31 | 8 | 0 | 2.858342 | 0.282023 | 1.616390 |
| 32 | 6 | 0 | 4.116234 | -0.075074 | 1.217226 |
| 33 | 6 | 0 | 4.656686 | -1.302067 | 1.989122 |
| 34 | 1 | 0 | -2.392031 | -3.391905 | -1.336025 |
| 35 | 1 | 0 | 0.890218 | 0.711179 | 3.596907 |
| 36 | 1 | 0 | 1.401561 | 4.023687 | -3.375450 |
| 37 | 1 | 0 | 2.472935 | 1.703138 | -2.329460 |
| 38 | 1 | 0 | -0.886035 | 4.375185 | -1.876270 |
| 39 | 1 | 0 | -4.357156 | 1.478914 | 0.577863 |
| 40 | 1 | 0 | -5.531781 | -0.148679 | -1.216793 |

| | | | | | |
|---|---|---|---|---|---|
| 41 | 1 | 0 | -4.195448 | -1.458946 | 2.136418 |
| 42 | 1 | 0 | -1.575736 | -0.839357 | 2.124935 |
| 43 | 1 | 0 | -4.698570 | -3.020490 | -0.006600 |
| 44 | 1 | 0 | -3.669578 | -0.827038 | -3.059449 |
| 45 | 1 | 0 | -1.366067 | 0.408385 | -2.384522 |
| 46 | 1 | 0 | -0.991908 | 2.404663 | 4.717006 |
| 47 | 1 | 0 | -2.084322 | 3.422276 | 0.030102 |
| 48 | 1 | 0 | -2.342118 | 3.363713 | 2.511990 |
| 49 | 1 | 0 | 0.640656 | -4.332862 | 0.378315 |
| 50 | 1 | 0 | 2.162452 | -3.397621 | 0.406368 |
| 51 | 1 | 0 | 1.022098 | -3.272964 | 1.758646 |
| 52 | 1 | 0 | 0.019735 | -3.431551 | -2.113785 |
| 53 | 1 | 0 | -0.206694 | -1.713986 | -2.534427 |
| 54 | 1 | 0 | 1.427978 | -2.344367 | -2.248682 |
| 55 | 1 | 0 | 4.849816 | 0.744860 | 1.367654 |
| 56 | 1 | 0 | 5.682960 | -1.556295 | 1.702751 |
| 57 | 1 | 0 | 4.631077 | -1.069139 | 3.057489 |
| 58 | 1 | 0 | 4.010714 | -2.171873 | 1.819632 |
| 59 | 1 | 0 | 6.567739 | -1.061367 | -2.348107 |
| 60 | 1 | 0 | 4.914911 | -1.752065 | -2.448840 |
| 61 | 1 | 0 | 5.168046 | -0.013526 | -2.747988 |

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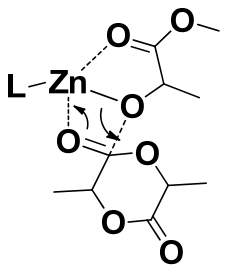


**TSI-II$^{monomer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.044848 | 1.757159 | -1.555872 |
| 2 | 6 | 0 | -4.861061 | 0.877797 | -2.322956 |
| 3 | 6 | 0 | -4.057205 | -0.225473 | -2.739997 |
| 4 | 6 | 0 | -2.743003 | -0.035882 | -2.228794 |
| 5 | 6 | 0 | -2.720296 | 1.198024 | -1.489596 |
| 6 | 26 | 0 | -4.097444 | -0.115634 | -0.655717 |
| 7 | 6 | 0 | -4.403639 | -2.017555 | 0.116186 |
| 8 | 6 | 0 | -3.427369 | -1.367238 | 0.942295 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | -4.073916 | -0.185527 | 1.437389 |
| 10 | 6 | 0 | -5.413551 | -0.123117 | 0.947680 |
| 11 | 6 | 0 | -5.621094 | -1.269855 | 0.124563 |
| 12 | 5 | 0 | -2.014844 | -1.994246 | 1.414315 |
| 13 | 7 | 0 | -1.293564 | -1.081094 | 2.463229 |
| 14 | 7 | 0 | -0.594723 | 0.055563 | 2.185973 |
| 15 | 6 | 0 | -0.306285 | 0.636282 | 3.362046 |
| 16 | 6 | 0 | -0.838016 | -0.106483 | 4.419857 |
| 17 | 6 | 0 | -1.450844 | -1.188688 | 3.798710 |
| 18 | 30 | 0 | 0.601624 | 0.177243 | 0.437052 |
| 19 | 8 | 0 | 1.500883 | 2.304152 | 0.855966 |
| 20 | 6 | 0 | 2.468374 | 2.588652 | 0.156605 |
| 21 | 8 | 0 | 3.088491 | 3.765786 | 0.225942 |
| 22 | 6 | 0 | 2.582856 | 4.716599 | 1.185541 |
| 23 | 15 | 0 | -1.230451 | 1.904787 | -0.737472 |
| 24 | 6 | 0 | -0.768686 | 3.201471 | -1.996391 |
| 25 | 8 | 0 | 2.265121 | -0.641756 | 1.442532 |
| 26 | 6 | 0 | 3.154536 | -0.730101 | 0.545789 |
| 27 | 6 | 0 | 4.565019 | -0.274870 | 0.919959 |
| 28 | 8 | 0 | 5.482275 | -0.290765 | -0.201102 |
| 29 | 6 | 0 | 5.291653 | -1.123740 | -1.249306 |
| 30 | 6 | 0 | 4.040594 | -2.002418 | -1.296389 |
| 31 | 8 | 0 | 3.181132 | -1.921929 | -0.157147 |
| 32 | 6 | 0 | 5.121626 | -1.136597 | 2.051584 |
| 33 | 6 | 0 | 4.411909 | -3.470387 | -1.495945 |
| 34 | 8 | 0 | 6.092155 | -1.136623 | -2.155108 |
| 35 | 8 | 0 | 2.563605 | 0.355255 | -0.734842 |
| 36 | 6 | 0 | 3.090830 | 1.643844 | -0.876273 |
| 37 | 6 | 0 | 2.870995 | 2.164430 | -2.307655 |
| 38 | 7 | 0 | -0.229932 | -1.562684 | -0.445615 |
| 39 | 7 | 0 | -1.065293 | -2.397226 | 0.230076 |
| 40 | 6 | 0 | -1.103138 | -3.589602 | -0.399356 |
| 41 | 6 | 0 | -0.278571 | -3.542332 | -1.518193 |
| 42 | 6 | 0 | 0.254100 | -2.250270 | -1.491817 |
| 43 | 6 | 0 | -1.872515 | 2.991899 | 0.618488 |
| 44 | 1 | 0 | -1.029113 | 3.539739 | 1.049951 |
| 45 | 1 | 0 | -4.376490 | 2.672079 | -1.083131 |
| 46 | 1 | 0 | 0.974987 | -1.783609 | -2.148587 |
| 47 | 1 | 0 | -0.776545 | 0.099246 | 5.478219 |
| 48 | 1 | 0 | 0.284526 | 1.542274 | 3.378906 |
| 49 | 1 | 0 | -1.996581 | -2.024006 | 4.212350 |
| 50 | 1 | 0 | -4.237863 | -2.929183 | -0.445175 |
| 51 | 1 | 0 | -6.520066 | -1.502963 | -0.432406 |
| 52 | 1 | 0 | -4.399987 | -1.084671 | -3.301704 |
| 53 | 1 | 0 | -1.914376 | -0.722544 | -2.327567 |
| 54 | 1 | 0 | -5.919432 | 1.001584 | -2.513675 |

| | | | | | |
|---|---|---|---|---|---|
| 55 | 1 | 0 | -6.128247 | 0.669216 | 1.132242 |
| 56 | 1 | 0 | -3.611470 | 0.545073 | 2.088929 |
| 57 | 1 | 0 | -0.082368 | -4.332154 | -2.228167 |
| 58 | 1 | 0 | -2.238431 | -3.031181 | 2.001545 |
| 59 | 1 | 0 | -1.713808 | -4.389308 | -0.006131 |
| 60 | 1 | 0 | -1.613632 | 3.869083 | -2.196788 |
| 61 | 1 | 0 | 0.076283 | 3.798256 | -1.636747 |
| 62 | 1 | 0 | -0.478720 | 2.720870 | -2.935739 |
| 63 | 1 | 0 | -2.618002 | 3.708462 | 0.258047 |
| 64 | 1 | 0 | -2.314500 | 2.371516 | 1.400204 |
| 65 | 1 | 0 | 3.255620 | 3.182918 | -2.423386 |
| 66 | 1 | 0 | 3.402970 | 1.507830 | -3.001547 |
| 67 | 1 | 0 | 1.808897 | 2.149618 | -2.565190 |
| 68 | 1 | 0 | 3.253784 | 5.572746 | 1.123528 |
| 69 | 1 | 0 | 1.561860 | 5.009932 | 0.928669 |
| 70 | 1 | 0 | 2.596203 | 4.285188 | 2.189029 |
| 71 | 1 | 0 | 4.173444 | 1.658419 | -0.693979 |
| 72 | 1 | 0 | 3.480612 | -1.642128 | -2.168469 |
| 73 | 1 | 0 | 5.019935 | -3.579102 | -2.396994 |
| 74 | 1 | 0 | 4.977009 | -3.848523 | -0.637762 |
| 75 | 1 | 0 | 3.498797 | -4.064232 | -1.595271 |
| 76 | 1 | 0 | 4.536186 | 0.768741 | 1.241927 |
| 77 | 1 | 0 | 6.142066 | -0.820105 | 2.287855 |
| 78 | 1 | 0 | 4.492178 | -1.029816 | 2.938538 |
| 79 | 1 | 0 | 5.134627 | -2.191662 | 1.761570 |

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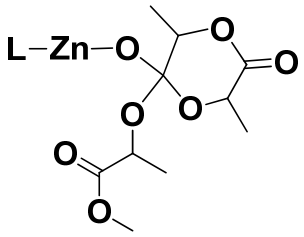


**II$^{monomer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.310689 | -2.645679 | 1.750021 |
| 2 | 7 | 0 | -0.725151 | -1.385975 | 1.531301 |
| 3 | 7 | 0 | -1.849018 | -1.197081 | 2.275602 |
| 4 | 6 | 0 | -2.131789 | -2.333204 | 2.943536 |
| 5 | 6 | 0 | -1.176505 | -3.295493 | 2.633618 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 30 | 0 | 0.255078 | 0.196017 | 0.552166 |
| 7 | 8 | 0 | 2.158244 | 0.486149 | 0.934737 |
| 8 | 6 | 0 | 3.031826 | -0.338071 | 0.378426 |
| 9 | 6 | 0 | 4.094608 | -0.846130 | 1.378931 |
| 10 | 8 | 0 | 4.980341 | -1.819530 | 0.760264 |
| 11 | 6 | 0 | 4.599937 | -2.570970 | -0.289616 |
| 12 | 6 | 0 | 3.197340 | -2.392233 | -0.884256 |
| 13 | 8 | 0 | 2.358958 | -1.495890 | -0.144560 |
| 14 | 8 | 0 | 3.710722 | 0.222952 | -0.779297 |
| 15 | 6 | 0 | 4.196473 | 1.536664 | -0.617890 |
| 16 | 6 | 0 | 5.344045 | 1.733311 | -1.615368 |
| 17 | 6 | 0 | 3.504420 | -1.442658 | 2.649332 |
| 18 | 8 | 0 | 5.371346 | -3.369133 | -0.772600 |
| 19 | 6 | 0 | 2.489643 | -3.739984 | -0.993062 |
| 20 | 5 | 0 | -2.717054 | 0.111918 | 2.283245 |
| 21 | 7 | 0 | -1.788445 | 1.355695 | 2.500531 |
| 22 | 7 | 0 | -0.694470 | 1.647030 | 1.744093 |
| 23 | 6 | 0 | -0.192277 | 2.805327 | 2.203414 |
| 24 | 6 | 0 | -0.973984 | 3.291414 | 3.255267 |
| 25 | 6 | 0 | -1.971436 | 2.334811 | 3.409016 |
| 26 | 6 | 0 | -3.702759 | 0.299243 | 1.017480 |
| 27 | 6 | 0 | -4.863572 | -0.497835 | 0.736474 |
| 28 | 6 | 0 | -5.645301 | 0.126986 | -0.282783 |
| 29 | 6 | 0 | -4.966911 | 1.320272 | -0.672491 |
| 30 | 6 | 0 | -3.781199 | 1.414630 | 0.117703 |
| 31 | 26 | 0 | -3.777372 | -0.339988 | -1.026690 |
| 32 | 6 | 0 | -2.034090 | -0.579352 | -2.123124 |
| 33 | 6 | 0 | -3.134051 | -0.285218 | -3.001664 |
| 34 | 6 | 0 | -4.112114 | -1.308345 | -2.845451 |
| 35 | 6 | 0 | -3.630256 | -2.243143 | -1.880994 |
| 36 | 6 | 0 | -2.356453 | -1.799299 | -1.430551 |
| 37 | 15 | 0 | -0.518869 | 0.370768 | -1.854901 |
| 38 | 6 | 0 | -0.904828 | 2.070645 | -2.456185 |
| 39 | 6 | 0 | 0.696213 | -0.244904 | -3.103620 |
| 40 | 6 | 0 | 3.107054 | 2.574587 | -0.892614 |
| 41 | 8 | 0 | 3.347790 | 3.707303 | -0.201937 |
| 42 | 6 | 0 | 2.473082 | 4.812603 | -0.479682 |
| 43 | 8 | 0 | 2.195193 | 2.454964 | -1.685273 |
| 44 | 1 | 0 | 0.005494 | 2.668486 | -2.374543 |
| 45 | 1 | 0 | -3.221591 | 0.578494 | -3.646782 |
| 46 | 1 | 0 | 0.589282 | -2.999574 | 1.268167 |
| 47 | 1 | 0 | -0.831058 | 4.193836 | 3.830780 |
| 48 | 1 | 0 | 0.716173 | 3.204112 | 1.772401 |
| 49 | 1 | 0 | -2.798296 | 2.281216 | 4.101889 |
| 50 | 1 | 0 | -5.108385 | -1.435431 | 1.221247 |
| 51 | 1 | 0 | -6.560430 | -0.257830 | -0.715054 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 1 | 0 | -4.161726 | -3.112666 | -1.517176 |
| 53 | 1 | 0 | -1.750772 | -2.269097 | -0.669077 |
| 54 | 1 | 0 | -5.073754 | -1.344080 | -3.340951 |
| 55 | 1 | 0 | -5.277118 | 2.007875 | -1.449278 |
| 56 | 1 | 0 | -3.051084 | 2.211975 | 0.059001 |
| 57 | 1 | 0 | -1.111980 | -4.306605 | 3.007146 |
| 58 | 1 | 0 | -3.387991 | 0.035050 | 3.288340 |
| 59 | 1 | 0 | -2.989324 | -2.374882 | 3.599129 |
| 60 | 1 | 0 | 0.322218 | -0.098604 | -4.122430 |
| 61 | 1 | 0 | 1.633193 | 0.300864 | -2.961685 |
| 62 | 1 | 0 | 0.876040 | -1.310742 | -2.939018 |
| 63 | 1 | 0 | -1.235085 | 2.053923 | -3.500276 |
| 64 | 1 | 0 | -1.691440 | 2.511541 | -1.839169 |
| 65 | 1 | 0 | 5.755437 | 2.745146 | -1.540134 |
| 66 | 1 | 0 | 6.135751 | 1.009356 | -1.403017 |
| 67 | 1 | 0 | 4.985985 | 1.568879 | -2.636547 |
| 68 | 1 | 0 | 2.857534 | 5.645457 | 0.109623 |
| 69 | 1 | 0 | 2.486887 | 5.056271 | -1.545385 |
| 70 | 1 | 0 | 1.448003 | 4.576495 | -0.180751 |
| 71 | 1 | 0 | 4.562935 | 1.709156 | 0.400367 |
| 72 | 1 | 0 | 3.358063 | -1.981671 | -1.888680 |
| 73 | 1 | 0 | 3.095737 | -4.421885 | -1.593474 |
| 74 | 1 | 0 | 2.342969 | -4.187178 | -0.003913 |
| 75 | 1 | 0 | 1.511226 | -3.613616 | -1.467890 |
| 76 | 1 | 0 | 4.758333 | -0.017470 | 1.642952 |
| 77 | 1 | 0 | 4.307751 | -1.819793 | 3.289820 |
| 78 | 1 | 0 | 2.941175 | -0.679270 | 3.191585 |
| 79 | 1 | 0 | 2.827776 | -2.269734 | 2.414458 |

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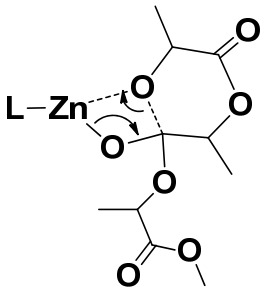


**TSII-III$^{monomer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.733163 | -2.074773 | 0.678073 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -4.105418 | -2.438658 | 0.769414 |
| 3 | 6 | 0 | -4.617726 | -2.583345 | -0.554786 |
| 4 | 6 | 0 | -3.560894 | -2.315901 | -1.471500 |
| 5 | 6 | 0 | -2.379989 | -1.997092 | -0.714499 |
| 6 | 26 | 0 | -3.898461 | -0.645441 | -0.283251 |
| 7 | 6 | 0 | -4.647090 | 0.905216 | 0.881851 |
| 8 | 6 | 0 | -3.402711 | 1.352532 | 0.323553 |
| 9 | 6 | 0 | -3.568392 | 1.256625 | -1.098836 |
| 10 | 6 | 0 | -4.883189 | 0.791703 | -1.405407 |
| 11 | 6 | 0 | -5.558729 | 0.575006 | -0.167342 |
| 12 | 5 | 0 | -2.206189 | 2.081826 | 1.131696 |
| 13 | 7 | 0 | -1.442843 | 1.160891 | 2.148249 |
| 14 | 7 | 0 | -0.503572 | 0.241278 | 1.804181 |
| 15 | 6 | 0 | -0.199051 | -0.452760 | 2.913147 |
| 16 | 6 | 0 | -0.952849 | 0.010872 | 3.996965 |
| 17 | 6 | 0 | -1.722184 | 1.039281 | 3.461925 |
| 18 | 30 | 0 | 0.496805 | 0.262353 | -0.076020 |
| 19 | 8 | 0 | 1.891393 | 0.082795 | -2.050692 |
| 20 | 6 | 0 | 2.931759 | -0.223045 | -1.457601 |
| 21 | 8 | 0 | 3.133298 | -1.572547 | -1.244226 |
| 22 | 6 | 0 | 3.984247 | -2.058546 | -0.207530 |
| 23 | 6 | 0 | 3.227067 | -2.136236 | 1.124244 |
| 24 | 8 | 0 | 4.070843 | -1.845825 | 2.133633 |
| 25 | 6 | 0 | 3.552296 | -2.011850 | 3.464240 |
| 26 | 15 | 0 | -0.731920 | -1.576674 | -1.332888 |
| 27 | 6 | 0 | 0.132568 | -3.203660 | -1.495269 |
| 28 | 7 | 0 | -1.200304 | 2.779471 | 0.154777 |
| 29 | 7 | 0 | -0.271904 | 2.131617 | -0.607696 |
| 30 | 6 | 0 | 0.247678 | 3.034816 | -1.456973 |
| 31 | 6 | 0 | -0.354724 | 4.280855 | -1.265687 |
| 32 | 6 | 0 | -1.262115 | 4.069450 | -0.234577 |
| 33 | 8 | 0 | 2.475391 | 0.314684 | 0.441100 |
| 34 | 6 | 0 | 3.207305 | 1.395975 | 0.969749 |
| 35 | 6 | 0 | 3.447373 | 2.472517 | -0.104868 |
| 36 | 8 | 0 | 3.312758 | 3.659196 | 0.067018 |
| 37 | 6 | 0 | 2.558364 | 2.016949 | 2.206454 |
| 38 | 6 | 0 | -0.996521 | -1.094511 | -3.094280 |
| 39 | 6 | 0 | 4.177313 | 0.662703 | -1.558122 |
| 40 | 8 | 0 | 3.828261 | 2.034941 | -1.344475 |
| 41 | 6 | 0 | 4.769631 | 0.577972 | -2.963117 |
| 42 | 6 | 0 | 4.440139 | -3.459774 | -0.617711 |
| 43 | 8 | 0 | 2.089957 | -2.530976 | 1.270917 |
| 44 | 1 | 0 | -0.461085 | -3.901990 | -2.094585 |
| 45 | 1 | 0 | 4.990184 | -3.412423 | -1.562158 |
| 46 | 1 | 0 | 4.207438 | 1.025807 | 1.268240 |
| 47 | 1 | 0 | -3.643969 | -2.319332 | -2.549990 |

| | | | | | |
|---|---|---|---|---|---|
| 48 | 1 | 0 | 0.536709 | -1.243953 | 2.856629 |
| 49 | 1 | 0 | -0.145161 | 5.205308 | -1.782353 |
| 50 | 1 | 0 | 1.038196 | 2.738226 | -2.132424 |
| 51 | 1 | 0 | -1.954711 | 4.744480 | 0.246642 |
| 52 | 1 | 0 | -4.862647 | 0.825209 | 1.940843 |
| 53 | 1 | 0 | -6.562271 | 0.186837 | -0.045723 |
| 54 | 1 | 0 | -4.673313 | -2.538318 | 1.685103 |
| 55 | 1 | 0 | -2.075580 | -1.859497 | 1.507759 |
| 56 | 1 | 0 | -5.642305 | -2.810934 | -0.819450 |
| 57 | 1 | 0 | -5.283216 | 0.602859 | -2.393807 |
| 58 | 1 | 0 | -2.808208 | 1.511568 | -1.826377 |
| 59 | 1 | 0 | -0.937232 | -0.337089 | 5.019332 |
| 60 | 1 | 0 | -2.674565 | 2.973420 | 1.804988 |
| 61 | 1 | 0 | -2.447679 | 1.693174 | 3.923610 |
| 62 | 1 | 0 | 1.105222 | -3.034611 | -1.964426 |
| 63 | 1 | 0 | 0.304451 | -3.621551 | -0.500434 |
| 64 | 1 | 0 | -1.448442 | -1.907957 | -3.671628 |
| 65 | 1 | 0 | -1.643575 | -0.215083 | -3.143643 |
| 66 | 1 | 0 | -0.022493 | -0.840490 | -3.519516 |
| 67 | 1 | 0 | 4.853708 | -1.414218 | -0.065002 |
| 68 | 1 | 0 | 5.094422 | -3.885448 | 0.149970 |
| 69 | 1 | 0 | 3.572896 | -4.113803 | -0.746046 |
| 70 | 1 | 0 | 4.408937 | -1.897071 | 4.128908 |
| 71 | 1 | 0 | 2.804687 | -1.243281 | 3.675549 |
| 72 | 1 | 0 | 3.101237 | -3.000553 | 3.579749 |
| 73 | 1 | 0 | 4.931167 | 0.371352 | -0.821587 |
| 74 | 1 | 0 | 3.192962 | 2.808528 | 2.615235 |
| 75 | 1 | 0 | 1.587128 | 2.455621 | 1.961041 |
| 76 | 1 | 0 | 2.410168 | 1.245409 | 2.967381 |
| 77 | 1 | 0 | 5.641952 | 1.233474 | -3.038110 |
| 78 | 1 | 0 | 5.075623 | -0.449168 | -3.187253 |
| 79 | 1 | 0 | 4.024128 | 0.892465 | -3.698325 |

