SUPPORTING INFORMATION

Tailoring Polyester Based-Diblock Copolymers for Boron-Enhanced Drug Delivery: Synthesis, Kinetics, and Nanoparticle Characterization

Robert Mundil [†,], Pavlína Marková [†], Martin Orságh [†], Ewa Pavlova [§], Zuzana Walterová [§], Petr Toman [§], Olga Kočková [§], and Mariusz Uchman [†,*]*

[†] Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova, 2030, 128 40 Prague 2, Czech Republic

[§] Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, 162 06 Prague 6, Czech Republic

EXPERIMENTAL SECTION AND METHODS

General Considerations and Materials

All operations were performed under dry nitrogen using vacuum/inert manifold and standard Schlenk techniques. Toluene (Acros Organics, 99.85%, Extra dry over molecular sieve) and benzyl alcohol (Acros Organics, 98+%, Extra dry) were used as received. Acetonitrile (Lach-Ner, G.R.) was dried over CaH_2 and distilled prior to use. 1,5,7-triazobicyclo[4.4.0]dec-5-ene (TBD) (Aldrich, 98%) was transferred to the Schlenk flask, stored under nitrogen, and used as received. Tin (II) 2-ethylhexanoate (stannous octoate, $SnOct_2$) (Sigma-Aldrich, 92.5-100%), 2,2-dimethoxy-2-phenylacetophenone (DMPA) (Sigma-Aldrich, 99%) and 1-thioglycerol (α-TG) (Sigma-Aldrich, ≥97%) were used as received. Poly(ethylene glycol) methyl ether (mPEG) (Aldrich, average M_n 5000) was dissolved in dry toluene at an elevated temperature (40 °C) and dried two times via azeotropic distillation just before use. ε-Caprolactone (ε-CL) (Sigma-Aldrich, 97%) was dried over CaH_2, distilled and stored in a fridge under nitrogen over molecular sieves. COSAN-dioxanate (Katchem Ltd., Czech Republic) and 3-pyridineboronic acid 1,3-propanediol ester (Sigma-Aldrich, 99%) were used as received. 3/7-(prop-2-ynyl)oxepan-2-one (PgCL) was synthesized according to the literature procedure.[1] In the case of kinetic experiments, the resulting mixture of both isomers (30% of 3-(prop-2-ynyl)oxepan-2-one) was separated by silica gel column chromatography using cyclohexane/ethyl acetate mixture of ratio 8/2 as the mobile phase. Spectra/Por 1 RC Dialysis Membrane Tubing (Spectrum Chemical Mfg. Corp., nominal molecular weight cut-off (MWCO) 3.5 and 6-8 kDa) was cut to approximately 15 cm long pieces. These were placed into a beaker filled with regular sink water and heated to 60 °C while stirring on a magnetic stirrer for 30 minutes. The softened tubing was thoroughly rinsed with deionized water and stored in a dilute sodium azide solution.

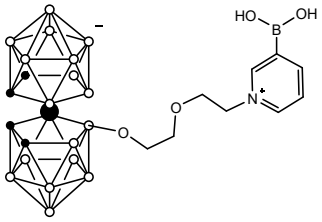
Synthesis of diblock copolymers mPEG-*b*-P(ε-CL-*co*-PgCL). In a standard procedure, ε-CL (33, 79 and 210 eq.) and PgCL (11, 26 and 70 eq.) were added to mPEG (1 eq.) in a 50 ml Schlenk flask equipped with a magnetic stir bar. The mixture was dissolved in dry toluene, carefully dried twice by azeotropic distillation and finally dissolved in 3 ml of dry toluene. Once heated to 110 °C, the reaction was initiated by $SnOct_2$ (0.5 eq.). After three hours, the polymerization was terminated by benzoic acid in toluene. The crude polymer was precipitated with cold diethyl ether, filtered off, and dried *in vacuo* until constant weight.

UV-initiated thiol-yne click reaction. In a typical click reaction, mPEG-*b*-P(ε-CL-*co*-PgCL) was introduced to a 50 ml Schlenk flask equipped with a magnetic stir bar. The propargylated diblock copolymer was dissolved in dry toluene and dried twice by azeotropic distillation. The diblock copolymer was finally dissolved in tetrahydrofuran (1 ml per 50 mg) at 25 °C (room temperature). DMPA (0.5 eq. to propargyl groups) and 1-thioglycerol (15 eq. to propargyl groups) were added, the final solution was purged with nitrogen for 15 minutes and irradiated for the allotted time at either 20 or 30 cm distance from UVAHAND 250 (Honle UV Technology) UV lamp. The crude reaction mixture was transferred into a dialysis membrane and dialyzed against deionized water. The desired product was subsequently isolated by lyophilization.

Kinetic investigation of ε-CL and 7-(prop-2-ynyl)oxepan-2-one copolymerization catalyzed by benzyl alcohol/1,5,7-triazobicyclo[4.4.0]dec-5-ene. In a typical kinetic experiment, ε-CL (0.10 g, 0.9 mmol, 12.5 eq.), 7-(prop-2-ynyl)oxepan-2-one (0.14 g, 0.9 mmol, 12.5 eq.) and solution of benzyl alcohol (7.5 µl, 0.07 mmol, 1 eq.) in toluene were introduced to the flame-dried Schlenk flask equipped with a magnetic stirring bar. Monomers and benzyl alcohol were dried via azeotropic distillation, and finally dissolved in the desired volume of toluene (5.3 ml). Then, an aliquot of the reaction mixture was transferred to the capped reaction vial designed for microwave

synthesis (Biotage). These vials were heated, sealed, allowed to cool down under vacuum, and filled with nitrogen prior to use. The calculated amount of catalyst, 1,5,7-triazobicyclo[4.4.0]dec-5-ene, (20.1 mg, 0.14 mmol, 2.0 eq.) was dissolved in dry toluene, and (co)polymerization was started by the addition of catalyst solution to the reaction vial. The reaction mixture was magnetically stirred at the controlled reaction temperature (30 °C) for an allotted polymerization time. Polymerization was quenched with a solution of benzoic acid in toluene and then a sample was taken for ^{1}H NMR analysis (monomer conversion determination). Toluene was evaporated via a rotary evaporator, the crude polymer was precipitated with hexane, extracted with cyclohexane/ethyl acetate, and dried *in vacuo* until constant weight.

Synthesis of COSAN-pyridinium-3-boronic acid conjugate (CosBA). COSAN-dioxanate (0.1 g, 0.24 mmol) and 3-pyridineboronic acid 1,3-propanediol ester (0.044 g, 0.27 mmol, 1.1 eq.) were weighted into the round-bottom flask, purged with nitrogen and finally dissolved in 3 ml of dried acetonitrile. Reaction mixture was stirred at 70 °C for 4 hours, followed by evaporation of acetonitrile on a rotary evaporator, providing the red oil. The red oily product was dissolved in 1 ml of acetone and evaporation resulted in the formation of orange foamy solid (97% yield). 1,3-propanediol protected COSAN-dioxanate-pyridinium-3-boronic acid in the form of orange solid was deprotected in the second step. The isolated protected compound was dissolved in acetone (5 ml), followed by the addition of 5 ml of 6% aqueous HCl. Water (5 ml) was added after 24 hours, and acetone was evaporated on the rotary evaporator. Residual water was removed by decantation and the whole procedure was repeated again. Resulting oily product was washed with water and dried *in vacuo* until constant weight (90% yield).



^{1}H NMR (400MHz, acetone-d_6) δ 9.32 (dt, J = 6.2, 1.5 Hz, 1H, pyr CH), 9.24 (d, J = 1.6 Hz, 1H, pyr CH), 8.98 (dt, J = 7.7, 1.4 Hz, 1H, pyr CH), 8.28 - 8.11 (m, 1H, pyr CH), 5.09 - 4.92 (m, 2H, pyrN-CH_2), 4.21 - 4.06 (m, 4H, CH-COSAN + OCH_2), 4.02 (s, 2H, CH-COSAN), 4.5 - 0.5 (m, 17H, BH), 3.63 (s, 4H, OCH_2CH_2OB). **MS** (MALDI-TOF, m/z): Calculated for $C_{13}H_{35}B_{19}CoNO_4Na$ ($M+Na^+$): 557.367, found: 557.230.

Preparation of nanoparticles. Polymer (10 mg) was dissolved overnight in 2 ml of THF/water (9/1, v/v) mixture and added dropwise into 4 ml of vigorously stirred water. (The same procedure but with addition of 2 mg of CosBA was used for drug encapsulation experiments.) THF was used as a nonselective solvent (good solvent for both blocks, in which polymer chains dissolve molecularly) and water as a selective solvent (a good solvent for PEG and simultaneously a poor solvent for P(ε-CL-*co*-PgCL), in which polymer chains spontaneously and reversibly form multimolecular micelles). Decreasing the content of initial common solvent by dropwise addition of the solution into an excess of water induced micelle formation and the remaining organic solvent was eliminated by dialysis. It was dialyzed against deionized water for 1 day and the dialysis fluid was exchanged at least 3 times. The aqueous solution was then filtered with 0.45 μm polyvinylidene difluoride (PVDF) membrane syringe filter and further diluted with deionized water to prepare 1 ml samples of different concentrations (0.2-1 g·ml^{-1}). Weeks later, no aggregation or precipitation was visible to the naked eye, suggesting high nanoparticle stability.

Methods

Size exclusion chromatography (SEC). SEC analysis was performed using a Deltachrom SDS 030 pump (Watrex Ltd., Prague, Czech Republic) at a flow rate of 0.5 ml·min^{-1} and a MIDAS autosampler (Spark Ltd., Emmen, Holland). Two PLgel 10-μm mixed B LS columns (Polymer Laboratories, Shropshire, UK) were used in a series, each of which separating in the molecular

weight range of approximately 5 x $10^2 \leq M \leq 1 \times 10^7$ (related to PS standards), according to the manufacturer's instructions. The following detectors were used: (i) a UV/VIS DeltaChrom UVD 200 detector (Watrex) at a flow cell volume of 8 µl and operating at a wavelength λ=264 nm, and (ii) an evaporative light-scattering photometer PL ELS 1000 (Polymer Laboratories) with nitrogen as a carrier gas, setting the temperatures of the nebulizer and evaporator to 100 °C and 180 °C, respectively. Tetrahydrofuran was used as the mobile phase at room temperature. M_w and M_n were determined by constructing a calibration curve with polystyrene standards with molecular weights ranging from 666 to 2 x 10^6. Data were collected into Clarity software (DataApex Ltd.).

Proton Nuclear Magnetic Resonance Spectroscopy. ^{1}H NMR spectra were recorded on a Bruker Avance MSL 400 MHz spectrometer at room temperature in $CDCl_3$ or in acetone-d_6. Approximately 5 mg of sample was directly dissolved into the NMR tube in 0.6 ml of NMR solvent. The chemical shifts were calibrated using the residual resonances of the solvent. Diffusion-ordered NMR spectroscopy (DOSY) and CosBA binding ^{1}H NMR experiments were performed using a Bruker Avance III 600MHz spectrometer equipped with a cryogenically cooled probe. For a CosBA binding experiments, 10 mg of polymer and 2 mg of CosBA (0.7 eq. respective to the diol containing ε-CL units) were dissolved in 0.6 ml of dry acetonitrile-d_3 with a drop of pyridine (20 eq. respective to the CosBA).

Light scattering. The light scattering measurements were performed on a photometer (ALV, Germany) consisting of a CGS-3 automatic goniometer, a 7004 multitau multibit autocorrelator, two high-QE APD pseudo cross-correlation detectors, and a 100 mW, 660 nm diode-pumped solid-state laser (Cobolt AB, Sweden). The photometer was operated using the ALV-Correlator software. Individual measurements were performed at different concentrations (0.2-1.0 g·ml^{-1}) and at 26 °C for 20 s, with scattering angles ranging from 50° to 150° and with an angular step of 10°.

Considering the probability distribution, each angle was measured three times, and only the averaged intensity values were used for further calculations. Both static light scattering (SLS) and dynamic light scattering (DLS) data were analyzed using ALV-Stat software.

The molar mass was calculated from angular averaged intensity values as: $(Kc/R(q,c))=1/M_w$, where M_w, stand for weight-averaged molar mass and $R(q,c)$ stands for the corrected Rayleigh ratio which depends on the polymer concentration c and on the magnitude of the scattering vector $q = (4\pi n/\lambda_0) \sin(\theta/2)$, where θ is the scattering angle, n is the refractive index of the solvent and λ_0 is the wavelength of the incident light. The contrast factor K is given by the relationship $K = 4\pi^2 n^2 (dn/dc)^2/(\lambda_0^4 N_A)$, where (dn/dc) is the refractive index increment of the polymer with respect to the solvent, and N_A is the Avogadro constant. The refractive index increments of **2b2** in THF was measured by the Optilab T-rEX refractive index detector (Wyatt Technology Corporation). First, the reference cuvette of the detector was purged with approximately 10 ml of THF. Then, pure solvent and 10 ml samples of increasing concentrations (up to 2.5 $g \cdot l^{-1}$) were consecutively injected into the detector with a plastic syringe by a mechanical pump (flow rate 1 $ml \cdot min^{-1}$) through 1 μm PTFE membrane syringe filter. The relative refractive index was plotted against time, and the change of the relative refractive index was determined by difference in heights between the plateaus corresponding to individual sample concentrations. The refractive index increment in THF was obtained by a linear fit of these changes plotted against the sample concentration. From these values, the refractive index increments of **2b2** in water were estimated using the Gladstone-Dale equation,[2] assuming the specific volume of the respective polymers is 1 $ml \cdot g^{-1}$ in both solvents: $v(n_0 - 1) = v_1 w_1 (n_1 - 1) + v_2 w_2 (n_2 - 1)$, where v_i represents the specific volume, w_i is the weight fraction and n_i stands for the refractive index.

Dynamic light scattering (DLS) measurements were evaluated by fitting the measured normalized time autocorrelation function of the scattered light intensity, $g^{(2)}(t,q)$, related to the electric field autocorrelation function, $g^{(1)}(t,q)$, by the Siegert relation, $g^{(2)}(t,q) = 1 + \beta|g^{(1)}(t,q)|^2$. The data were fitted using the constrained regularization algorithm (CONTIN), which provides the distribution of relaxation times τ, $A(\tau,q)$ as the inverse Laplace transform of $g^{(1)}(t,q)$ function. The $A(\tau,q)$ distributions can be recalculated to the distributions of apparent hydrodynamic radii, R_h, using the relationship $R_h = k_B T q^2 \tau / 6\pi\eta$, where k_B is the Boltzmann constant, T is the temperature, and η is the viscosity of the solvent.

Transmission electron microscopy. Transmission electron microscopy (TEM) micrographs were acquired under a JEOL NEOARM transmission electron microscope operating at an acceleration voltage of 200 kV and equipped with a TemCamXF416R 4k × 4k CMOS camera (TVIPS, Germany). Approximately 100 µl of aqueous nanoparticle dispersion (**2b2**, 11.2 $g \cdot l^{-1}$) was applied to a copper TEM grid coated with an electron-transparent carbon film. After 1 min, the solution was removed by touching the bottom of the TEM grid with filter paper and the grid was dried prior to insertion into the microscope holder. Samples were negatively stained with the uranyl acetate. Obtained images were analyzed using ImageJ software to assess the particle size.

Cryogenic TEM. Cryo-TEM micrographs of synthesized nanoparticles were obtained with a TEM microscope Tecnai G2 Spirit Twin 12 (FEI, Czech Republic) using the bright field imaging mode at the accelerating voltage 120 kV. 3 µl of the sample **2b2** solution (11.2 $g \cdot l^{-1}$) was applied to an electron microscopy grid covered with a holey carbon supporting film (Electron Microscopy Science), which was hydrophilized just before the experiment via glow discharge (Expanded Plasma Cleaner, Harrick Plasma, USA). The excess of the solution was removed by blotting (Whatman no. 1 filter paper) for ∼1 s, and the grid was immediately plunged into liquid ethane

held at -181 °C. The frozen sample was then transferred into the microscope and observed at -173 °C. Recorded images were processed via ImageJ software to determine the size of particles.

Quantum chemical calculations. The ground state molecular geometries of the reactants, intermediates, and products of the TBD-catalyzed ring-opening polymerization (ROP) (Scheme 1) were determined by means of the minimization of the total energy calculated using the hybrid Density Functional Theory (DFT) method B3LYP[3-4] and the Pople basis set 6-311G(d). This method was previously successfully used for an extensive theoretical and experimental study of similar reactions by Nifant'ev et al.[5] Solvation effects (toluene solution) were described by means of the polarizable continuum model (PCM) using the integral equation formalism variant.[6-7] For each reactant, different initial geometries were considered to find the lowest-energy conformer. Each obtained equilibrium geometry was checked by the normal mode analysis showing no imaginary frequency. The transition states on the TBD-catalyzed ROP reaction path were found using the Berny algorithm with an initial guess obtained from the relaxed potential energy surface scans along the appropriate internal coordinates. All obtained transition states were confirmed by the normal mode analysis showing just one imaginary frequency and intrinsic reaction coordinate (IRC) calculations performed on both sides of the transition state. IRC calculations were followed by the geometry optimizations, which proved that reaction proceeds from the given transition state to the expected reaction intermediate. Thermodynamic parameters were calculated for the room temperature 298.15 K and pressure 1 atm. All calculations were performed using the Gaussian 16 program package.[8]

Thiol-yne click functionalization of mPEG-*b*-P(ε-CL-*co*-PgCL

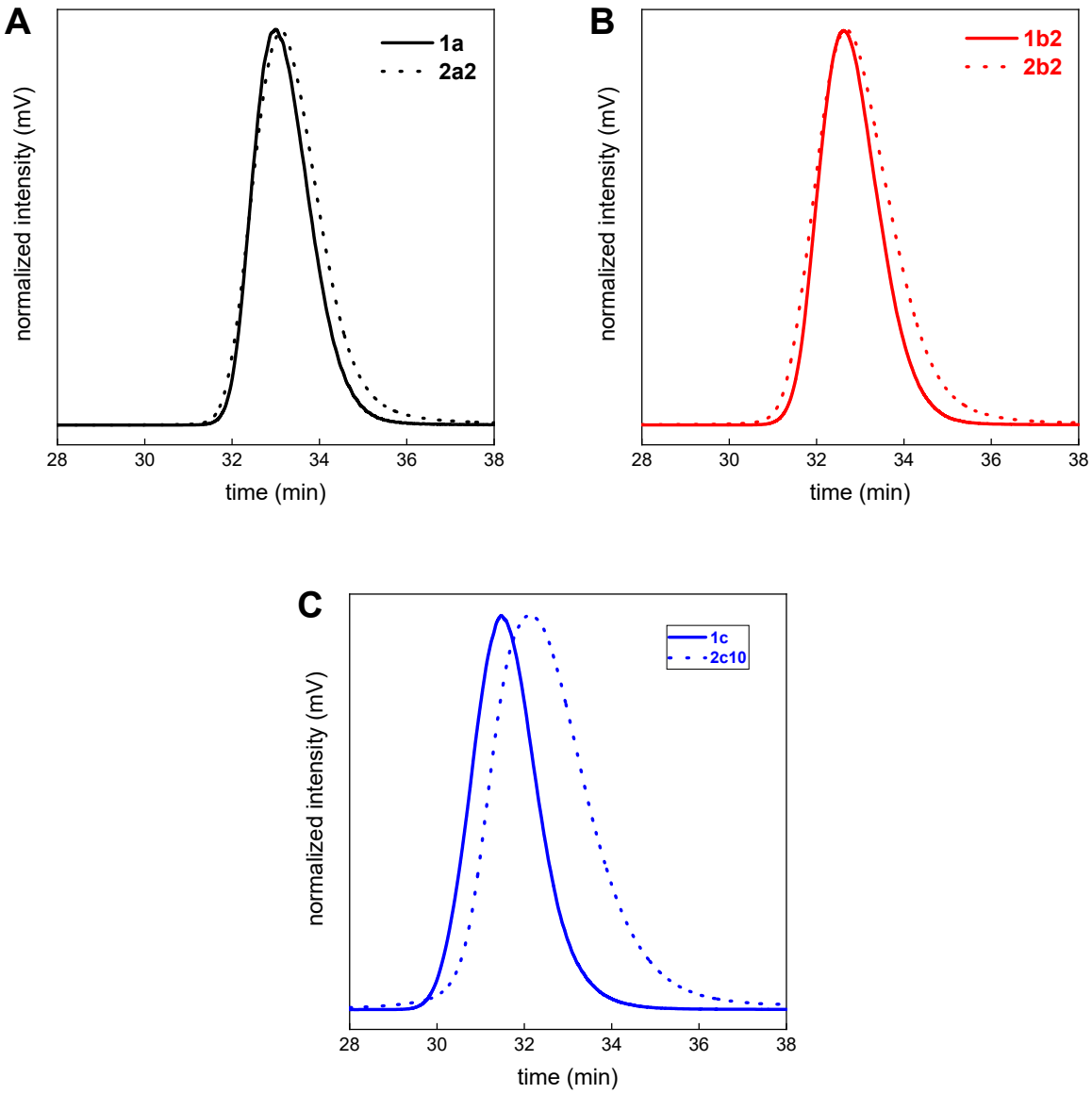


Figure S1: SEC-ELS chromatograms showing direct comparison between mPEG-*b*-P(ε-CL-*co*-PgCL) copolymers and their corresponding analogs modified via thiol-yne click reaction