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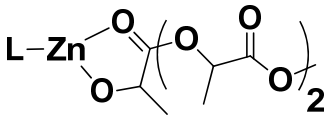


**III$^{monomer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.063621 | 0.973258 | 2.133342 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 7 | 0 | -1.192981 | -0.291779 | 2.621437 |
| 3 | 6 | 0 | -1.166928 | -0.250261 | 3.969113 |
| 4 | 6 | 0 | -1.009942 | 1.067732 | 4.382621 |
| 5 | 6 | 0 | -0.942614 | 1.793842 | 3.189989 |
| 6 | 5 | 0 | -1.534223 | -1.559076 | 1.762386 |
| 7 | 7 | 0 | -0.496391 | -1.718212 | 0.589441 |
| 8 | 7 | 0 | -0.068627 | -0.724392 | -0.235130 |
| 9 | 6 | 0 | 0.781499 | -1.276735 | -1.115087 |
| 10 | 6 | 0 | 0.900899 | -2.651529 | -0.880691 |
| 11 | 6 | 0 | 0.076408 | -2.880577 | 0.216200 |
| 12 | 30 | 0 | -0.445073 | 1.337382 | 0.153539 |
| 13 | 8 | 0 | 1.818684 | 1.455042 | 0.697521 |
| 14 | 6 | 0 | 2.267123 | 2.486626 | 0.207443 |
| 15 | 8 | 0 | 3.572779 | 2.782559 | 0.247437 |
| 16 | 6 | 0 | 4.432265 | 1.791459 | 0.844485 |
| 17 | 6 | 0 | 5.852880 | 2.345717 | 0.798983 |
| 18 | 6 | 0 | -3.096104 | -1.580668 | 1.344194 |
| 19 | 6 | 0 | -3.840269 | -2.737859 | 0.932232 |
| 20 | 6 | 0 | -5.235793 | -2.433294 | 0.904602 |
| 21 | 6 | 0 | -5.383056 | -1.065792 | 1.284584 |
| 22 | 6 | 0 | -4.076443 | -0.550801 | 1.544486 |
| 23 | 26 | 0 | -4.230171 | -1.219877 | -0.430436 |
| 24 | 6 | 0 | -4.031253 | -1.985885 | -2.362555 |
| 25 | 6 | 0 | -5.275494 | -1.298845 | -2.234267 |
| 26 | 6 | 0 | -5.001804 | 0.053922 | -1.879037 |
| 27 | 6 | 0 | -3.577031 | 0.212523 | -1.776398 |
| 28 | 6 | 0 | -2.985050 | -1.064338 | -2.077258 |
| 29 | 15 | 0 | -2.604829 | 1.665960 | -1.306518 |
| 30 | 6 | 0 | -2.180785 | 2.479485 | -2.917287 |
| 31 | 8 | 0 | 0.069393 | 3.108205 | -0.490192 |
| 32 | 6 | 0 | 1.380157 | 3.519883 | -0.494032 |
| 33 | 6 | 0 | 1.915796 | 3.777581 | -1.919748 |
| 34 | 6 | 0 | -3.836805 | 2.850140 | -0.599499 |
| 35 | 6 | 0 | 4.343666 | 0.481881 | 0.060581 |
| 36 | 8 | 0 | 4.087484 | 0.383880 | -1.116849 |
| 37 | 8 | 0 | 4.654185 | -0.549265 | 0.873379 |
| 38 | 6 | 0 | 4.756811 | -1.836306 | 0.248013 |
| 39 | 6 | 0 | 4.731147 | -2.881782 | 1.359721 |
| 40 | 6 | 0 | 6.055049 | -1.887522 | -0.560943 |
| 41 | 8 | 0 | 6.952718 | -1.079711 | -0.496744 |
| 42 | 8 | 0 | 6.067436 | -2.985462 | -1.339843 |
| 43 | 6 | 0 | 7.250467 | -3.162034 | -2.140072 |
| 44 | 1 | 0 | -3.316226 | 3.784944 | -0.369214 |
| 45 | 1 | 0 | -3.852269 | 0.463493 | 1.850593 |
| 46 | 1 | 0 | -3.073499 | 2.793401 | -3.469168 |
| 47 | 1 | 0 | 3.787508 | -2.810476 | 1.907712 |

| | | | | | |
|---|---|---|---|---|---|
| 48 | 1 | 0 | 1.522593 | 4.457554 | 0.083379 |
| 49 | 1 | 0 | -5.743074 | 0.817566 | -1.685083 |
| 50 | 1 | 0 | 1.283571 | -0.658644 | -1.847468 |
| 51 | 1 | 0 | -0.946941 | 1.439683 | 5.394450 |
| 52 | 1 | 0 | -0.802431 | 2.855516 | 3.033418 |
| 53 | 1 | 0 | -1.271006 | -1.161629 | 4.539434 |
| 54 | 1 | 0 | -3.407805 | -3.697621 | 0.674972 |
| 55 | 1 | 0 | -6.032334 | -3.103100 | 0.605495 |
| 56 | 1 | 0 | -3.905370 | -3.036576 | -2.589174 |
| 57 | 1 | 0 | -1.928232 | -1.288393 | -2.049311 |
| 58 | 1 | 0 | -6.258901 | -1.737355 | -2.345846 |
| 59 | 1 | 0 | -6.312244 | -0.511835 | 1.331815 |
| 60 | 1 | 0 | 1.495926 | -3.371580 | -1.423172 |
| 61 | 1 | 0 | -1.315645 | -2.503350 | 2.489770 |
| 62 | 1 | 0 | -0.138649 | -3.788456 | 0.760612 |
| 63 | 1 | 0 | -1.542038 | 3.339350 | -2.698551 |
| 64 | 1 | 0 | -1.611902 | 1.778016 | -3.535728 |
| 65 | 1 | 0 | -4.653551 | 3.062977 | -1.297939 |
| 66 | 1 | 0 | -4.253466 | 2.444792 | 0.326509 |
| 67 | 1 | 0 | 3.913083 | -1.973731 | -0.433233 |
| 68 | 1 | 0 | 4.816829 | -3.883464 | 0.929799 |
| 69 | 1 | 0 | 5.557944 | -2.722752 | 2.059229 |
| 70 | 1 | 0 | 7.088258 | -4.082090 | -2.701707 |
| 71 | 1 | 0 | 7.380117 | -2.313969 | -2.817021 |
| 72 | 1 | 0 | 8.134091 | -3.249756 | -1.502511 |
| 73 | 1 | 0 | 4.107204 | 1.604913 | 1.871113 |
| 74 | 1 | 0 | 2.943230 | 4.155625 | -1.912805 |
| 75 | 1 | 0 | 1.884865 | 2.853575 | -2.508182 |
| 76 | 1 | 0 | 1.266746 | 4.514284 | -2.402450 |
| 77 | 1 | 0 | 5.914892 | 3.268332 | 1.383384 |
| 78 | 1 | 0 | 6.550126 | 1.609924 | 1.209129 |
| 79 | 1 | 0 | 6.139926 | 2.558658 | -0.234760 |

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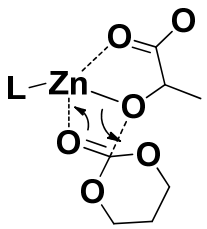


**TSI-II$^{monomer}$- propagation-TMC**

Standard orientation:

---

| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.597896 | 2.063711 | -1.416935 |
| 2 | 6 | 0 | -4.546486 | 1.295644 | -2.151389 |
| 3 | 6 | 0 | -3.891947 | 0.120709 | -2.629861 |
| 4 | 6 | 0 | -2.539500 | 0.154521 | -2.188538 |
| 5 | 6 | 0 | -2.341317 | 1.362264 | -1.433359 |
| 6 | 26 | 0 | -3.810592 | 0.188149 | -0.546582 |
| 7 | 6 | 0 | -3.659991 | 0.051934 | 1.538469 |
| 8 | 6 | 0 | -3.200676 | -1.183517 | 0.971165 |
| 9 | 6 | 0 | -4.304293 | -1.681969 | 0.201309 |
| 10 | 6 | 0 | -5.414528 | -0.789408 | 0.310474 |
| 11 | 6 | 0 | -5.010160 | 0.295909 | 1.143637 |
| 12 | 5 | 0 | -1.847550 | -1.995374 | 1.323590 |
| 13 | 7 | 0 | -0.998070 | -2.406633 | 0.067488 |
| 14 | 7 | 0 | -0.090072 | -1.627209 | -0.580517 |
| 15 | 6 | 0 | 0.256765 | -2.275619 | -1.703167 |
| 16 | 6 | 0 | -0.439287 | -3.483487 | -1.807005 |
| 17 | 6 | 0 | -1.215341 | -3.525319 | -0.653962 |
| 18 | 30 | 0 | 0.957169 | -0.040309 | 0.374035 |
| 19 | 8 | 0 | 2.964880 | 0.090674 | -0.954901 |
| 20 | 6 | 0 | 3.638001 | 1.306760 | -0.816077 |
| 21 | 6 | 0 | 3.639720 | 2.074699 | -2.149179 |
| 22 | 15 | 0 | -0.750548 | 1.872070 | -0.728064 |
| 23 | 6 | 0 | -1.222914 | 3.044244 | 0.627313 |
| 24 | 8 | 0 | 2.645362 | -0.931415 | 1.171523 |
| 25 | 6 | 0 | 3.417210 | -1.122411 | 0.184444 |
| 26 | 8 | 0 | 4.763579 | -0.911415 | 0.456566 |
| 27 | 6 | 0 | 5.742966 | -1.278031 | -0.526202 |
| 28 | 6 | 0 | 5.442016 | -2.635683 | -1.144273 |
| 29 | 6 | 0 | 4.002726 | -2.597654 | -1.636103 |
| 30 | 8 | 0 | 3.139059 | -2.263546 | -0.549341 |
| 31 | 8 | 0 | 1.976831 | 1.937783 | 0.875340 |
| 32 | 6 | 0 | 3.037364 | 2.164910 | 0.301763 |
| 33 | 8 | 0 | 3.796784 | 3.219739 | 0.596767 |
| 34 | 6 | 0 | 3.338935 | 4.075579 | 1.662239 |
| 35 | 7 | 0 | -0.184141 | -0.170737 | 2.157648 |
| 36 | 7 | 0 | -0.986967 | -1.246256 | 2.394046 |
| 37 | 6 | 0 | -1.094392 | -1.434367 | 3.725563 |
| 38 | 6 | 0 | -0.341558 | -0.469923 | 4.385211 |
| 39 | 6 | 0 | 0.218395 | 0.288666 | 3.353441 |
| 40 | 6 | 0 | -0.143041 | 3.078938 | -2.013101 |
| 41 | 1 | 0 | -3.800001 | 2.996194 | -0.907162 |
| 42 | 1 | 0 | 1.005868 | -1.849594 | -2.355473 |
| 43 | 1 | 0 | -0.208032 | -0.350825 | 5.450205 |
| 44 | 1 | 0 | 0.907079 | 1.121277 | 3.399582 |

| | | | | | |
|---|---|---|---|---|---|
| 45 | 1 | 0 | -1.706942 | -2.236908 | 4.109520 |
| 46 | 1 | 0 | -4.292192 | -2.589865 | -0.390007 |
| 47 | 1 | 0 | -6.370963 | -0.892287 | -0.186987 |
| 48 | 1 | 0 | -4.357368 | -0.684569 | -3.183163 |
| 49 | 1 | 0 | -1.796276 | -0.614098 | -2.345044 |
| 50 | 1 | 0 | -5.593486 | 1.538231 | -2.281307 |
| 51 | 1 | 0 | -5.606061 | 1.164007 | 1.396860 |
| 52 | 1 | 0 | -3.070162 | 0.696273 | 2.178114 |
| 53 | 1 | 0 | -0.374093 | -4.228111 | -2.586602 |
| 54 | 1 | 0 | -2.160575 | -3.044299 | 1.845378 |
| 55 | 1 | 0 | -1.906349 | -4.274170 | -0.294982 |
| 56 | 1 | 0 | -0.902057 | 3.834451 | -2.244088 |
| 57 | 1 | 0 | 0.760688 | 3.583321 | -1.654736 |
| 58 | 1 | 0 | 0.103619 | 2.541039 | -2.934035 |
| 59 | 1 | 0 | -1.875667 | 3.850584 | 0.275913 |
| 60 | 1 | 0 | -1.729326 | 2.489686 | 1.420200 |
| 61 | 1 | 0 | -0.308538 | 3.478785 | 1.042054 |
| 62 | 1 | 0 | 4.170036 | 3.028414 | -2.060909 |
| 63 | 1 | 0 | 4.138696 | 1.461462 | -2.905317 |
| 64 | 1 | 0 | 2.617454 | 2.263558 | -2.488928 |
| 65 | 1 | 0 | 4.114345 | 4.832396 | 1.777687 |
| 66 | 1 | 0 | 2.386275 | 4.540430 | 1.395707 |
| 67 | 1 | 0 | 3.219217 | 3.500234 | 2.582962 |
| 68 | 1 | 0 | 4.678080 | 1.145017 | -0.506742 |
| 69 | 1 | 0 | 3.656812 | -3.570835 | -1.994019 |
| 70 | 1 | 0 | 3.884101 | -1.860672 | -2.442405 |
| 71 | 1 | 0 | 6.137276 | -2.837151 | -1.968412 |
| 72 | 1 | 0 | 5.555155 | -3.427441 | -0.395200 |
| 73 | 1 | 0 | 6.697845 | -1.264358 | 0.006417 |
| 74 | 1 | 0 | 5.780018 | -0.512294 | -1.315524 |

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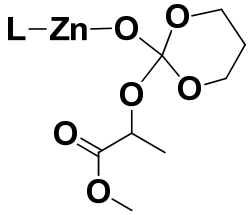


**II$^{monomer}$- propagation-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

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| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.508932 | -0.607161 | 4.115799 |
| 2 | 7 | 0 | 1.443749 | -0.123793 | 2.858785 |
| 3 | 7 | 0 | 0.309347 | -0.583172 | 2.262514 |
| 4 | 6 | 0 | -0.335619 | -1.339852 | 3.164958 |
| 5 | 6 | 0 | 0.390842 | -1.397640 | 4.358058 |
| 6 | 5 | 0 | 2.520371 | 0.762288 | 2.145004 |
| 7 | 6 | 0 | 3.433248 | -0.097017 | 1.125994 |
| 8 | 6 | 0 | 4.691551 | 0.318631 | 0.573368 |
| 9 | 6 | 0 | 5.348116 | -0.796902 | -0.030602 |
| 10 | 6 | 0 | 4.492135 | -1.929046 | 0.116890 |
| 11 | 6 | 0 | 3.325214 | -1.493818 | 0.815224 |
| 12 | 26 | 0 | 3.553458 | -0.446806 | -0.987367 |
| 13 | 6 | 0 | 1.839834 | -0.476835 | -2.154958 |
| 14 | 6 | 0 | 2.867593 | -1.276104 | -2.764590 |
| 15 | 6 | 0 | 3.986998 | -0.435042 | -3.027390 |
| 16 | 6 | 0 | 3.664671 | 0.885326 | -2.591967 |
| 17 | 6 | 0 | 2.349328 | 0.865762 | -2.050555 |
| 18 | 15 | 0 | 0.208586 | -0.983919 | -1.561954 |
| 19 | 6 | 0 | -0.943610 | -0.755498 | -2.988080 |
| 20 | 30 | 0 | -0.467320 | 0.293481 | 0.516174 |
| 21 | 8 | 0 | -2.401886 | 0.237803 | 0.797497 |
| 22 | 6 | 0 | -3.115733 | 0.944796 | -0.043627 |
| 23 | 8 | 0 | -2.247659 | 1.699805 | -0.906370 |
| 24 | 6 | 0 | -2.909582 | 2.596000 | -1.811025 |
| 25 | 6 | 0 | -3.826747 | 3.538616 | -1.033859 |
| 26 | 6 | 0 | -4.744734 | 2.705689 | -0.139591 |
| 27 | 8 | 0 | -3.978381 | 1.814691 | 0.671315 |
| 28 | 8 | 0 | -3.910798 | 0.149037 | -0.953047 |
| 29 | 6 | 0 | -4.650295 | -0.865281 | -0.302774 |
| 30 | 6 | 0 | -3.778268 | -2.095192 | -0.039457 |
| 31 | 8 | 0 | -2.906683 | -2.515095 | -0.773845 |
| 32 | 7 | 0 | 1.825618 | 2.034813 | 1.538171 |
| 33 | 6 | 0 | 2.252453 | 3.306567 | 1.668214 |
| 34 | 6 | 0 | 1.392350 | 4.150668 | 0.973491 |
| 35 | 6 | 0 | 0.427960 | 3.291941 | 0.438963 |
| 36 | 7 | 0 | 0.699430 | 2.019513 | 0.774105 |
| 37 | 6 | 0 | 0.297370 | -2.818703 | -1.397659 |
| 38 | 6 | 0 | -5.807383 | -1.265259 | -1.223431 |
| 39 | 8 | 0 | -4.178904 | -2.734118 | 1.078330 |
| 40 | 6 | 0 | -3.504579 | -3.966778 | 1.369865 |
| 41 | 1 | 0 | 2.484675 | -2.120381 | 1.085512 |
| 42 | 1 | 0 | -4.416095 | 4.153323 | -1.726197 |
| 43 | 1 | 0 | 2.817196 | -2.339541 | -2.955634 |
| 44 | 1 | 0 | -0.454788 | 3.508731 | -0.145297 |
| 45 | 1 | 0 | 0.137073 | -1.920245 | 5.268297 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 1 | 0 | -1.295580 | -1.770592 | 2.913627 |
| 47 | 1 | 0 | 2.345931 | -0.353431 | 4.749670 |
| 48 | 1 | 0 | 5.083609 | 1.328219 | 0.607232 |
| 49 | 1 | 0 | 6.300095 | -0.777789 | -0.546243 |
| 50 | 1 | 0 | 4.324280 | 1.742740 | -2.620266 |
| 51 | 1 | 0 | 1.836177 | 1.703164 | -1.598802 |
| 52 | 1 | 0 | 4.934448 | -0.754605 | -3.441804 |
| 53 | 1 | 0 | 4.680018 | -2.926267 | -0.261048 |
| 54 | 1 | 0 | 1.448814 | 5.225680 | 0.888098 |
| 55 | 1 | 0 | 3.227183 | 1.187239 | 3.031963 |
| 56 | 1 | 0 | 3.132725 | 3.523177 | 2.255692 |
| 57 | 1 | 0 | -0.626925 | -1.352824 | -3.849765 |
| 58 | 1 | 0 | -1.943916 | -1.054771 | -2.663324 |
| 59 | 1 | 0 | -0.966343 | 0.300794 | -3.268781 |
| 60 | 1 | 0 | 0.593797 | -3.287297 | -2.342303 |
| 61 | 1 | 0 | 1.017395 | -3.090843 | -0.621995 |
| 62 | 1 | 0 | -0.697293 | -3.173987 | -1.117314 |
| 63 | 1 | 0 | -6.401424 | -2.066996 | -0.772181 |
| 64 | 1 | 0 | -6.457138 | -0.402503 | -1.397648 |
| 65 | 1 | 0 | -5.418147 | -1.610910 | -2.186421 |
| 66 | 1 | 0 | -4.002451 | -4.372852 | 2.250974 |
| 67 | 1 | 0 | -3.583905 | -4.660327 | 0.528233 |
| 68 | 1 | 0 | -2.447044 | -3.784437 | 1.581929 |
| 69 | 1 | 0 | -5.035150 | -0.504699 | 0.656403 |
| 70 | 1 | 0 | -2.113698 | 3.136047 | -2.333254 |
| 71 | 1 | 0 | -3.478061 | 2.014779 | -2.547736 |
| 72 | 1 | 0 | -3.223608 | 4.210805 | -0.411382 |
| 73 | 1 | 0 | -5.305566 | 3.332981 | 0.559204 |
| 74 | 1 | 0 | -5.462049 | 2.141750 | -0.752416 |

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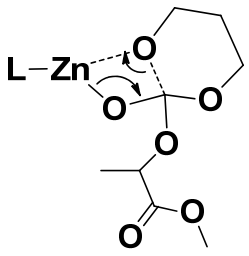


**TSII-III$^{monomer}$- propagation-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.230574 | 0.498284 | 1.760162 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 7 | 0 | -1.288013 | 1.253828 | 2.154284 |
| 3 | 6 | 0 | -1.422604 | 1.167629 | 3.493970 |
| 4 | 6 | 0 | -0.431658 | 0.330722 | 3.996122 |
| 5 | 6 | 0 | 0.295869 | -0.055325 | 2.864621 |
| 6 | 5 | 0 | -2.261203 | 1.995892 | 1.177864 |
| 7 | 7 | 0 | -1.448747 | 2.801706 | 0.103627 |
| 8 | 7 | 0 | -0.461828 | 2.285636 | -0.679814 |
| 9 | 6 | 0 | -0.144992 | 3.221619 | -1.591130 |
| 10 | 6 | 0 | -0.939093 | 4.358748 | -1.413167 |
| 11 | 6 | 0 | -1.748024 | 4.044510 | -0.326368 |
| 12 | 30 | 0 | 0.637037 | 0.550577 | -0.199450 |
| 13 | 8 | 0 | 2.583342 | 0.571651 | 0.459234 |
| 14 | 6 | 0 | 3.217070 | 1.649206 | 1.116976 |
| 15 | 6 | 0 | 3.272262 | 2.899063 | 0.224706 |
| 16 | 6 | 0 | 4.036896 | 2.626963 | -1.086441 |
| 17 | 8 | 0 | 4.236555 | 1.217217 | -1.322489 |
| 18 | 6 | 0 | 3.101732 | 0.463602 | -1.353942 |
| 19 | 8 | 0 | 3.400045 | -0.871350 | -1.428052 |
| 20 | 6 | 0 | 4.424797 | -1.391944 | -0.577709 |
| 21 | 6 | 0 | 5.023647 | -2.609515 | -1.280056 |
| 22 | 6 | 0 | -3.385450 | 1.060836 | 0.489341 |
| 23 | 6 | 0 | -4.458919 | 0.395495 | 1.171017 |
| 24 | 6 | 0 | -5.408108 | -0.092031 | 0.221034 |
| 25 | 6 | 0 | -4.925094 | 0.244953 | -1.078587 |
| 26 | 6 | 0 | -3.689241 | 0.939154 | -0.908031 |
| 27 | 26 | 0 | -3.581309 | -0.994627 | -0.100622 |
| 28 | 6 | 0 | -3.984071 | -3.024157 | -0.344783 |
| 29 | 6 | 0 | -3.383093 | -2.799023 | 0.930370 |
| 30 | 6 | 0 | -2.105743 | -2.209084 | 0.721301 |
| 31 | 6 | 0 | -1.900961 | -2.070999 | -0.695754 |
| 32 | 6 | 0 | -3.076259 | -2.579889 | -1.348702 |
| 33 | 15 | 0 | -0.389955 | -1.406067 | -1.432709 |
| 34 | 6 | 0 | 0.689108 | -2.876710 | -1.730448 |
| 35 | 8 | 0 | 2.049907 | 0.843880 | -1.923104 |
| 36 | 6 | 0 | 3.828896 | -1.814416 | 0.770223 |
| 37 | 8 | 0 | 4.683913 | -1.498480 | 1.766403 |
| 38 | 6 | 0 | 4.303227 | -1.935435 | 3.079739 |
| 39 | 8 | 0 | 2.805679 | -2.444029 | 0.930919 |
| 40 | 6 | 0 | -0.856257 | -0.906965 | -3.147813 |
| 41 | 1 | 0 | 4.237264 | 1.349092 | 1.403641 |
| 42 | 1 | 0 | -3.256366 | -2.592724 | -2.415311 |
| 43 | 1 | 0 | 1.163912 | -0.694322 | 2.773389 |
| 44 | 1 | 0 | -0.925039 | 5.277150 | -1.981188 |
| 45 | 1 | 0 | 0.643316 | 3.017565 | -2.302673 |
| 46 | 1 | 0 | -2.520941 | 4.614976 | 0.167745 |
| 47 | 1 | 0 | -4.535860 | 0.274465 | 2.245100 |

| | | | | | |
|---|---|---|---|---|---|
| 48 | 1 | 0 | -6.305294 | -0.656133 | 0.443439 |
| 49 | 1 | 0 | -3.840967 | -2.992643 | 1.891551 |
| 50 | 1 | 0 | -1.418743 | -1.883584 | 1.489502 |
| 51 | 1 | 0 | -4.976868 | -3.418591 | -0.519367 |
| 52 | 1 | 0 | -5.393016 | -0.010799 | -2.021109 |
| 53 | 1 | 0 | -3.074378 | 1.328214 | -1.709967 |
| 54 | 1 | 0 | -0.258907 | 0.057752 | 5.026733 |
| 55 | 1 | 0 | -2.815837 | 2.834486 | 1.855182 |
| 56 | 1 | 0 | -2.209494 | 1.711956 | 3.995649 |
| 57 | 1 | 0 | 0.141352 | -3.664775 | -2.257776 |
| 58 | 1 | 0 | 1.551372 | -2.555589 | -2.321247 |
| 59 | 1 | 0 | 1.063438 | -3.250181 | -0.774484 |
| 60 | 1 | 0 | -1.240634 | -1.753013 | -3.727341 |
| 61 | 1 | 0 | -1.613583 | -0.119839 | -3.114657 |
| 62 | 1 | 0 | 0.038933 | -0.511832 | -3.636923 |
| 63 | 1 | 0 | 2.676232 | 1.882955 | 2.045350 |
| 64 | 1 | 0 | 3.755714 | 3.721335 | 0.767617 |
| 65 | 1 | 0 | 2.248245 | 3.218911 | 0.005822 |
| 66 | 1 | 0 | 5.056073 | 3.018224 | -1.045495 |
| 67 | 1 | 0 | 3.529215 | 3.065134 | -1.951138 |
| 68 | 1 | 0 | 5.188241 | -0.633183 | -0.405848 |
| 69 | 1 | 0 | 5.816725 | -3.050030 | -0.666517 |
| 70 | 1 | 0 | 4.250975 | -3.364948 | -1.451632 |
| 71 | 1 | 0 | 5.448206 | -2.309495 | -2.242379 |
| 72 | 1 | 0 | 5.169253 | -1.747605 | 3.715446 |
| 73 | 1 | 0 | 3.443635 | -1.359925 | 3.434618 |
| 74 | 1 | 0 | 4.047060 | -2.997771 | 3.075217 |

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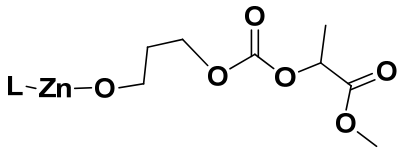


**III$^{monomer}$- propagation-TMC**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.589721 | 0.973657 | 1.874738 |
| 2 | 7 | 0 | -1.669669 | 1.800030 | 1.859547 |
| 3 | 6 | 0 | -1.974485 | 2.156980 | 3.124050 |
| 4 | 6 | 0 | -1.075609 | 1.553115 | 3.996421 |
| 5 | 6 | 0 | -0.220403 | 0.830845 | 3.158553 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 5 | 0 | -2.488555 | 2.174198 | 0.580162 |
| 7 | 7 | 0 | -1.538673 | 2.666092 | -0.567198 |
| 8 | 7 | 0 | -0.436215 | 2.002177 | -1.012965 |
| 9 | 6 | 0 | -0.016702 | 2.628030 | -2.126328 |
| 10 | 6 | 0 | -0.855272 | 3.708419 | -2.419359 |
| 11 | 6 | 0 | -1.802966 | 3.692495 | -1.402209 |
| 12 | 30 | 0 | 0.582251 | 0.549760 | 0.153664 |
| 13 | 8 | 0 | 2.427941 | 0.726194 | 0.682051 |
| 14 | 6 | 0 | 3.040355 | 1.943533 | 0.991516 |
| 15 | 6 | 0 | 3.276308 | 2.838501 | -0.244353 |
| 16 | 6 | 0 | 4.352673 | 2.325722 | -1.210549 |
| 17 | 8 | 0 | 4.519065 | 0.885989 | -1.183126 |
| 18 | 6 | 0 | 3.507405 | 0.137334 | -1.626449 |
| 19 | 8 | 0 | 3.666612 | -1.171184 | -1.342883 |
| 20 | 6 | 0 | 4.594649 | -1.598671 | -0.321316 |
| 21 | 6 | 0 | 5.070365 | -2.993060 | -0.713566 |
| 22 | 6 | 0 | -3.506977 | 1.027872 | 0.078633 |
| 23 | 6 | 0 | -4.547762 | 0.430392 | 0.864671 |
| 24 | 6 | 0 | -5.438275 | -0.296463 | 0.016404 |
| 25 | 6 | 0 | -4.946208 | -0.183774 | -1.317951 |
| 26 | 6 | 0 | -3.764273 | 0.615599 | -1.271690 |
| 27 | 26 | 0 | -3.548369 | -1.114258 | -0.102262 |
| 28 | 6 | 0 | -3.807731 | -3.181763 | -0.053723 |
| 29 | 6 | 0 | -3.351045 | -2.720458 | 1.217837 |
| 30 | 6 | 0 | -2.093896 | -2.081962 | 1.032135 |
| 31 | 6 | 0 | -1.758037 | -2.147400 | -0.364340 |
| 32 | 6 | 0 | -2.831929 | -2.832737 | -1.030522 |
| 33 | 15 | 0 | -0.203742 | -1.535472 | -1.057842 |
| 34 | 6 | 0 | 0.859428 | -3.039796 | -1.191013 |
| 35 | 8 | 0 | 2.582323 | 0.513084 | -2.319522 |
| 36 | 6 | 0 | 3.873562 | -1.645831 | 1.033272 |
| 37 | 8 | 0 | 4.601812 | -1.019795 | 1.972544 |
| 38 | 6 | 0 | 4.012054 | -0.988214 | 3.281832 |
| 39 | 8 | 0 | 2.853557 | -2.263237 | 1.251327 |
| 40 | 6 | 0 | -0.555146 | -1.153544 | -2.828210 |
| 41 | 1 | 0 | 4.013091 | 1.747527 | 1.478004 |
| 42 | 1 | 0 | -2.902492 | -3.025633 | -2.092793 |
| 43 | 1 | 0 | 0.643299 | 0.227570 | 3.403721 |
| 44 | 1 | 0 | -0.781778 | 4.404439 | -3.241825 |
| 45 | 1 | 0 | 0.865722 | 2.265123 | -2.636301 |
| 46 | 1 | 0 | -2.651974 | 4.333987 | -1.215945 |
| 47 | 1 | 0 | -4.638907 | 0.510829 | 1.941347 |
| 48 | 1 | 0 | -6.298922 | -0.872057 | 0.333637 |
| 49 | 1 | 0 | -3.890761 | -2.796258 | 2.152675 |
| 50 | 1 | 0 | -1.506064 | -1.592865 | 1.796254 |
| 51 | 1 | 0 | -4.754072 | -3.669216 | -0.250358 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 1 | 0 | -5.369634 | -0.652855 | -2.197413 |
| 53 | 1 | 0 | -3.160384 | 0.886469 | -2.129532 |
| 54 | 1 | 0 | -1.040553 | 1.638720 | 5.072368 |
| 55 | 1 | 0 | -3.137181 | 3.149730 | 0.893316 |
| 56 | 1 | 0 | -2.806440 | 2.819748 | 3.312827 |
| 57 | 1 | 0 | 0.314255 | -3.846469 | -1.692397 |
| 58 | 1 | 0 | 1.756251 | -2.780415 | -1.758857 |
| 59 | 1 | 0 | 1.175276 | -3.356041 | -0.195252 |
| 60 | 1 | 0 | -0.922488 | -2.034286 | -3.365470 |
| 61 | 1 | 0 | -1.295689 | -0.353834 | -2.892300 |
| 62 | 1 | 0 | 0.377839 | -0.811117 | -3.285451 |
| 63 | 1 | 0 | 2.449293 | 2.537075 | 1.715226 |
| 64 | 1 | 0 | 3.584218 | 3.843138 | 0.079681 |
| 65 | 1 | 0 | 2.323521 | 2.956852 | -0.768127 |
| 66 | 1 | 0 | 5.344048 | 2.678941 | -0.917631 |
| 67 | 1 | 0 | 4.158058 | 2.636606 | -2.241524 |
| 68 | 1 | 0 | 5.425130 | -0.898498 | -0.262566 |
| 69 | 1 | 0 | 5.794252 | -3.362361 | 0.020948 |
| 70 | 1 | 0 | 4.225583 | -3.686435 | -0.749651 |
| 71 | 1 | 0 | 5.552634 | -2.962103 | -1.695082 |
| 72 | 1 | 0 | 4.746131 | -0.499846 | 3.923510 |
| 73 | 1 | 0 | 3.086339 | -0.409858 | 3.240498 |
| 74 | 1 | 0 | 3.800346 | -2.000652 | 3.635691 |

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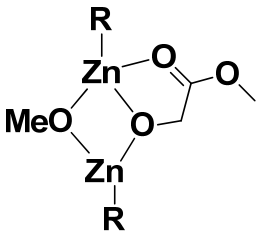


**Cat$^{dimer}$- propagation**

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 6.309591 | -0.904268 | 0.681297 |
| 2 | 6 | 0 | 4.645782 | 0.363386 | 0.305860 |
| 3 | 6 | 0 | 4.261714 | -1.019746 | 0.295680 |
| 4 | 6 | 0 | 4.571502 | -1.615816 | 1.557874 |
| 5 | 1 | 0 | 5.541057 | -0.736304 | 3.381123 |
| 6 | 6 | 0 | 5.211965 | 0.598093 | 1.603967 |
| 7 | 6 | 0 | 5.163384 | -0.604975 | 2.374828 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 5 | 0 | 4.506686 | 1.419599 | -0.906032 |
| 9 | 7 | 0 | 4.067895 | 2.831356 | -0.371670 |
| 10 | 7 | 0 | 2.859769 | 3.085920 | 0.200881 |
| 11 | 7 | 0 | 3.457761 | 0.907050 | -1.952256 |
| 12 | 1 | 0 | 2.327795 | 1.589211 | 2.900450 |
| 13 | 30 | 0 | 1.217889 | 1.771532 | -0.056292 |
| 14 | 8 | 0 | -0.740853 | 1.012110 | -0.507774 |
| 15 | 8 | 0 | 0.765074 | 0.937571 | 1.708399 |
| 16 | 6 | 0 | 1.593852 | 0.775031 | 2.842485 |
| 17 | 30 | 0 | -1.005086 | 0.163460 | 1.278665 |
| 18 | 7 | 0 | -2.444392 | 0.765803 | 2.658096 |
| 19 | 7 | 0 | -3.469035 | -0.079598 | 2.951810 |
| 20 | 7 | 0 | -1.390513 | -1.865893 | 1.487948 |
| 21 | 7 | 0 | -2.613434 | -2.262824 | 1.939558 |
| 22 | 5 | 0 | -3.847038 | -1.290356 | 2.021374 |
| 23 | 6 | 0 | -5.162945 | 0.553871 | -1.160320 |
| 24 | 6 | 0 | -5.035203 | 0.411547 | 0.256708 |
| 25 | 6 | 0 | -4.245568 | -0.752046 | 0.554515 |
| 26 | 6 | 0 | -3.909760 | -1.328617 | -0.718432 |
| 27 | 6 | 0 | -4.466044 | -0.534307 | -1.767879 |
| 28 | 6 | 0 | -8.017237 | -1.392940 | -1.105112 |
| 29 | 6 | 0 | -7.857881 | -1.514039 | 0.317183 |
| 30 | 6 | 0 | -7.023865 | -2.637633 | 0.593796 |
| 31 | 6 | 0 | -6.649287 | -3.222575 | -0.651520 |
| 32 | 1 | 0 | -7.138438 | -2.639462 | -2.754189 |
| 33 | 6 | 0 | -7.253396 | -2.456914 | -1.693598 |
| 34 | 15 | 0 | -9.214781 | -0.309683 | -1.972598 |
| 35 | 6 | 0 | 7.788224 | -0.482787 | -0.707547 |
| 36 | 6 | 0 | 7.395325 | -1.860126 | -0.826094 |
| 37 | 6 | 0 | 7.652488 | -2.475350 | 0.447798 |
| 38 | 6 | 0 | 8.198968 | -1.492973 | 1.325245 |
| 39 | 6 | 0 | 8.287021 | -0.260750 | 0.608417 |
| 40 | 15 | 0 | 6.744847 | -2.582383 | -2.378344 |
| 41 | 6 | 0 | 2.889165 | 4.356076 | 0.634999 |
| 42 | 6 | 0 | 4.129950 | 4.938337 | 0.359519 |
| 43 | 6 | 0 | 4.841981 | 3.930900 | -0.283538 |
| 44 | 6 | 0 | -0.598440 | -2.950763 | 1.473957 |
| 45 | 6 | 0 | -1.309000 | -4.073074 | 1.908928 |
| 46 | 6 | 0 | -2.580415 | -3.584688 | 2.194727 |
| 47 | 8 | 0 | -0.027277 | 3.594906 | -0.557365 |
| 48 | 6 | 0 | -1.625787 | 1.873007 | -1.138409 |
| 49 | 6 | 0 | -1.118049 | 3.304669 | -1.046394 |
| 50 | 8 | 0 | -1.947600 | 4.206985 | -1.555258 |
| 51 | 6 | 0 | -1.507339 | 5.581750 | -1.535515 |
| 52 | 6 | 0 | 5.796904 | -4.059117 | -1.743077 |
| 53 | 6 | 0 | 8.277520 | -3.472973 | -2.985792 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 7 | 0 | 2.128943 | 0.808761 | -1.675948 |
| 55 | 6 | 0 | 1.552037 | 0.175250 | -2.710819 |
| 56 | 6 | 0 | 2.513390 | -0.156077 | -3.670159 |
| 57 | 6 | 0 | 3.707695 | 0.327658 | -3.142662 |
| 58 | 6 | 0 | -2.422557 | 1.712331 | 3.611052 |
| 59 | 6 | 0 | -3.453998 | 1.496814 | 4.529564 |
| 60 | 6 | 0 | -4.087552 | 0.345537 | 4.069614 |
| 61 | 26 | 0 | -5.982337 | -1.261035 | -0.554211 |
| 62 | 6 | 0 | -9.010888 | 1.293371 | -1.040211 |
| 63 | 6 | 0 | -8.280777 | 0.102425 | -3.534196 |
| 64 | 1 | 0 | 8.458955 | -1.644276 | 2.365274 |
| 65 | 1 | 0 | 5.634756 | 1.537387 | 1.939937 |
| 66 | 1 | 0 | -4.395835 | -0.737636 | -2.828868 |
| 67 | 1 | 0 | -5.987846 | -4.068446 | -0.787003 |
| 68 | 1 | 0 | -8.214321 | -0.786374 | -4.170089 |
| 69 | 1 | 0 | -7.963746 | 1.601743 | -0.959432 |
| 70 | 1 | 0 | -3.702568 | 2.083199 | 5.401543 |
| 71 | 1 | 0 | 8.027671 | -4.062114 | -3.875824 |
| 72 | 1 | 0 | -3.343471 | -2.240748 | -0.859590 |
| 73 | 1 | 0 | 4.907413 | -3.720493 | -1.203914 |
| 74 | 1 | 0 | 6.390894 | -4.698538 | -1.079546 |
| 75 | 1 | 0 | 4.461419 | 5.941195 | 0.584748 |
| 76 | 1 | 0 | 8.626242 | 0.685761 | 1.009069 |
| 77 | 1 | 0 | 7.668315 | 0.268790 | -1.476876 |
| 78 | 1 | 0 | 7.439745 | -3.503038 | 0.710971 |
| 79 | 1 | 0 | 4.418827 | -2.651675 | 1.834104 |
| 80 | 1 | 0 | 3.822559 | -1.530423 | -0.552297 |
| 81 | 1 | 0 | 2.369717 | -0.671138 | -4.608356 |
| 82 | 1 | 0 | 5.530959 | 1.612935 | -1.516877 |
| 83 | 1 | 0 | 9.035573 | -2.736443 | -3.271787 |
| 84 | 1 | 0 | 8.704613 | -4.138476 | -2.226402 |
| 85 | 1 | 0 | 5.469599 | -4.659760 | -2.599022 |
| 86 | 1 | 0 | 0.486156 | -0.006031 | -2.692035 |
| 87 | 1 | 0 | 4.718160 | 0.277158 | -3.520998 |
| 88 | 1 | 0 | 2.013874 | 4.785070 | 1.103531 |
| 89 | 1 | 0 | 5.844662 | 3.918596 | -0.685357 |
| 90 | 1 | 0 | -2.643987 | 1.846517 | -0.721768 |
| 91 | 1 | 0 | -1.664621 | 2.484124 | 3.586995 |
| 92 | 1 | 0 | -4.935762 | -0.198924 | 4.458649 |
| 93 | 1 | 0 | 0.432913 | -2.864109 | 1.158112 |
| 94 | 1 | 0 | -0.954041 | -5.088067 | 2.007091 |
| 95 | 1 | 0 | -3.463985 | -4.086704 | 2.561389 |
| 96 | 1 | 0 | -4.714536 | -1.894593 | 2.605144 |
| 97 | 1 | 0 | -5.478214 | 1.069800 | 0.994396 |
| 98 | 1 | 0 | -5.702498 | 1.336039 | -1.678483 |
| 99 | 1 | 0 | -6.681957 | -2.946184 | 1.572510 |

| | | | | | |
|---|---|---|---|---|---|
| 100 | 1 | 0 | -8.286064 | -0.852399 | 1.058870 |
| 101 | 1 | 0 | -8.841995 | 0.862409 | -4.089155 |
| 102 | 1 | 0 | -7.269365 | 0.470408 | -3.333935 |
| 103 | 1 | 0 | -9.583280 | 2.073937 | -1.553694 |
| 104 | 1 | 0 | -9.427033 | 1.189405 | -0.032889 |
| 105 | 1 | 0 | 0.994872 | 0.789784 | 3.765867 |
| 106 | 1 | 0 | 2.152301 | -0.170305 | 2.807929 |
| 107 | 1 | 0 | -1.738021 | 1.644746 | -2.213333 |
| 108 | 1 | 0 | -2.305753 | 6.145616 | -2.016704 |
| 109 | 1 | 0 | -1.364268 | 5.917730 | -0.505798 |
| 110 | 1 | 0 | -0.570376 | 5.686764 | -2.087103 |