Kinetics and modeling of ε-CL and 7-(prop-2-ynyl)oxepan-2-one copolymerization

Table S1: Copolymerization of ε-CL and 7-(prop-2-ynyl)oxepan-2-one in toluene catalyzed by BnOH/TBD at 30 °C [a]

time (h)	conv. ε-CL [b] (%)	conv. 7-is. [b] (%)	M_n [c] (kg.mol^{-1})	$Đ^{RI}$ [c]	M_n [d] (kg.mol^{-1})
1	12.2	28.6			0.8
2	22.0	49.3	1.3	1.15	1.4
3	32.0	65.4	1.5	1.20	1.9
4	41.6	78.1	1.8	1.15	2.3
5	50.0	86.2	2.1	1.18	2.6

[a] n_{BnOH} = 10.5 µmol (1 eq.), ε-CL/7-is/BnOH/TBD = 12.5/12.5/1/2, c_M = 0.27M; [b] determined by ^{1}H NMR; [c] apparent number-average molecular weights (M_n) and dispersities ($Đ$) determined by SEC-ELS with PS calibration in THF at 25 °C; [d] M_n

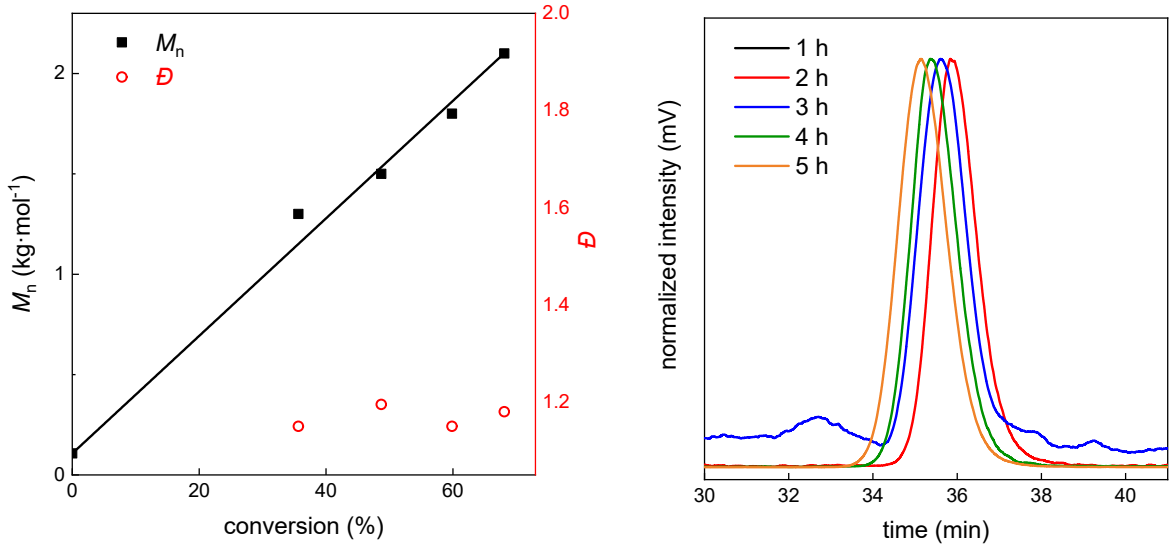


Figure S2: Kinetics of copolymerization of ε-CL with 7-(prop-2-ynyl)oxepan-2-one in toluene catalyzed by BnOH/TBD at 30 °C: The apparent number-average molecular weights (M_n) and dispersities ($Đ$) determined by SEC-ELS with PS calibration plotted vs. monomer conversion (left). Corresponding SEC-ELS chromatograms (right).

Copolymerization parameters

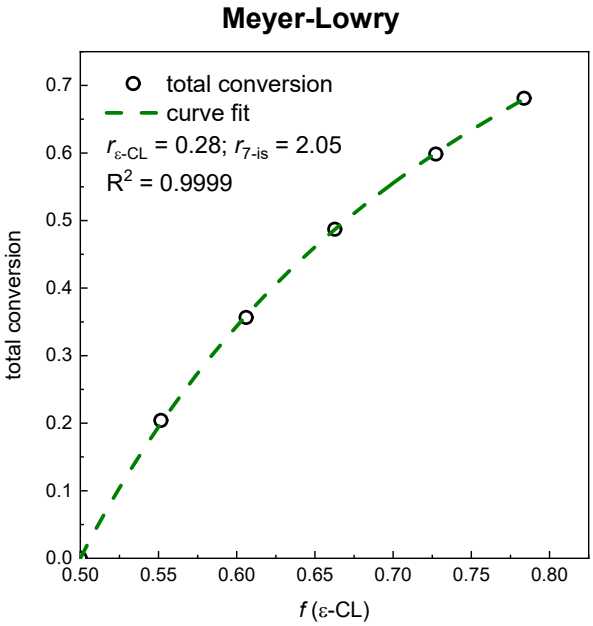


Figure S3: The Meyer-Lowry evaluation of the ε-CL and 7-(prop-2-ynyl)oxepan-2-one copolymerization in toluene catalyzed by BnOH/TBD at 30 °C.

Table S2: Data obtained from determined copolymerization parameters (integrated Ideal Model) and used for construction of simulated copolymer composition profiles

f (ε-CL)	total conversion [a]	F (ε-CL) [b]	f (ε-CL)	total conversion [a]	F (ε-CL) [b]
0.500	0.000	0.264	0.775	0.677	0.552
0.525	0.099	0.284	0.800	0.712	0.589
0.550	0.187	0.305	0.825	0.745	0.628
0.575	0.266	0.327	0.850	0.777	0.670
0.600	0.336	0.350	0.875	0.807	0.715
0.625	0.399	0.374	0.900	0.837	0.763
0.650	0.456	0.400	0.925	0.867	0.816
0.675	0.508	0.427	0.950	0.898	0.872
0.700	0.555	0.455	0.975	0.934	0.933
0.725	0.599	0.486	1.000	1.000	1.000
0.750	0.639	0.518			

[a] $total\ conversion = 1 - \left(\frac{f}{f_0}\right)^{\frac{1}{r-1}} \cdot \left(\frac{1-f}{1-f_0}\right)^{\frac{r}{1-r}}$, $(f_0 = 0.5)$[9]

[b] $F = \frac{rf}{rf - f + 1}$

Quantum chemical validation of kinetics and copolymer structure

Table S3: Gibbs free energies (in kcal·mol^{-1}) of reaction intermediates and transition states for the TBD-catalyzed ROP calculated by the PCM-B3LYP/6-311G(d) method. For each isomer, the highest-energy transition state is shown in bold. All values are with respect to the Gibbs free energy of the ground state of the system, i.e. complex BnOH-TBD.

a) Initial step of the polymerization

	I1	TS12	I2	TS23	I3	TSr	I3r	TSr2	I3r2	TS34	I4	I5
						Vacuum						
ε-CL	2.47	**21.46**	16.11	18.35	16.40	18.73	14.72	16.82	14.92	21.07	4.17	-1.54
3-is *	2.39	**23.02**	20.01	21.58	19.05	20.54	14.95	16.70	15.45	20.61	5.41	1.21
7-is *	2.54	21.23	15.83	18.44	16.68	20.44	15.56	–	–	**21.33**	4.04	0.13
						Toluene						
ε-CL	4.64	22.33	19.00	20.75	19.30	21.47	17.63	19.61	18.32	**22.60**	7.47	1.21
3-is *	4.79	**26.57**	22.65	23.95	21.67	23.27	18.09	19.16	18.21	22.24	8.03	2.88
7-is *	5.05	21.58	18.30	21.13	18.75	**22.70**	17.93	–	–	21.95	6.67	1.40

b) Next step of the polymerization *(calculated only in toluene solution)*

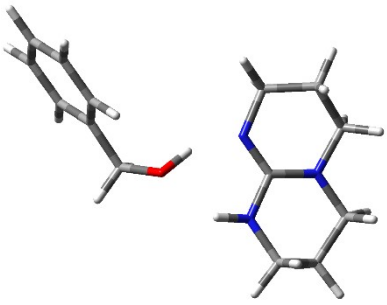
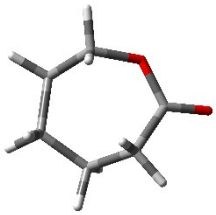
Addition of another unit	to the chain end	I1	TS12	I2	TS2r	I2r	TS23	I3	TSr	I3r	TSr2	I3r2	TS34	I4	I5
								Toluene							
ε-CL	ε-CL	6.66	**24.87**	20.30	21.86	19.78	23.75	21.87	22.37	18.41	–	–	23.16	6.82	2.65
ε-CL	3-is	8.42	**25.71**	23.27	24.59	22.38	23.15	21.81	23.48	20.37	22.72	20.04	25.22	7.00	3.64
ε-CL	7-is	7.50	**26.30**	22.30	–	–	24.49	22.01	24.44	21.08	22.48	20.50	24.05	9.00	2.80
3-is	ε-CL	6.36	**25.87**	24.78	–	–	25.24	18.28	19.82	18.47	–	–	22.30	8.48	3.77
3-is	3-is *	8.68	**27.68**	25.82	–	–	26.82	20.48	21.83	20.37	–	–	23.18	10.19	5.60
3-is	7-is *	8.44	28.37	26.96	–	–	**29.70**	27.43	27.69	20.85	22.30	20.99	24.04	10.48	4.68
7-is	ε-CL	6.77	**24.16**	19.25	21.84	18.63	21.65	19.63	21.75	18.32	–	–	22.66	5.44	-0.03
7-is	3-is *	8.36	**25.44**	21.48	–	–	23.08	20.70	23.41	22.98	–	–	24.41	6.92	3.93
7-is	7-is *	7.40	**25.96**	23.05	–	–	24.13	22.41	24.37	22.42	23.65	21.18	23.77	9.12	4.22

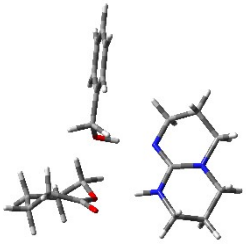
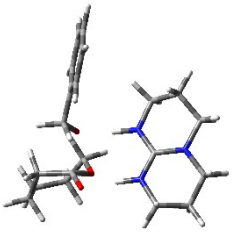
*) Data for 3- and 7-isomer polymerization are taken from our previous paper[10]

Table S4: Thermodynamic data

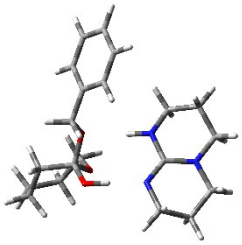
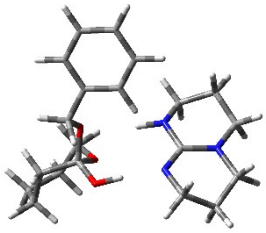
a) Initial step of the ε-CL polymerization

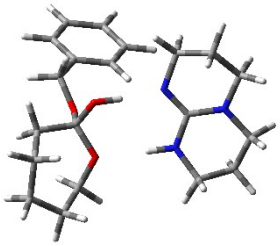
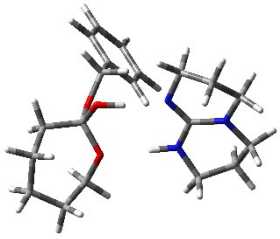
Optimized molecular conformations (in vacuum) and thermodynamic parameters (electronic energies (with the nuclear repulsion) E_{DFT}, sum of electronic and zero-point energies E_0, sum of electronic and thermal energies E_{298}, sum of electronic and thermal enthalpies H_{298}, and sum of electronic and thermal free energies G_{298}) in vacuum and toluene solution calculated by the PCM-B3LYP/6-311G(d) method

State	**BnOH–TBD**	**ε-CL**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-493092.1104	-241722.1152
E_0 (kcal/mol)	-492878.1956	-241623.8527
E_{298} (kcal/mol)	-492867.4037	-241619.3215
H_{298} (kcal/mol)	-492866.8113	-241618.7285
G_{298} (kcal/mol)	-492908.9316	-241643.6431
Toluene		
E_{DFT} (kcal/mol)	-493094.9932	-241725.0684
E_0 (kcal/mol)	-492881.2691	-241626.8039
E_{298} (kcal/mol)	-492870.4509	-241622.2840
H_{298} (kcal/mol)	-492869.8579	-241621.6916
G_{298} (kcal/mol)	-492912.2512	-241646.5567

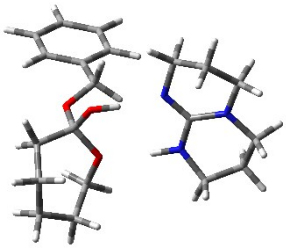
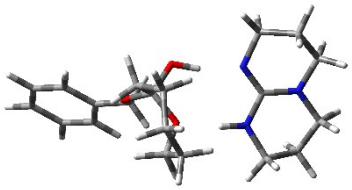
State	**I1**	**TS12**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-734821.9444	-734807.3864
E_0 (kcal/mol)	-734509.6142	-734494.9920
E_{298} (kcal/mol)	-734492.8459	-734479.5778
H_{298} (kcal/mol)	-734492.2535	-734478.9855

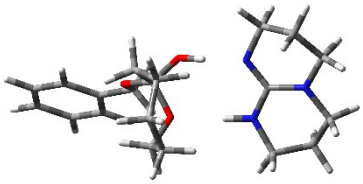
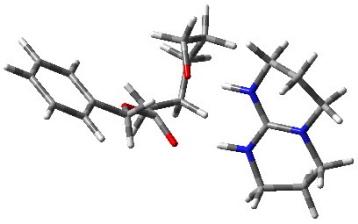
G_{298} (kcal/mol)	-734550.1068	-734531.1102
Toluene		
E_{DFT} (kcal/mol)	-734825.4678	-734812.6276
E_0 (kcal/mol)	-734513.3717	-734500.2417
E_{298} (kcal/mol)	-734496.5595	-734484.7498
H_{298} (kcal/mol)	-734495.9671	-734484.1574
G_{298} (kcal/mol)	-734554.1630	-734536.4804

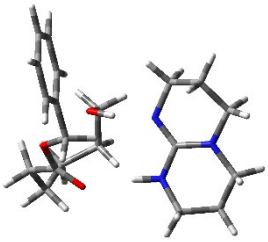
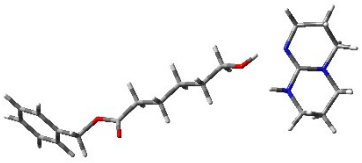
State	**I2**	**TS23**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-734812.4160	-734812.0071
E_0 (kcal/mol)	-734498.9302	-734498.5305
E_{298} (kcal/mol)	-734483.2375	-734483.3636
H_{298} (kcal/mol)	-734482.6451	-734482.7712
G_{298} (kcal/mol)	-734536.4672	-734534.2201
Toluene		
E_{DFT} (kcal/mol)	-734815.9097	-734815.5064
E_0 (kcal/mol)	-734502.5547	-734502.2391
E_{298} (kcal/mol)	-734486.8846	-734487.0621
H_{298} (kcal/mol)	-734486.2922	-734486.4698
G_{298} (kcal/mol)	-734539.8081	-734538.0623

State	**I3**	**TS3r**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-734812.6996	-734810.9058
E_0 (kcal/mol)	-734499.1015	-734497.4255
E_{298} (kcal/mol)	-734483.4565	-734482.2322
H_{298} (kcal/mol)	-734482.8641	-734481.6398
G_{298} (kcal/mol)	-734536.1792	-734533.8486
Toluene		
E_{DFT} (kcal/mol)	-734816.2859	-734814.5648
E_0 (kcal/mol)	-734502.8603	-734501.2696

E_{298} (kcal/mol)	-734487.2441	-734486.0977
H_{298} (kcal/mol)	-734486.6518	-734485.5053
G_{298} (kcal/mol)	-734539.5081	-734537.3351

State	**I3r**	**TS3r2**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-734813.9256	-734812.6021
E_0 (kcal/mol)	-734500.3622	-734499.3714
E_{298} (kcal/mol)	-734484.6795	-734484.1994
H_{298} (kcal/mol)	-734484.0871	-734483.6071
G_{298} (kcal/mol)	-734537.8528	-734535.7594
Toluene		
E_{DFT} (kcal/mol)	-734817.4927	-734816.2733
E_0 (kcal/mol)	-734504.1147	-734503.1634
E_{298} (kcal/mol)	-734488.4558	-734488.0266
H_{298} (kcal/mol)	-734487.8635	-734487.4343
G_{298} (kcal/mol)	-734541.1742	-734539.1956

State	**I3r2**	**TS34**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-734813.3399	-734805.8451
E_0 (kcal/mol)	-734499.9085	-734494.2490
E_{298} (kcal/mol)	-734484.1831	-734478.6108
H_{298} (kcal/mol)	-734483.5908	-734478.0185
G_{298} (kcal/mol)	-734537.6551	-734531.5093
Toluene		
E_{DFT} (kcal/mol)	-734816.8049	-734811.2779
E_0 (kcal/mol)	-734503.4590	-734499.6148
E_{298} (kcal/mol)	-734487.8114	-734483.9516
H_{298} (kcal/mol)	-734487.2190	-734483.3592
G_{298} (kcal/mol)	-734540.4839	-734536.2043

State	I4	I5
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-734823.0823	-734823.0232
E_0 (kcal/mol)	-734510.1727	-734510.7688
E_{298} (kcal/mol)	-734493.6366	-734493.7062
H_{298} (kcal/mol)	-734493.0436	-734493.1132
G_{298} (kcal/mol)	-734548.4031	-734554.1103
Toluene		
E_{DFT} (kcal/mol)	-734826.0918	-734827.4903
E_0 (kcal/mol)	-734513.3253	-734515.4312
E_{298} (kcal/mol)	-734496.7904	-734498.3736
H_{298} (kcal/mol)	-734496.1981	-734497.7813
G_{298} (kcal/mol)	-734551.3342	-734557.5930

b) Next step of the polymerization *(calculated only in toluene solution)*

Thermodynamic parameters of DFT-optimized structures in the second step of the TBD catalyzed ROP of ε-CL/3-isomer/7-isomer in toluene solution calculated by the PCM-B3LYP/6-311G(d) method: electronic energies (with the nuclear repulsion) E_{DFT}, sum of electronic and zero-point energies E_0, sum of electronic and thermal energies E_{298}, sum of electronic and thermal enthalpies H_{298}, and sum of electronic and thermal free energies G_{298}

Addition of another ε-CL unit to the ε-CL chain end		
State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-976557.7593	-976543.9082
E_0 (kcal/mol)	-976147.2458	-976133.3728
E_{298} (kcal/mol)	-976124.2080	-976111.7143
H_{298} (kcal/mol)	-976123.6157	-976111.1220
G_{298} (kcal/mol)	-976198.7078	-976180.4988
State	**I2**	**TS2r**
Toluene		
E_{DFT} (kcal/mol)	-976548.3000	-976548.2925
E_0 (kcal/mol)	-976136.6083	-976136.6635
E_{298} (kcal/mol)	-976114.7402	-976115.3445
H_{298} (kcal/mol)	-976114.1478	-976114.7521
G_{298} (kcal/mol)	-976185.0658	-976183.5058

State	**I2r**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-976549.7460	-976546.2078
E_0 (kcal/mol)	-976137.9122	-976134.8449
E_{298} (kcal/mol)	-976116.0730	-976113.4400
H_{298} (kcal/mol)	-976115.4806	-976112.8476
G_{298} (kcal/mol)	-976185.5841	-976181.6113

State	**I3**	**TS3r**
Toluene		
E_{DFT} (kcal/mol)	-976546.6705	-976546.0198
E_0 (kcal/mol)	-976135.1091	-976134.8286
E_{298} (kcal/mol)	-976113.1312	-976113.2994
H_{298} (kcal/mol)	-976112.5389	-976112.7070
G_{298} (kcal/mol)	-976183.4901	-976182.9950

State	**I3r**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-976550.4311	-976544.8153
E_0 (kcal/mol)	-976138.7681	-976134.6592
E_{298} (kcal/mol)	-976116.8687	-976112.8250
H_{298} (kcal/mol)	-976116.2763	-976112.2326
G_{298} (kcal/mol)	-976186.9565	-976182.2075