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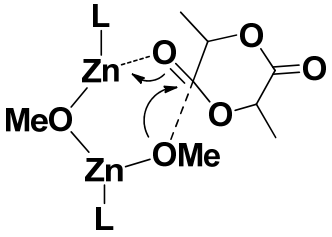


**TSI-II$^{dimer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -7.991529 | -1.523847 | 0.591329 |
| 2 | 6 | 0 | -8.513708 | -1.303121 | -0.715488 |
| 3 | 6 | 0 | -8.235489 | -2.463036 | -1.500679 |
| 4 | 6 | 0 | -7.548185 | -3.400668 | -0.674440 |
| 5 | 6 | 0 | -7.391580 | -2.829365 | 0.635584 |
| 6 | 26 | 0 | -6.459315 | -1.635295 | -0.800265 |
| 7 | 6 | 0 | -5.590292 | 0.033453 | -1.680377 |
| 8 | 6 | 0 | -5.023653 | -0.130100 | -0.370820 |
| 9 | 6 | 0 | -4.429609 | -1.436999 | -0.366913 |
| 10 | 6 | 0 | -4.613902 | -2.054396 | -1.642661 |
| 11 | 6 | 0 | -5.336574 | -1.136036 | -2.463177 |
| 12 | 5 | 0 | -5.065376 | 0.929625 | 0.844412 |
| 13 | 7 | 0 | -4.768366 | 2.378569 | 0.300671 |
| 14 | 6 | 0 | -5.673628 | 3.358901 | 0.115225 |
| 15 | 6 | 0 | -5.088949 | 4.388489 | -0.615960 |
| 16 | 6 | 0 | -3.783410 | 3.946078 | -0.845848 |
| 17 | 7 | 0 | -3.596091 | 2.734398 | -0.294757 |
| 18 | 30 | 0 | -1.835096 | 1.690206 | 0.162837 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 7 | 0 | -2.671258 | 0.558331 | 1.720374 |
| 20 | 7 | 0 | -4.014803 | 0.539562 | 1.939920 |
| 21 | 6 | 0 | -4.264739 | -0.066047 | 3.117847 |
| 22 | 6 | 0 | -3.058497 | -0.450680 | 3.694660 |
| 23 | 6 | 0 | -2.090085 | -0.032047 | 2.777510 |
| 24 | 15 | 0 | -6.633695 | -3.525246 | 2.150560 |
| 25 | 6 | 0 | -8.006116 | -4.673413 | 2.704775 |
| 26 | 8 | 0 | -0.513777 | 2.951828 | 1.059601 |
| 27 | 6 | 0 | -0.481889 | 4.307280 | 0.742493 |
| 28 | 6 | 0 | -0.112788 | 4.560410 | -0.718058 |
| 29 | 8 | 0 | 0.576330 | 5.706293 | -0.872266 |
| 30 | 6 | 0 | 0.882491 | 6.088805 | -2.226794 |
| 31 | 8 | 0 | -1.051786 | 0.600521 | -1.295801 |
| 32 | 6 | 0 | -1.678032 | 0.537664 | -2.571795 |
| 33 | 8 | 0 | -0.435089 | 3.836909 | -1.642698 |
| 34 | 30 | 0 | 0.847862 | 0.174185 | -1.029978 |
| 35 | 8 | 0 | 0.786145 | 0.805586 | 0.915818 |
| 36 | 6 | 0 | 1.160976 | 1.932426 | 1.343366 |
| 37 | 6 | 0 | 1.223356 | 2.121258 | 2.851926 |
| 38 | 8 | 0 | 1.572598 | 3.467936 | 3.235497 |
| 39 | 6 | 0 | 2.466788 | 4.174434 | 2.519007 |
| 40 | 6 | 0 | 2.832956 | 3.706028 | 1.112069 |
| 41 | 8 | 0 | 2.045050 | 2.606201 | 0.584929 |
| 42 | 6 | 0 | 2.191344 | 1.131136 | 3.503630 |
| 43 | 8 | 0 | 2.938352 | 5.196854 | 2.954166 |
| 44 | 6 | 0 | 4.313665 | 3.349047 | 0.996664 |
| 45 | 7 | 0 | 2.157732 | 0.854228 | -2.472618 |
| 46 | 7 | 0 | 3.110009 | 0.022417 | -2.976963 |
| 47 | 6 | 0 | 3.610593 | 0.562125 | -4.104218 |
| 48 | 6 | 0 | 2.970567 | 1.773136 | -4.354168 |
| 49 | 6 | 0 | 2.059265 | 1.906790 | -3.303042 |
| 50 | 5 | 0 | 3.590944 | -1.293631 | -2.249492 |
| 51 | 6 | 0 | 4.313829 | -0.947743 | -0.854288 |
| 52 | 6 | 0 | 3.934757 | -1.339137 | 0.475925 |
| 53 | 6 | 0 | 4.876265 | -0.816174 | 1.416191 |
| 54 | 6 | 0 | 5.858909 | -0.087020 | 0.679676 |
| 55 | 6 | 0 | 5.518558 | -0.180062 | -0.704548 |
| 56 | 26 | 0 | 5.836696 | -2.081706 | 0.085813 |
| 57 | 6 | 0 | 7.416698 | -3.010531 | -0.905474 |
| 58 | 6 | 0 | 6.199193 | -3.716628 | -1.137342 |
| 59 | 6 | 0 | 5.697210 | -4.151819 | 0.124760 |
| 60 | 6 | 0 | 6.607994 | -3.713133 | 1.131746 |
| 61 | 6 | 0 | 7.689463 | -3.006345 | 0.504804 |
| 62 | 15 | 0 | 9.257154 | -2.505056 | 1.310523 |
| 63 | 6 | 0 | 8.635499 | -1.745940 | 2.897527 |
| 64 | 7 | 0 | 1.234569 | -1.839255 | -1.353434 |

| | | | | | |
|---|---|---|---|---|---|
| 65 | 7 | 0 | 2.349490 | -2.229876 | -2.033343 |
| 66 | 6 | 0 | 2.220080 | -3.523801 | -2.382316 |
| 67 | 6 | 0 | 0.993320 | -3.999500 | -1.928254 |
| 68 | 6 | 0 | 0.409460 | -2.898831 | -1.295982 |
| 69 | 6 | 0 | 9.696370 | -0.962543 | 0.357202 |
| 70 | 6 | 0 | -5.466532 | -4.795756 | 1.439013 |
| 71 | 1 | 0 | -5.666507 | -1.309438 | -3.479778 |
| 72 | 1 | 0 | -1.528064 | 1.468692 | -3.136865 |
| 73 | 1 | 0 | 6.492351 | -3.873844 | 2.195936 |
| 74 | 1 | 0 | -8.466053 | -2.590902 | -2.550723 |
| 75 | 1 | 0 | -6.146514 | 0.900645 | -2.015464 |
| 76 | 1 | 0 | 4.868399 | -0.978923 | 2.486535 |
| 77 | 1 | 0 | 4.767552 | -4.679070 | 0.295291 |
| 78 | 1 | 0 | 8.234306 | -2.530111 | 3.547826 |
| 79 | 1 | 0 | 8.868392 | -0.248473 | 0.297535 |
| 80 | 1 | 0 | 3.136369 | 2.446584 | -5.181960 |
| 81 | 1 | 0 | -7.661580 | -5.264786 | 3.561124 |
| 82 | 1 | 0 | 3.090633 | -1.970108 | 0.723584 |
| 83 | 1 | 0 | -4.656332 | -4.287575 | 0.908073 |
| 84 | 1 | 0 | -5.955569 | -5.495120 | 0.750771 |
| 85 | 1 | 0 | -5.543926 | 5.315739 | -0.931166 |
| 86 | 1 | 0 | -8.992738 | -0.397864 | -1.065226 |
| 87 | 1 | 0 | -8.004162 | -0.814339 | 1.408671 |
| 88 | 1 | 0 | -7.175819 | -4.364584 | -0.995060 |
| 89 | 1 | 0 | -4.293911 | -3.049095 | -1.926478 |
| 90 | 1 | 0 | -3.939642 | -1.890306 | 0.485619 |
| 91 | 1 | 0 | -2.911543 | -0.959504 | 4.635630 |
| 92 | 1 | 0 | -6.132208 | 1.009262 | 1.405837 |
| 93 | 1 | 0 | -8.865441 | -4.078588 | 3.031389 |
| 94 | 1 | 0 | -8.333405 | -5.354374 | 1.910368 |
| 95 | 1 | 0 | -5.028586 | -5.371281 | 2.262049 |
| 96 | 1 | 0 | -1.013533 | -0.127746 | 2.808747 |
| 97 | 1 | 0 | -5.282046 | -0.201978 | 3.453684 |
| 98 | 1 | 0 | -2.972633 | 4.419963 | -1.381330 |
| 99 | 1 | 0 | -6.674021 | 3.250375 | 0.508198 |
| 100 | 1 | 0 | 0.199628 | 4.871840 | 1.389625 |
| 101 | 1 | 0 | 1.332013 | 2.682365 | -3.099629 |
| 102 | 1 | 0 | 4.387806 | 0.047716 | -4.650503 |
| 103 | 1 | 0 | -0.556553 | -2.804315 | -0.817832 |
| 104 | 1 | 0 | 0.584635 | -4.991607 | -2.048963 |
| 105 | 1 | 0 | 3.009338 | -4.017726 | -2.930108 |
| 106 | 1 | 0 | 4.310212 | -1.847627 | -3.046263 |
| 107 | 1 | 0 | 6.094729 | 0.242340 | -1.518990 |
| 108 | 1 | 0 | 6.721039 | 0.419535 | 1.093284 |
| 109 | 1 | 0 | 5.718562 | -3.847326 | -2.097574 |
| 110 | 1 | 0 | 8.024981 | -2.541766 | -1.667943 |

| | | | | | |
|---|---|---|---|---|---|
| 111 | 1 | 0 | 9.479990 | -1.284594 | 3.421417 |
| 112 | 1 | 0 | 7.857062 | -0.995247 | 2.728222 |
| 113 | 1 | 0 | 10.554104 | -0.484240 | 0.843006 |
| 114 | 1 | 0 | 10.003435 | -1.232628 | -0.658467 |
| 115 | 1 | 0 | -1.264111 | -0.293054 | -3.160477 |
| 116 | 1 | 0 | -2.754033 | 0.363474 | -2.461057 |
| 117 | 1 | 0 | -1.476783 | 4.763710 | 0.887951 |
| 118 | 1 | 0 | 1.344124 | 7.073412 | -2.154014 |
| 119 | 1 | 0 | 1.576743 | 5.373867 | -2.676346 |
| 120 | 1 | 0 | -0.029200 | 6.131744 | -2.827642 |
| 121 | 1 | 0 | 2.613752 | 4.557486 | 0.461676 |
| 122 | 1 | 0 | 0.215529 | 1.977800 | 3.237072 |
| 123 | 1 | 0 | 4.913906 | 4.206338 | 1.313005 |
| 124 | 1 | 0 | 4.567128 | 2.483787 | 1.615539 |
| 125 | 1 | 0 | 4.550296 | 3.100812 | -0.041211 |
| 126 | 1 | 0 | 2.223646 | 1.320777 | 4.580406 |
| 127 | 1 | 0 | 1.851816 | 0.107083 | 3.328635 |
| 128 | 1 | 0 | 3.203735 | 1.225535 | 3.098872 |

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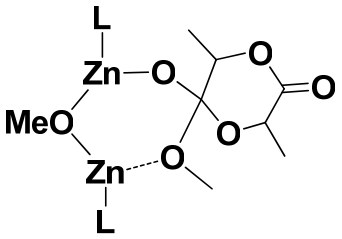


**II$^{dimer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -6.439149 | -1.675951 | -0.866812 |
| 2 | 6 | 0 | -5.008215 | -0.181038 | -0.398539 |
| 3 | 6 | 0 | -5.619676 | 0.051992 | -1.677048 |
| 4 | 15 | 0 | -6.530553 | -3.685633 | 2.018083 |
| 5 | 6 | 0 | -4.619416 | -2.021251 | -1.795599 |
| 6 | 6 | 0 | -4.398129 | -1.478037 | -0.492258 |
| 7 | 6 | 0 | -7.320822 | -2.939754 | 0.543559 |
| 8 | 6 | 0 | -7.496963 | -3.463642 | -0.783484 |
| 9 | 6 | 0 | -8.216665 | -2.507027 | -1.558655 |
| 10 | 6 | 0 | -8.495020 | -1.381882 | -0.724309 |
| 11 | 6 | 0 | -7.940597 | -1.642871 | 0.561712 |
| 12 | 6 | 0 | 6.043872 | -0.187243 | 0.719348 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 6 | 0 | 4.950943 | -0.829157 | 1.377391 |
| 14 | 6 | 0 | 4.441171 | -0.709882 | -0.906749 |
| 15 | 6 | 0 | 6.064203 | -3.601733 | -1.447484 |
| 16 | 6 | 0 | 6.141756 | -3.970370 | 0.826802 |
| 17 | 1 | 0 | 8.095328 | -2.676089 | -1.565600 |
| 18 | 6 | 0 | 7.324354 | -3.140327 | -0.964588 |
| 19 | 15 | 0 | 8.881976 | -3.240097 | 1.509932 |
| 20 | 30 | 0 | 0.875609 | 0.497855 | -1.123789 |
| 21 | 7 | 0 | 2.306266 | 1.324653 | -2.357255 |
| 22 | 7 | 0 | 3.289775 | 0.559337 | -2.905336 |
| 23 | 7 | 0 | 1.344908 | -1.476786 | -1.591527 |
| 24 | 6 | 0 | 2.353704 | -3.028104 | -2.794047 |
| 25 | 7 | 0 | 2.476414 | -1.787588 | -2.284670 |
| 26 | 5 | 0 | 3.732515 | -0.850708 | -2.343482 |
| 27 | 6 | 0 | 0.515927 | -2.530671 | -1.688097 |
| 28 | 6 | 0 | 1.114203 | -3.549178 | -2.434466 |
| 29 | 6 | 0 | 3.280397 | 2.502850 | -4.003693 |
| 30 | 8 | 0 | -1.052569 | 0.735127 | -1.523651 |
| 31 | 30 | 0 | -1.784444 | 1.439238 | 0.170257 |
| 32 | 7 | 0 | -3.491636 | 2.628599 | -0.141893 |
| 33 | 7 | 0 | -4.680411 | 2.276442 | 0.420151 |
| 34 | 6 | 0 | -5.550845 | 3.296464 | 0.290644 |
| 35 | 6 | 0 | -4.924653 | 4.348995 | -0.370177 |
| 36 | 6 | 0 | -3.632412 | 3.877198 | -0.619282 |
| 37 | 8 | 0 | 0.344856 | 1.012218 | 0.775421 |
| 38 | 6 | 0 | 0.704112 | 2.167765 | 1.340299 |
| 39 | 6 | 0 | 1.013684 | 2.014423 | 2.839901 |
| 40 | 8 | 0 | 1.533968 | 3.247952 | 3.400624 |
| 41 | 6 | 0 | 2.525354 | 3.896659 | 2.752518 |
| 42 | 6 | 0 | 2.719809 | 3.637990 | 1.257817 |
| 43 | 8 | 0 | 1.747639 | 2.773108 | 0.627210 |
| 44 | 8 | 0 | -0.542376 | 3.010827 | 1.216058 |
| 45 | 6 | 0 | -0.448175 | 4.414086 | 1.079013 |
| 46 | 6 | 0 | -0.036343 | 4.839729 | -0.328066 |
| 47 | 8 | 0 | -0.308268 | 4.236680 | -1.345724 |
| 48 | 6 | 0 | -5.379165 | -1.065589 | -2.535491 |
| 49 | 6 | 0 | 5.733416 | -0.126927 | -0.673625 |
| 50 | 6 | 0 | 3.974719 | -1.145917 | 0.380997 |
| 51 | 6 | 0 | 5.330148 | -4.115336 | -0.337750 |
| 52 | 6 | 0 | 7.391141 | -3.371272 | 0.450820 |
| 53 | 6 | 0 | 2.287247 | 2.494133 | -3.020882 |
| 54 | 6 | 0 | 3.886322 | 1.254367 | -3.892001 |
| 55 | 5 | 0 | -5.022993 | 0.806989 | 0.875670 |
| 56 | 7 | 0 | -3.980136 | 0.329897 | 1.942635 |
| 57 | 7 | 0 | -2.638918 | 0.316655 | 1.707174 |
| 58 | 6 | 0 | -2.062338 | -0.324750 | 2.738032 |

| | | | | | |
|---|---|---|---|---|---|
| 59 | 6 | 0 | -3.032437 | -0.744177 | 3.651857 |
| 60 | 6 | 0 | -4.233800 | -0.306457 | 3.102198 |
| 61 | 26 | 0 | 5.766575 | -2.108499 | -0.037274 |
| 62 | 6 | 0 | 9.710487 | -1.723133 | 0.808698 |
| 63 | 6 | 0 | 8.170328 | -2.525396 | 3.079751 |
| 64 | 6 | 0 | 1.955599 | 0.859532 | 3.160489 |
| 65 | 6 | 0 | 4.126601 | 3.134816 | 0.936304 |
| 66 | 8 | 0 | 3.188483 | 4.730906 | 3.319897 |
| 67 | 6 | 0 | -1.703016 | 0.681382 | -2.780969 |
| 68 | 6 | 0 | -7.881740 | -4.871529 | 2.543951 |
| 69 | 6 | 0 | -5.359209 | -4.914409 | 1.243114 |
| 70 | 8 | 0 | 0.610834 | 6.016494 | -0.292998 |
| 71 | 6 | 0 | 0.954706 | 6.590885 | -1.570023 |
| 72 | 1 | 0 | 4.250114 | 3.074310 | -0.148170 |
| 73 | 1 | 0 | -5.741502 | -1.183417 | -3.548964 |
| 74 | 1 | 0 | -1.588431 | 1.625895 | -3.333279 |
| 75 | 1 | 0 | 5.855284 | -4.254325 | 1.831423 |
| 76 | 1 | 0 | -8.468989 | -2.599175 | -2.607442 |
| 77 | 1 | 0 | -6.197510 | 0.929262 | -1.942402 |
| 78 | 1 | 0 | 4.891079 | -1.070135 | 2.431199 |
| 79 | 1 | 0 | 4.318566 | -4.498917 | -0.364941 |
| 80 | 1 | 0 | 7.535339 | -3.271001 | 3.569235 |
| 81 | 1 | 0 | 9.029031 | -0.870920 | 0.718756 |
| 82 | 1 | 0 | 3.519390 | 3.290479 | -4.702818 |
| 83 | 1 | 0 | -7.519037 | -5.490802 | 3.372566 |
| 84 | 1 | 0 | 3.050579 | -1.680074 | 0.561204 |
| 85 | 1 | 0 | -4.553938 | -4.379794 | 0.730957 |
| 86 | 1 | 0 | -5.847633 | -5.586723 | 0.527957 |
| 87 | 1 | 0 | -5.346062 | 5.308445 | -0.631256 |
| 88 | 1 | 0 | -8.995718 | -0.472067 | -1.028922 |
| 89 | 1 | 0 | -7.944793 | -0.964151 | 1.405047 |
| 90 | 1 | 0 | -7.117374 | -4.409239 | -1.147325 |
| 91 | 1 | 0 | -4.297364 | -2.992378 | -2.149750 |
| 92 | 1 | 0 | -3.875077 | -1.975347 | 0.314865 |
| 93 | 1 | 0 | -2.889973 | -1.288334 | 4.573478 |
| 94 | 1 | 0 | -6.087295 | 0.883952 | 1.441681 |
| 95 | 1 | 0 | -8.744685 | -4.301373 | 2.903344 |
| 96 | 1 | 0 | -8.209668 | -5.525666 | 1.727603 |
| 97 | 1 | 0 | -4.913477 | -5.522369 | 2.038228 |
| 98 | 1 | 0 | -0.988875 | -0.448857 | 2.755346 |
| 99 | 1 | 0 | -5.250591 | -0.423609 | 3.445955 |
| 100 | 1 | 0 | -2.800852 | 4.353318 | -1.120121 |
| 101 | 1 | 0 | -6.557646 | 3.198035 | 0.669771 |
| 102 | 1 | 0 | 0.210851 | 4.858040 | 1.827750 |
| 103 | 1 | 0 | 1.553049 | 3.245351 | -2.760247 |
| 104 | 1 | 0 | 4.702119 | 0.813195 | -4.445912 |

| | | | | | |
|---|---|---|---|---|---|
| 105 | 1 | 0 | -0.464106 | -2.488722 | -1.231714 |
| 106 | 1 | 0 | 0.706312 | -4.516314 | -2.687934 |
| 107 | 1 | 0 | 3.155861 | -3.455478 | -3.377671 |
| 108 | 1 | 0 | 4.467002 | -1.304423 | -3.188980 |
| 109 | 1 | 0 | 6.385965 | 0.270404 | -1.441823 |
| 110 | 1 | 0 | 6.954113 | 0.163557 | 1.187641 |
| 111 | 1 | 0 | 5.711017 | -3.519093 | -2.466437 |
| 112 | 1 | 0 | 8.993485 | -2.293486 | 3.764805 |
| 113 | 1 | 0 | 7.579674 | -1.621358 | 2.900788 |
| 114 | 1 | 0 | 10.546979 | -1.450783 | 1.461750 |
| 115 | 1 | 0 | 10.125612 | -1.950815 | -0.178460 |
| 116 | 1 | 0 | -1.281260 | -0.127005 | -3.395287 |
| 117 | 1 | 0 | -2.773614 | 0.481647 | -2.654935 |
| 118 | 1 | 0 | -1.456491 | 4.805713 | 1.257183 |
| 119 | 1 | 0 | 1.378045 | 7.568871 | -1.343116 |
| 120 | 1 | 0 | 1.690258 | 5.964079 | -2.080376 |
| 121 | 1 | 0 | 0.064545 | 6.687375 | -2.196055 |
| 122 | 1 | 0 | 2.593897 | 4.626428 | 0.800271 |
| 123 | 1 | 0 | 0.061290 | 1.873211 | 3.352964 |
| 124 | 1 | 0 | 4.860807 | 3.834003 | 1.346092 |
| 125 | 1 | 0 | 4.308878 | 2.139894 | 1.350270 |
| 126 | 1 | 0 | 2.173516 | 0.862401 | 4.232898 |
| 127 | 1 | 0 | 1.487948 | -0.090685 | 2.893256 |
| 128 | 1 | 0 | 2.897275 | 0.930338 | 2.609421 |

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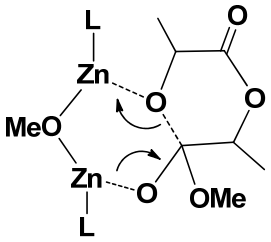


**TSII-III$^{dimer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.360794 | 2.856715 | -1.985050 |
| 2 | 7 | 0 | -2.859980 | 2.103044 | -0.988714 |
| 3 | 7 | 0 | -4.219529 | 2.149374 | -1.088916 |
| 4 | 6 | 0 | -4.557753 | 2.910449 | -2.146596 |
| 5 | 6 | 0 | -3.400151 | 3.383162 | -2.756465 |
| 6 | 30 | 0 | -1.990118 | 1.431643 | 0.775962 |
| 7 | 8 | 0 | -1.034962 | -0.237068 | 1.225293 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 30 | 0 | 0.957233 | -0.381710 | 1.188210 |
| 9 | 7 | 0 | 1.736908 | -1.859502 | 2.448755 |
| 10 | 7 | 0 | 2.531560 | -2.838594 | 1.934496 |
| 11 | 6 | 0 | 2.685109 | -3.811071 | 2.853659 |
| 12 | 6 | 0 | 1.973900 | -3.472574 | 4.000941 |
| 13 | 6 | 0 | 1.391428 | -2.241137 | 3.691199 |
| 14 | 5 | 0 | 3.245733 | -2.738063 | 0.531369 |
| 15 | 6 | 0 | 4.309555 | -1.528664 | 0.517557 |
| 16 | 6 | 0 | 4.576855 | -0.607933 | -0.553229 |
| 17 | 6 | 0 | 5.605949 | 0.302989 | -0.156891 |
| 18 | 6 | 0 | 6.008417 | -0.048630 | 1.165985 |
| 19 | 6 | 0 | 5.218700 | -1.169321 | 1.572044 |
| 20 | 26 | 0 | 6.328180 | -1.649618 | -0.117847 |
| 21 | 6 | 0 | 8.289494 | -2.318941 | 0.093721 |
| 22 | 6 | 0 | 8.104505 | -1.835760 | -1.245546 |
| 23 | 6 | 0 | 7.045834 | -2.617513 | -1.820086 |
| 24 | 6 | 0 | 6.599556 | -3.568505 | -0.854615 |
| 25 | 6 | 0 | 7.369838 | -3.384390 | 0.330767 |
| 26 | 15 | 0 | 9.216124 | -0.682101 | -2.136195 |
| 27 | 6 | 0 | 9.472777 | 0.656262 | -0.861639 |
| 28 | 5 | 0 | -5.180206 | 1.368598 | -0.127563 |
| 29 | 6 | 0 | -4.980040 | -0.223432 | -0.275638 |
| 30 | 6 | 0 | -4.311598 | -0.938503 | -1.327680 |
| 31 | 6 | 0 | -4.397565 | -2.344587 | -1.083191 |
| 32 | 6 | 0 | -5.128187 | -2.526797 | 0.129634 |
| 33 | 6 | 0 | -5.487736 | -1.230795 | 0.614517 |
| 34 | 26 | 0 | -6.298348 | -1.551661 | -1.274376 |
| 35 | 6 | 0 | -7.883755 | -0.459504 | -2.036022 |
| 36 | 6 | 0 | -8.378189 | -1.483086 | -1.157082 |
| 37 | 6 | 0 | -7.946002 | -2.740920 | -1.703751 |
| 38 | 6 | 0 | -7.206183 | -2.489351 | -2.896814 |
| 39 | 6 | 0 | -7.171293 | -1.077238 | -3.104931 |
| 40 | 15 | 0 | -9.368877 | -1.125662 | 0.342833 |
| 41 | 6 | 0 | -9.145210 | -2.701769 | 1.317101 |
| 42 | 7 | 0 | -3.675540 | 1.747424 | 1.945786 |
| 43 | 6 | 0 | -3.828268 | 2.114253 | 3.229901 |
| 44 | 6 | 0 | -5.165394 | 2.423943 | 3.488514 |
| 45 | 6 | 0 | -5.805356 | 2.227130 | 2.267650 |
| 46 | 7 | 0 | -4.900335 | 1.826659 | 1.355185 |
| 47 | 8 | 0 | -0.500189 | 2.769526 | 1.176425 |
| 48 | 6 | 0 | 0.615037 | 2.779773 | 0.609339 |
| 49 | 6 | 0 | 1.520025 | 3.998380 | 0.839139 |
| 50 | 6 | 0 | 1.151922 | 4.773018 | 2.100115 |
| 51 | 8 | 0 | 0.627335 | 2.131853 | -0.602388 |
| 52 | 6 | 0 | 1.809471 | 2.015023 | -1.391328 |
| 53 | 6 | 0 | 1.986486 | 3.206614 | -2.321415 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 8 | 0 | 3.088354 | 3.038067 | -3.065686 |
| 55 | 6 | 0 | 3.385529 | 4.098752 | -3.994969 |
| 56 | 8 | 0 | 1.238485 | 4.157991 | -2.396870 |
| 57 | 6 | 0 | -11.090510 | -1.445383 | -0.322796 |
| 58 | 6 | 0 | -1.763526 | -1.456359 | 1.375962 |
| 59 | 8 | 0 | 1.697159 | 1.424732 | 1.536356 |
| 60 | 6 | 0 | 2.878826 | 1.709936 | 2.247850 |
| 61 | 6 | 0 | 3.572702 | 2.972039 | 1.726930 |
| 62 | 8 | 0 | 4.703196 | 3.258646 | 2.034220 |
| 63 | 7 | 0 | 1.290225 | -1.480427 | -0.571754 |
| 64 | 7 | 0 | 2.154991 | -2.530876 | -0.578033 |
| 65 | 6 | 0 | 1.942899 | -3.274214 | -1.681246 |
| 66 | 6 | 0 | 0.911001 | -2.704995 | -2.421455 |
| 67 | 6 | 0 | 0.528321 | -1.587017 | -1.674310 |
| 68 | 6 | 0 | 2.676876 | 1.760961 | 3.770069 |
| 69 | 6 | 0 | 8.022241 | 0.179919 | -3.281868 |
| 70 | 8 | 0 | 2.933858 | 3.732069 | 0.776791 |
| 71 | 1 | 0 | 5.310322 | -1.686375 | 2.519763 |
| 72 | 1 | 0 | -9.404418 | -3.601795 | 0.747113 |
| 73 | 1 | 0 | -5.388408 | -3.475711 | 0.581331 |
| 74 | 1 | 0 | -3.324246 | 4.023087 | -3.622862 |
| 75 | 1 | 0 | 1.351747 | 4.643100 | -0.029256 |
| 76 | 1 | 0 | 2.371300 | 0.771220 | 4.124386 |
| 77 | 1 | 0 | -0.259108 | -0.867886 | -1.858755 |
| 78 | 1 | 0 | 3.292475 | -4.675584 | 2.628421 |
| 79 | 1 | 0 | 1.889607 | -4.037849 | 4.917013 |
| 80 | 1 | 0 | -8.106783 | -2.782549 | 1.651972 |
| 81 | 1 | 0 | -5.599212 | 3.063367 | -2.389416 |
| 82 | 1 | 0 | -1.292986 | 3.000513 | -2.076477 |
| 83 | 1 | 0 | -3.846961 | -0.481376 | -2.192645 |
| 84 | 1 | 0 | -4.010450 | -3.129793 | -1.720239 |
| 85 | 1 | 0 | -6.653970 | -0.564714 | -3.905581 |
| 86 | 1 | 0 | -7.995137 | 0.604750 | -1.874984 |
| 87 | 1 | 0 | -8.117355 | -3.715343 | -1.265966 |
| 88 | 1 | 0 | -6.718720 | -3.235546 | -3.511192 |
| 89 | 1 | 0 | -6.072868 | -1.033589 | 1.504470 |
| 90 | 1 | 0 | -5.605768 | 2.747798 | 4.419667 |
| 91 | 1 | 0 | -6.295411 | 1.757153 | -0.376236 |
| 92 | 1 | 0 | -11.814418 | -1.382624 | 0.497945 |
| 93 | 1 | 0 | -11.345298 | -0.672481 | -1.055289 |
| 94 | 1 | 0 | -11.180061 | -2.426990 | -0.802748 |
| 95 | 1 | 0 | -9.786990 | -2.658952 | 2.203942 |
| 96 | 1 | 0 | -2.971392 | 2.143075 | 3.890182 |
| 97 | 1 | 0 | -6.842880 | 2.336543 | 1.986864 |
| 98 | 1 | 0 | -2.812635 | -1.253878 | 1.616204 |
| 99 | 1 | 0 | -1.737870 | -2.053345 | 0.455185 |

| | | | | | |
|---|---|---|---|---|---|
| 100 | 1 | 0 | -1.336825 | -2.058789 | 2.189699 |
| 101 | 1 | 0 | 0.496231 | -3.056171 | -3.354552 |
| 102 | 1 | 0 | 2.539791 | -4.156194 | -1.862333 |
| 103 | 1 | 0 | 0.740890 | -1.615911 | 4.288961 |
| 104 | 1 | 0 | 3.716621 | -3.833509 | 0.338378 |
| 105 | 1 | 0 | 4.094353 | -0.624791 | -1.522687 |
| 106 | 1 | 0 | 6.015394 | 1.106312 | -0.754238 |
| 107 | 1 | 0 | 6.781121 | 0.436041 | 1.747780 |
| 108 | 1 | 0 | 8.997701 | -1.928491 | 0.813273 |
| 109 | 1 | 0 | 5.779893 | -4.263220 | -0.978023 |
| 110 | 1 | 0 | 7.246592 | -3.921477 | 1.262159 |
| 111 | 1 | 0 | 6.639966 | -2.494371 | -2.815863 |
| 112 | 1 | 0 | 10.034825 | 1.476220 | -1.322489 |
| 113 | 1 | 0 | 8.531972 | 1.042799 | -0.457053 |
| 114 | 1 | 0 | 10.078001 | 0.267131 | -0.036374 |
| 115 | 1 | 0 | 8.545699 | 1.009812 | -3.769552 |
| 116 | 1 | 0 | 7.699150 | -0.511607 | -4.066883 |
| 117 | 1 | 0 | 7.138534 | 0.563232 | -2.761806 |
| 118 | 1 | 0 | 1.844542 | 5.612792 | 2.208939 |
| 119 | 1 | 0 | 0.133211 | 5.158736 | 2.020188 |
| 120 | 1 | 0 | 1.205561 | 4.148398 | 2.994604 |
| 121 | 1 | 0 | 3.611943 | 2.036134 | 4.267725 |
| 122 | 1 | 0 | 1.899060 | 2.478037 | 4.050527 |
| 123 | 1 | 0 | 3.621993 | 0.925506 | 2.047105 |
| 124 | 1 | 0 | 1.678814 | 1.112137 | -1.993815 |
| 125 | 1 | 0 | 2.693751 | 1.875222 | -0.770561 |
| 126 | 1 | 0 | 4.296799 | 3.789283 | -4.505880 |
| 127 | 1 | 0 | 2.565187 | 4.222329 | -4.706282 |
| 128 | 1 | 0 | 3.543232 | 5.037435 | -3.458431 |

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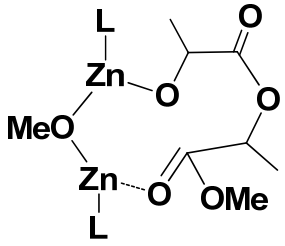


**III$^{dimer}$- propagation-LA**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

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| | | | | | |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -6.369700 | -1.171401 | -1.398475 |
| 2 | 6 | 0 | -5.024627 | -0.186561 | -0.090394 |
| 3 | 6 | 0 | -5.615261 | -1.337686 | 0.534633 |
| 4 | 6 | 0 | -4.355108 | -0.683608 | -1.261227 |
| 5 | 6 | 0 | -4.523148 | -2.100729 | -1.346154 |
| 6 | 6 | 0 | -5.306183 | -2.509257 | -0.224646 |
| 7 | 6 | 0 | -7.903297 | 0.136160 | -1.872076 |
| 8 | 6 | 0 | -8.451307 | -1.077179 | -1.331380 |
| 9 | 6 | 0 | -8.023026 | -2.144485 | -2.194447 |
| 10 | 6 | 0 | -7.233126 | -1.591622 | -3.245455 |
| 11 | 6 | 0 | -7.163069 | -0.179167 | -3.048760 |
| 12 | 7 | 0 | -4.697776 | 1.467105 | 1.924370 |
| 13 | 7 | 0 | -4.258180 | 2.292390 | -0.453515 |
| 14 | 7 | 0 | -2.897785 | 2.205869 | -0.507221 |
| 15 | 30 | 0 | -1.854474 | 1.196044 | 0.979509 |
| 16 | 8 | 0 | -0.996006 | -0.606206 | 0.964393 |
| 17 | 30 | 0 | 0.964338 | -0.707591 | 0.855123 |
| 18 | 7 | 0 | 1.779344 | -2.110777 | 2.169853 |
| 19 | 6 | 0 | 1.336847 | -2.563159 | 3.357384 |
| 20 | 6 | 0 | 1.965885 | -3.766474 | 3.683319 |
| 21 | 6 | 0 | 2.807056 | -4.015553 | 2.602462 |
| 22 | 7 | 0 | 2.681217 | -3.019779 | 1.705225 |
| 23 | 7 | 0 | 1.548475 | -1.708707 | -0.875276 |
| 24 | 6 | 0 | 1.466857 | -2.904426 | -2.779478 |
| 25 | 7 | 0 | 2.513088 | -2.669253 | -0.822124 |
| 26 | 5 | 0 | 3.514020 | -2.814305 | 0.380756 |
| 27 | 6 | 0 | 4.460753 | -1.520883 | 0.511142 |
| 28 | 6 | 0 | 5.334053 | -1.219127 | 1.613690 |
| 29 | 6 | 0 | 6.005410 | 0.018907 | 1.370868 |
| 30 | 6 | 0 | 5.562844 | 0.505791 | 0.105353 |
| 31 | 6 | 0 | 4.628558 | -0.440366 | -0.421524 |
| 32 | 26 | 0 | 6.474290 | -1.353164 | -0.120049 |
| 33 | 6 | 0 | 8.138491 | -1.226861 | -1.416251 |
| 34 | 6 | 0 | 7.828551 | -2.891331 | 0.183544 |
| 35 | 6 | 0 | 8.530847 | -1.684357 | -0.113025 |
| 36 | 6 | 0 | 6.987118 | -3.191392 | -0.927362 |
| 37 | 15 | 0 | 8.942513 | 0.105439 | -2.385293 |
| 38 | 8 | 0 | -0.264318 | 2.263124 | 1.547259 |
| 39 | 8 | 0 | 1.790157 | 1.136052 | 1.390485 |
| 40 | 6 | 0 | 2.692017 | 1.405405 | 2.479462 |
| 41 | 6 | 0 | 3.529833 | 2.642355 | 2.161495 |
| 42 | 8 | 0 | 4.584389 | 2.858005 | 2.705971 |
| 43 | 6 | 0 | 2.013655 | 1.460096 | 3.850303 |
| 44 | 8 | 0 | 3.078916 | 3.447695 | 1.168070 |
| 45 | 6 | 0 | 1.646847 | 3.606931 | 0.976581 |
| 46 | 6 | 0 | 1.098140 | 4.589103 | 2.005786 |

| | | | | | |
|---|---|---|---|---|---|
| 47 | 6 | 0 | 0.860993 | 2.255601 | 0.909078 |
| 48 | 8 | 0 | 0.647355 | 1.796673 | -0.447355 |
| 49 | 6 | 0 | 1.725554 | 1.835668 | -1.372039 |
| 50 | 6 | 0 | 1.565873 | 2.961447 | -2.386584 |
| 51 | 8 | 0 | 2.460513 | 2.804828 | -3.376823 |
| 52 | 6 | 0 | 2.453673 | 3.823529 | -4.395242 |
| 53 | 6 | 0 | 7.172276 | -2.169462 | -1.906100 |
| 54 | 6 | 0 | 0.906008 | -1.854607 | -2.048766 |
| 55 | 6 | 0 | 2.478868 | -3.391884 | -1.957327 |
| 56 | 6 | 0 | -4.671941 | 3.250107 | -1.304813 |
| 57 | 6 | 0 | -3.563965 | 3.812076 | -1.930595 |
| 58 | 6 | 0 | -2.471701 | 3.128162 | -1.388020 |
| 59 | 6 | 0 | -5.489785 | 1.697378 | 2.988412 |
| 60 | 6 | 0 | -4.722538 | 1.639666 | 4.148641 |
| 61 | 6 | 0 | -3.431345 | 1.364166 | 3.692179 |
| 62 | 7 | 0 | -3.423560 | 1.252729 | 2.352846 |
| 63 | 6 | 0 | 9.214678 | 1.404164 | -1.074198 |
| 64 | 6 | 0 | 7.485444 | 0.846684 | -3.284937 |
| 65 | 6 | 0 | -1.742607 | -1.819931 | 1.025279 |
| 66 | 5 | 0 | -5.143624 | 1.338372 | 0.416310 |
| 67 | 15 | 0 | -9.488758 | -1.124296 | 0.178641 |
| 68 | 6 | 0 | -11.189194 | -1.238065 | -0.599640 |
| 69 | 8 | 0 | 0.770321 | 3.874193 | -2.322020 |
| 70 | 6 | 0 | -9.297053 | -2.905737 | 0.701218 |
| 71 | 1 | 0 | 5.483283 | -1.849908 | 2.482056 |
| 72 | 1 | 0 | -9.542291 | -3.618404 | -0.095113 |
| 73 | 1 | 0 | -5.635972 | -3.518065 | -0.010161 |
| 74 | 1 | 0 | -3.551105 | 4.606559 | -2.661853 |
| 75 | 1 | 0 | 1.569043 | 4.072146 | -0.006334 |
| 76 | 1 | 0 | 1.591118 | 0.479149 | 4.088895 |
| 77 | 1 | 0 | 0.074079 | -1.207469 | -2.294419 |
| 78 | 1 | 0 | 3.488781 | -4.831659 | 2.411927 |
| 79 | 1 | 0 | 1.829050 | -4.371300 | 4.567196 |
| 80 | 1 | 0 | -8.267877 | -3.081568 | 1.027633 |
| 81 | 1 | 0 | -5.726143 | 3.464361 | -1.404221 |
| 82 | 1 | 0 | -1.413578 | 3.261320 | -1.569723 |
| 83 | 1 | 0 | -3.833888 | -0.070601 | -1.985848 |
| 84 | 1 | 0 | -4.155061 | -2.743607 | -2.135925 |
| 85 | 1 | 0 | -6.603323 | 0.520983 | -3.655196 |
| 86 | 1 | 0 | -8.000945 | 1.115838 | -1.422999 |
| 87 | 1 | 0 | -8.231547 | -3.196673 | -2.053718 |
| 88 | 1 | 0 | -6.737253 | -2.150697 | -4.028776 |
| 89 | 1 | 0 | -6.226610 | -1.314488 | 1.428784 |
| 90 | 1 | 0 | -5.053160 | 1.783458 | 5.166477 |
| 91 | 1 | 0 | -6.265779 | 1.781696 | 0.380221 |
| 92 | 1 | 0 | -11.937927 | -1.395194 | 0.185418 |

| | | | | | |
|---|---|---|---|---|---|
| 93 | 1 | 0 | -11.422063 | -0.293297 | -1.101677 |
| 94 | 1 | 0 | -11.263438 | -2.051611 | -1.330829 |
| 95 | 1 | 0 | -9.961967 | -3.096124 | 1.550883 |
| 96 | 1 | 0 | -2.510768 | 1.251046 | 4.249624 |
| 97 | 1 | 0 | -6.544591 | 1.882765 | 2.846209 |
| 98 | 1 | 0 | -2.784314 | -1.614264 | 1.291042 |
| 99 | 1 | 0 | -1.738330 | -2.338849 | 0.057642 |
| 100 | 1 | 0 | -1.322867 | -2.498206 | 1.781974 |
| 101 | 1 | 0 | 1.178169 | -3.264740 | -3.755490 |
| 102 | 1 | 0 | 3.176545 | -4.203815 | -2.101969 |
| 103 | 1 | 0 | 0.587651 | -2.006482 | 3.905079 |
| 104 | 1 | 0 | 4.097651 | -3.857345 | 0.208768 |
| 105 | 1 | 0 | 4.144144 | -0.371224 | -1.387254 |
| 106 | 1 | 0 | 5.887179 | 1.421427 | -0.370312 |
| 107 | 1 | 0 | 6.726587 | 0.496520 | 2.020384 |
| 108 | 1 | 0 | 9.231117 | -1.186770 | 0.545250 |
| 109 | 1 | 0 | 6.284064 | -4.011411 | -0.988464 |
| 110 | 1 | 0 | 7.889532 | -3.450789 | 1.107946 |
| 111 | 1 | 0 | 6.656329 | -2.107857 | -2.855584 |
| 112 | 1 | 0 | 9.562112 | 2.323849 | -1.557824 |
| 113 | 1 | 0 | 8.309657 | 1.616625 | -0.496132 |
| 114 | 1 | 0 | 10.003008 | 1.076425 | -0.388684 |
| 115 | 1 | 0 | 7.820793 | 1.747840 | -3.810437 |
| 116 | 1 | 0 | 7.121701 | 0.141871 | -4.039833 |
| 117 | 1 | 0 | 6.659876 | 1.102848 | -2.613477 |
| 118 | 1 | 0 | 1.690320 | 5.508361 | 1.964105 |
| 119 | 1 | 0 | 0.055810 | 4.821160 | 1.778291 |
| 120 | 1 | 0 | 1.140383 | 4.192464 | 3.023535 |
| 121 | 1 | 0 | 2.761367 | 1.708672 | 4.609895 |
| 122 | 1 | 0 | 1.208983 | 2.197394 | 3.878305 |
| 123 | 1 | 0 | 3.403341 | 0.575432 | 2.465710 |
| 124 | 1 | 0 | 1.751384 | 0.883520 | -1.909852 |
| 125 | 1 | 0 | 2.692106 | 1.941531 | -0.868844 |
| 126 | 1 | 0 | 3.230974 | 3.533084 | -5.101646 |
| 127 | 1 | 0 | 1.478702 | 3.862605 | -4.887263 |
| 128 | 1 | 0 | 2.674972 | 4.800214 | -3.957586 |