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-976559.0777	-976561.4381
E_0 (kcal/mol)	-976148.0509	-976150.8766
E_{298} (kcal/mol)	-976125.2359	-976127.6681
H_{298} (kcal/mol)	-976124.6435	-976127.0758
G_{298} (kcal/mol)	-976198.5447	-976202.7170

Addition of another ε-CL unit to the 3-isomer chain end

State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1049021.3610	-1049007.4121
E_0 (kcal/mol)	-1048586.9962	-1048573.2989
E_{298} (kcal/mol)	-1048561.9611	-1048549.4875
H_{298} (kcal/mol)	-1048561.3687	-1048548.8951
G_{298} (kcal/mol)	-1048641.4057	-1048624.1109

State	**I2**	**TS2r**
Toluene		
E_{DFT} (kcal/mol)	-1049011.4507	-1049011.4256
E_0 (kcal/mol)	-1048576.1089	-1048576.1303
E_{298} (kcal/mol)	-1048552.1864	-1048552.7254
H_{298} (kcal/mol)	-1048551.5940	-1048552.1330
G_{298} (kcal/mol)	-1048626.5532	-1048625.2323

State	**I2r**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1049012.7871	-1049012.3841
E_0 (kcal/mol)	-1048577.2573	-1048577.1751
E_{298} (kcal/mol)	-1048553.3291	-1048553.6623
H_{298} (kcal/mol)	-1048552.7367	-1048553.0699
G_{298} (kcal/mol)	-1048627.4486	-1048626.6749

State	**I3**	**TS3r**
Toluene		
E_{DFT} (kcal/mol)	-1049012.5510	-1049011.4206
E_0 (kcal/mol)	-1048577.2102	-1048576.2376
E_{298} (kcal/mol)	-1048553.2161	-1048552.7191
H_{298} (kcal/mol)	-1048552.6238	-1048552.1268
G_{298} (kcal/mol)	-1048628.0109	-1048626.3417

State	**I3r**	**TSr2**
Toluene		
E_{DFT} (kcal/mol)	-1049014.2466	-1049013.0298
E_0 (kcal/mol)	-1048578.8461	-1048577.8553
E_{298} (kcal/mol)	-1048554.8803	-1048554.4203
H_{298} (kcal/mol)	-1048554.2873	-1048553.8273
G_{298} (kcal/mol)	-1048629.4516	-1048627.1054

State	**I3r2**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1049013.6905	-1049008.2023
E_0 (kcal/mol)	-1048578.4608	-1048574.3099
E_{298} (kcal/mol)	-1048554.4322	-1048550.3992
H_{298} (kcal/mol)	-1048553.8399	-1048549.8069
G_{298} (kcal/mol)	-1048629.7905	-1048624.6073

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1049022.8284	-1049025.1433
E_0 (kcal/mol)	-1048588.2205	-1048591.0022
E_{298} (kcal/mol)	-1048563.2613	-1048565.6841
H_{298} (kcal/mol)	-1048562.6683	-1048565.0911
G_{298} (kcal/mol)	-1048642.8245	-1048646.1904

Addition of another ε-CL unit to the 7-isomer chain end

State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1049023.8998	-1049010.0880
E_0 (kcal/mol)	-1048590.0836	-1048575.8604
E_{298} (kcal/mol)	-1048564.9826	-1048552.1161
H_{298} (kcal/mol)	-1048564.3902	-1048551.5237
G_{298} (kcal/mol)	-1048644.5024	-1048625.6966

State	**I2**	**TS23**
Toluene		

E_{DFT} (kcal/mol)	-1049013.5984	-1049013.5982
E_0 (kcal/mol)	-1048578.5857	-1048578.6221
E_{298} (kcal/mol)	-1048554.5678	-1048555.1714
H_{298} (kcal/mol)	-1048553.9748	-1048554.5791
G_{298} (kcal/mol)	-1048629.6995	-1048627.5107

State	**I3**	**TS3r**
Toluene		
E_{DFT} (kcal/mol)	-1049014.2332	-1049013.0953
E_0 (kcal/mol)	-1048579.2371	-1048578.2738
E_{298} (kcal/mol)	-1048555.2417	-1048554.8269
H_{298} (kcal/mol)	-1048554.6494	-1048554.2339
G_{298} (kcal/mol)	-1048629.9881	-1048627.5547

State	**I3r**	**TS3r2**
Toluene		
E_{DFT} (kcal/mol)	-1049015.2628	-1049014.5745
E_0 (kcal/mol)	-1048580.2712	-1048579.8953
E_{298} (kcal/mol)	-1048556.2683	-1048556.3882
H_{298} (kcal/mol)	-1048555.6760	-1048555.7958
G_{298} (kcal/mol)	-1048630.9175	-1048629.5169

State	**I3r2**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1049015.2524	-1049011.3625
E_0 (kcal/mol)	-1048580.3478	-1048577.5560
E_{298} (kcal/mol)	-1048556.3160	-1048553.6585
H_{298} (kcal/mol)	-1048555.7237	-1048553.0655
G_{298} (kcal/mol)	-1048631.5004	-1048627.9456

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1049024.5476	-1049028.0558
E_0 (kcal/mol)	-1048590.2932	-1048594.2007
E_{298} (kcal/mol)	-1048565.3716	-1048568.9177
H_{298} (kcal/mol)	-1048564.7792	-1048568.3247
G_{298} (kcal/mol)	-1048643.0014	-1048649.1962

Addition of another 3-isomer unit to the ε-CL chain end

State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1049022.6854	-1049008.4644
E_0 (kcal/mol)	-1048588.8430	-1048574.2772
E_{298} (kcal/mol)	-1048563.6253	-1048550.4965
H_{298} (kcal/mol)	-1048563.0329	-1048549.9041
G_{298} (kcal/mol)	-1048643.4645	-1048623.9597

State	**I2**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1049010.3404	-1049010.1788
E_0 (kcal/mol)	-1048575.1488	-1048575.3402

E_{298} (kcal/mol)	-1048551.2357	-1048551.8005
H_{298} (kcal/mol)	-1048550.6433	-1048551.2075
G_{298} (kcal/mol)	-1048625.0415	-1048624.5834
State	**I3**	**TS3r**
Toluene		
E_{DFT} (kcal/mol)	-1049015.9230	-1049014.8565
E_0 (kcal/mol)	-1048580.9401	-1048580.1426
E_{298} (kcal/mol)	-1048556.8601	-1048556.5689
H_{298} (kcal/mol)	-1048556.2677	-1048555.9765
G_{298} (kcal/mol)	-1048631.5469	-1048630.0013
State	**I3r**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1049015.5954	-1049010.1816
E_0 (kcal/mol)	-1048580.6063	-1048576.8500
E_{298} (kcal/mol)	-1048556.5275	-1048552.7643
H_{298} (kcal/mol)	-1048555.9351	-1048552.1720
G_{298} (kcal/mol)	-1048631.3586	-1048627.5214
State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1049023.0575	-1049025.2892
E_0 (kcal/mol)	-1048588.6152	-1048591.0970
E_{298} (kcal/mol)	-1048563.5838	-1048565.7989
H_{298} (kcal/mol)	-1048562.9915	-1048565.2066
G_{298} (kcal/mol)	-1048641.3498	-1048646.0530
Addition of another 7-isomer unit to the ε-CL chain end		
State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1049025.3446	-1049011.4546
E_0 (kcal/mol)	-1048591.5344	-1048577.7768
E_{298} (kcal/mol)	-1048566.3844	-1048553.8907
H_{298} (kcal/mol)	-1048565.7920	-1048553.2983
G_{298} (kcal/mol)	-1048645.2247	-1048627.8389
State	**I2**	**TS2r**
Toluene		
E_{DFT} (kcal/mol)	-1049015.8072	-1049015.8113
E_0 (kcal/mol)	-1048580.8962	-1048580.8968
E_{298} (kcal/mol)	-1048556.8199	-1048557.4110
H_{298} (kcal/mol)	-1048556.2275	-1048556.8187
G_{298} (kcal/mol)	-1048632.7486	-1048630.1620
State	**I2r**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1049017.2405	-1049015.8058
E_0 (kcal/mol)	-1048582.2767	-1048581.0098
E_{298} (kcal/mol)	-1048558.2080	-1048557.4129
H_{298} (kcal/mol)	-1048557.6156	-1048556.8205

G_{298} (kcal/mol)	-1048633.3685	-1048630.3521
State	**I3**	**TS3r**
Toluene		
E_{DFT} (kcal/mol)	-1049016.4407	-1049015.0023
E_0 (kcal/mol)	-1048581.5532	-1048580.3478
E_{298} (kcal/mol)	-1048557.4562	-1048556.6957
H_{298} (kcal/mol)	-1048556.8638	-1048556.1033
G_{298} (kcal/mol)	-1048632.3677	-1048630.2454
State	**I3r**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1049017.7514	-1049013.2396
E_0 (kcal/mol)	-1048582.8120	-1048579.3331
E_{298} (kcal/mol)	-1048558.7282	-1048555.4112
H_{298} (kcal/mol)	-1048558.1358	-1048554.8188
G_{298} (kcal/mol)	-1048633.6735	-1048629.3387
State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1049028.2553	-1049030.6416
E_0 (kcal/mol)	-1048593.9076	-1048596.7778
E_{298} (kcal/mol)	-1048568.9428	-1048571.4898
H_{298} (kcal/mol)	-1048568.3498	-1048570.8975
G_{298} (kcal/mol)	-1048646.5557	-1048652.0319

A note on artefact intermediate states

The geometry optimization in all standard quantum chemical methods is based on the minimization of the total electronic energy of the molecule plus the nuclear repulsion energy (here E_{DFT}). However, the Gibbs free energy G includes also the zero-point energy and thermal corrections. Consequently, some shallow intermediate states (local minima of E_{DFT}) found by the geometry optimization and IRC calculations do not need to be local minima of G. Consequently, such intermediate states should be considered either thermally unstable at the given temperature, or even artefacts of the method if it happens at zero temperature due to zero-point energy corrections. Such artefact intermediate states (not shown in Table S4) were found for all isomers between TS12 and I2 and between I3 and TS34.

Encapsulation of model drug

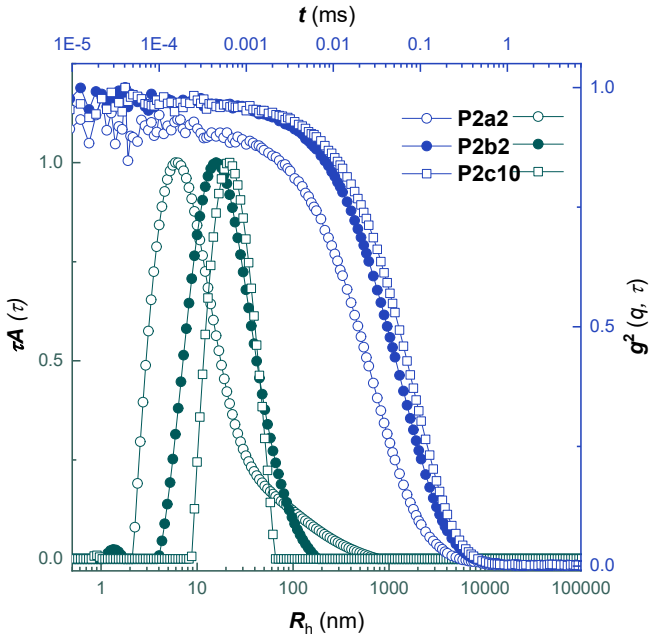


Figure S4: Autocorrelation functions at 130° (blue) and the corresponding apparent size distributions of loaded nanoparticles (green)

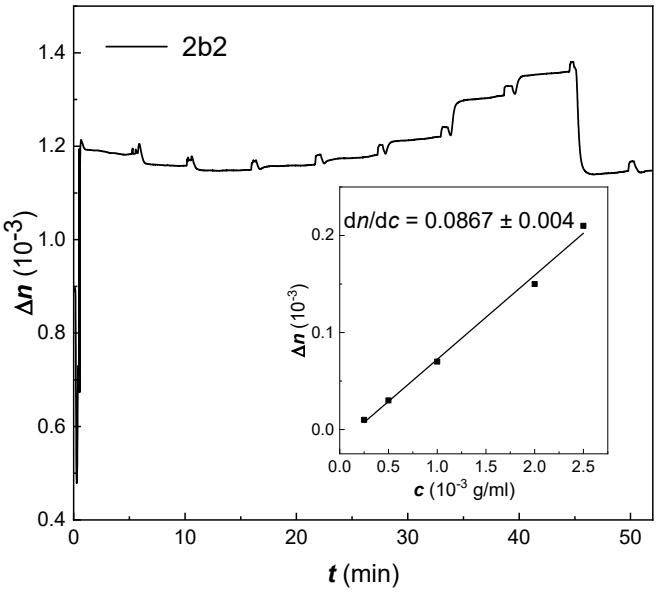


Figure S5: Determination of d*n*/d*c* with the linear fit in inset

Optimized Cartesian coordinates

Table S5: Cartesian coordinates (in Angstroms) of all intermediates and transition states of the initial step of the TBD-catalyzed ROP of ε-CL (Scheme 1) optimized in vacuum and toluene using the (PCM-)B3LYP/6-311G(d) method

```
39 atoms
complex BnO-TBD in vacuum
N     -3.241467     0.563143     0.190145
C     -1.998784     0.003327    -0.020043
N     -1.946517    -1.367762    -0.145904
C     -3.119525    -2.160628    -0.454968
C     -4.255264    -1.689893     0.444854
C     -4.487622    -0.200415     0.219037
C     -2.196368     2.728578    -0.374120
C     -0.915255     2.095487     0.167159
N     -0.880107     0.663219    -0.069861
C     -3.400262     2.017324     0.233253
H     -2.881710    -3.210250    -0.267729
H     -3.417030    -2.078313    -1.513158
H     -3.980603    -1.875185     1.487316
H     -5.178528    -2.237925     0.237310
H     -5.032534    -0.046343    -0.725312
H     -5.121627     0.207917     1.014998
H     -4.313270     2.276294    -0.315818
H     -3.553460     2.340114     1.272755
H     -2.215512     2.621284    -1.463764
H     -2.246122     3.797885    -0.147075
H     -0.825789     2.310374     1.243866
H     -0.037156     2.543775    -0.305724
H     -1.034403    -1.706653    -0.434929
O      0.957556    -1.235363    -0.771667
C      1.872263    -1.470210     0.280752
C      3.162800    -0.675918     0.167688
H      2.109790    -2.540237     0.255359
H      1.407699    -1.270102     1.256859
C      3.608331    -0.210695    -1.071240
C      3.946542    -0.432011     1.299087
C      4.812625     0.482629    -1.176503
H      2.993092    -0.390773    -1.945525
C      5.153348     0.255989     1.196408
H      3.606883    -0.778357     2.272468
H      5.144536     0.841072    -2.146473
C      5.590987     0.716297    -0.044447
H      5.748323     0.440104     2.086015
H      6.528670     1.257244    -0.126712
```

```
H      0.472038    -0.388379    -0.583552


18 atoms
ε-CL in vacuum
O      2.499434    -0.087899    -0.406435
O      0.773420     1.240263    -0.078821
C      1.378077     0.024628     0.009116
C      0.596173    -1.139251     0.600195
H      0.284515    -0.907540     1.625743
H      1.311017    -1.959413     0.661023
C     -0.629448    -1.563671    -0.235108
H     -0.349520    -1.598522    -1.294209
H     -0.888287    -2.590296     0.041781
C     -1.865170    -0.678760    -0.040769
H     -2.197822    -0.761644     1.002463
H     -2.685841    -1.071870    -0.650133
C     -1.656511     0.801857    -0.375973
H     -1.434201     0.931416    -1.441310
H     -2.591089     1.343434    -0.189174
C     -0.552720     1.488010     0.424372
H     -0.605536     1.227651     1.487605
H     -0.648471     2.570982     0.347269


57 atoms
ε-CL, structure I1 in vacuum
O     -2.397324     0.781183    -1.711365
O     -2.754832     0.541123     0.439565
C     -2.813390     0.071331    -0.822221
C     -3.437672    -1.284012    -1.083851
H     -2.768943    -2.044685    -0.668368
H     -3.423087    -1.402913    -2.167400
C     -4.869284    -1.468438    -0.543314
H     -5.471152    -0.583054    -0.780518
H     -5.327865    -2.297611    -1.091395
C     -4.948590    -1.775048     0.956238
H     -4.412182    -2.712514     1.152013
H     -5.993203    -1.960877     1.229084
C     -4.380450    -0.679559     1.863966
H     -4.981668     0.234120     1.787476
H     -4.451710    -1.007485     2.907875
C     -2.924868    -0.319364     1.589843
H     -2.284280    -1.195276     1.468837
H     -2.520920     0.279568     2.405793
O     -0.309474    -1.339532    -0.047709
C      0.434709    -1.884796    -1.114543
```

C	1.633263	-2.717219	-0.684481
H	0.771007	-1.094248	-1.798988
H	-0.246417	-2.524648	-1.690101
C	1.718519	-3.241119	0.606637
C	2.656523	-3.004413	-1.593387
C	2.801282	-4.035785	0.981371
H	0.928784	-3.009789	1.312264
C	3.737592	-3.800860	-1.224000
H	2.609266	-2.596411	-2.600474
H	2.853313	-4.434392	1.990399
C	3.813771	-4.320505	0.067723
H	4.524721	-4.011025	-1.942100
H	4.657348	-4.938516	0.359387
H	0.120979	-0.479452	0.225976
N	1.841658	3.168498	0.363415
C	0.949556	2.146630	0.095149
N	-0.056352	2.425386	-0.783415
C	-0.169557	3.657311	-1.534003
C	0.298412	4.814147	-0.659646
C	1.712341	4.519486	-0.175635
C	3.346395	1.422846	1.257251
C	2.036083	0.737672	1.640153
N	1.007839	0.962360	0.637255
C	3.088571	2.914700	1.085477
H	-1.214607	3.772931	-1.827149
H	0.423937	3.626732	-2.461280
H	-0.378051	4.917762	0.194196
H	0.289988	5.757812	-1.212688
H	2.426735	4.659443	-1.002273
H	2.002260	5.228380	0.609662
H	3.911043	3.385669	0.531448
H	3.044862	3.410857	2.065625
H	3.707956	0.992075	0.318186
H	4.123756	1.267771	2.011800
H	1.708403	1.102478	2.627924
H	2.185315	-0.340292	1.742523
H	-0.773796	1.723670	-0.914799

57 atoms
ε-CL, structure TS12 in vacuum

O	1.720761	-0.634484	-1.638691
O	2.241480	-0.743881	0.514964
C	2.175598	0.002184	-0.663316
C	3.318799	0.995252	-0.899996
H	3.193286	1.887289	-0.282638
H	3.220144	1.305287	-1.941149

C	4.714350	0.388039	-0.660814
H	4.740966	-0.638948	-1.042283
H	5.444086	0.951471	-1.252959
C	5.159642	0.429645	0.808762
H	5.148792	1.476401	1.141576
H	6.203712	0.102560	0.880882
C	4.311943	-0.408563	1.774200
H	4.478216	-1.476332	1.588646
H	4.643277	-0.216558	2.803049
C	2.806454	-0.158752	1.690582
H	2.553578	0.903314	1.739175
H	2.304480	-0.654921	2.526058
O	0.830936	1.160469	-0.084232
C	0.329129	1.945201	-1.125372
C	-0.881288	2.760218	-0.700103
H	0.062531	1.330217	-2.000846
H	1.098148	2.655468	-1.481627
C	-0.935628	3.334568	0.575376
C	-1.951989	2.979295	-1.571639
C	-2.024538	4.112111	0.963706
H	-0.111710	3.155970	1.257801
C	-3.044056	3.757571	-1.188031
H	-1.930374	2.533762	-2.563003
H	-2.045080	4.555884	1.955194
C	-3.084658	4.327612	0.082635
H	-3.865382	3.915417	-1.881208
H	-3.933279	4.934248	0.384036
H	-0.276147	0.019770	0.310682
N	-2.254001	-2.629223	0.343852
C	-1.222115	-1.808094	-0.005602
N	-0.372766	-2.171609	-0.967381
C	-0.506235	-3.411448	-1.710798
C	-1.090383	-4.488216	-0.804994
C	-2.396190	-3.979473	-0.206759
C	-3.330092	-0.701596	1.465662
C	-1.910437	-0.202011	1.699812
N	-1.056891	-0.635859	0.606469
C	-3.303417	-2.213438	1.279250
H	0.487678	-3.684822	-2.068558
H	-1.142470	-3.271535	-2.595701
H	-0.377133	-4.716492	-0.007416
H	-1.277378	-5.411179	-1.359881
H	-3.191539	-3.981745	-0.964822
H	-2.726668	-4.637339	0.604079
H	-4.262018	-2.567771	0.885042
H	-3.147932	-2.716805	2.243245
H	-3.738318	-0.217784	0.573692

```
H     -3.979696    -0.448549     2.307443
H     -1.529209    -0.572190     2.661900
H     -1.873061     0.887314     1.728871
H      0.459349    -1.562020    -1.181549


57 atoms
ε-CL, structure I2 in vacuum
O     -1.239299     1.294519    -1.550937
O     -1.647111     1.470656     0.645702
C     -1.919493     0.728236    -0.515525
C     -3.411288     0.649048    -0.884715
H     -3.877551    -0.181222    -0.344324
H     -3.452775     0.400929    -1.946927
C     -4.195711     1.944832    -0.623698
H     -3.583016     2.803960    -0.913771
H     -5.071404     1.955480    -1.281667
C     -4.687664     2.090835     0.825424
H     -5.284247     1.203895     1.079273
H     -5.376673     2.941012     0.886728
C     -3.586780     2.275002     1.877466
H     -3.133558     3.267206     1.772309
H     -4.031852     2.239564     2.880192
C     -2.456616     1.250722     1.803339
H     -2.827768     0.220944     1.825927
H     -1.785664     1.371896     2.657815
O     -1.393326    -0.598727    -0.196111
C     -1.375328    -1.541907    -1.273855
C     -0.737787    -2.819198    -0.786647
H     -0.822406    -1.125890    -2.119898
H     -2.400905    -1.742252    -1.609087
C     -1.349229    -3.575761     0.219524
C      0.470884    -3.268029    -1.322220
C     -0.769487    -4.756382     0.673508
H     -2.285168    -3.231479     0.648803
C      1.052828    -4.453983    -0.874348
H      0.962852    -2.682188    -2.092582
H     -1.257567    -5.334358     1.452270
C      0.434091    -5.200723     0.124728
H      1.990141    -4.791978    -1.305430
H      0.884488    -6.124495     0.474355
H      0.537740    -0.196894     0.321704
N      3.397522     1.322070     0.258576
C      2.099319     1.016133    -0.102028
N      1.407379     1.663209    -0.992175
C      2.045503     2.761594    -1.695845
C      3.017338     3.521734    -0.795303
```

C	4.038867	2.542071	-0.230582
C	3.589493	-0.812934	1.507436
C	2.081516	-0.698337	1.686396
N	1.530020	-0.077775	0.499412
C	4.166202	0.573895	1.250520
H	1.263246	3.431210	-2.064914
H	2.580673	2.394416	-2.586494
H	2.456405	3.984800	0.023117
H	3.532116	4.320869	-1.337659
H	4.786914	2.284584	-0.994258
H	4.584842	2.998656	0.603983
H	5.200060	0.494337	0.893103
H	4.203964	1.143266	2.192582
H	3.796915	-1.471957	0.659350
H	4.061688	-1.246192	2.393689
H	1.853900	-0.126614	2.601065
H	1.622427	-1.682923	1.796076
H	-0.274333	1.436213	-1.296703

57 atoms
ε-CL, structure TS23 in vacuum

O	1.265493	-0.906874	-1.622981
O	1.556172	-1.454585	0.536566
C	1.979560	-0.590728	-0.501421
C	3.477614	-0.688738	-0.833895
H	4.042344	-0.049438	-0.147854
H	3.594733	-0.261099	-1.831828
C	4.045482	-2.116215	-0.805694
H	3.315976	-2.805070	-1.242625
H	4.928009	-2.151412	-1.453540
C	4.465726	-2.583739	0.596846
H	5.190670	-1.863043	0.999074
H	5.004970	-3.534256	0.513263
C	3.319886	-2.757706	1.601506
H	2.714333	-3.629540	1.329059
H	3.736731	-2.965329	2.595421
C	2.372576	-1.564495	1.706872
H	2.901960	-0.625339	1.896518
H	1.676855	-1.716755	2.536694
O	1.636271	0.716114	0.005701
C	1.831017	1.810363	-0.896291
C	0.955146	2.963697	-0.475812
H	1.570878	1.485527	-1.908328
H	2.884031	2.119064	-0.895916
C	1.507646	4.166058	-0.032786
C	-0.438159	2.840104	-0.532594

C	0.690049	5.233115	0.340207
H	2.587801	4.270850	0.022741
C	-1.255749	3.901493	-0.158232
H	-0.873837	1.904247	-0.867585
H	1.135467	6.162794	0.680937
C	-0.694214	5.102584	0.278015
H	-2.335104	3.794695	-0.210589
H	-1.333804	5.930918	0.567153
H	-0.407838	-0.285871	0.846632
N	-3.396957	-1.254694	0.112911
C	-2.083051	-0.883825	-0.087248
N	-1.465303	-0.922889	-1.231226
C	-2.220453	-1.336411	-2.402283
C	-3.245979	-2.416075	-2.061415
C	-4.159651	-1.901024	-0.955622
C	-3.356061	-0.287065	2.398902
C	-1.863503	-0.588268	2.359552
N	-1.402783	-0.392987	0.999900
C	-4.073686	-1.194833	1.407080
H	-1.514560	-1.702077	-3.153348
H	-2.732802	-0.473737	-2.857095
H	-2.719369	-3.312937	-1.719060
H	-3.844224	-2.696718	-2.933702
H	-4.894335	-1.192014	-1.363111
H	-4.729730	-2.727784	-0.514956
H	-5.098224	-0.840310	1.241928
H	-4.157420	-2.210875	1.823104
H	-3.511733	0.762374	2.132898
H	-3.766117	-0.445015	3.400268
H	-1.674496	-1.611221	2.724144
H	-1.309385	0.095156	3.006700
H	0.284854	-0.918780	-1.416487

57 atoms
ε-CL, structure I3 in vacuum

O	-0.824112	-0.887103	1.662637
O	-0.930694	-1.892032	-0.348091
C	-1.647647	-1.101224	0.595140
C	-2.935310	-1.780512	1.098231
H	-3.758115	-1.535504	0.419110
H	-3.168193	-1.312652	2.057138
C	-2.838391	-3.304762	1.266036
H	-1.862913	-3.563844	1.689124
H	-3.585949	-3.620040	2.001984
C	-3.095184	-4.085602	-0.033894
H	-4.073730	-3.782855	-0.430362

H	-3.185056	-5.152765	0.199056
C	-2.034416	-3.913321	-1.129342
H	-1.113278	-4.431610	-0.838540
H	-2.383438	-4.393455	-2.052480
C	-1.665247	-2.464704	-1.437789
H	-2.536271	-1.846781	-1.671404
H	-1.000841	-2.420245	-2.305457
O	-1.938951	0.100123	-0.128596
C	-2.523329	1.163783	0.616486
C	-2.207307	2.481257	-0.051792
H	-2.117855	1.154021	1.634323
H	-3.611529	1.033126	0.688426
C	-3.169811	3.489685	-0.126903
C	-0.931006	2.723560	-0.570671
C	-2.865645	4.724917	-0.697865
H	-4.169142	3.308972	0.260683
C	-0.628637	3.954015	-1.147082
H	-0.187099	1.936268	-0.523352
H	-3.626296	5.497973	-0.750173
C	-1.592856	4.960230	-1.210822
H	0.364577	4.129243	-1.549948
H	-1.354526	5.918510	-1.662097
H	0.947226	-1.318947	-0.686755
N	3.758962	0.081849	0.085007
C	2.413800	-0.216557	0.145871
N	1.588858	0.247517	1.038225
C	2.094408	1.203600	2.009066
C	3.536579	0.894352	2.407190
C	4.400909	0.849743	1.152441
C	3.930153	-1.001254	-2.143523
C	2.763193	-1.858115	-1.668299
N	1.911541	-1.034782	-0.834657
C	4.667742	-0.446618	-0.930376
H	1.441309	1.178207	2.885890
H	2.032585	2.228427	1.610924
H	3.567422	-0.076503	2.912658
H	3.933658	1.640952	3.101737
H	4.612871	1.867617	0.795564
H	5.369265	0.384132	1.371888
H	5.346814	0.358366	-1.236195
H	5.295907	-1.232731	-0.483494
H	3.541073	-0.182831	-2.756062
H	4.624491	-1.581239	-2.757906
H	3.139494	-2.747531	-1.136817
H	2.171744	-2.215174	-2.514583
H	0.048330	-0.485916	1.366881

57 atoms
ε-CL, structure TS3r in vacuum

O	-0.546635	1.351883	-1.708405
O	-0.686858	1.853243	0.480136
C	-1.420569	1.387487	-0.663084
C	-2.603419	2.294705	-1.030600
H	-3.470824	1.996484	-0.435753
H	-2.840523	2.046888	-2.068141
C	-2.344370	3.800461	-0.881342
H	-1.326447	4.031319	-1.211238
H	-3.015530	4.339847	-1.558530
C	-2.588214	4.322699	0.544000
H	-3.615246	4.064210	0.834875
H	-2.545139	5.417934	0.541090
C	-1.618160	3.799924	1.611779
H	-0.628468	4.248251	1.466518
H	-1.962965	4.120534	2.603312
C	-1.431781	2.284103	1.625421
H	-2.380092	1.742912	1.688850
H	-0.838652	1.991421	2.497162
O	-1.954757	0.106681	-0.294835
C	-1.658032	-1.020688	-1.122424
C	-2.169005	-2.254029	-0.420169
H	-0.579212	-1.101799	-1.281944
H	-2.132302	-0.912596	-2.104488
C	-3.192078	-3.029077	-0.966938
C	-1.611586	-2.642788	0.803557
C	-3.647092	-4.175329	-0.314392
H	-3.640392	-2.733344	-1.911352
C	-2.064965	-3.782023	1.459740
H	-0.818430	-2.040429	1.236014
H	-4.443445	-4.767811	-0.754411
C	-3.084935	-4.553979	0.901020
H	-1.622483	-4.072669	2.407926
H	-3.438099	-5.444185	1.412356
H	0.921256	0.776653	0.887444
N	3.741643	-0.546404	0.041685
C	2.460870	-0.057043	-0.098887
N	1.843018	0.094853	-1.232829
C	2.517163	-0.331155	-2.448473
C	4.024815	-0.100311	-2.369917
C	4.571558	-0.806967	-1.135210
C	3.453209	-0.687856	2.504217
C	2.463851	0.454877	2.316818
N	1.778148	0.254185	1.054487
C	4.420273	-0.707937	1.326446
H	2.087254	0.220706	-3.289031

```
H      2.318812    -1.396206    -2.646702
H      4.219814     0.974763    -2.297675
H      4.536782    -0.469391    -3.263751
H      4.634969    -1.890514    -1.308276
H      5.588789    -0.461545    -0.916204
H      4.972325    -1.655103     1.306255
H      5.170249     0.089310     1.444437
H      2.900290    -1.630190     2.555383
H      4.015573    -0.576794     3.435418
H      2.991497     1.421733     2.359717
H      1.717006     0.458867     3.114082
H      0.324776     0.927387    -1.451269
```

```
57 atoms
ε-CL, structure I3r in vacuum
O      0.197167     1.018950     1.793519
O      0.310574     1.684698    -0.352979
C      1.081640     1.448969     0.845090
C      1.805746     2.698941     1.362106
H      2.790311     2.758457     0.890343
H      1.978964     2.508338     2.422965
C      1.042322     4.015642     1.167441
H     -0.020474     3.858147     1.377800
H      1.397747     4.733770     1.914178
C      1.236772     4.643294    -0.223109
H      2.314113     4.759095    -0.401735
H      0.823654     5.658537    -0.222230
C      0.615498     3.866578    -1.391674
H     -0.476984     3.953481    -1.354892
H      0.930756     4.321547    -2.339440
C      0.957831     2.378943    -1.425113
H      2.035682     2.195673    -1.390924
H      0.585249     1.926131    -2.349146
O      2.109815     0.516933     0.545208
C      1.687662    -0.819847     0.294630
C      2.876979    -1.662373    -0.098730
H      0.931663    -0.839641    -0.497571
H      1.219647    -1.227407     1.198088
C      2.686185    -2.810529    -0.873205
C      4.169211    -1.347904     0.329161
C      3.759381    -3.633359    -1.206449
H      1.687654    -3.062058    -1.221542
C      5.245052    -2.166100    -0.009272
H      4.324477    -0.452849     0.919344
H      3.592543    -4.520328    -1.810194
C      5.045136    -3.312772    -0.775266
```

H	6.244112	-1.906062	0.327541
H	5.884539	-3.949005	-1.038125
H	-1.380460	0.756810	-0.780418
N	-3.806208	-1.258221	-0.080987
C	-2.602844	-0.599604	0.058059
N	-1.812065	-0.701281	1.084107
C	-2.182399	-1.617203	2.150204
C	-3.695755	-1.666568	2.352497
C	-4.363356	-2.029688	1.031101
C	-3.963875	-0.538792	-2.452888
C	-3.121153	0.650641	-2.009737
N	-2.197686	0.191043	-0.991415
C	-4.684287	-1.118658	-1.241243
H	-1.682813	-1.293273	3.067403
H	-1.806791	-2.630502	1.936866
H	-4.044047	-0.683239	2.685202
H	-3.977514	-2.393610	3.120161
H	-4.251028	-3.103599	0.825708
H	-5.440038	-1.828070	1.079192
H	-5.094570	-2.106539	-1.482258
H	-5.541061	-0.480307	-0.975396
H	-3.306797	-1.291583	-2.897920
H	-4.698874	-0.245128	-3.207424
H	-3.774275	1.462723	-1.650584
H	-2.540110	1.049793	-2.844396
H	-0.508506	0.407615	1.429868

57 atoms
ε-CL, structure TS3r2 in vacuum

O	-0.315615	0.668220	-1.484586
O	-0.160068	1.117972	0.717505
C	-0.970794	1.300178	-0.459461
C	-1.232311	2.776377	-0.799056
H	-2.096209	3.134079	-0.231402
H	-1.530557	2.770722	-1.849099
C	-0.028361	3.702719	-0.583314
H	0.890166	3.188099	-0.885757
H	-0.126978	4.565565	-1.250419
C	0.092470	4.226334	0.857188
H	-0.849639	4.723621	1.123386
H	0.863251	5.004514	0.897538
C	0.415303	3.164229	1.916346
H	1.455185	2.834529	1.807053
H	0.334317	3.610400	2.915791
C	-0.466110	1.918046	1.864967
H	-1.533448	2.157637	1.879830

H	-0.268877	1.283295	2.734168
O	-2.250657	0.741561	-0.239495
C	-2.293747	-0.678635	-0.119516
C	-3.729960	-1.142290	-0.107569
H	-1.787727	-0.996011	0.800083
H	-1.753634	-1.121702	-0.962312
C	-4.080934	-2.306427	0.581661
C	-4.721879	-0.454176	-0.811596
C	-5.390066	-2.782407	0.560196
H	-3.322845	-2.846350	1.143441
C	-6.032934	-0.924141	-0.827996
H	-4.458478	0.457024	-1.335159
H	-5.644118	-3.688327	1.102234
C	-6.372360	-2.090986	-0.145404
H	-6.793083	-0.376088	-1.376624
H	-7.394745	-2.455726	-0.159198
H	1.256917	-0.248753	0.984450
N	4.030702	-1.417459	-0.167942
C	2.783345	-0.829240	-0.171817
N	2.211192	-0.301206	-1.210662
C	2.896118	-0.377714	-2.489865
C	4.411950	-0.282343	-2.326841
C	4.879152	-1.363647	-1.358978
C	3.647945	-2.289454	2.123677
C	2.719677	-1.092667	2.286914
N	2.079592	-0.843090	1.010661
C	4.657032	-1.992503	1.020508
H	2.525186	0.432059	-3.124143
H	2.639544	-1.314718	-3.008465
H	4.668505	0.705079	-1.928705
H	4.928654	-0.395939	-3.284666
H	4.884092	-2.345669	-1.852713
H	5.908049	-1.167353	-1.034988
H	5.173661	-2.913044	0.724279
H	5.431493	-1.305852	1.396565
H	3.050602	-3.167504	1.861658
H	4.178671	-2.508422	3.054341
H	3.290005	-0.222191	2.651489
H	1.941961	-1.301067	3.025693
H	0.599171	0.330825	-1.250405

57 atoms
ε-CL, structure I3r2 in vacuum

O	0.280094	0.249595	1.368137
O	0.368795	0.446976	-0.867716
C	0.924040	0.942204	0.374885

C	0.808886	2.473174	0.513144
H	1.680719	2.936235	0.041216
H	0.901453	2.666834	1.583786
C	-0.479839	3.096054	-0.043376
H	-1.337599	2.455275	0.187259
H	-0.656438	4.042993	0.478376
C	-0.417619	3.391281	-1.551158
H	0.457552	4.026170	-1.743748
H	-1.290039	3.989353	-1.838858
C	-0.350421	2.156833	-2.459437
H	-1.318043	1.641329	-2.456422
H	-0.172890	2.476099	-3.494387
C	0.717148	1.134736	-2.074106
H	1.708621	1.586692	-1.972526
H	0.794830	0.363682	-2.846199
O	2.298156	0.665418	0.424120
C	2.649312	-0.714161	0.533260
C	4.146074	-0.866552	0.406411
H	2.141392	-1.290367	-0.247030
H	2.304349	-1.097479	1.498264
C	4.682883	-2.108428	0.052132
C	5.019347	0.190337	0.673068
C	6.060370	-2.294832	-0.026877
H	4.015571	-2.938507	-0.166365
C	6.398493	0.007060	0.588412
H	4.609613	1.156946	0.939318
H	6.458613	-3.265991	-0.304872
C	6.925015	-1.234837	0.240912
H	7.064054	0.839725	0.795634
H	7.999419	-1.375634	0.175359
H	-1.268340	-0.686063	-0.776485
N	-4.293728	-1.090551	0.297110
C	-2.985549	-0.655061	0.279431
N	-2.451512	0.132593	1.168213
C	-3.263373	0.534039	2.304201
C	-4.728291	0.722957	1.914579
C	-5.243301	-0.561831	1.276534
C	-3.792435	-2.759301	-1.466358
C	-2.704730	-1.788724	-1.908852
N	-2.187209	-1.116500	-0.735326
C	-4.863973	-1.991240	-0.702209
H	-2.852168	1.463213	2.708986
H	-3.191702	-0.209842	3.113352
H	-4.805776	1.548166	1.198848
H	-5.346736	0.978362	2.780393
H	-5.438751	-1.321712	2.046403
H	-6.195270	-0.378972	0.763901

H	-5.534762	-2.689702	-0.188362
H	-5.487544	-1.416905	-1.404904
H	-3.347573	-3.524347	-0.823372
H	-4.245391	-3.262449	-2.325095
H	-3.112960	-1.082699	-2.650578
H	-1.879839	-2.319238	-2.390339
H	-0.715799	0.271869	1.264549

57 atoms
ε-CL, structure TS34 in vacuum

O	-0.147106	0.531611	-1.646804
O	-0.176173	0.985753	0.784714
C	-0.922041	1.219360	-0.951747
C	-0.968795	2.737985	-1.074830
H	-1.799444	3.126299	-0.480918
H	-1.237636	2.911984	-2.123284
C	0.334360	3.480546	-0.739468
H	1.186247	2.816808	-0.916942
H	0.449064	4.315058	-1.440843
C	0.387626	4.065965	0.683060
H	-0.525356	4.655710	0.843276
H	1.214219	4.786108	0.734400
C	0.544480	3.066415	1.837243
H	1.560813	2.650243	1.823218
H	0.447242	3.611028	2.787268
C	-0.437661	1.884678	1.819190
H	-1.473998	2.258486	1.756381
H	-0.375127	1.366602	2.793908
O	-2.203404	0.763543	-0.706385
C	-2.342428	-0.651809	-0.686662
C	-3.768412	-1.026973	-0.364619
H	-1.659819	-1.051526	0.072151
H	-2.039648	-1.069299	-1.651280
C	-4.226192	-2.311379	-0.677143
C	-4.642338	-0.141010	0.269309
C	-5.521115	-2.707762	-0.354356
H	-3.561879	-3.008052	-1.182837
C	-5.941713	-0.533486	0.586910
H	-4.297999	0.859201	0.501092
H	-5.858509	-3.708633	-0.606953
C	-6.386081	-1.817466	0.280150
H	-6.609961	0.169350	1.075730
H	-7.398647	-2.121045	0.527690
H	1.038801	0.072932	0.905275
N	3.902401	-1.415435	0.130429
C	2.729432	-0.735377	-0.005037