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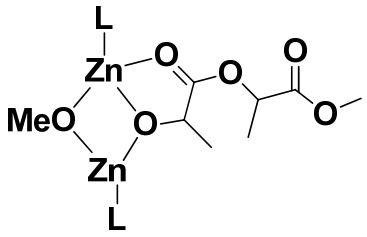

**$IV^{dimer}$- propagation-LA**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.484444 | -0.702227 | -3.019145 |
| 2 | 7 | 0 | 4.022138 | 0.131801 | -2.067165 |
| 3 | 7 | 0 | 2.705769 | -0.131978 | -1.839447 |
| 4 | 6 | 0 | 2.352673 | -1.131344 | -2.665819 |
| 5 | 6 | 0 | 3.447876 | -1.532544 | -3.435835 |
| 6 | 5 | 0 | 4.874875 | 1.094396 | -1.169505 |
| 7 | 6 | 0 | 5.123214 | 0.435216 | 0.283186 |
| 8 | 6 | 0 | 5.584130 | 1.099010 | 1.469606 |
| 9 | 6 | 0 | 5.702202 | 0.153646 | 2.535765 |
| 10 | 6 | 0 | 5.325048 | -1.124168 | 2.021233 |
| 11 | 6 | 0 | 4.977211 | -0.946030 | 0.645628 |
| 12 | 26 | 0 | 6.957970 | -0.382692 | 0.985725 |
| 13 | 6 | 0 | 8.884030 | -0.461362 | 1.771681 |
| 14 | 6 | 0 | 8.547515 | -1.712026 | 1.174792 |
| 15 | 6 | 0 | 8.258735 | -1.493415 | -0.216438 |
| 16 | 6 | 0 | 8.417595 | -0.085178 | -0.455449 |
| 17 | 6 | 0 | 8.808031 | 0.544924 | 0.761232 |
| 18 | 15 | 0 | 7.808136 | -2.684002 | -1.532746 |
| 19 | 6 | 0 | 7.070755 | -4.083299 | -0.542681 |
| 20 | 30 | 0 | 1.505941 | 1.025833 | -0.563418 |
| 21 | 7 | 0 | 2.866170 | 2.642539 | -0.621772 |
| 22 | 7 | 0 | 4.149295 | 2.482333 | -1.048006 |
| 23 | 6 | 0 | 4.711336 | 3.693781 | -1.228413 |
| 24 | 6 | 0 | 3.780089 | 4.678845 | -0.916399 |
| 25 | 6 | 0 | 2.636141 | 3.964678 | -0.549317 |
| 26 | 30 | 0 | -0.554811 | -0.602414 | 0.964757 |
| 27 | 8 | 0 | -0.305671 | -0.086310 | -0.948562 |
| 28 | 6 | 0 | -1.279553 | 0.520121 | -1.744521 |
| 29 | 6 | 0 | -1.236939 | 0.017111 | -3.199152 |
| 30 | 7 | 0 | -0.842399 | -2.577271 | 1.542429 |
| 31 | 7 | 0 | -2.022367 | -2.936871 | 2.123066 |
| 32 | 6 | 0 | -1.909479 | -4.187234 | 2.610610 |
| 33 | 6 | 0 | -0.628647 | -4.665050 | 2.351111 |
| 34 | 6 | 0 | 0.002737 | -3.612204 | 1.683193 |
| 35 | 5 | 0 | -3.305419 | -2.027720 | 2.089737 |
| 36 | 7 | 0 | -2.956970 | -0.653153 | 2.775663 |
| 37 | 7 | 0 | -1.974171 | 0.154396 | 2.300012 |
| 38 | 6 | 0 | -1.925488 | 1.236564 | 3.093251 |
| 39 | 6 | 0 | -2.906214 | 1.148267 | 4.088176 |
| 40 | 6 | 0 | -3.531221 | -0.073490 | 3.845803 |

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|---|---|---|---|---|---|
| 41 | 6 | 0 | -3.792075 | -1.782555 | 0.573826 |
| 42 | 6 | 0 | -4.688944 | -0.755188 | 0.120197 |
| 43 | 6 | 0 | -4.881895 | -0.876653 | -1.290854 |
| 44 | 6 | 0 | -4.118637 | -1.998355 | -1.736477 |
| 45 | 6 | 0 | -3.455170 | -2.547718 | -0.595756 |
| 46 | 26 | 0 | -5.516956 | -2.614637 | -0.335937 |
| 47 | 6 | 0 | -6.024166 | -4.612593 | -0.102985 |
| 48 | 6 | 0 | -6.369485 | -3.878032 | 1.069377 |
| 49 | 6 | 0 | -7.308365 | -2.871583 | 0.695739 |
| 50 | 6 | 0 | -7.563902 | -2.975496 | -0.713609 |
| 51 | 6 | 0 | -6.751603 | -4.055909 | -1.197639 |
| 52 | 15 | 0 | -8.900021 | -2.124220 | -1.635916 |
| 53 | 6 | 0 | -8.762666 | -0.384382 | -0.976769 |
| 54 | 6 | 0 | -8.115769 | -1.904126 | -3.314343 |
| 55 | 8 | 0 | 1.097826 | 0.430589 | 1.302679 |
| 56 | 6 | 0 | 1.884353 | 0.569186 | 2.469847 |
| 57 | 8 | 0 | -0.049201 | 2.545539 | -1.233390 |
| 58 | 6 | 0 | -1.055508 | 2.029396 | -1.716956 |
| 59 | 8 | 0 | -2.034797 | 2.741942 | -2.267187 |
| 60 | 6 | 0 | -1.905798 | 4.184084 | -2.227617 |
| 61 | 6 | 0 | -2.025226 | 4.726876 | -0.806213 |
| 62 | 8 | 0 | -2.706834 | 3.883127 | 0.001753 |
| 63 | 6 | 0 | -3.091456 | 4.412875 | 1.264410 |
| 64 | 6 | 0 | -3.021889 | 4.754061 | -3.098307 |
| 65 | 6 | 0 | 9.487814 | -3.438303 | -1.879909 |
| 66 | 8 | 0 | -1.602808 | 5.808964 | -0.475230 |
| 67 | 1 | 0 | 9.114565 | -0.297861 | 2.816804 |
| 68 | 1 | 0 | 5.831047 | 2.151722 | 1.538513 |
| 69 | 1 | 0 | -4.073293 | -2.380237 | -2.748310 |
| 70 | 1 | 0 | -6.687088 | -4.385025 | -2.226631 |
| 71 | 1 | 0 | -5.304699 | -5.418885 | -0.163425 |
| 72 | 1 | 0 | -8.032525 | -2.875553 | -3.812470 |
| 73 | 1 | 0 | -7.741223 | 0.005995 | -1.023757 |
| 74 | 1 | 0 | -3.114037 | 1.846202 | 4.886117 |
| 75 | 1 | 0 | -0.252324 | 0.202600 | -3.641958 |
| 76 | 1 | 0 | -2.002467 | 0.505003 | -3.810951 |
| 77 | 1 | 0 | 9.375377 | -4.263065 | -2.593245 |
| 78 | 1 | 0 | -2.818568 | -3.423632 | -0.604820 |
| 79 | 1 | 0 | 6.119160 | -3.762920 | -0.109043 |
| 80 | 1 | 0 | 7.727161 | -4.432376 | 0.262998 |
| 81 | 1 | 0 | 3.910555 | 5.749918 | -0.960871 |
| 82 | 1 | 0 | 6.051554 | 0.360891 | 3.539533 |
| 83 | 1 | 0 | 8.968207 | 1.605538 | 0.905524 |
| 84 | 1 | 0 | 8.220035 | 0.414424 | -1.394671 |
| 85 | 1 | 0 | 8.490704 | -2.659524 | 1.694114 |
| 86 | 1 | 0 | 5.334580 | -2.060478 | 2.565269 |

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|---|---|---|---|---|---|
| 87 | 1 | 0 | 4.669549 | -1.732944 | -0.031772 |
| 88 | 1 | 0 | 3.487647 | -2.308344 | -4.185953 |
| 89 | 1 | 0 | 5.889949 | 1.320576 | -1.784612 |
| 90 | 1 | 0 | 10.136211 | -2.684012 | -2.337638 |
| 91 | 1 | 0 | 9.975799 | -3.816185 | -0.973645 |
| 92 | 1 | 0 | 6.873822 | -4.924713 | -1.216311 |
| 93 | 1 | 0 | 1.335156 | -1.494776 | -2.652848 |
| 94 | 1 | 0 | 5.522384 | -0.667446 | -3.315654 |
| 95 | 1 | 0 | 1.658418 | 4.327569 | -0.264538 |
| 96 | 1 | 0 | 5.733835 | 3.768594 | -1.568809 |
| 97 | 1 | 0 | -2.295336 | 0.347496 | -1.358205 |
| 98 | 1 | 0 | -1.177031 | 1.997289 | 2.915230 |
| 99 | 1 | 0 | -4.339598 | -0.569491 | 4.363235 |
| 100 | 1 | 0 | 1.013069 | -3.541996 | 1.302103 |
| 101 | 1 | 0 | -0.217805 | -5.628846 | 2.612015 |
| 102 | 1 | 0 | -2.749401 | -4.651434 | 3.106689 |
| 103 | 1 | 0 | -4.112969 | -2.557633 | 2.814498 |
| 104 | 1 | 0 | -5.159385 | -0.012587 | 0.753157 |
| 105 | 1 | 0 | -5.505053 | -0.242179 | -1.907279 |
| 106 | 1 | 0 | -5.948934 | -4.014454 | 2.056522 |
| 107 | 1 | 0 | -7.745076 | -2.140639 | 1.363811 |
| 108 | 1 | 0 | -8.771633 | -1.275962 | -3.927271 |
| 109 | 1 | 0 | -7.122211 | -1.447778 | -3.260562 |
| 110 | 1 | 0 | -9.427410 | 0.264310 | -1.557987 |
| 111 | 1 | 0 | -9.103985 | -0.356460 | 0.063169 |
| 112 | 1 | 0 | -1.421580 | -1.060549 | -3.198254 |
| 113 | 1 | 0 | -0.918784 | 4.464802 | -2.601117 |
| 114 | 1 | 0 | -2.928090 | 5.842669 | -3.140160 |
| 115 | 1 | 0 | -2.944136 | 4.349917 | -4.111719 |
| 116 | 1 | 0 | -4.000021 | 4.504639 | -2.678601 |
| 117 | 1 | 0 | -3.260010 | 3.548820 | 1.911588 |
| 118 | 1 | 0 | -2.288843 | 5.030027 | 1.680252 |
| 119 | 6 | 0 | -4.369235 | 5.243698 | 1.094811 |
| 120 | 1 | 0 | 1.245387 | 0.602683 | 3.365752 |
| 121 | 1 | 0 | 2.595007 | -0.259849 | 2.582548 |
| 122 | 1 | 0 | 2.467237 | 1.498694 | 2.433632 |
| 123 | 8 | 0 | -4.870709 | 5.455270 | 0.020103 |
| 124 | 8 | 0 | -4.933647 | 5.742129 | 2.217224 |
| 125 | 6 | 0 | -4.346991 | 5.521527 | 3.505590 |
| 126 | 1 | 0 | -4.998398 | 6.036627 | 4.212305 |
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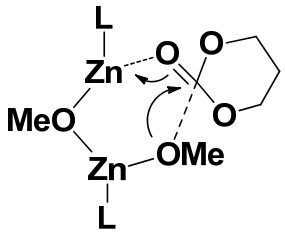


**TSI-II$^{dimer}$- propagation-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 1.253637 | 1.331692 | 2.934404 |
| 2 | 6 | 0 | 1.207341 | 1.705995 | 1.638910 |
| 3 | 8 | 0 | 2.147417 | 2.608053 | 1.242529 |
| 4 | 6 | 0 | 3.235435 | 2.799540 | 2.178616 |
| 5 | 6 | 0 | 2.697173 | 3.250379 | 3.533455 |
| 6 | 6 | 0 | 1.502912 | 2.352031 | 3.923527 |
| 7 | 8 | 0 | 0.815488 | 0.815914 | 0.834757 |
| 8 | 30 | 0 | 0.981215 | 0.649293 | -1.179172 |
| 9 | 7 | 0 | 2.382937 | 1.643621 | -2.321120 |
| 10 | 6 | 0 | 2.338840 | 2.850640 | -2.910710 |
| 11 | 6 | 0 | 3.359951 | 2.957484 | -3.858848 |
| 12 | 6 | 0 | 4.010909 | 1.727875 | -3.804508 |
| 13 | 7 | 0 | 3.412412 | 0.951196 | -2.882414 |
| 14 | 5 | 0 | 3.858097 | -0.487420 | -2.402466 |
| 15 | 6 | 0 | 4.403167 | -0.438589 | -0.889509 |
| 16 | 6 | 0 | 5.635089 | 0.175213 | -0.477082 |
| 17 | 6 | 0 | 5.792715 | 0.033903 | 0.935508 |
| 18 | 6 | 0 | 4.661546 | -0.688664 | 1.425862 |
| 19 | 6 | 0 | 3.815833 | -0.973562 | 0.308986 |
| 20 | 26 | 0 | 5.682332 | -1.841493 | 0.037370 |
| 21 | 6 | 0 | 7.294474 | -2.782309 | -0.891821 |
| 22 | 6 | 0 | 6.062263 | -3.308893 | -1.379884 |
| 23 | 6 | 0 | 5.354206 | -3.866129 | -0.274382 |
| 24 | 6 | 0 | 6.154382 | -3.683823 | 0.892891 |
| 25 | 6 | 0 | 7.371042 | -3.017336 | 0.522762 |
| 26 | 15 | 0 | 8.855656 | -2.814174 | 1.577563 |
| 27 | 6 | 0 | 9.566179 | -1.220121 | 0.917176 |
| 28 | 30 | 0 | -1.601250 | 1.698351 | 0.445356 |
| 29 | 8 | 0 | -0.349446 | 2.827734 | 1.619552 |
| 30 | 6 | 0 | -0.219870 | 4.205883 | 1.526829 |
| 31 | 6 | 0 | 0.089483 | 4.698987 | 0.115711 |
| 32 | 8 | 0 | -0.157143 | 4.083118 | -0.905024 |
| 33 | 7 | 0 | -2.436265 | 0.361827 | 1.821797 |
| 34 | 6 | 0 | -1.846127 | -0.328374 | 2.811303 |

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|---|---|---|---|---|---|
| 35 | 6 | 0 | -2.812834 | -0.901876 | 3.643147 |
| 36 | 6 | 0 | -4.025266 | -0.500037 | 3.092378 |
| 37 | 7 | 0 | -3.782605 | 0.260931 | 2.006665 |
| 38 | 5 | 0 | -4.835806 | 0.793031 | 0.979407 |
| 39 | 6 | 0 | -4.799863 | -0.083075 | -0.375177 |
| 40 | 6 | 0 | -4.171053 | -1.359024 | -0.564852 |
| 41 | 6 | 0 | -4.388547 | -1.810031 | -1.903489 |
| 42 | 6 | 0 | -5.165835 | -0.815222 | -2.570200 |
| 43 | 6 | 0 | -5.419941 | 0.233219 | -1.631223 |
| 44 | 26 | 0 | -6.213744 | -1.561559 | -0.952536 |
| 45 | 6 | 0 | -7.090757 | -2.920958 | 0.371670 |
| 46 | 6 | 0 | -7.253071 | -3.364061 | -0.986312 |
| 47 | 6 | 0 | -7.978087 | -2.369184 | -1.706007 |
| 48 | 6 | 0 | -8.272432 | -1.299819 | -0.806010 |
| 49 | 6 | 0 | -7.723831 | -1.633919 | 0.465682 |
| 50 | 15 | 0 | -6.309766 | -3.755650 | 1.802365 |
| 51 | 6 | 0 | -5.084282 | -4.885819 | 0.963210 |
| 52 | 7 | 0 | -3.388017 | 2.789220 | 0.165790 |
| 53 | 7 | 0 | -4.562028 | 2.313921 | 0.663713 |
| 54 | 6 | 0 | -5.484472 | 3.295939 | 0.636968 |
| 55 | 6 | 0 | -4.908754 | 4.448901 | 0.112260 |
| 56 | 6 | 0 | -3.590270 | 4.075701 | -0.164202 |
| 57 | 8 | 0 | -0.947378 | 0.992903 | -1.301160 |
| 58 | 6 | 0 | -1.641325 | 1.245022 | -2.513032 |
| 59 | 6 | 0 | -7.633072 | -5.023188 | 2.195089 |
| 60 | 7 | 0 | 1.439694 | -1.228828 | -1.937582 |
| 61 | 7 | 0 | 2.633839 | -1.456156 | -2.551975 |
| 62 | 6 | 0 | 2.576129 | -2.634306 | -3.201546 |
| 63 | 6 | 0 | 1.316645 | -3.196926 | -3.015407 |
| 64 | 6 | 0 | 0.638105 | -2.269395 | -2.219741 |
| 65 | 6 | 0 | 8.106976 | -2.203147 | 3.174000 |
| 66 | 8 | 0 | 0.621513 | 5.933456 | 0.136489 |
| 67 | 6 | 0 | 0.882666 | 6.538506 | -1.141810 |
| 68 | 1 | 0 | -5.530519 | -0.864982 | -3.588504 |
| 69 | 1 | 0 | -1.550246 | 2.298217 | -2.817108 |
| 70 | 1 | 0 | 5.879914 | -3.985804 | 1.895492 |
| 71 | 1 | 0 | -8.222653 | -2.399185 | -2.760322 |
| 72 | 1 | 0 | -6.012655 | 1.118197 | -1.830295 |
| 73 | 1 | 0 | 4.493877 | -1.003053 | 2.448407 |
| 74 | 1 | 0 | 4.365948 | -4.305918 | -0.305680 |
| 75 | 1 | 0 | 7.535405 | -3.010137 | 3.643992 |
| 76 | 1 | 0 | 8.817839 | -0.424944 | 0.837610 |
| 77 | 1 | 0 | 3.590505 | 3.796829 | -4.498100 |
| 78 | 1 | 0 | -7.270633 | -5.695378 | 2.981544 |
| 79 | 1 | 0 | 2.898641 | -1.545314 | 0.356525 |
| 80 | 1 | 0 | -4.286027 | -4.290431 | 0.511109 |

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| 81 | 1 | 0 | -5.538965 | -5.514489 | 0.188391 |
| 82 | 1 | 0 | -5.377314 | 5.409441 | -0.043112 |
| 83 | 1 | 0 | -8.779539 | -0.377393 | -1.057703 |
| 84 | 1 | 0 | -7.733021 | -1.005598 | 1.346848 |
| 85 | 1 | 0 | -6.864033 | -4.283565 | -1.403653 |
| 86 | 1 | 0 | -4.054377 | -2.748630 | -2.327496 |
| 87 | 1 | 0 | -3.630206 | -1.898585 | 0.202322 |
| 88 | 1 | 0 | -2.659724 | -1.518562 | 4.516299 |
| 89 | 1 | 0 | -5.902971 | 0.781016 | 1.545360 |
| 90 | 1 | 0 | -8.524623 | -4.512382 | 2.573448 |
| 91 | 1 | 0 | -7.916063 | -5.619719 | 1.319789 |
| 92 | 1 | 0 | -4.636116 | -5.540204 | 1.719222 |
| 93 | 1 | 0 | -0.767276 | -0.357028 | 2.873199 |
| 94 | 1 | 0 | -5.040866 | -0.722438 | 3.384283 |
| 95 | 1 | 0 | -2.780237 | 4.652133 | -0.589294 |
| 96 | 1 | 0 | -6.488085 | 3.102789 | 0.986827 |
| 97 | 1 | 0 | 0.565231 | 4.595735 | 2.187507 |
| 98 | 1 | 0 | 1.571101 | 3.555321 | -2.620114 |
| 99 | 1 | 0 | 4.859721 | 1.352450 | -4.357358 |
| 100 | 1 | 0 | -0.377267 | -2.282179 | -1.846027 |
| 101 | 1 | 0 | 0.948282 | -4.133240 | -3.407280 |
| 102 | 1 | 0 | 3.433058 | -2.990586 | -3.754443 |
| 103 | 1 | 0 | 4.691325 | -0.844683 | -3.201093 |
| 104 | 1 | 0 | 6.348628 | 0.647542 | -1.141536 |
| 105 | 1 | 0 | 6.632482 | 0.382630 | 1.522407 |
| 106 | 1 | 0 | 5.707860 | -3.244129 | -2.399547 |
| 107 | 1 | 0 | 8.041435 | -2.275763 | -1.489078 |
| 108 | 1 | 0 | 8.916912 | -1.931100 | 3.860086 |
| 109 | 1 | 0 | 7.446972 | -1.341934 | 3.029054 |
| 110 | 1 | 0 | 10.374333 | -0.895211 | 1.581882 |
| 111 | 1 | 0 | 10.003804 | -1.393116 | -0.071379 |
| 112 | 1 | 0 | -1.238250 | 0.617876 | -3.321385 |
| 113 | 1 | 0 | -2.704712 | 1.004502 | -2.402303 |
| 114 | 1 | 0 | -1.156266 | 4.703046 | 1.834079 |
| 115 | 1 | 0 | 1.201617 | 7.557829 | -0.923217 |
| 116 | 1 | 0 | 1.676277 | 5.996571 | -1.663303 |
| 117 | 1 | 0 | -0.019098 | 6.540733 | -1.759453 |
| 118 | 1 | 0 | 3.875575 | 3.551502 | 1.715579 |
| 119 | 1 | 0 | 3.792688 | 1.860861 | 2.253579 |
| 120 | 1 | 0 | 3.498084 | 3.189278 | 4.278660 |
| 121 | 1 | 0 | 2.385073 | 4.298335 | 3.478860 |
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| 123 | 1 | 0 | 0.581006 | 2.925500 | 4.045257 |