N	2.385242	-0.215419	-1.190104
C	3.148872	-0.452857	-2.402724
C	4.630702	-0.515987	-2.058270
C	4.851178	-1.567437	-0.976936
C	3.057776	-2.319184	2.269123
C	2.218400	-1.051383	2.360871
N	1.908409	-0.565375	1.026988
C	4.278001	-2.052072	1.395904
H	2.933436	0.363201	-3.094264
H	2.829524	-1.383637	-2.891958
H	4.962378	0.463019	-1.699639
H	5.226476	-0.766958	-2.939343
H	4.761324	-2.577724	-1.398870
H	5.861256	-1.481775	-0.563781
H	4.787556	-2.990625	1.156641
H	5.001962	-1.418925	1.926574
H	2.458030	-3.123100	1.831626
H	3.379699	-2.646870	3.260793
H	2.750946	-0.285085	2.941169
H	1.272330	-1.240014	2.871837
H	1.413517	0.148982	-1.301300

57 atoms
ε-CL, structure I4 in vacuum

O	0.008236	1.684999	-1.615703
O	-0.504028	1.249286	1.419282
C	-1.062616	2.012990	-1.147113
C	-1.411934	3.392120	-0.634972
H	-2.052454	3.269388	0.239902
H	-2.046921	3.841853	-1.408830
C	-0.207038	4.300593	-0.352079
H	0.618187	4.007293	-1.007878
H	-0.477825	5.320128	-0.647030
C	0.288176	4.374357	1.104247
H	-0.557188	4.623590	1.760386
H	0.957474	5.241410	1.155191
C	1.048695	3.170990	1.698099
H	1.714103	2.729843	0.946877
H	1.704176	3.556194	2.491066
C	0.206064	2.060133	2.337702
H	-0.532402	2.508023	3.013804
H	0.866831	1.435226	2.955478
O	-2.132315	1.207226	-1.104505
C	-1.934945	-0.186893	-1.443595
C	-3.016199	-0.992248	-0.774962
H	-0.945208	-0.487707	-1.096220

H	-1.966039	-0.292941	-2.531146
C	-3.846152	-1.834713	-1.514844
C	-3.179505	-0.920172	0.614558
C	-4.821577	-2.606128	-0.882616
H	-3.733307	-1.889087	-2.594309
C	-4.157532	-1.684030	1.243422
H	-2.539268	-0.257718	1.189420
H	-5.460927	-3.257433	-1.470495
C	-4.979493	-2.531062	0.497994
H	-4.279936	-1.619785	2.320324
H	-5.740914	-3.126229	0.992609
H	0.095422	0.519055	1.121166
N	3.203017	-1.882900	0.082370
C	2.220166	-0.916507	0.036391
N	2.406624	0.122724	-0.846388
C	3.355785	0.040228	-1.940674
C	4.661024	-0.521470	-1.394551
C	4.391077	-1.884867	-0.769974
C	1.577526	-3.278660	1.304472
C	0.997109	-1.949007	1.779788
N	1.156979	-0.898756	0.786383
C	3.036900	-3.072345	0.918182
H	3.495712	1.045488	-2.343553
H	2.989091	-0.591872	-2.765779
H	5.057379	0.166989	-0.642475
H	5.409803	-0.623774	-2.184850
H	4.272689	-2.642080	-1.560420
H	5.247376	-2.199693	-0.161762
H	3.409665	-3.936351	0.355649
H	3.664611	-2.984142	1.816352
H	1.010635	-3.628455	0.435351
H	1.504098	-4.049510	2.077588
H	1.478031	-1.659547	2.728064
H	-0.069131	-2.052728	1.998436
H	1.571558	0.675156	-1.008924

57 atoms
ε-CL, structure I5 in vacuum

O	-4.153405	1.386211	-1.764408
O	3.168674	-0.805456	-1.444127
C	-4.181539	0.550517	-0.895482
C	-2.988454	-0.211526	-0.356551
H	-3.226637	-1.280269	-0.395505
H	-2.903346	0.022935	0.711406
C	-1.685454	0.096409	-1.092325
H	-1.801870	-0.150110	-2.152888

H	-1.498977	1.174515	-1.059886
C	-0.486380	-0.659212	-0.511416
H	-0.687575	-1.738456	-0.537719
H	-0.373832	-0.401530	0.550417
C	0.822695	-0.367873	-1.249913
H	0.732222	-0.651302	-2.304634
H	1.028200	0.709281	-1.238162
C	2.021509	-1.099040	-0.663180
H	1.825506	-2.182552	-0.660049
H	2.173688	-0.796675	0.384627
O	-5.315670	0.173453	-0.261597
C	-6.530085	0.848527	-0.686765
C	-7.671420	0.307976	0.126480
H	-6.669272	0.672031	-1.755094
H	-6.397663	1.922758	-0.543169
C	-7.999004	0.880105	1.358888
C	-8.410082	-0.788771	-0.325398
C	-9.043929	0.368999	2.123947
H	-7.430342	1.731941	1.720699
C	-9.456368	-1.303107	0.436202
H	-8.163088	-1.242613	-1.280847
H	-9.289661	0.824964	3.077722
C	-9.775303	-0.724279	1.663017
H	-10.023947	-2.153301	0.071557
H	-10.592431	-1.121824	2.256519
H	3.960394	-1.207489	-1.006745
N	7.138257	0.268183	0.776551
C	5.934371	-0.045165	0.179102
N	5.137317	1.011015	-0.204675
C	5.659939	2.352307	-0.370023
C	6.523114	2.673682	0.843439
C	7.630502	1.632484	0.958154
C	7.773624	-2.085635	0.387088
C	6.273834	-2.362299	0.484983
N	5.484660	-1.249617	-0.011649
C	8.090355	-0.787789	1.121272
H	4.815566	3.041514	-0.443110
H	6.251025	2.463584	-1.293841
H	5.894950	2.656750	1.738805
H	6.967041	3.669794	0.762106
H	8.416021	1.839626	0.214720
H	8.108806	1.696443	1.942835
H	9.096288	-0.438023	0.860403
H	8.083709	-0.949671	2.208590
H	8.050866	-1.989657	-0.667949
H	8.364729	-2.903467	0.810628
H	6.010129	-2.586946	1.531042

```
H      6.013052    -3.254253    -0.092042
H      4.336462     0.723420    -0.760065


39 atoms
complex BnO-TBD in toluene
N     -3.208356     0.586107     0.216068
C     -1.991466    -0.004781    -0.030156
N     -1.975904    -1.378001    -0.155718
C     -3.178630    -2.139609    -0.441518
C     -4.280639    -1.639517     0.483110
C     -4.476374    -0.143811     0.266753
C     -2.125393     2.726365    -0.372715
C     -0.843577     2.059306     0.123114
N     -0.854440     0.624739    -0.112941
C     -3.325408     2.045162     0.274451
H     -2.964653    -3.195171    -0.261125
H     -3.493867    -2.044545    -1.492549
H     -3.991883    -1.836874     1.519562
H     -5.222295    -2.160595     0.291693
H     -5.032705     0.030232    -0.666331
H     -5.080949     0.279701     1.076450
H     -4.249849     2.331243    -0.239281
H     -3.431283     2.363254     1.320615
H     -2.185591     2.624052    -1.461356
H     -2.138363     3.795335    -0.140548
H     -0.710984     2.272211     1.195548
H      0.029081     2.483916    -0.380958
H     -1.087991    -1.734022    -0.490760
O      0.962042    -1.252785    -0.880184
C      1.861224    -1.523619     0.177342
C      3.140548    -0.703709     0.132146
H      2.119395    -2.586927     0.107436
H      1.374899    -1.379499     1.152353
C      3.597441    -0.153034    -1.067270
C      3.904107    -0.520723     1.289402
C      4.791889     0.564962    -1.109450
H      3.000222    -0.285645    -1.962293
C      5.100891     0.191668     1.249934
H      3.556325    -0.934268     2.233049
H      5.131761     0.989990    -2.049197
C      5.549432     0.738100     0.047756
H      5.679361     0.327479     2.158782
H      6.478803     1.298119     0.015245
H      0.450867    -0.426172    -0.654126
```

18 atoms
ε-CL in toluene

O	2.500347	-0.086963	-0.407845
O	0.776958	1.237257	-0.076844
C	1.375078	0.023543	0.010100
C	0.596045	-1.139396	0.599986
H	0.285025	-0.904627	1.624546
H	1.308796	-1.961211	0.662562
C	-0.630731	-1.563635	-0.234891
H	-0.352219	-1.600850	-1.294183
H	-0.888094	-2.589263	0.045654
C	-1.865371	-0.677682	-0.040378
H	-2.197791	-0.758891	1.002729
H	-2.685549	-1.070431	-0.650216
C	-1.655398	0.802098	-0.377746
H	-1.432796	0.930544	-1.443123
H	-2.588802	1.345157	-0.191667
C	-0.555397	1.489287	0.424587
H	-0.605456	1.230087	1.487139
H	-0.646913	2.571839	0.344125

57 atoms
ε-CL, structure I1 in toluene

O	2.281395	-0.994730	-1.689467
O	2.702861	-0.799738	0.452810
C	2.777569	-0.327951	-0.804973
C	3.512296	0.968195	-1.074302
H	2.934848	1.782577	-0.625198
H	3.471513	1.105919	-2.154854
C	4.973841	1.010597	-0.584820
H	5.481086	0.076835	-0.854628
H	5.486118	1.802026	-1.140433
C	5.133661	1.286087	0.914001
H	4.697652	2.267669	1.139821
H	6.200001	1.365493	1.151049
C	4.494447	0.236705	1.828604
H	5.000226	-0.729799	1.719439
H	4.633317	0.539612	2.872867
C	3.001957	0.024888	1.606772
H	2.447323	0.960987	1.517721
H	2.571173	-0.542849	2.430755
O	0.385866	1.269036	0.013580
C	-0.278311	1.892972	-1.062677
C	-1.337780	2.904091	-0.648686
H	-0.735190	1.143798	-1.723055
H	0.480999	2.411706	-1.661986

C	-1.400413	3.391230	0.657686
C	-2.250655	3.391333	-1.590719
C	-2.353801	4.344554	1.017055
H	-0.696470	3.008416	1.387453
C	-3.201750	4.345204	-1.236760
H	-2.219652	3.017182	-2.611448
H	-2.389912	4.711561	2.038588
C	-3.256733	4.826558	0.071782
H	-3.904299	4.709812	-1.980198
H	-3.999245	5.567677	0.350791
H	-0.122666	0.443284	0.260070
N	-2.182728	-3.027674	0.336600
C	-1.186744	-2.102169	0.101273
N	-0.167884	-2.490607	-0.720419
C	-0.164881	-3.717715	-1.490488
C	-0.786368	-4.824628	-0.648770
C	-2.176486	-4.384465	-0.209322
C	-3.548050	-1.139824	1.162997
C	-2.195368	-0.571052	1.585614
N	-1.152022	-0.908036	0.628864
C	-3.421693	-2.651002	1.020147
H	0.870376	-3.946543	-1.749763
H	-0.719103	-3.609655	-2.435675
H	-0.155247	-5.010628	0.225441
H	-0.860553	-5.756976	-1.215067
H	-2.873497	-4.442236	-1.059188
H	-2.564961	-5.061143	0.560642
H	-4.265880	-3.054803	0.447804
H	-3.450015	-3.133042	2.007214
H	-3.837178	-0.694236	0.205736
H	-4.332926	-0.902806	1.887523
H	-1.941756	-0.945557	2.591096
H	-2.247088	0.517977	1.666683
H	0.590043	-1.836233	-0.866388

57 atoms
ε-CL, structure TS12 in toluene

O	1.685589	-0.767415	-1.651566
O	2.183261	-0.933985	0.502307
C	2.175230	-0.176173	-0.666522
C	3.370491	0.758473	-0.877285
H	3.291911	1.640682	-0.239228
H	3.293989	1.099648	-1.910463
C	4.730812	0.070607	-0.649857
H	4.704114	-0.947960	-1.053833
H	5.490988	0.606827	-1.228467

C	5.173363	0.055079	0.820828
H	5.223223	1.093327	1.175415
H	6.195599	-0.335296	0.887605
C	4.273838	-0.750855	1.766482
H	4.375782	-1.822864	1.559580
H	4.612784	-0.600926	2.799424
C	2.787364	-0.405916	1.688492
H	2.603569	0.668925	1.754702
H	2.254091	-0.883267	2.514729
O	0.881840	1.077995	-0.075414
C	0.426691	1.882563	-1.117704
C	-0.663552	2.852090	-0.686167
H	0.051125	1.281257	-1.963898
H	1.253952	2.488718	-1.533975
C	-0.683854	3.372912	0.612073
C	-1.647962	3.274720	-1.585875
C	-1.655348	4.295738	0.997869
H	0.071885	3.038638	1.314019
C	-2.620679	4.198597	-1.205734
H	-1.653727	2.873346	-2.596350
H	-1.651711	4.692125	2.009343
C	-2.628231	4.713849	0.089976
H	-3.376643	4.512161	-1.919858
H	-3.385467	5.431999	0.389389
H	-0.309201	-0.009091	0.330028
N	-2.469305	-2.501337	0.331657
C	-1.387300	-1.753431	-0.009211
N	-0.575833	-2.154205	-0.992800
C	-0.813124	-3.361044	-1.769534
C	-1.468576	-4.413169	-0.884548
C	-2.722969	-3.822807	-0.253810
C	-3.384456	-0.532804	1.524040
C	-1.929667	-0.140886	1.745550
N	-1.124329	-0.610960	0.628362
C	-3.468277	-2.037083	1.301669
H	0.151890	-3.701825	-2.147081
H	-1.446670	-3.145553	-2.639983
H	-0.765784	-4.720868	-0.104780
H	-1.734487	-5.300676	-1.463539
H	-3.525635	-3.739553	-0.997950
H	-3.091616	-4.473590	0.544994
H	-4.455670	-2.313501	0.919112
H	-3.326639	-2.575249	2.247742
H	-3.773347	-0.000133	0.651470
H	-3.999262	-0.256539	2.383904
H	-1.561854	-0.558911	2.692271
H	-1.813450	0.942043	1.797665

H 0.294251 -1.613891 -1.189535

57 atoms
ε-CL, structure I2 in toluene
O 1.089296 -1.402810 -1.549465
O 1.474279 -1.613334 0.648541
C 1.824608 -0.903371 -0.513095
C 3.317935 -0.981094 -0.877260
H 3.865099 -0.201246 -0.338118
H 3.390357 -0.741154 -1.939661
C 3.967215 -2.348514 -0.608356
H 3.274940 -3.145397 -0.898099
H 4.839892 -2.447878 -1.262653
C 4.436797 -2.538341 0.843116
H 5.118170 -1.714847 1.096324
H 5.036077 -3.453466 0.909220
C 3.319252 -2.606996 1.891445
H 2.769169 -3.549373 1.789065
H 3.761786 -2.611828 2.895553
C 2.300181 -1.473684 1.810473
H 2.774806 -0.487696 1.829360
H 1.617779 -1.521653 2.662747
O 1.433879 0.467481 -0.200773
C 1.538106 1.411436 -1.275723
C 1.049523 2.752624 -0.788983
H 0.947748 1.066526 -2.128311
H 2.583024 1.490366 -1.598937
C 1.767304 3.455077 0.186023
C -0.125831 3.314450 -1.292446
C 1.323470 4.692870 0.642299
H 2.680309 3.026136 0.587906
C -0.571718 4.557367 -0.842022
H -0.698267 2.774105 -2.040060
H 1.892684 5.227590 1.396299
C 0.151656 5.248941 0.126734
H -1.484453 4.982814 -1.247239
H -0.192811 6.216449 0.478094
H -0.551730 0.262157 0.320082
N -3.523250 -1.014148 0.252973
C -2.210917 -0.807255 -0.112363
N -1.575527 -1.493751 -1.018888
C -2.304591 -2.527495 -1.735857
C -3.335513 -3.217034 -0.844865
C -4.269054 -2.163831 -0.261696
C -3.531941 1.098619 1.557080
C -2.036422 0.859216 1.712504

N	-1.549921	0.229486	0.499336
C	-4.221467	-0.229547	1.271720
H	-1.581009	-3.254784	-2.115750
H	-2.808594	-2.105277	-2.619966
H	-2.816097	-3.740764	-0.035619
H	-3.916709	-3.959246	-1.400199
H	-4.989066	-1.825648	-1.019956
H	-4.853670	-2.586041	0.563652
H	-5.247051	-0.057858	0.925293
H	-4.296732	-0.819153	2.197811
H	-3.696922	1.796192	0.730762
H	-3.956698	1.542507	2.461405
H	-1.843999	0.244423	2.606089
H	-1.498425	1.800186	1.842867
H	0.110089	-1.428592	-1.300686

57 atoms
ε-CL, structure TS23 in toluene

O	1.116888	-1.093257	-1.612211
O	1.353829	-1.609052	0.560147
C	1.867247	-0.826543	-0.498538
C	3.345315	-1.096026	-0.825299
H	3.976551	-0.502440	-0.156681
H	3.510292	-0.713039	-1.834590
C	3.756455	-2.575038	-0.752239
H	2.957734	-3.196299	-1.169503
H	4.629423	-2.723396	-1.396726
C	4.124931	-3.042784	0.664717
H	4.921883	-2.391074	1.047427
H	4.559783	-4.047208	0.610251
C	2.966906	-3.064129	1.670367
H	2.272521	-3.875188	1.422762
H	3.359066	-3.284271	2.671256
C	2.153676	-1.773978	1.738324
H	2.782147	-0.893145	1.902074
H	1.444285	-1.824898	2.568262
O	1.668701	0.526133	-0.031658
C	1.993729	1.565150	-0.962857
C	1.320656	2.843573	-0.531098
H	1.648799	1.269536	-1.958155
H	3.079933	1.709868	-1.006500
C	2.066860	3.938965	-0.092565
C	-0.075101	2.948028	-0.567624
C	1.437493	5.122444	0.295435
H	3.150307	3.867980	-0.053510
C	-0.706025	4.125809	-0.178602

H	-0.662131	2.097268	-0.898205
H	2.032037	5.966106	0.631952
C	0.049000	5.217984	0.253077
H	-1.788897	4.194781	-0.214780
H	-0.443993	6.137197	0.553838
H	-0.482640	-0.144943	0.812071
N	-3.538968	-0.896320	0.118387
C	-2.201608	-0.650261	-0.094292
N	-1.584352	-0.812718	-1.230359
C	-2.369754	-1.234423	-2.380460
C	-3.489273	-2.194002	-1.982229
C	-4.355435	-1.530643	-0.918827
C	-3.419022	0.177468	2.355836
C	-1.955420	-0.241972	2.334178
N	-1.483113	-0.148205	0.964902
C	-4.208442	-0.716568	1.407646
H	-1.696318	-1.709796	-3.099509
H	-2.801328	-0.361501	-2.895172
H	-3.048174	-3.112419	-1.581094
H	-4.107298	-2.471695	-2.841218
H	-5.017324	-0.780881	-1.373763
H	-5.001738	-2.271720	-0.435041
H	-5.199785	-0.288642	1.220080
H	-4.372986	-1.700973	1.870632
H	-3.493196	1.222460	2.041402
H	-3.837558	0.099039	3.362639
H	-1.846454	-1.258390	2.744547
H	-1.347157	0.424913	2.948633
H	0.138779	-0.985429	-1.403800

57 atoms
ε-CL, structure I3 in toluene

O	0.821251	-0.892546	-1.647857
O	0.928376	-1.892016	0.363498
C	1.646476	-1.105025	-0.578032
C	2.937231	-1.779390	-1.077135
H	3.753393	-1.544583	-0.386859
H	3.182504	-1.299344	-2.026928
C	2.840471	-3.301410	-1.265396
H	1.867928	-3.555912	-1.698467
H	3.592815	-3.607077	-2.000258
C	3.087038	-4.098690	0.026177
H	4.064564	-3.804730	0.431193
H	3.172756	-5.163232	-0.219309
C	2.021123	-3.933786	1.117441
H	1.098117	-4.442576	0.816030

H	2.362140	-4.427235	2.036156
C	1.660405	-2.487717	1.445381
H	2.536111	-1.879987	1.688100
H	0.994327	-2.451551	2.311420
O	1.932651	0.103094	0.140455
C	2.530371	1.157814	-0.609742
C	2.213437	2.483274	0.041985
H	2.133929	1.140376	-1.630721
H	3.617858	1.021000	-0.669967
C	3.189660	3.476103	0.148617
C	0.922923	2.749250	0.513382
C	2.885258	4.718785	0.704612
H	4.198813	3.277782	-0.202642
C	0.619762	3.986713	1.075089
H	0.166869	1.975324	0.439900
H	3.656063	5.479455	0.781582
C	1.598402	4.977194	1.170555
H	-0.384483	4.180161	1.440072
H	1.359845	5.940998	1.609481
H	-0.943787	-1.271279	0.737418
N	-3.758809	0.080702	-0.088301
C	-2.414318	-0.207054	-0.132809
N	-1.588610	0.226469	-1.044068
C	-2.102808	1.136434	-2.055963
C	-3.541268	0.798001	-2.442355
C	-4.406156	0.799761	-1.187740
C	-3.931173	-0.918595	2.180701
C	-2.751444	-1.778493	1.746070
N	-1.904199	-0.975841	0.883830
C	-4.668245	-0.420280	0.943496
H	-1.448006	1.081410	-2.930394
H	-2.053127	2.177846	-1.701295
H	-3.564117	-0.193278	-2.907020
H	-3.942827	1.512047	-3.167468
H	-4.625180	1.829241	-0.872654
H	-5.370034	0.317755	-1.386950
H	-5.357317	0.388247	1.212969
H	-5.282458	-1.229737	0.521871
H	-3.557569	-0.072898	2.765185
H	-4.621709	-1.484290	2.811727
H	-3.112292	-2.690992	1.245479
H	-2.159140	-2.094435	2.607566
H	-0.055732	-0.493404	-1.350226

57 atoms
ε-CL, structure TS3r in toluene

O	-0.496618	1.355371	-1.686374
O	-0.632498	1.861699	0.499009
C	-1.374286	1.418792	-0.643476
C	-2.532153	2.356114	-1.015389
H	-3.407264	2.083158	-0.419935
H	-2.776937	2.112512	-2.052341
C	-2.237249	3.855787	-0.868108
H	-1.214552	4.064799	-1.198596
H	-2.896470	4.408977	-1.545708
C	-2.467325	4.385360	0.556723
H	-3.499956	4.151860	0.848364
H	-2.397337	5.479062	0.551743
C	-1.509472	3.840391	1.624196
H	-0.508538	4.262422	1.477118
H	-1.844294	4.172375	2.615048
C	-1.364605	2.320539	1.644502
H	-2.328304	1.807896	1.711065
H	-0.777793	2.014693	2.515017
O	-1.944152	0.148783	-0.279514
C	-1.686548	-0.980166	-1.120586
C	-2.248040	-2.199991	-0.433299
H	-0.611062	-1.099677	-1.276405
H	-2.153710	-0.842921	-2.102150
C	-3.348066	-2.883901	-0.953321
C	-1.666893	-2.663899	0.753070
C	-3.856025	-4.013777	-0.310561
H	-3.813867	-2.530224	-1.868786
C	-2.172129	-3.787540	1.399554
H	-0.813005	-2.134462	1.165198
H	-4.711035	-4.535417	-0.729369
C	-3.269422	-4.467691	0.867770
H	-1.709731	-4.137404	2.317533
H	-3.662788	-5.345667	1.370559
H	0.950109	0.709170	0.915067
N	3.744153	-0.632510	0.029563
C	2.471736	-0.127121	-0.093612
N	1.849110	0.058057	-1.223289
C	2.514681	-0.351265	-2.451212
C	4.025037	-0.141132	-2.374097
C	4.566803	-0.880225	-1.156884
C	3.472877	-0.813171	2.493117
C	2.489706	0.338273	2.332635
N	1.793961	0.163733	1.068952
C	4.431353	-0.819933	1.308697
H	2.088933	0.222776	-3.279148

H	2.303213	-1.409522	-2.670369
H	4.235253	0.929495	-2.281435
H	4.527538	-0.499427	-3.277297
H	4.614218	-1.960381	-1.351103
H	5.588286	-0.552712	-0.933840
H	4.976043	-1.769846	1.267021
H	5.185919	-0.029140	1.432163
H	2.915817	-1.753587	2.534867
H	4.042749	-0.719205	3.421156
H	3.022593	1.300786	2.385979
H	1.747149	0.333416	3.133416
H	0.364512	0.901742	-1.424693

57 atoms
ε-CL, structure I3r in toluene

O	0.232925	1.026769	1.762902
O	0.281712	1.725859	-0.373608
C	1.088050	1.471520	0.791002
C	1.836291	2.709500	1.304145
H	2.802901	2.774313	0.797481
H	2.049025	2.501351	2.354744
C	1.074654	4.034158	1.160567
H	0.018875	3.882182	1.408145
H	1.463902	4.736396	1.905375
C	1.220499	4.683823	-0.225625
H	2.290970	4.797330	-0.442161
H	0.812325	5.700332	-0.192066
C	0.552106	3.928935	-1.382125
H	-0.537890	4.016503	-1.302385
H	0.832047	4.399196	-2.333141
C	0.890734	2.442532	-1.456400
H	1.968966	2.258808	-1.465074
H	0.482360	2.007555	-2.373203
O	2.104586	0.536592	0.449852
C	1.665012	-0.787118	0.152744
C	2.860647	-1.656950	-0.150416
H	0.975947	-0.778831	-0.698371
H	1.114623	-1.188228	1.010881
C	4.079793	-1.469249	0.508298
C	2.749037	-2.702223	-1.071737
C	5.160153	-2.310545	0.252038
H	4.178091	-0.652762	1.214152
C	3.826271	-3.550262	-1.323815
H	1.811136	-2.853820	-1.599309
H	6.101370	-2.149394	0.768785
C	5.037310	-3.356303	-0.662369

H	3.721547	-4.356396	-2.043475
H	5.879816	-4.011289	-0.860882
H	-1.382540	0.726508	-0.803956
N	-3.781806	-1.290217	-0.041282
C	-2.591453	-0.611749	0.078526
N	-1.810077	-0.652052	1.119613
C	-2.183430	-1.522628	2.224222
C	-3.698078	-1.583347	2.409885
C	-4.342508	-2.018533	1.099392
C	-3.926221	-0.683643	-2.446787
C	-3.098743	0.533119	-2.053735
N	-2.179902	0.130569	-1.004110
C	-4.652159	-1.212507	-1.215748
H	-1.700144	-1.150242	3.131899
H	-1.792958	-2.539849	2.063530
H	-4.065122	-0.590945	2.691751
H	-3.978537	-2.277898	3.207150
H	-4.210670	-3.098158	0.945046
H	-5.421822	-1.831060	1.123436
H	-5.050530	-2.214302	-1.411953
H	-5.514913	-0.570117	-0.985019
H	-3.259947	-1.450779	-2.851979
H	-4.657217	-0.431409	-3.219398
H	-3.761114	1.354405	-1.737460
H	-2.512132	0.897605	-2.899892
H	-0.497446	0.429947	1.412254

57 atoms
ε-CL, structure TS3r2 in toluene

O	0.389340	0.610239	1.411933
O	0.117199	1.195048	-0.743308
C	0.981955	1.319201	0.395208
C	1.243921	2.773586	0.817018
H	2.062786	3.184519	0.219753
H	1.611195	2.706935	1.842980
C	0.016096	3.690997	0.741565
H	-0.874689	3.142885	1.067757
H	0.147943	4.509421	1.456943
C	-0.205733	4.305031	-0.650100
H	0.709099	4.837389	-0.941882
H	-0.990212	5.067801	-0.588973
C	-0.579261	3.307682	-1.754048
H	-1.602340	2.945758	-1.598929
H	-0.574893	3.820435	-2.724047
C	0.328831	2.083825	-1.848814
H	1.387260	2.352182	-1.916407

H	0.085572	1.504930	-2.744008
O	2.260643	0.793918	0.082430
C	2.305005	-0.605587	-0.194585
C	3.720972	-1.108068	-0.048685
H	1.937722	-0.801366	-1.208476
H	1.643093	-1.125474	0.505181
C	4.563953	-0.610936	0.950272
C	4.198966	-2.116910	-0.889610
C	5.852345	-1.116432	1.106319
H	4.205070	0.181600	1.596572
C	5.485586	-2.629827	-0.730762
H	3.560244	-2.505070	-1.678668
H	6.495614	-0.717992	1.885012
C	6.317772	-2.129913	0.268645
H	5.839992	-3.413107	-1.393799
H	7.322188	-2.522859	0.391156
H	-1.270601	-0.215049	-1.028724
N	-3.965515	-1.483502	0.191766
C	-2.731054	-0.877164	0.167022
N	-2.121863	-0.379094	1.203737
C	-2.754715	-0.517509	2.506467
C	-4.276853	-0.443307	2.408595
C	-4.764210	-1.494988	1.419262
C	-3.672828	-2.253228	-2.150764
C	-2.766666	-1.038733	-2.302037
N	-2.074583	-0.833889	-1.042186
C	-4.636480	-2.017403	-0.994179
H	-2.372631	0.273564	3.157883
H	-2.463435	-1.469396	2.977329
H	-4.566974	0.553816	2.060822
H	-4.750376	-0.604079	3.381538
H	-4.728660	-2.495458	1.871647
H	-5.808437	-1.307406	1.145422
H	-5.127482	-2.955991	-0.713973
H	-5.433490	-1.325264	-1.304619
H	-3.055968	-3.134942	-1.954441
H	-4.240962	-2.437440	-3.066282
H	-3.361035	-0.160707	-2.601870
H	-2.018101	-1.204565	-3.080171
H	-0.536820	0.274787	1.202900

57 atoms
ε-CL, structure I3r2 in toluene

O	0.520340	-0.085759	1.056808
O	0.235932	0.910375	-0.935736
C	0.987949	0.958731	0.293353

C	0.897692	2.320121	1.009291
H	1.662918	2.986634	0.600715
H	1.187515	2.117585	2.042401
C	-0.476844	3.002842	0.956772
H	-1.271066	2.257629	1.073693
H	-0.559542	3.675565	1.817102
C	-0.701158	3.832472	-0.317917
H	0.116014	4.560756	-0.404906
H	-1.618428	4.422320	-0.208716
C	-0.792074	3.023929	-1.618151
H	-1.734870	2.465194	-1.643865
H	-0.815996	3.711614	-2.472814
C	0.341904	2.024007	-1.832650
H	1.327641	2.489568	-1.736016
H	0.282532	1.599653	-2.838644
O	2.357275	0.769800	0.031297
C	2.712111	-0.478608	-0.578620
C	4.128420	-0.834558	-0.200098
H	2.617548	-0.396706	-1.666602
H	2.018533	-1.249463	-0.235046
C	4.539506	-0.782688	1.136711
C	5.043434	-1.253604	-1.168175
C	5.833911	-1.147586	1.494417
H	3.836264	-0.449093	1.891952
C	6.340130	-1.625816	-0.812255
H	4.742126	-1.287492	-2.211714
H	6.138663	-1.101655	2.535493
C	6.739274	-1.572777	0.520756
H	7.038801	-1.948486	-1.578036
H	7.748889	-1.856834	0.800589
H	-1.342180	-0.327899	-1.092067
N	-4.139554	-1.312203	0.184742
C	-2.853873	-0.826520	0.138204
N	-2.179380	-0.399945	1.169995
C	-2.797237	-0.501721	2.482767
C	-4.306135	-0.275207	2.418809
C	-4.914828	-1.257679	1.425829
C	-3.946666	-2.135637	-2.147840
C	-2.938070	-1.009704	-2.333244
N	-2.226078	-0.826367	-1.082543
C	-4.872356	-1.790728	-0.988022
H	-2.326906	0.234166	3.141416
H	-2.593970	-1.487221	2.930446
H	-4.503085	0.751249	2.091798
H	-4.773929	-0.404432	3.399196
H	-4.974537	-2.262655	1.865606
H	-5.938820	-0.960688	1.172723

H	-5.450015	-2.672748	-0.690196
H	-5.600561	-1.027770	-1.301270
H	-3.409590	-3.065135	-1.937776
H	-4.538420	-2.286592	-3.054421
H	-3.455045	-0.092426	-2.657452
H	-2.209158	-1.260880	-3.106969
H	-0.485144	-0.135087	1.069450

57 atoms
ε-CL, structure TS34 in toluene

O	-0.270760	0.654891	-1.550467
O	-0.105332	0.922487	0.952120
C	-1.007752	1.283699	-0.775503
C	-1.058497	2.803228	-0.751172
H	-1.809922	3.128190	-0.028533
H	-1.449533	3.076219	-1.739481
C	0.281654	3.516720	-0.508211
H	1.101697	2.858926	-0.811101
H	0.334042	4.390469	-1.167770
C	0.489852	4.014589	0.933057
H	-0.398273	4.590427	1.227843
H	1.319182	4.733492	0.935257
C	0.771176	2.949220	2.001432
H	1.771604	2.526051	1.839765
H	0.798977	3.442592	2.983804
C	-0.223834	1.777133	2.043917
H	-1.253281	2.172185	2.126996
H	-0.053158	1.221863	2.986727
O	-2.254198	0.794624	-0.447071
C	-2.389473	-0.622756	-0.502926
C	-3.832517	-1.009137	-0.292907
H	-1.749353	-1.062202	0.267696
H	-2.031171	-0.981106	-1.473620
C	-4.881407	-0.151361	-0.635800
C	-4.140905	-2.274494	0.217134
C	-6.206693	-0.552493	-0.476312
H	-4.652054	0.836597	-1.017204
C	-5.464760	-2.680360	0.370817
H	-3.336280	-2.947892	0.500994
H	-7.009466	0.128223	-0.743202
C	-6.504549	-1.818786	0.024378
H	-5.684110	-3.665938	0.770123
H	-7.537109	-2.129604	0.148993
H	1.119187	-0.010712	0.946394
N	3.933196	-1.416780	-0.088673
C	2.755863	-0.741915	-0.107569

N	2.344077	-0.134257	-1.232622
C	3.038177	-0.278815	-2.503549
C	4.536197	-0.363760	-2.247175
C	4.815583	-1.489802	-1.259633
C	3.218775	-2.479948	2.024736
C	2.372498	-1.234719	2.253810
N	1.987596	-0.655378	0.975422
C	4.385973	-2.134797	1.108493
H	2.788118	0.586603	-3.118905
H	2.690368	-1.171821	-3.039897
H	4.890804	0.587421	-1.839361
H	5.078450	-0.550372	-3.176864
H	4.695101	-2.467329	-1.744067
H	5.846936	-1.433333	-0.899834
H	4.890538	-3.045837	0.775027
H	5.130559	-1.527823	1.639287
H	2.605004	-3.260395	1.564928
H	3.598502	-2.870658	2.971635
H	2.926976	-0.505011	2.858961
H	1.457012	-1.474348	2.797692
H	1.376721	0.225337	-1.259930

57 atoms
ε-CL, structure I4 in toluene

O	-0.006819	1.707860	-1.617617
O	-0.448074	1.267091	1.456963
C	-1.063479	2.035941	-1.116780
C	-1.400287	3.416647	-0.601845
H	-2.020475	3.301133	0.288508
H	-2.051771	3.863146	-1.363743
C	-0.191134	4.328166	-0.350690
H	0.611274	4.051209	-1.041120
H	-0.480598	5.349371	-0.620407
C	0.357698	4.384214	1.086811
H	-0.463252	4.623971	1.776416
H	1.027225	5.251613	1.123052
C	1.140607	3.173622	1.636432
H	1.755116	2.723721	0.848181
H	1.846130	3.552003	2.388356
C	0.326132	2.073567	2.328422
H	-0.364149	2.532415	3.046883
H	1.015959	1.442327	2.906402
O	-2.128539	1.225811	-1.039236
C	-1.936219	-0.166134	-1.398361
C	-3.032097	-0.970743	-0.753580
H	-0.953552	-0.478630	-1.041345

H	-1.954978	-0.256207	-2.487095
C	-3.887693	-1.764571	-1.518430
C	-3.186633	-0.945817	0.638744
C	-4.879917	-2.532671	-0.907613
H	-3.781154	-1.783943	-2.599459
C	-4.180822	-1.705828	1.247322
H	-2.526562	-0.321566	1.233428
H	-5.538549	-3.146145	-1.514318
C	-5.028833	-2.503535	0.476306
H	-4.294990	-1.678178	2.326520
H	-5.802465	-3.096644	0.953788
H	0.123876	0.523396	1.134409
N	3.178377	-1.916558	0.072249
C	2.206085	-0.944423	0.023878
N	2.398295	0.091425	-0.863847
C	3.340750	-0.007481	-1.965593
C	4.642206	-0.582669	-1.425598
C	4.360693	-1.938614	-0.791058
C	1.549952	-3.291769	1.313641
C	0.978461	-1.955020	1.778933
N	1.142832	-0.911526	0.777101
C	3.009082	-3.097026	0.922147
H	3.490863	0.994140	-2.373442
H	2.959663	-0.639043	-2.783672
H	5.054890	0.104975	-0.681594
H	5.382013	-0.699354	-2.221798
H	4.224458	-2.699044	-1.574332
H	5.216440	-2.260010	-0.186758
H	3.376255	-3.967532	0.367431
H	3.639480	-3.000909	1.816881
H	0.979276	-3.647304	0.449258
H	1.474526	-4.054123	2.094593
H	1.462606	-1.661866	2.724202
H	-0.088067	-2.051248	2.000728
H	1.564137	0.643717	-1.027878

57 atoms
ε-CL, structure I5 in toluene

O	4.160685	1.887777	-1.343338
O	-3.204146	-0.155334	-1.836272
C	4.146883	0.843257	-0.736746
C	2.925769	-0.011020	-0.468817
H	2.814545	-0.094689	0.618718
H	3.146724	-1.027367	-0.813167
C	1.648338	0.526284	-1.111774
H	1.468019	1.547550	-0.760895

H	1.792592	0.604668	-2.194423
C	0.427272	-0.349313	-0.814186
H	0.287842	-0.421321	0.272753
H	0.620470	-1.372942	-1.160958
C	-0.858256	0.172725	-1.461568
H	-1.058137	1.197308	-1.125514
H	-0.737018	0.223774	-2.549681
C	-2.076568	-0.687288	-1.157734
H	-2.253476	-0.719062	-0.071367
H	-1.885344	-1.722139	-1.481435
O	5.250910	0.283576	-0.197220
C	6.494871	1.016302	-0.384158
C	7.596594	0.231127	0.268362
H	6.382687	2.007470	0.058594
H	6.661732	1.143482	-1.455209
C	8.260597	-0.778955	-0.434496
C	7.960061	0.482839	1.594304
C	9.268220	-1.522597	0.174660
H	7.986352	-0.982883	-1.465437
C	8.968218	-0.258143	2.207098
H	7.450770	1.264998	2.149725
H	9.777876	-2.301690	-0.382972
C	9.624163	-1.262751	1.497598
H	9.243195	-0.050041	3.236065
H	10.411699	-1.839063	1.972343
H	-4.009806	-0.665161	-1.558465
N	-7.049663	-0.081635	0.842465
C	-5.962383	-0.061043	-0.001053
N	-5.338096	1.151552	-0.183865
C	-5.533589	2.277017	0.709645
C	-7.024776	2.397575	0.996510
C	-7.529454	1.085205	1.584178
C	-6.830249	-2.541432	0.830480
C	-6.233791	-2.340650	-0.561900
N	-5.506184	-1.086445	-0.662986
C	-7.710879	-1.345606	1.172971
H	-5.155732	3.174573	0.215508
H	-4.975824	2.164239	1.653060
H	-7.549534	2.619632	0.062820
H	-7.226822	3.211494	1.697747
H	-7.218354	1.001432	2.636373
H	-8.625041	1.065258	1.578625
H	-7.944027	-1.337348	2.243778
H	-8.669380	-1.408396	0.639662
H	-6.017617	-2.623156	1.560155
H	-7.419220	-3.461616	0.888279
H	-7.038178	-2.383017	-1.313401

```
H     -5.548389    -3.158014    -0.804356
H     -4.480835     1.088376    -0.721805
```

Table S6: Cartesian coordinates (in Angstroms) of all intermediates and transition states of the second step of the TBD-catalyzed ROP of ε-CL/3-isomer/7-isomer (i.e. addition of another ε-CL/3-isomer/7-isomer unit to the ε-CL/3-isomer/7-isomer chain end) optimized in toluene using the PCM-B3LYP/6-311G(d) method

```
75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure
I1, in toluene
O     -3.529169     1.334479     2.030701
O     -4.588971     2.091564     0.267171
C     -3.552853     2.140729     1.123200
C     -2.501189     3.217760     0.960430
H     -1.935125     2.997999     0.049764
H     -1.817853     3.086500     1.799617
C     -3.036073     4.663456     0.927472
H     -3.779673     4.801038     1.721323
H     -2.204132     5.329246     1.176684
C     -3.617375     5.095505    -0.422996
H     -2.828002     5.030856    -1.182691
H     -3.900874     6.152027    -0.368364
C     -4.824581     4.276894    -0.890510
H     -5.677572     4.429439    -0.218912
H     -5.141532     4.636852    -1.876159
C     -4.568705     2.779826    -1.008922
H     -3.629632     2.546795    -1.514656
H     -5.374723     2.296664    -1.559826
N     -5.602347    -3.072734    -0.049667
C     -4.864417    -1.910499     0.054029
N     -4.900151    -1.263157     1.255974
C     -5.504120    -1.805744     2.455439
C     -6.776597    -2.549589     2.070014
C     -6.431867    -3.606933     1.029382
C     -4.275377    -3.565401    -2.077705
C     -4.245008    -2.044400    -2.215951
N     -4.166489    -1.391882    -0.918816
C     -5.466137    -3.954764    -1.210244
H     -5.718479    -0.973769     3.128950
H     -4.820244    -2.484909     2.987868
H     -7.499477    -1.838197     1.659502
```