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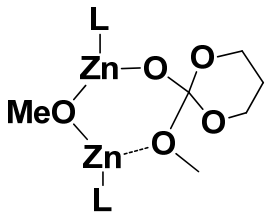


**II$^{dimer}$- propagation-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -6.273438 | -1.558100 | -0.970202 |
| 2 | 6 | 0 | -5.444836 | 0.232931 | -1.617881 |
| 3 | 6 | 0 | -4.822430 | -0.125433 | -0.374240 |
| 4 | 6 | 0 | -4.224456 | -1.411546 | -0.597643 |
| 5 | 6 | 0 | -4.463449 | -1.827270 | -1.944007 |
| 6 | 6 | 0 | -7.784544 | -1.616643 | 0.448021 |
| 7 | 6 | 0 | -7.170300 | -2.912117 | 0.345728 |
| 8 | 6 | 0 | -7.339172 | -3.344016 | -1.015092 |
| 9 | 6 | 0 | -8.049388 | -2.333912 | -1.728362 |
| 10 | 6 | 0 | -8.328027 | -1.266179 | -0.821501 |
| 11 | 15 | 0 | -6.399009 | -3.765143 | 1.770970 |
| 12 | 5 | 0 | -4.822214 | 0.724564 | 0.996767 |
| 13 | 7 | 0 | -4.505766 | 2.242177 | 0.700216 |
| 14 | 7 | 0 | -3.328232 | 2.681900 | 0.177977 |
| 15 | 6 | 0 | -3.489657 | 3.979854 | -0.129324 |
| 16 | 6 | 0 | -4.785534 | 4.396755 | 0.189233 |
| 17 | 6 | 0 | -5.390752 | 3.257885 | 0.712268 |
| 18 | 1 | 0 | -1.563969 | 2.136587 | -3.118379 |
| 19 | 7 | 0 | -2.422375 | 0.222900 | 1.768737 |
| 20 | 6 | 0 | -2.766392 | -1.012286 | 3.613500 |
| 21 | 6 | 0 | -1.813694 | -0.467819 | 2.747103 |
| 22 | 6 | 0 | -3.987800 | -0.591680 | 3.095785 |
| 23 | 6 | 0 | 5.267116 | -3.902542 | -0.387817 |
| 24 | 6 | 0 | 5.996958 | -3.313649 | -1.462477 |
| 25 | 6 | 0 | 6.075987 | -3.821737 | 0.784819 |
| 26 | 6 | 0 | 7.252177 | -2.870301 | -0.950299 |
| 27 | 1 | 0 | 8.019783 | -2.363402 | -1.520442 |
| 28 | 15 | 0 | 8.810873 | -3.100021 | 1.511271 |
| 29 | 6 | 0 | 5.873989 | -0.101513 | 1.043516 |
| 30 | 6 | 0 | 5.729430 | 0.129535 | -0.358675 |
| 31 | 6 | 0 | 4.473278 | -0.402230 | -0.809420 |
| 32 | 6 | 0 | 3.857174 | -0.980862 | 0.354261 |
| 33 | 6 | 0 | 4.710827 | -0.801317 | 1.487876 |
| 34 | 30 | 0 | -1.603684 | 1.485588 | 0.335015 |

| | | | | | |
|---|---|---|---|---|---|
| 35 | 30 | 0 | 0.998448 | 0.781488 | -1.159327 |
| 36 | 7 | 0 | 1.507493 | -1.078410 | -1.940064 |
| 37 | 7 | 0 | 2.706717 | -1.278951 | -2.553870 |
| 38 | 6 | 0 | 2.646173 | -2.413239 | -3.277324 |
| 39 | 6 | 0 | 1.379893 | -2.974508 | -3.140931 |
| 40 | 6 | 0 | 0.700198 | -2.091522 | -2.297203 |
| 41 | 7 | 0 | 2.491823 | 1.806077 | -2.146025 |
| 42 | 7 | 0 | 3.528928 | 1.134669 | -2.718799 |
| 43 | 6 | 0 | 4.185776 | 1.968893 | -3.546168 |
| 44 | 6 | 0 | 3.566587 | 3.215928 | -3.525362 |
| 45 | 6 | 0 | 2.502515 | 3.058776 | -2.633380 |
| 46 | 8 | 0 | 0.499210 | 1.056068 | 0.774498 |
| 47 | 6 | 0 | 0.850597 | 2.037131 | 1.596729 |
| 48 | 8 | 0 | 1.134006 | 1.497179 | 2.848981 |
| 49 | 8 | 0 | 1.879654 | 2.876929 | 1.140644 |
| 50 | 6 | 0 | 1.742403 | 2.380094 | 3.800400 |
| 51 | 6 | 0 | 3.068526 | 2.959248 | 3.251109 |
| 52 | 6 | 0 | 3.156083 | 2.625470 | 1.761066 |
| 53 | 8 | 0 | -0.367770 | 2.898082 | 1.687225 |
| 54 | 6 | 0 | -0.242105 | 4.303929 | 1.710848 |
| 55 | 6 | 0 | 0.087187 | 4.891340 | 0.343107 |
| 56 | 8 | 0 | 0.603087 | 6.122644 | 0.478067 |
| 57 | 6 | 0 | 0.890308 | 6.827629 | -0.743662 |
| 58 | 6 | 0 | -5.223121 | -0.800235 | -2.581551 |
| 59 | 7 | 0 | -3.763729 | 0.152712 | 1.995508 |
| 60 | 6 | 0 | 7.319439 | -3.187656 | 0.448520 |
| 61 | 6 | 0 | -5.201348 | -4.918276 | 0.923234 |
| 62 | 6 | 0 | -7.746023 | -5.005747 | 2.168808 |
| 63 | 8 | 0 | -0.942909 | 1.005182 | -1.478067 |
| 64 | 6 | 0 | -1.639036 | 1.119443 | -2.704454 |
| 65 | 5 | 0 | 3.941402 | -0.341435 | -2.326428 |
| 66 | 26 | 0 | 5.684599 | -1.914718 | 0.035652 |
| 67 | 6 | 0 | 9.582189 | -1.501293 | 0.937099 |
| 68 | 6 | 0 | 8.085439 | -2.550302 | 3.140169 |
| 69 | 8 | 0 | -0.138785 | 4.353748 | -0.722227 |
| 70 | 1 | 0 | -5.597617 | -0.819417 | -3.597299 |
| 71 | 1 | 0 | 5.789311 | -4.165907 | 1.770223 |
| 72 | 1 | 0 | -8.294067 | -2.353435 | -2.782888 |
| 73 | 1 | 0 | -6.017750 | 1.135861 | -1.792467 |
| 74 | 1 | 0 | 4.522453 | -1.162738 | 2.490822 |
| 75 | 1 | 0 | 4.260476 | -4.296272 | -0.440231 |
| 76 | 1 | 0 | 7.482985 | -3.359650 | 3.565445 |
| 77 | 1 | 0 | 8.866778 | -0.673152 | 0.907025 |
| 78 | 1 | 0 | 3.844781 | 4.098375 | -4.082329 |
| 79 | 1 | 0 | -7.393950 | -5.685244 | 2.953653 |
| 80 | 1 | 0 | 2.914461 | -1.512085 | 0.364992 |

| | | | | | |
|---|---|---|---|---|---|
| 81 | 1 | 0 | -4.391359 | -4.339271 | 0.470597 |
| 82 | 1 | 0 | -5.672172 | -5.534109 | 0.147778 |
| 83 | 1 | 0 | -5.222367 | 5.375896 | 0.059358 |
| 84 | 1 | 0 | -8.821528 | -0.334789 | -1.067142 |
| 85 | 1 | 0 | -7.785813 | -0.994793 | 1.333813 |
| 86 | 1 | 0 | -6.962904 | -4.265943 | -1.438739 |
| 87 | 1 | 0 | -4.154599 | -2.763700 | -2.391256 |
| 88 | 1 | 0 | -3.692765 | -1.983043 | 0.152700 |
| 89 | 1 | 0 | -2.598635 | -1.621255 | 4.489325 |
| 90 | 1 | 0 | -5.880537 | 0.732301 | 1.578279 |
| 91 | 1 | 0 | -8.625423 | -4.477071 | 2.551031 |
| 92 | 1 | 0 | -8.044754 | -5.596369 | 1.294714 |
| 93 | 1 | 0 | -4.765221 | -5.585075 | 1.675381 |
| 94 | 1 | 0 | -0.733780 | -0.509815 | 2.777078 |
| 95 | 1 | 0 | -4.998336 | -0.789054 | 3.421427 |
| 96 | 1 | 0 | -2.667902 | 4.529728 | -0.566643 |
| 97 | 1 | 0 | -6.391601 | 3.096714 | 1.085568 |
| 98 | 1 | 0 | 0.501918 | 4.645776 | 2.432675 |
| 99 | 1 | 0 | 1.740241 | 3.758802 | -2.317331 |
| 100 | 1 | 0 | 5.050433 | 1.618671 | -4.090961 |
| 101 | 1 | 0 | -0.320580 | -2.116879 | -1.939519 |
| 102 | 1 | 0 | 1.007982 | -3.880905 | -3.594917 |
| 103 | 1 | 0 | 3.505933 | -2.742485 | -3.842348 |
| 104 | 1 | 0 | 4.780629 | -0.660134 | -3.135330 |
| 105 | 1 | 0 | 6.466371 | 0.607256 | -0.993049 |
| 106 | 1 | 0 | 6.723868 | 0.177954 | 1.652110 |
| 107 | 1 | 0 | 5.642481 | -3.171222 | -2.473939 |
| 108 | 1 | 0 | 8.905009 | -2.348561 | 3.838974 |
| 109 | 1 | 0 | 7.459454 | -1.657372 | 3.045064 |
| 110 | 1 | 0 | 10.405764 | -1.247308 | 1.613664 |
| 111 | 1 | 0 | 10.008403 | -1.636067 | -0.062345 |
| 112 | 1 | 0 | -1.228245 | 0.419337 | -3.446733 |
| 113 | 1 | 0 | -2.700578 | 0.879849 | -2.570835 |
| 114 | 1 | 0 | -1.220355 | 4.690670 | 2.019835 |
| 115 | 1 | 0 | 1.196134 | 7.828039 | -0.437762 |
| 116 | 1 | 0 | 1.699668 | 6.330234 | -1.284432 |
| 117 | 1 | 0 | 0.003036 | 6.871064 | -1.379999 |
| 118 | 1 | 0 | 3.864740 | 3.265477 | 1.232455 |
| 119 | 1 | 0 | 3.442503 | 1.583082 | 1.599143 |
| 120 | 1 | 0 | 3.934877 | 2.535369 | 3.771365 |
| 121 | 1 | 0 | 3.098074 | 4.045080 | 3.397361 |
| 122 | 1 | 0 | 1.900401 | 1.760647 | 4.685266 |
| 123 | 1 | 0 | 1.035729 | 3.172338 | 4.075231 |

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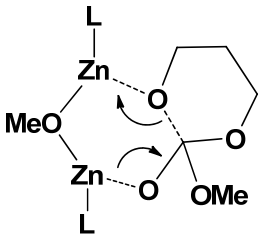


**TSII-III$^{dimer}$- propagation-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.646521 | -0.717629 | 3.321432 |
| 2 | 7 | 0 | 3.519417 | -0.906842 | 1.997450 |
| 3 | 7 | 0 | 4.722300 | -1.349157 | 1.536641 |
| 4 | 6 | 0 | 5.592423 | -1.414932 | 2.562155 |
| 5 | 6 | 0 | 4.948036 | -1.017502 | 3.730601 |
| 6 | 30 | 0 | 1.817377 | -1.022299 | 0.814980 |
| 7 | 8 | 0 | 0.506685 | -1.814613 | 2.140441 |
| 8 | 6 | 0 | -0.672493 | -2.166208 | 1.870346 |
| 9 | 8 | 0 | -0.899369 | -2.602224 | 0.600530 |
| 10 | 6 | 0 | -2.231707 | -2.970360 | 0.263062 |
| 11 | 6 | 0 | -2.315717 | -3.081239 | -1.248188 |
| 12 | 8 | 0 | -3.598457 | -3.255276 | -1.610783 |
| 13 | 6 | 0 | -3.836293 | -3.375860 | -3.027074 |
| 14 | 5 | 0 | 5.028637 | -1.576356 | 0.014066 |
| 15 | 6 | 0 | 5.042182 | -0.165467 | -0.768076 |
| 16 | 6 | 0 | 4.912932 | 0.043932 | -2.182454 |
| 17 | 6 | 0 | 5.010291 | 1.439767 | -2.473692 |
| 18 | 6 | 0 | 5.214836 | 2.124660 | -1.237511 |
| 19 | 6 | 0 | 5.236712 | 1.139785 | -0.200080 |
| 20 | 26 | 0 | 6.758364 | 0.789609 | -1.577563 |
| 21 | 6 | 0 | 8.612772 | 0.828244 | -0.621064 |
| 22 | 6 | 0 | 8.551394 | 1.840227 | -1.640599 |
| 23 | 6 | 0 | 8.313974 | 1.207644 | -2.896543 |
| 24 | 6 | 0 | 8.227256 | -0.199916 | -2.672618 |
| 25 | 6 | 0 | 8.403451 | -0.432951 | -1.278178 |
| 26 | 15 | 0 | 8.918669 | 0.976291 | 1.178780 |
| 27 | 6 | 0 | 10.781940 | 1.173610 | 1.175521 |
| 28 | 8 | 0 | 0.831060 | 0.576838 | 0.181415 |
| 29 | 6 | 0 | 1.438511 | 1.451268 | -0.771407 |
| 30 | 30 | 0 | -1.134784 | 0.766008 | 0.442201 |
| 31 | 8 | 0 | -1.657582 | -0.576507 | 1.793178 |
| 32 | 6 | 0 | -2.379546 | -0.329719 | 2.991434 |
| 33 | 6 | 0 | -1.560655 | -0.804821 | 4.197634 |

| | | | | | |
|---|---|---|---|---|---|
| 34 | 6 | 0 | -1.328318 | -2.321736 | 4.137050 |
| 35 | 8 | 0 | -1.429166 | -2.822071 | 2.780826 |
| 36 | 7 | 0 | -2.048596 | 0.801356 | -1.447230 |
| 37 | 7 | 0 | -2.998889 | 1.741009 | -1.717321 |
| 38 | 6 | 0 | -3.218485 | 1.779458 | -3.045261 |
| 39 | 6 | 0 | -2.394945 | 0.847411 | -3.669808 |
| 40 | 6 | 0 | -1.673898 | 0.265818 | -2.621873 |
| 41 | 5 | 0 | -3.761785 | 2.531093 | -0.597370 |
| 42 | 7 | 0 | -2.710589 | 3.319600 | 0.275106 |
| 43 | 7 | 0 | -1.686605 | 2.718305 | 0.940554 |
| 44 | 6 | 0 | -1.048864 | 3.674909 | 1.637074 |
| 45 | 6 | 0 | -1.667056 | 4.912162 | 1.439365 |
| 46 | 6 | 0 | -2.713972 | 4.634667 | 0.565081 |
| 47 | 6 | 0 | -4.637076 | 1.533460 | 0.316769 |
| 48 | 6 | 0 | -4.910053 | 0.139949 | 0.098394 |
| 49 | 6 | 0 | -5.744065 | -0.355397 | 1.148829 |
| 50 | 6 | 0 | -6.015621 | 0.731052 | 2.033410 |
| 51 | 6 | 0 | -5.342495 | 1.881617 | 1.518903 |
| 52 | 26 | 0 | -6.720384 | 1.173474 | 0.132682 |
| 53 | 6 | 0 | -8.438013 | 0.463806 | -0.871425 |
| 54 | 6 | 0 | -7.591367 | 1.206624 | -1.762087 |
| 55 | 6 | 0 | -7.442392 | 2.532919 | -1.258362 |
| 56 | 6 | 0 | -8.188024 | 2.627474 | -0.046974 |
| 57 | 6 | 0 | -8.794408 | 1.357903 | 0.194400 |
| 58 | 15 | 0 | -9.174344 | -1.179458 | -1.212473 |
| 59 | 6 | 0 | -7.681987 | -2.161260 | -1.757199 |
| 60 | 6 | 0 | -9.398162 | -1.856348 | 0.511401 |
| 61 | 7 | 0 | 2.615455 | -2.314480 | -0.590108 |
| 62 | 7 | 0 | 3.959046 | -2.549779 | -0.604823 |
| 63 | 6 | 0 | 4.204177 | -3.630578 | -1.370493 |
| 64 | 6 | 0 | 3.000763 | -4.121273 | -1.867285 |
| 65 | 6 | 0 | 2.030174 | -3.263480 | -1.341654 |
| 66 | 6 | 0 | 8.449907 | 2.754504 | 1.496221 |
| 67 | 8 | 0 | -1.386676 | -3.031070 | -2.024094 |
| 68 | 1 | 0 | -5.383390 | 2.873810 | 1.952424 |
| 69 | 1 | 0 | 8.961111 | 3.459487 | 0.830134 |
| 70 | 1 | 0 | 5.356271 | 3.190927 | -1.113564 |
| 71 | 1 | 0 | 2.852215 | -4.977192 | -2.508723 |
| 72 | 1 | 0 | -0.922741 | -0.511539 | -2.648715 |
| 73 | 1 | 0 | -3.461031 | 5.282131 | 0.129482 |
| 74 | 1 | 0 | -1.393818 | 5.868200 | 1.860375 |
| 75 | 1 | 0 | 7.369388 | 2.877291 | 1.378391 |
| 76 | 1 | 0 | 5.219617 | -3.971554 | -1.511166 |
| 77 | 1 | 0 | 0.953883 | -3.275924 | -1.458363 |
| 78 | 1 | 0 | 4.786417 | -0.739988 | -2.919535 |
| 79 | 1 | 0 | 4.976901 | 1.891933 | -3.456874 |

| | | | | | |
|---|---|---|---|---|---|
| 80 | 1 | 0 | 8.016393 | -0.951777 | -3.422032 |
| 81 | 1 | 0 | 8.340151 | -1.392396 | -0.781698 |
| 82 | 1 | 0 | 8.634293 | 2.907250 | -1.482023 |
| 83 | 1 | 0 | 8.179432 | 1.710425 | -3.845853 |
| 84 | 1 | 0 | 5.396904 | 1.340063 | 0.852192 |
| 85 | 1 | 0 | 5.364177 | -0.960379 | 4.725291 |
| 86 | 1 | 0 | 6.073251 | -2.180160 | -0.030730 |
| 87 | 1 | 0 | 11.125857 | 1.393810 | 2.192826 |
| 88 | 1 | 0 | 11.246040 | 0.233468 | 0.859839 |
| 89 | 1 | 0 | 11.118634 | 1.972971 | 0.505000 |
| 90 | 1 | 0 | 8.711407 | 3.006063 | 2.530019 |
| 91 | 1 | 0 | 2.794559 | -0.391595 | 3.902939 |
| 92 | 1 | 0 | 6.613777 | -1.719614 | 2.387593 |
| 93 | 1 | 0 | 0.993003 | 2.453701 | -0.705057 |
| 94 | 1 | 0 | 2.512512 | 1.547372 | -0.582317 |
| 95 | 1 | 0 | 1.303450 | 1.085096 | -1.798443 |
| 96 | 1 | 0 | -2.319703 | 0.635567 | -4.726073 |
| 97 | 1 | 0 | -3.945740 | 2.466616 | -3.452748 |
| 98 | 1 | 0 | -0.180132 | 3.423350 | 2.231414 |
| 99 | 1 | 0 | -4.403915 | 3.385109 | -1.161008 |
| 100 | 1 | 0 | -4.558929 | -0.442093 | -0.743930 |
| 101 | 1 | 0 | -6.117455 | -1.366329 | 1.245459 |
| 102 | 1 | 0 | -6.646226 | 0.698083 | 2.912947 |
| 103 | 1 | 0 | -9.406762 | 1.105925 | 1.050415 |
| 104 | 1 | 0 | -6.819432 | 3.307998 | -1.683819 |
| 105 | 1 | 0 | -8.243797 | 3.491225 | 0.602821 |
| 106 | 1 | 0 | -7.128884 | 0.820100 | -2.661217 |
| 107 | 1 | 0 | -9.694503 | -2.908547 | 0.437483 |
| 108 | 1 | 0 | -8.491203 | -1.777288 | 1.119730 |
| 109 | 1 | 0 | -10.210276 | -1.321577 | 1.014642 |
| 110 | 1 | 0 | -7.985366 | -3.204080 | -1.904925 |
| 111 | 1 | 0 | -7.329035 | -1.779198 | -2.721008 |
| 112 | 1 | 0 | -6.857998 | -2.118970 | -1.037804 |
| 113 | 1 | 0 | -2.497612 | -3.933081 | 0.714294 |
| 114 | 1 | 0 | -2.934204 | -2.211754 | 0.617792 |
| 115 | 1 | 0 | -2.114832 | -2.869838 | 4.660780 |
| 116 | 1 | 0 | -0.357875 | -2.609261 | 4.551999 |
| 117 | 1 | 0 | -2.081196 | -0.553944 | 5.130262 |
| 118 | 1 | 0 | -0.603124 | -0.274389 | 4.198129 |
| 119 | 1 | 0 | -3.348342 | -0.849155 | 2.959197 |
| 120 | 1 | 0 | -2.594124 | 0.742482 | 3.078697 |
| 121 | 1 | 0 | -4.909781 | -3.534146 | -3.126790 |
| 122 | 1 | 0 | -3.532402 | -2.458392 | -3.537054 |
| 123 | 1 | 0 | -3.278775 | -4.221749 | -3.436761 |