H	-7.232865	-3.028958	2.940402
H	-5.913108	-4.450329	1.510285
H	-7.346526	-4.015259	0.583844
H	-5.356790	-4.984786	-0.848811
H	-6.394053	-3.923663	-1.798105
H	-3.344510	-3.898901	-1.607256
H	-4.350734	-4.062377	-3.049704
H	-5.138652	-1.713218	-2.770460
H	-3.383182	-1.726676	-2.809996
H	-4.408694	-0.380229	1.320954
O	5.409442	1.730343	-1.328634
O	-2.148958	0.491044	-1.002687
C	5.347038	0.716948	-0.673913
C	4.076405	0.008918	-0.253671
H	4.055300	-0.004283	0.842551
H	4.163543	-1.041835	-0.551078
C	2.806003	0.642517	-0.818104
H	2.768382	1.697091	-0.526702
H	2.853430	0.637528	-1.912288
C	1.533842	-0.071388	-0.351053
H	1.492437	-0.059489	0.746069
H	1.583329	-1.130021	-0.638310
C	0.253586	0.550231	-0.915983
H	0.205132	1.610621	-0.639535
H	0.270250	0.518276	-2.011802
C	-1.014893	-0.140725	-0.432516
H	-1.061157	-0.105088	0.667622
H	-0.984740	-1.203821	-0.714855
O	6.434836	0.064626	-0.210876
C	7.722943	0.658852	-0.537242
C	8.795729	-0.201821	0.066362
H	7.743560	1.675759	-0.141245
H	7.810494	0.719325	-1.623285
C	9.377134	-1.236431	-0.672062
C	9.213705	0.005582	1.384435
C	10.358465	-2.047645	-0.106572
H	9.059896	-1.406792	-1.696749
C	10.193832	-0.803583	1.953727
H	8.768509	0.806678	1.967284
H	10.804347	-2.845191	-0.692058
C	10.768534	-1.832184	1.208132
H	10.511588	-0.629990	2.976757
H	11.534990	-2.461260	1.649214
H	-2.925524	-0.122355	-0.904754

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure TS12, in toluene

O	-3.264365	1.089312	1.816346
O	-4.428868	1.826091	0.079621
C	-3.223271	1.769715	0.772770
C	-2.359376	3.033152	0.734071
H	-1.888857	3.151874	-0.242190
H	-1.560692	2.861794	1.457571
C	-3.140041	4.313410	1.092311
H	-3.849018	4.104929	1.901823
H	-2.434983	5.052214	1.488906
C	-3.861879	4.939560	-0.110400
H	-3.110870	5.173695	-0.876693
H	-4.298217	5.900263	0.187126
C	-4.960102	4.072639	-0.739944
H	-5.819069	4.004031	-0.061896
H	-5.323849	4.561881	-1.652443
C	-4.537739	2.646064	-1.089872
H	-3.606373	2.610600	-1.659812
H	-5.313539	2.171749	-1.696514
N	-5.456764	-2.936373	-0.059768
C	-4.691450	-1.828472	0.128674
N	-4.597903	-1.276847	1.344106
C	-5.255362	-1.832735	2.516586
C	-6.572576	-2.476095	2.103092
C	-6.306794	-3.491585	0.999493
C	-4.290781	-3.300957	-2.216958
C	-4.141385	-1.785002	-2.245378
N	-4.021876	-1.282845	-0.886311
C	-5.475632	-3.667712	-1.332178
H	-5.414317	-1.014385	3.219958
H	-4.609662	-2.569083	3.012897
H	-7.257607	-1.702511	1.744044
H	-7.047327	-2.975179	2.951151
H	-5.829423	-4.390596	1.410460
H	-7.246810	-3.809663	0.538112
H	-5.464003	-4.737699	-1.101566
H	-6.420856	-3.460284	-1.849961
H	-3.373799	-3.748093	-1.821851
H	-4.449713	-3.700061	-3.221591
H	-4.999722	-1.328356	-2.756680
H	-3.244995	-1.480620	-2.787539
H	-4.097968	-0.372007	1.459060

O	5.285855	1.246708	-1.879740
O	-2.306093	0.703002	-0.531502
C	5.232770	0.479116	-0.948327
C	3.968845	-0.053807	-0.308003
H	4.062467	0.068207	0.776358
H	3.951223	-1.137940	-0.474222
C	2.691116	0.599429	-0.833151
H	2.738900	1.679505	-0.656541
H	2.643277	0.478152	-1.920067
C	1.424734	0.026493	-0.188854
H	1.489554	0.136096	0.902004
H	1.379014	-1.054859	-0.378127
C	0.136470	0.687377	-0.687834
H	0.176881	1.765422	-0.492146
H	0.055808	0.577870	-1.776920
C	-1.134832	0.114278	-0.046639
H	-1.079303	0.220820	1.050664
H	-1.150880	-0.977814	-0.234182
O	6.329432	-0.026697	-0.342345
C	7.610714	0.404040	-0.881216
C	8.696248	-0.232334	-0.060979
H	7.653072	1.493726	-0.839830
H	7.663611	0.105499	-1.929766
C	9.242200	-1.463271	-0.435696
C	9.162448	0.387762	1.102295
C	10.235912	-2.063317	0.334587
H	8.887244	-1.953830	-1.337376
C	10.155146	-0.209010	1.875563
H	8.745134	1.344390	1.402876
H	10.653934	-3.017505	0.030399
C	10.694175	-1.436509	1.492251
H	10.510370	0.284432	2.774478
H	11.470324	-1.901020	2.091919
H	-3.378220	-0.443888	-0.714689

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure I2, in toluene

O	-3.505620	1.238961	1.663335
O	-4.344331	1.920341	-0.303820
C	-3.174404	1.827261	0.474879
C	-2.499264	3.179248	0.760477
H	-1.871796	3.454437	-0.091579

H	-1.827788	3.017254	1.606558
C	-3.476220	4.323689	1.075936
H	-4.294019	3.946193	1.697681
H	-2.951308	5.071555	1.679858
C	-4.024767	5.023418	-0.178092
H	-3.173977	5.386744	-0.770119
H	-4.582830	5.917105	0.123492
C	-4.925973	4.160723	-1.070982
H	-5.886119	3.984403	-0.572815
H	-5.150427	4.707249	-1.995690
C	-4.348758	2.795321	-1.437551
H	-3.346903	2.871271	-1.872119
H	-4.987481	2.308548	-2.178874
N	-5.549130	-2.996274	0.029211
C	-4.753534	-1.886742	0.214985
N	-4.673975	-1.206351	1.322023
C	-5.434025	-1.673395	2.470780
C	-6.769130	-2.287804	2.056036
C	-6.509371	-3.406783	1.055411
C	-4.459011	-3.462045	-2.154850
C	-4.210664	-1.960349	-2.195660
N	-3.955066	-1.509368	-0.839767
C	-5.632306	-3.745572	-1.225116
H	-5.596219	-0.824769	3.141768
H	-4.852879	-2.412311	3.045190
H	-7.390846	-1.513977	1.593957
H	-7.317038	-2.682154	2.917038
H	-6.136179	-4.303608	1.569155
H	-7.440261	-3.694197	0.553352
H	-5.674939	-4.813656	-0.982598
H	-6.578021	-3.500327	-1.731334
H	-3.556980	-3.961854	-1.789836
H	-4.681030	-3.854387	-3.150827
H	-5.072510	-1.447058	-2.650882
H	-3.334886	-1.722368	-2.803162
H	-3.953917	0.352677	1.490667
O	5.251791	1.283770	-1.728130
O	-2.308121	0.969153	-0.316410
C	5.202002	0.539036	-0.778142
C	3.945530	0.129362	-0.038871
H	4.074590	0.405143	1.013998
H	3.897881	-0.965457	-0.044785
C	2.671050	0.741290	-0.617589
H	2.755342	1.832848	-0.604111

H	2.583211	0.462673	-1.672807
C	1.412045	0.308105	0.139650
H	1.507043	0.588356	1.196863
H	1.335569	-0.786963	0.124738
C	0.129237	0.916248	-0.436770
H	0.193717	2.009910	-0.413716
H	0.025096	0.634831	-1.491199
C	-1.119869	0.468200	0.314557
H	-1.092883	0.779500	1.360870
H	-1.190537	-0.625471	0.312216
O	6.290648	-0.043812	-0.233441
C	7.566054	0.272893	-0.860520
C	8.639778	-0.486549	-0.135237
H	7.719830	1.351864	-0.804134
H	7.509755	-0.004079	-1.914614
C	8.969840	-1.789844	-0.519187
C	9.310146	0.089330	0.947722
C	9.951018	-2.503866	0.164209
H	8.455234	-2.246904	-1.359384
C	10.292688	-0.621261	1.633538
H	9.061576	1.101087	1.254691
H	10.200097	-3.513538	-0.145962
C	10.614717	-1.919915	1.242449
H	10.808254	-0.161249	2.470325
H	11.382026	-2.473784	1.773656
H	-3.506097	-0.605605	-0.721206

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure TS2r, in toluene

O	-3.499472	1.149355	1.690982
O	-4.329272	1.827953	-0.281228
C	-3.170158	1.766322	0.516766
C	-2.549089	3.137914	0.832445
H	-1.913361	3.444654	-0.002826
H	-1.891041	2.989879	1.691260
C	-3.570847	4.244345	1.141211
H	-4.385794	3.832147	1.744419
H	-3.082919	5.003039	1.762439
C	-4.120933	4.939001	-0.114806
H	-3.272846	5.337808	-0.687579
H	-4.714506	5.809683	0.186302
C	-4.976164	4.056187	-1.032807

H	-5.938110	3.841195	-0.553543
H	-5.203582	4.605377	-1.955213
C	-4.345230	2.716124	-1.404520
H	-3.339327	2.832223	-1.820508
H	-4.953645	2.216320	-2.162481
N	-5.360865	-3.135254	-0.034429
C	-4.614364	-1.997272	0.181143
N	-4.591016	-1.323651	1.294858
C	-5.363487	-1.828494	2.418981
C	-6.661270	-2.492225	1.963702
C	-6.330217	-3.592243	0.963116
C	-4.192677	-3.541551	-2.189586
C	-4.002392	-2.031081	-2.214042
N	-3.803300	-1.580213	-0.848730
C	-5.379975	-3.877186	-1.295739
H	-5.577864	-0.991596	3.090051
H	-4.769633	-2.547807	3.005138
H	-7.300748	-1.740264	1.489899
H	-7.216028	-2.914593	2.806837
H	-5.934534	-4.477102	1.480795
H	-7.235168	-3.913237	0.434641
H	-5.388280	-4.948010	-1.061867
H	-6.319721	-3.664267	-1.827086
H	-3.282523	-4.008512	-1.801864
H	-4.370744	-3.934953	-3.193937
H	-4.870494	-1.548690	-2.690686
H	-3.119770	-1.754664	-2.794770
H	-3.918125	0.252820	1.498742
O	5.246801	1.160778	-1.890302
O	-2.259023	0.953787	-0.271187
C	5.231666	0.525245	-0.862952
C	3.997271	0.162501	-0.064264
H	4.146770	0.517713	0.961482
H	3.961956	-0.930348	0.012807
C	2.703101	0.715204	-0.658682
H	2.774015	1.805720	-0.728234
H	2.596334	0.357885	-1.688045
C	1.465558	0.327208	0.156313
H	1.580852	0.684210	1.188070
H	1.399518	-0.766613	0.222173
C	0.165344	0.882242	-0.434206
H	0.219992	1.975299	-0.493264
H	0.041087	0.523599	-1.462717
C	-1.064866	0.486776	0.374382

H	-1.011929	0.872283	1.394651
H	-1.136048	-0.604303	0.452252
O	6.344389	0.038008	-0.274756
C	7.601264	0.319803	-0.953972
C	8.710220	-0.295981	-0.149817
H	7.710814	1.402139	-1.040532
H	7.548993	-0.094565	-1.962251
C	9.123471	-1.608151	-0.398138
C	9.331148	0.426051	0.873717
C	10.138011	-2.188245	0.359769
H	8.647949	-2.178161	-1.190979
C	10.345882	-0.150378	1.634023
H	9.018028	1.446325	1.075266
H	10.451847	-3.206582	0.154409
C	10.751281	-1.459475	1.377745
H	10.821995	0.422106	2.423471
H	11.544089	-1.908818	1.967031
H	-3.393896	-0.660401	-0.712401

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure I2r, in toluene

O	-3.760084	1.232266	1.673662
O	-4.685521	1.508278	-0.349995
C	-3.622817	1.899711	0.487981
C	-3.564148	3.410440	0.773205
H	-3.014025	3.909283	-0.030904
H	-2.970633	3.529568	1.681727
C	-4.936505	4.078026	0.955113
H	-5.588830	3.417649	1.534984
H	-4.801886	4.982701	1.557682
C	-5.608877	4.482214	-0.366821
H	-4.918914	5.133688	-0.920033
H	-6.489928	5.096308	-0.148396
C	-6.034341	3.317962	-1.270191
H	-6.887214	2.792931	-0.824992
H	-6.379875	3.712918	-2.233938
C	-4.945201	2.279797	-1.528117
H	-4.022022	2.732571	-1.903499
H	-5.283887	1.562425	-2.280015
N	-4.099790	-3.448957	0.033714
C	-3.732542	-2.138712	0.248372
N	-3.958715	-1.472129	1.343146

C	-4.599314	-2.165890	2.449449
C	-5.620614	-3.191256	1.961755
C	-4.933719	-4.158315	1.005848
C	-2.780414	-3.516605	-2.071983
C	-3.043100	-2.017629	-2.122148
N	-3.034412	-1.514555	-0.760206
C	-3.847048	-4.179513	-1.209169
H	-5.082090	-1.419809	3.087369
H	-3.847338	-2.667786	3.078893
H	-6.431309	-2.669785	1.442363
H	-6.063883	-3.746569	2.793729
H	-4.317178	-4.877451	1.562748
H	-5.678086	-4.741827	0.452169
H	-3.544571	-5.200600	-0.949707
H	-4.786484	-4.264381	-1.775714
H	-1.787478	-3.689434	-1.646911
H	-2.798152	-3.955652	-3.073004
H	-3.997500	-1.817667	-2.634462
H	-2.260700	-1.499235	-2.680291
H	-3.842909	0.242901	1.501990
O	4.660672	-0.927776	-1.733234
O	-2.443015	1.459349	-0.234684
C	4.834055	-0.238150	-0.756455
C	3.752677	0.475202	0.027643
H	4.043910	1.527130	0.120676
H	3.772776	0.079990	1.050125
C	2.361046	0.335567	-0.586769
H	2.374536	0.732364	-1.607484
H	2.113245	-0.726284	-0.682912
C	1.280432	1.048560	0.231816
H	1.538429	2.111059	0.330445
H	1.269199	0.644079	1.252036
C	-0.115463	0.914807	-0.384921
H	-0.117992	1.337044	-1.396673
H	-0.378118	-0.143834	-0.484784
C	-1.189966	1.609593	0.439393
H	-0.948463	2.674633	0.551564
H	-1.258842	1.172071	1.440315
O	6.049085	-0.008857	-0.215534
C	7.174792	-0.654567	-0.875811
C	8.428093	-0.255281	-0.150934
H	7.188560	-0.339572	-1.920441
H	7.015189	-1.734025	-0.851873
C	8.895270	-1.009607	0.929370

C	9.134578	0.889248	-0.532166
C	10.046432	-0.629453	1.615279
H	8.354080	-1.900666	1.233987
C	10.286161	1.272821	0.151072
H	8.780506	1.482547	-1.370200
H	10.400416	-1.225624	2.450101
C	10.744206	0.513224	1.226638
H	10.827292	2.161539	-0.157205
H	11.643100	0.808925	1.757934
H	-2.923636	-0.513870	-0.630404

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure TS23, in toluene

O	-2.762887	0.393903	1.144105
O	-3.649891	1.341444	-0.692184
C	-2.646352	1.474571	0.298845
C	-2.745142	2.800258	1.086589
H	-2.247031	3.600261	0.528897
H	-2.164453	2.647661	1.998726
C	-4.178324	3.225776	1.440691
H	-4.770581	2.341896	1.701447
H	-4.148107	3.849956	2.340094
C	-4.870140	4.027830	0.326354
H	-4.245822	4.899974	0.090913
H	-5.816918	4.430107	0.704297
C	-5.150435	3.247517	-0.964343
H	-5.958525	2.526570	-0.795564
H	-5.506979	3.939248	-1.737847
C	-3.956972	2.473026	-1.517853
H	-3.070042	3.100274	-1.642400
H	-4.199468	2.060887	-2.500598
N	-6.671449	-2.448571	0.165546
C	-5.634154	-1.544785	0.133403
N	-5.097936	-0.986896	1.181570
C	-5.576726	-1.389465	2.494151
C	-7.072610	-1.697164	2.482612
C	-7.353921	-2.756411	1.423703
C	-6.341417	-2.962380	-2.239972
C	-5.787893	-1.547132	-2.338263
N	-5.101025	-1.242788	-1.096755
C	-7.259994	-3.056788	-1.028006
H	-5.355708	-0.585099	3.201749

H	-5.025073	-2.272765	2.853055
H	-7.626416	-0.782202	2.246878
H	-7.418574	-2.050151	3.458630
H	-7.041079	-3.748043	1.778656
H	-8.428999	-2.817254	1.220052
H	-7.480304	-4.105997	-0.801417
H	-8.223577	-2.572940	-1.247756
H	-5.508528	-3.663974	-2.137557
H	-6.898441	-3.230957	-3.141386
H	-6.604652	-0.838187	-2.549552
H	-5.067662	-1.464551	-3.155224
H	-3.657789	-0.064728	1.083230
O	5.801760	-0.254291	-2.233601
O	-1.418695	1.410283	-0.419673
C	5.882353	-0.092289	-1.039181
C	4.741570	0.281750	-0.116420
H	5.013474	1.219564	0.381865
H	4.699658	-0.466216	0.683210
C	3.396099	0.406449	-0.828986
H	3.479504	1.145269	-1.632629
H	3.157557	-0.542392	-1.320575
C	2.259314	0.797447	0.120316
H	2.506072	1.747637	0.612073
H	2.181776	0.053129	0.923367
C	0.908474	0.923540	-0.590192
H	0.972755	1.675715	-1.385092
H	0.649629	-0.022456	-1.078094
C	-0.224267	1.302955	0.352719
H	-0.000071	2.258697	0.848125
H	-0.355446	0.542211	1.127818
O	7.034891	-0.224200	-0.348404
C	8.210140	-0.580904	-1.130058
C	9.378249	-0.679560	-0.191110
H	8.362889	0.183942	-1.893348
H	8.012323	-1.527001	-1.636848
C	9.663979	-1.882177	0.462227
C	10.184359	0.434369	0.060331
C	10.734348	-1.971063	1.348860
H	9.044037	-2.753947	0.274118
C	11.256346	0.349490	0.945922
H	9.971302	1.373658	-0.441678
H	10.947297	-2.911287	1.847188
C	11.533074	-0.854382	1.591924
H	11.876565	1.220879	1.129512