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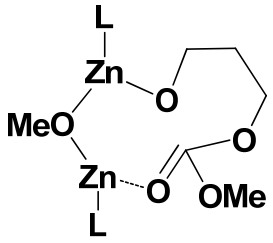


**III$^{dimer}$- propagation-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.646295 | 1.197053 | 3.154714 |
| 2 | 7 | 0 | -3.530978 | 1.224459 | 1.816133 |
| 3 | 7 | 0 | -4.762000 | 1.518605 | 1.311838 |
| 4 | 6 | 0 | -5.635471 | 1.653041 | 2.327458 |
| 5 | 6 | 0 | -4.965882 | 1.454823 | 3.532126 |
| 6 | 30 | 0 | -1.854757 | 1.282929 | 0.598191 |
| 7 | 8 | 0 | -0.702431 | 2.496679 | 1.835222 |
| 8 | 6 | 0 | 0.380177 | 3.008845 | 1.524368 |
| 9 | 8 | 0 | 0.661617 | 3.234297 | 0.245556 |
| 10 | 6 | 0 | 2.031622 | 3.465891 | -0.111626 |
| 11 | 5 | 0 | -5.086267 | 1.515379 | -0.225348 |
| 12 | 6 | 0 | -4.998625 | 0.014653 | -0.808237 |
| 13 | 6 | 0 | -4.870764 | -0.376329 | -2.184321 |
| 14 | 6 | 0 | -4.849504 | -1.802958 | -2.278099 |
| 15 | 6 | 0 | -4.977583 | -2.323639 | -0.955048 |
| 16 | 6 | 0 | -5.071362 | -1.211230 | -0.062957 |
| 17 | 26 | 0 | -6.636236 | -1.180655 | -1.438664 |
| 18 | 6 | 0 | -8.474133 | -1.198794 | -0.447144 |
| 19 | 6 | 0 | -8.336623 | -2.366290 | -1.274948 |
| 20 | 6 | 0 | -8.162766 | -1.947468 | -2.627216 |
| 21 | 6 | 0 | -8.191798 | -0.519970 | -2.654793 |
| 22 | 6 | 0 | -8.375373 | -0.060178 | -1.318860 |
| 23 | 15 | 0 | -8.756932 | -1.051085 | 1.356319 |
| 24 | 6 | 0 | -10.595351 | -1.404808 | 1.425909 |
| 25 | 8 | 0 | -0.721963 | -0.263753 | 0.181920 |
| 26 | 6 | 0 | -1.336498 | -1.329807 | -0.548971 |
| 27 | 30 | 0 | 1.254221 | -0.486104 | 0.562145 |
| 28 | 8 | 0 | 1.837808 | 1.044202 | 1.578586 |
| 29 | 6 | 0 | 2.389547 | 1.007900 | 2.865170 |
| 30 | 6 | 0 | 1.404840 | 1.579215 | 3.906048 |
| 31 | 6 | 0 | 1.165404 | 3.084828 | 3.767095 |
| 32 | 8 | 0 | 1.222932 | 3.548861 | 2.380622 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 7 | 0 | 2.108806 | -0.876912 | -1.327463 |
| 34 | 7 | 0 | 2.967625 | -1.922400 | -1.485008 |
| 35 | 6 | 0 | 3.192739 | -2.117428 | -2.798424 |
| 36 | 6 | 0 | 2.466666 | -1.180948 | -3.528069 |
| 37 | 6 | 0 | 1.796526 | -0.430122 | -2.556002 |
| 38 | 5 | 0 | 3.640656 | -2.669601 | -0.280454 |
| 39 | 7 | 0 | 2.510282 | -3.221720 | 0.672211 |
| 40 | 7 | 0 | 1.591166 | -2.426827 | 1.284654 |
| 41 | 6 | 0 | 0.863659 | -3.213794 | 2.094738 |
| 42 | 6 | 0 | 1.316386 | -4.534169 | 2.025581 |
| 43 | 6 | 0 | 2.360848 | -4.487740 | 1.107086 |
| 44 | 6 | 0 | 4.642463 | -1.709425 | 0.533503 |
| 45 | 6 | 0 | 4.933635 | -0.318244 | 0.328489 |
| 46 | 6 | 0 | 5.879795 | 0.120734 | 1.305210 |
| 47 | 6 | 0 | 6.202748 | -0.998462 | 2.129152 |
| 48 | 6 | 0 | 5.449908 | -2.113649 | 1.651144 |
| 49 | 26 | 0 | 6.704448 | -1.407900 | 0.156219 |
| 50 | 6 | 0 | 8.448822 | -0.756816 | -0.838657 |
| 51 | 6 | 0 | 7.473745 | -1.244038 | -1.773352 |
| 52 | 6 | 0 | 7.182585 | -2.607248 | -1.466752 |
| 53 | 6 | 0 | 7.966260 | -2.978845 | -0.335497 |
| 54 | 6 | 0 | 8.739493 | -1.843817 | 0.053632 |
| 55 | 15 | 0 | 9.370613 | 0.822202 | -0.962436 |
| 56 | 6 | 0 | 8.004509 | 2.017613 | -1.398894 |
| 57 | 6 | 0 | 9.620341 | 1.253003 | 0.835758 |
| 58 | 7 | 0 | -2.729959 | 2.317954 | -0.958553 |
| 59 | 7 | 0 | -4.086008 | 2.465589 | -0.983737 |
| 60 | 6 | 0 | -4.404830 | 3.404454 | -1.895023 |
| 61 | 6 | 0 | -3.238748 | 3.890246 | -2.479009 |
| 62 | 6 | 0 | -2.211779 | 3.179685 | -1.851617 |
| 63 | 6 | 0 | -8.129426 | -2.695829 | 1.975765 |
| 64 | 1 | 0 | 5.502161 | -3.119297 | 2.050808 |
| 65 | 1 | 0 | -8.584367 | -3.551400 | 1.462914 |
| 66 | 1 | 0 | -5.025912 | -3.370342 | -0.682891 |
| 67 | 1 | 0 | -3.150310 | 4.649072 | -3.242188 |
| 68 | 1 | 0 | 1.117192 | 0.403379 | -2.673414 |
| 69 | 1 | 0 | 3.009627 | -5.267172 | 0.734766 |
| 70 | 1 | 0 | 0.940916 | -5.396371 | 2.556325 |
| 71 | 1 | 0 | -7.043979 | -2.746223 | 1.850510 |
| 72 | 1 | 0 | -5.440929 | 3.656905 | -2.068092 |
| 73 | 1 | 0 | -1.139473 | 3.237183 | -1.988917 |
| 74 | 1 | 0 | -4.822327 | 0.305434 | -3.024863 |
| 75 | 1 | 0 | -4.788268 | -2.383330 | -3.190052 |
| 76 | 1 | 0 | -8.048412 | 0.102660 | -3.528328 |
| 77 | 1 | 0 | -8.390418 | 0.973548 | -0.998652 |
| 78 | 1 | 0 | -8.327547 | -3.391415 | -0.929479 |

| | | | | | |
|---|---|---|---|---|---|
| 79 | 1 | 0 | -7.992895 | -2.597298 | -3.476249 |
| 80 | 1 | 0 | -5.196985 | -1.276545 | 1.010474 |
| 81 | 1 | 0 | -5.378449 | 1.495044 | 4.529095 |
| 82 | 1 | 0 | -6.168952 | 2.036685 | -0.339951 |
| 83 | 1 | 0 | -10.915596 | -1.462629 | 2.472695 |
| 84 | 1 | 0 | -11.141233 | -0.582386 | 0.952080 |
| 85 | 1 | 0 | -10.861987 | -2.340017 | 0.919788 |
| 86 | 1 | 0 | -8.353701 | -2.775639 | 3.045220 |
| 87 | 1 | 0 | -2.775627 | 1.005888 | 3.767778 |
| 88 | 1 | 0 | -6.676343 | 1.856959 | 2.124133 |
| 89 | 1 | 0 | -0.613064 | -1.788015 | -1.235572 |
| 90 | 1 | 0 | -1.709749 | -2.109475 | 0.128628 |
| 91 | 1 | 0 | -2.181098 | -0.967321 | -1.145771 |
| 92 | 1 | 0 | 2.418211 | -1.074413 | -4.601720 |
| 93 | 1 | 0 | 3.852288 | -2.909247 | -3.122378 |
| 94 | 1 | 0 | 0.052526 | -2.791864 | 2.673774 |
| 95 | 1 | 0 | 4.172996 | -3.652960 | -0.739027 |
| 96 | 1 | 0 | 4.516604 | 0.297113 | -0.457730 |
| 97 | 1 | 0 | 6.290417 | 1.117815 | 1.394120 |
| 98 | 1 | 0 | 6.916019 | -1.009121 | 2.943645 |
| 99 | 1 | 0 | 9.419081 | -1.805480 | 0.895250 |
| 100 | 1 | 0 | 6.452370 | -3.230971 | -1.964142 |
| 101 | 1 | 0 | 7.945020 | -3.936340 | 0.168622 |
| 102 | 1 | 0 | 7.021339 | -0.668646 | -2.570587 |
| 103 | 1 | 0 | 10.040503 | 2.263004 | 0.899690 |
| 104 | 1 | 0 | 8.692645 | 1.206677 | 1.415220 |
| 105 | 1 | 0 | 10.348443 | 0.566235 | 1.279793 |
| 106 | 1 | 0 | 8.404565 | 3.037143 | -1.361267 |
| 107 | 1 | 0 | 7.671258 | 1.831708 | -2.425435 |
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| 109 | 6 | 0 | 2.151783 | 3.251640 | -1.608667 |
| 110 | 1 | 0 | 2.337236 | 4.482379 | 0.153892 |
| 111 | 1 | 0 | 2.647431 | 2.733688 | 0.419401 |
| 112 | 1 | 0 | 1.968337 | 3.660640 | 4.231277 |
| 113 | 1 | 0 | 0.208062 | 3.398591 | 4.192414 |
| 114 | 1 | 0 | 1.784342 | 1.408081 | 4.923229 |
| 115 | 1 | 0 | 0.457513 | 1.037230 | 3.815922 |
| 116 | 1 | 0 | 3.327061 | 1.592550 | 2.901105 |
| 117 | 1 | 0 | 2.660770 | -0.014142 | 3.176788 |
| 118 | 8 | 0 | 1.252499 | 2.954061 | -2.364224 |
| 119 | 8 | 0 | 3.430944 | 3.424892 | -1.972075 |
| 120 | 6 | 0 | 3.726238 | 3.194919 | -3.364654 |
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| 123 | 1 | 0 | 3.117614 | 3.846709 | -3.995939 |

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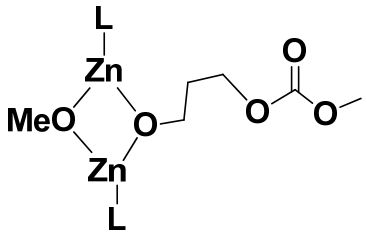


**IV$^{dimer}$- propagation-TMC**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.959063 | -1.320097 | 2.119882 |
| 2 | 6 | 0 | 7.593588 | -0.461461 | 1.172747 |
| 3 | 6 | 0 | 7.973254 | -1.237265 | 0.025761 |
| 4 | 6 | 0 | 7.547313 | -2.584612 | 0.283036 |
| 5 | 6 | 0 | 6.931392 | -2.635131 | 1.568537 |
| 6 | 26 | 0 | 5.887562 | -1.326096 | 0.344147 |
| 7 | 6 | 0 | 4.473508 | -1.931648 | -1.063635 |
| 8 | 6 | 0 | 3.899750 | -2.049365 | 0.248252 |
| 9 | 6 | 0 | 3.953786 | -0.728056 | 0.814326 |
| 10 | 6 | 0 | 4.535656 | 0.178168 | -0.125807 |
| 11 | 6 | 0 | 4.851113 | -0.573547 | -1.298597 |
| 12 | 5 | 0 | 3.340804 | -3.397274 | 0.927145 |
| 13 | 7 | 0 | 2.400220 | -4.161460 | -0.082006 |
| 14 | 7 | 0 | 1.263546 | -3.608870 | -0.587527 |
| 15 | 6 | 0 | 0.756966 | -4.481329 | -1.475458 |
| 16 | 6 | 0 | 1.575327 | -5.610141 | -1.564843 |
| 17 | 6 | 0 | 2.603396 | -5.359984 | -0.659867 |
| 18 | 15 | 0 | 9.069377 | -0.689565 | -1.337616 |
| 19 | 6 | 0 | 8.440163 | 1.038550 | -1.649342 |
| 20 | 30 | 0 | 0.461048 | -1.942111 | 0.361387 |
| 21 | 8 | 0 | -1.533390 | -1.887144 | 0.584717 |
| 22 | 6 | 0 | -2.405762 | -2.868921 | 1.107865 |
| 23 | 30 | 0 | -1.875784 | -0.226946 | -0.433590 |
| 24 | 8 | 0 | 0.136162 | -0.219342 | -0.577443 |
| 25 | 6 | 0 | 0.969063 | 0.670393 | -1.293870 |
| 26 | 6 | 0 | 1.197973 | 1.973309 | -0.517126 |
| 27 | 6 | 0 | 2.013442 | 2.983130 | -1.316886 |
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| 30 | 8 | 0 | 4.083246 | 3.571411 | 0.374863 |
| 31 | 7 | 0 | -2.829695 | 1.438060 | 0.351333 |
| 32 | 7 | 0 | -3.979087 | 1.884763 | -0.228872 |
| 33 | 6 | 0 | -4.332469 | 3.056246 | 0.332837 |

| | | | | | |
|---|---|---|---|---|---|
| 34 | 6 | 0 | -3.391267 | 3.398743 | 1.299937 |
| 35 | 6 | 0 | -2.466699 | 2.352318 | 1.268110 |
| 36 | 5 | 0 | -4.803341 | 1.032983 | -1.262784 |
| 37 | 7 | 0 | -3.874375 | 0.647975 | -2.471898 |
| 38 | 7 | 0 | -2.732197 | -0.075714 | -2.320288 |
| 39 | 6 | 0 | -2.233666 | -0.296917 | -3.548448 |
| 40 | 6 | 0 | -3.064259 | 0.273664 | -4.516774 |
| 41 | 6 | 0 | -4.089890 | 0.863911 | -3.783384 |
| 42 | 6 | 0 | -5.382181 | -0.291552 | -0.548912 |
| 43 | 6 | 0 | -5.683020 | -0.453890 | 0.847021 |
| 44 | 6 | 0 | -6.218978 | -1.759551 | 1.075005 |
| 45 | 6 | 0 | -6.262656 | -2.430954 | -0.184367 |
| 46 | 6 | 0 | -5.755515 | -1.531020 | -1.171992 |
| 47 | 26 | 0 | -7.434596 | -0.725455 | -0.246548 |
| 48 | 6 | 0 | -8.827671 | 0.742197 | 0.262986 |
| 49 | 6 | 0 | -8.562738 | 0.757557 | -1.149487 |
| 50 | 6 | 0 | -8.914385 | -0.510432 | -1.695876 |
| 51 | 6 | 0 | -9.390239 | -1.331093 | -0.628780 |
| 52 | 6 | 0 | -9.338819 | -0.565403 | 0.573229 |
| 53 | 15 | 0 | -8.541449 | 2.192455 | 1.345422 |
| 54 | 6 | 0 | -8.429592 | 1.395048 | 3.028867 |
| 55 | 7 | 0 | 1.384878 | -2.302874 | 2.184564 |
| 56 | 7 | 0 | 2.513725 | -3.063026 | 2.220695 |
| 57 | 6 | 0 | 2.791424 | -3.379640 | 3.499269 |
| 58 | 6 | 0 | 1.822595 | -2.820338 | 4.328015 |
| 59 | 6 | 0 | 0.957888 | -2.160500 | 3.450360 |
| 60 | 6 | 0 | 8.325455 | -1.577617 | -2.800591 |
| 61 | 6 | 0 | -10.287992 | 2.859475 | 1.463003 |
| 62 | 8 | 0 | 3.100120 | 5.577054 | 0.796813 |
| 63 | 6 | 0 | 4.190844 | 5.895223 | 1.658334 |
| 64 | 1 | 0 | 7.658740 | -3.422275 | -0.393241 |
| 65 | 1 | 0 | -9.695385 | -2.366690 | -0.709620 |
| 66 | 1 | 0 | -5.690561 | -1.739997 | -2.232983 |
| 67 | 1 | 0 | 4.712407 | 1.233886 | 0.033502 |
| 68 | 1 | 0 | 7.741910 | 0.603947 | 1.291558 |
| 69 | 1 | 0 | 6.533837 | -1.014684 | 3.067142 |
| 70 | 1 | 0 | 8.724874 | 1.690592 | -0.817241 |
| 71 | 1 | 0 | 7.246675 | -1.415265 | -2.889526 |
| 72 | 1 | 0 | 1.442366 | -6.481073 | -2.189107 |
| 73 | 1 | 0 | -10.312576 | 3.688697 | 2.179455 |
| 74 | 1 | 0 | 3.638102 | -0.466777 | 1.816713 |
| 75 | 1 | 0 | -7.508948 | 0.808375 | 3.099936 |
| 76 | 1 | 0 | -9.282499 | 0.744523 | 3.255276 |
| 77 | 1 | 0 | -2.940404 | 0.264563 | -5.589389 |
| 78 | 1 | 0 | -6.645164 | -3.427738 | -0.363967 |
| 79 | 1 | 0 | -8.795708 | -0.814245 | -2.727906 |

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|---|---|---|---|---|---|
| 80 | 1 | 0 | -8.118013 | 1.582333 | -1.690658 |
| 81 | 1 | 0 | -9.608830 | -0.924402 | 1.557515 |
| 82 | 1 | 0 | -6.561798 | -2.155740 | 2.022488 |
| 83 | 1 | 0 | -5.547749 | 0.310584 | 1.602033 |
| 84 | 1 | 0 | -3.380900 | 4.276813 | 1.928044 |
| 85 | 1 | 0 | -5.638437 | 1.776266 | -1.715603 |
| 86 | 1 | 0 | -10.593635 | 3.249435 | 0.486626 |
| 87 | 1 | 0 | -11.009491 | 2.096136 | 1.777038 |
| 88 | 1 | 0 | -8.388731 | 2.185110 | 3.786856 |
| 89 | 1 | 0 | -1.562648 | 2.211108 | 1.845597 |
| 90 | 1 | 0 | -5.238585 | 3.554140 | 0.019999 |
| 91 | 1 | 0 | -1.308101 | -0.845072 | -3.665279 |
| 92 | 1 | 0 | -4.958865 | 1.420107 | -4.103673 |
| 93 | 1 | 0 | -0.165599 | -4.254002 | -1.993326 |
| 94 | 1 | 0 | 3.466657 | -5.950862 | -0.390055 |
| 95 | 1 | 0 | 0.054907 | -1.600880 | 3.655408 |
| 96 | 1 | 0 | 1.755568 | -2.887634 | 5.403596 |
| 97 | 1 | 0 | 3.658881 | -3.980084 | 3.731792 |
| 98 | 1 | 0 | 4.181847 | -4.199112 | 1.255340 |
| 99 | 1 | 0 | 4.611802 | -2.749854 | -1.760167 |
| 100 | 1 | 0 | 5.309393 | -0.185832 | -2.198888 |
| 101 | 1 | 0 | 6.470309 | -3.506717 | 2.014070 |
| 102 | 1 | 0 | 8.921145 | 1.428490 | -2.553420 |
| 103 | 1 | 0 | 7.352837 | 1.074951 | -1.769185 |
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| 105 | 1 | 0 | 8.514421 | -2.652589 | -2.713694 |
| 106 | 1 | 0 | -2.616509 | -3.659008 | 0.371020 |
| 107 | 1 | 0 | -1.962318 | -3.344945 | 1.994895 |
| 108 | 1 | 0 | -3.363836 | -2.424247 | 1.403868 |
| 109 | 1 | 0 | 1.935054 | 0.191696 | -1.501395 |
| 110 | 1 | 0 | 0.505687 | 0.903322 | -2.267447 |
| 111 | 1 | 0 | 0.226963 | 2.417436 | -0.263565 |
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| 113 | 1 | 0 | 3.013818 | 2.605733 | -1.540967 |
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| 115 | 6 | 0 | 5.487145 | 6.270885 | 0.948996 |
| 116 | 1 | 0 | 3.856896 | 6.756333 | 2.242409 |
| 117 | 1 | 0 | 4.413264 | 5.067569 | 2.335944 |
| 118 | 8 | 0 | 6.517056 | 6.454032 | 1.558148 |
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| 120 | 6 | 0 | 6.538915 | 6.752568 | -1.093065 |
| 121 | 1 | 0 | 6.239671 | 6.831833 | -2.138074 |
| 122 | 1 | 0 | 6.937207 | 7.703581 | -0.730620 |
| 123 | 1 | 0 | 7.296091 | 5.974787 | -0.965534 |

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