H 12.369596 -0.923048 2.279873
H -4.472487 -0.446550 -1.076240

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure I3, in toluene
O -2.660350 -0.283528 0.523298
O -3.487440 1.404094 -0.702404
C -2.534773 1.069236 0.299509
C -2.708125 1.909481 1.590679
H -2.151176 2.846597 1.484173
H -2.214319 1.346999 2.386293
C -4.159204 2.221935 1.991989
H -4.792559 1.345858 1.817634
H -4.184419 2.409903 3.071064
C -4.739930 3.456753 1.283293
H -4.077000 4.310779 1.476761
H -5.702111 3.714813 1.740411
C -4.940429 3.310871 -0.230359
H -5.772622 2.626175 -0.431185
H -5.227596 4.281149 -0.654740
C -3.722253 2.789457 -0.988362
H -2.821223 3.373312 -0.780518
H -3.897205 2.841525 -2.065951
N -7.099372 -2.093449 -0.147555
C -5.951812 -1.335423 -0.103273
N -5.203415 -1.177405 0.954730
C -5.562022 -1.905752 2.160820
C -7.075875 -2.030820 2.319954
C -7.653811 -2.685106 1.071232
C -7.136547 -1.947620 -2.623174
C -6.405879 -0.624428 -2.437452
N -5.554892 -0.731903 -1.268262
C -7.910739 -2.272213 -1.351958
H -5.129779 -1.383309 3.019503
H -5.111530 -2.910998 2.155861
H -7.508164 -1.032885 2.448952
H -7.340670 -2.621571 3.201886
H -7.456893 -3.766061 1.076995
H -8.742407 -2.561392 1.043500
H -8.257787 -3.311240 -1.375451
H -8.809541 -1.640862 -1.286404
H -6.404933 -2.734133 -2.829698

H	-7.827155	-1.899859	-3.469186
H	-7.134797	0.196728	-2.347370
H	-5.773137	-0.401794	-3.299296
H	-3.605036	-0.542876	0.746263
O	6.116166	0.801783	-2.125639
O	-1.273983	1.315017	-0.295250
C	6.113024	0.372273	-0.996584
C	4.901070	0.252801	-0.096828
H	5.099945	0.843522	0.805000
H	4.841660	-0.785577	0.247793
C	3.598736	0.689778	-0.765079
H	3.701109	1.721262	-1.117305
H	3.430486	0.084178	-1.661642
C	2.390388	0.577025	0.169560
H	2.564404	1.188746	1.064641
H	2.298498	-0.457706	0.524220
C	1.079997	1.004934	-0.497805
H	1.157816	2.041524	-0.845612
H	0.892286	0.392192	-1.386133
C	-0.120754	0.887137	0.429347
H	0.026411	1.513050	1.320881
H	-0.257252	-0.146516	0.759640
O	7.223210	-0.068065	-0.366748
C	8.459595	-0.002188	-1.132373
C	9.568810	-0.529906	-0.267995
H	8.629560	1.034585	-1.427170
H	8.332965	-0.593482	-2.041056
C	9.830097	-1.902372	-0.209291
C	10.342976	0.339049	0.505891
C	10.844840	-2.397211	0.605890
H	9.234628	-2.586556	-0.806741
C	11.360099	-0.151872	1.321822
H	10.148825	1.407003	0.468187
H	11.039339	-3.464309	0.640065
C	11.612490	-1.521654	1.373141
H	11.956276	0.534088	1.914882
H	12.406132	-1.905525	2.006014
H	-4.777912	-0.087429	-1.169173

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure TS3r, in toluene

O	2.663221	-0.020534	-0.801426

O	3.460973	1.332281	0.801264
C	2.605725	1.271750	-0.344874
C	2.983528	2.315889	-1.420153
H	2.514923	3.269763	-1.159919
H	2.492353	1.976086	-2.336053
C	4.487238	2.524873	-1.657329
H	5.013596	1.566000	-1.602467
H	4.631796	2.897121	-2.677555
C	5.116546	3.539187	-0.688141
H	4.568602	4.486851	-0.776323
H	6.142862	3.755561	-1.006466
C	5.141454	3.111093	0.784991
H	5.873622	2.307519	0.926486
H	5.482308	3.952826	1.401011
C	3.805360	2.616372	1.336490
H	2.994393	3.329209	1.161298
H	3.876891	2.472953	2.417780
N	6.841542	-2.328785	0.068016
C	5.762779	-1.475828	0.036677
N	5.145663	-1.094475	-1.048674
C	5.579728	-1.656933	-2.317328
C	7.088787	-1.889654	-2.348357
C	7.478855	-2.775845	-1.171925
C	6.625843	-2.559237	2.528064
C	6.014053	-1.165274	2.485580
N	5.285248	-1.023652	1.239690
C	7.506012	-2.754878	1.300134
H	5.281968	-0.971929	-3.116724
H	5.059734	-2.606829	-2.518705
H	7.603667	-0.926068	-2.272733
H	7.404217	-2.359671	-3.284517
H	7.204169	-3.821130	-1.369741
H	8.564185	-2.756170	-1.021514
H	7.774859	-3.811498	1.191959
H	8.448577	-2.200013	1.419762
H	5.823014	-3.302228	2.538242
H	7.224348	-2.698276	3.432139
H	6.804545	-0.405667	2.593944
H	5.311583	-1.020368	3.309219
H	3.611088	-0.341442	-0.919199
O	-6.218431	1.731542	1.415792
O	1.291837	1.563689	0.106330
C	-6.123557	0.802341	0.649674
C	-4.839375	0.287449	0.034445

H	-4.964589	0.296860	-1.054241
H	-4.744766	-0.771046	0.302718
C	-3.600116	1.075347	0.455386
H	-3.728326	2.127227	0.179611
H	-3.515851	1.061919	1.546901
C	-2.313591	0.528243	-0.170680
H	-2.406983	0.539171	-1.264535
H	-2.190402	-0.525594	0.110754
C	-1.067420	1.315845	0.244629
H	-1.175353	2.367687	-0.043766
H	-0.962287	1.302735	1.335433
C	0.209805	0.763464	-0.370968
H	0.157044	0.803437	-1.466785
H	0.358828	-0.281805	-0.087902
O	-7.181553	0.076636	0.228713
C	-8.478538	0.472965	0.757867
C	-9.514981	-0.449507	0.182739
H	-8.660369	1.513507	0.483564
H	-8.438713	0.414345	1.846911
C	-9.829849	-1.651349	0.823922
C	-10.164967	-0.131032	-1.013160
C	-10.776082	-2.518023	0.282297
H	-9.330865	-1.908662	1.753694
C	-11.112134	-0.994954	-1.558091
H	-9.928044	0.800010	-1.519787
H	-11.013752	-3.446286	0.791756
C	-11.419345	-2.190645	-0.910585
H	-11.611957	-0.734130	-2.485371
H	-12.159314	-2.863290	-1.332182
H	4.578305	-0.299155	1.166876

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure I3r, in toluene

O	2.967856	0.697646	-1.406007
O	3.069136	1.092703	0.802067
C	2.784524	1.698046	-0.480453
C	3.638515	2.952141	-0.754841
H	3.134213	3.822121	-0.323563
H	3.604560	3.085814	-1.838248
C	5.091461	2.892062	-0.261154
H	5.507522	1.894436	-0.437676
H	5.688016	3.583599	-0.866023

C	5.256080	3.290855	1.214504
H	4.822574	4.290239	1.353193
H	6.322973	3.392197	1.444524
C	4.626628	2.327320	2.228405
H	5.205298	1.396985	2.266651
H	4.682324	2.768196	3.231723
C	3.173606	1.954910	1.941324
H	2.541053	2.837188	1.802265
H	2.758384	1.390533	2.781074
N	6.339493	-2.627256	-0.192169
C	5.402988	-1.620005	-0.219822
N	5.271862	-0.749068	-1.181916
C	6.130129	-0.881826	-2.348253
C	7.519769	-1.394090	-1.975432
C	7.378469	-2.710152	-1.220541
C	5.191805	-3.684013	1.736614
C	4.719038	-2.275656	2.072083
N	4.521427	-1.553386	0.829897
C	6.459580	-3.597854	0.896169
H	6.200206	0.094806	-2.836068
H	5.676616	-1.560956	-3.087316
H	8.018005	-0.654472	-1.339772
H	8.144784	-1.542274	-2.860973
H	7.143521	-3.528760	-1.914655
H	8.322043	-2.972257	-0.728717
H	6.688254	-4.574714	0.455767
H	7.316158	-3.330691	1.532998
H	4.405317	-4.201795	1.179868
H	5.394468	-4.257606	2.644821
H	5.451314	-1.781272	2.730250
H	3.767464	-2.299521	2.607818
H	3.845562	0.224022	-1.286302
O	-6.151922	2.315747	0.177998
O	1.453935	2.138523	-0.521784
C	-5.945866	1.139195	-0.002424
C	-4.588789	0.495836	-0.194462
H	-4.616297	-0.067542	-1.133872
H	-4.467949	-0.260458	0.589833
C	-3.431234	1.492665	-0.180658
H	-3.579982	2.231846	-0.974613
H	-3.449708	2.055976	0.757957
C	-2.069104	0.813597	-0.352627
H	-2.059161	0.247054	-1.292667
H	-1.927992	0.073728	0.446308

C	-0.901117	1.804433	-0.343157
H	-1.022699	2.533311	-1.152564
H	-0.903205	2.376484	0.591920
C	0.447185	1.118950	-0.502434
H	0.489792	0.545340	-1.432241
H	0.635892	0.429058	0.327125
O	-6.927091	0.213233	-0.055383
C	-8.283581	0.708957	0.127285
C	-9.218782	-0.463925	0.052338
H	-8.490435	1.446373	-0.650003
H	-8.337945	1.214409	1.093162
C	-9.483832	-1.233188	1.189614
C	-9.820818	-0.817828	-1.158264
C	-10.334091	-2.333731	1.119365
H	-9.021253	-0.966907	2.135560
C	-10.673212	-1.917459	-1.232522
H	-9.621545	-0.227787	-2.048079
H	-10.533989	-2.920695	2.010006
C	-10.930951	-2.677653	-0.093100
H	-11.137078	-2.179245	-2.178024
H	-11.596719	-3.532893	-0.148560
H	3.944445	-0.718218	0.835952

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure TS34, in toluene

O	-3.252122	-1.036627	-1.579450
O	-3.417662	-1.216949	0.907000
C	-3.040159	-2.006896	-0.827701
C	-3.958007	-3.222952	-0.804492
H	-3.530614	-3.985533	-0.149502
H	-3.893429	-3.627369	-1.822306
C	-5.428203	-2.956194	-0.443948
H	-5.681472	-1.920981	-0.692138
H	-6.061560	-3.584499	-1.080876
C	-5.793610	-3.268625	1.018118
H	-5.441064	-4.283500	1.248230
H	-6.887081	-3.311782	1.102795
C	-5.263235	-2.301878	2.085581
H	-5.796504	-1.344971	2.007813
H	-5.505481	-2.710826	3.077172
C	-3.757616	-1.997978	2.008420
H	-3.189519	-2.946309	2.010268

H	-3.465363	-1.485231	2.944914
N	-5.320767	3.092436	-0.025163
C	-4.786389	1.846027	-0.081109
N	-4.875533	1.120982	-1.207069
C	-5.408601	1.661683	-2.448466
C	-6.540875	2.627377	-2.128466
C	-6.038620	3.689096	-1.158181
C	-4.008573	3.498661	2.028953
C	-4.067067	1.993204	2.250732
N	-4.172748	1.308170	0.971172
C	-5.194117	3.928474	1.174093
H	-5.759175	0.823431	-3.052404
H	-4.622615	2.170513	-3.022477
H	-7.374132	2.077228	-1.681398
H	-6.908851	3.108157	-3.037673
H	-5.379149	4.400777	-1.671369
H	-6.877852	4.261710	-0.753020
H	-5.069188	4.962978	0.842525
H	-6.126162	3.883562	1.751943
H	-3.073662	3.758487	1.523388
H	-4.030729	4.032094	2.982110
H	-4.916328	1.738151	2.898703
H	-3.164001	1.631761	2.746021
H	-4.308720	0.255496	-1.270125
O	5.848827	-2.470501	0.276347
O	-1.749724	-2.429599	-0.595432
C	5.629533	-1.312115	0.013584
C	4.273374	-0.712797	-0.292657
H	4.323483	-0.281714	-1.299446
H	4.126456	0.141334	0.377790
C	3.121793	-1.710247	-0.179306
H	3.308481	-2.556604	-0.848037
H	3.102709	-2.128694	0.832419
C	1.764727	-1.079272	-0.505140
H	1.791507	-0.661840	-1.520292
H	1.587880	-0.228271	0.165769
C	0.599728	-2.067046	-0.391149
H	0.759490	-2.913016	-1.069922
H	0.560839	-2.484529	0.621255
C	-0.740544	-1.424808	-0.711799
H	-0.749990	-1.008841	-1.724100
H	-0.972760	-0.615817	-0.012439
O	6.594821	-0.369295	-0.046966
C	7.950193	-0.825333	0.224352

C	8.865811	0.361325	0.126574
H	8.206263	-1.599442	-0.501080
H	7.969890	-1.276272	1.217985
C	9.106324	1.166525	1.243980
C	9.473686	0.691832	-1.087996
C	9.938662	2.279343	1.150895
H	8.639181	0.918761	2.192709
C	10.307189	1.803767	-1.185263
H	9.293639	0.073310	-1.962437
H	10.119963	2.894021	2.026702
C	10.541039	2.599779	-0.065027
H	10.775876	2.047095	-2.133333
H	11.192758	3.464462	-0.138286
H	-3.861446	0.279630	0.920109

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure I4, in toluene

O	-3.249518	-1.315805	-1.613573
O	-3.805260	-1.339918	1.480976
C	-2.984626	-2.331701	-1.003822
C	-3.951917	-3.436092	-0.644905
H	-3.705967	-3.756090	0.367935
H	-3.697536	-4.285736	-1.290110
C	-5.440068	-3.066848	-0.791198
H	-5.520716	-2.056847	-1.200855
H	-5.890817	-3.726092	-1.539707
C	-6.280729	-3.169363	0.495138
H	-6.043031	-4.108105	1.014171
H	-7.330942	-3.261993	0.193745
C	-6.198870	-2.001391	1.492765
H	-6.432591	-1.060967	0.978890
H	-6.993760	-2.145822	2.237392
C	-4.885402	-1.818193	2.262276
H	-4.570357	-2.776679	2.692295
H	-5.071789	-1.139859	3.108413
N	-4.922764	3.330253	-0.085598
C	-4.603552	1.993869	0.014215
N	-4.721457	1.236846	-1.130993
C	-4.771367	1.846599	-2.448813
C	-5.764260	2.998975	-2.398698
C	-5.320316	3.990095	-1.330329
C	-3.792893	3.619777	2.087803

C	-4.200572	2.169944	2.339320
N	-4.241588	1.392396	1.110373
C	-4.736314	4.226246	1.056896
H	-5.086085	1.082457	-3.162067
H	-3.784935	2.211371	-2.776521
H	-6.756430	2.604478	-2.160500
H	-5.828099	3.508200	-3.363913
H	-4.480589	4.594334	-1.705138
H	-6.132012	4.689789	-1.100528
H	-4.334327	5.173876	0.681272
H	-5.710411	4.452766	1.512215
H	-2.765802	3.644859	1.708396
H	-3.819706	4.211057	3.007933
H	-5.180338	2.150322	2.843019
H	-3.496741	1.688017	3.024540
H	-4.268207	0.332234	-1.076322
O	5.753486	-2.403923	0.845281
O	-1.738221	-2.644669	-0.618785
C	5.573528	-1.333600	0.315055
C	4.247745	-0.810370	-0.196648
H	4.376408	-0.556394	-1.254884
H	4.051020	0.143500	0.305949
C	3.089916	-1.786936	0.000790
H	3.323718	-2.732110	-0.499826
H	2.996277	-2.027888	1.064506
C	1.761406	-1.235747	-0.525714
H	1.863234	-0.994724	-1.591830
H	1.533432	-0.288044	-0.021366
C	0.595874	-2.210831	-0.330214
H	0.810677	-3.157571	-0.838325
H	0.477369	-2.445389	0.732876
C	-0.713796	-1.653180	-0.857212
H	-0.666099	-1.441593	-1.928686
H	-0.999913	-0.731976	-0.343889
O	6.557216	-0.434628	0.101603
C	7.885832	-0.820364	0.556051
C	8.829739	0.301453	0.229833
H	8.165883	-1.748888	0.055768
H	7.839140	-1.016838	1.628593
C	9.020813	1.353062	1.131135
C	9.514172	0.322896	-0.988813
C	9.879377	2.405260	0.822156
H	8.494261	1.346301	2.081051
C	10.374217	1.373191	-1.301450

H	9.373300	-0.488914	-1.696475
H	10.021580	3.213703	1.532009
C	10.558047	2.416796	-0.395739
H	10.902422	1.375828	-2.249434
H	11.230168	3.234150	-0.636402
H	-3.948552	-0.374917	1.306053

75 atoms
addition of another ε-CL unit to the ε-CL chain end, structure I5, in toluene

O	0.770891	0.484172	-0.694008
O	7.943226	-2.425518	-0.434730
C	0.580482	-0.662578	-0.365284
C	1.650601	-1.711010	-0.145998
H	1.420826	-2.561599	-0.797961
H	1.536310	-2.093520	0.874834
C	3.070081	-1.200094	-0.386859
H	3.147640	-0.814407	-1.408712
H	3.263995	-0.345254	0.269197
C	4.132016	-2.280330	-0.158698
H	3.928058	-3.135822	-0.816573
H	4.046914	-2.663355	0.866920
C	5.560087	-1.782165	-0.400135
H	5.653175	-1.400283	-1.424084
H	5.779867	-0.939147	0.264853
C	6.616862	-2.868104	-0.186412
H	6.434882	-3.703150	-0.871408
H	6.531522	-3.268898	0.835148
N	9.596642	1.898007	0.364600
C	9.018408	0.673788	0.118768
N	8.666707	0.400414	-1.185622
C	9.213011	1.143064	-2.306555
C	9.142292	2.625983	-1.967003
C	9.909232	2.879979	-0.675016
C	10.266506	0.980186	2.555875
C	9.026655	0.098977	2.412922
N	8.746003	-0.223349	1.023340
C	10.089577	2.230306	1.702702
H	8.614419	0.914477	-3.190855
H	10.252269	0.855742	-2.531799
H	8.093785	2.913675	-1.847137
H	9.568556	3.234976	-2.768502
H	10.991515	2.867189	-0.872735

H	9.673310	3.876267	-0.284417
H	11.045142	2.754814	1.591121
H	9.396346	2.932144	2.186468
H	11.144868	0.421932	2.215125
H	10.440240	1.265482	3.597707
H	8.164121	0.605732	2.874433
H	9.159562	-0.837023	2.963483
H	8.389430	-0.563781	-1.331739
O	-8.210828	-2.063463	0.416908
O	-0.647508	-1.176430	-0.143412
C	-8.122548	-0.881037	0.185724
C	-6.835553	-0.121287	-0.059574
H	-6.815155	0.734084	0.624505
H	-6.896476	0.314653	-1.063596
C	-5.583118	-0.982917	0.090190
H	-5.551549	-1.403851	1.100523
H	-5.649894	-1.839511	-0.587928
C	-4.295707	-0.200445	-0.186162
H	-4.236972	0.659475	0.493216
H	-4.333235	0.217152	-1.200448
C	-3.036472	-1.060178	-0.033213
H	-2.982546	-1.467780	0.982178
H	-3.084451	-1.918419	-0.712349
C	-1.767955	-0.276867	-0.318219
H	-1.648648	0.569869	0.362745
H	-1.749629	0.113572	-1.338932
O	-9.187528	-0.056582	0.108249
C	-10.490640	-0.674172	0.313007
C	-11.534901	0.398899	0.196472
H	-10.498023	-1.146558	1.296555
H	-10.621817	-1.456083	-0.437130
C	-12.066216	0.739622	-1.051170
C	-11.976066	1.087510	1.329981
C	-13.020012	1.748000	-1.164602
H	-11.730842	0.210499	-1.938404
C	-12.930686	2.096267	1.220909
H	-11.570381	0.830809	2.304220
H	-13.427001	2.000585	-2.138371
C	-13.454292	2.428230	-0.027536
H	-13.267439	2.620580	2.109352
H	-14.200251	3.211675	-0.113955
H	8.206218	-1.767630	0.259474

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I1, in toluene

O	-4.868019	-1.021951	1.785603
O	-5.453393	-0.750262	-0.310797
C	-5.042924	-1.538340	0.701976
C	-4.873113	-3.024641	0.468373
H	-4.020794	-3.163340	-0.204158
H	-4.587514	-3.438370	1.435526
C	-6.117386	-3.752749	-0.078169
H	-7.008327	-3.425775	0.470820
H	-6.002115	-4.818017	0.144320
C	-6.336015	-3.591193	-1.586153
H	-5.469358	-4.009082	-2.114199
H	-7.197374	-4.195851	-1.889602
C	-6.549898	-2.147058	-2.049500
H	-7.484166	-1.745150	-1.640145
H	-6.661500	-2.133719	-3.139900
C	-5.418736	-1.191005	-1.691437
H	-4.429327	-1.602983	-1.899553
H	-5.517616	-0.259601	-2.248113
N	-3.217306	3.770086	0.287416
C	-3.172431	2.395800	0.388913
N	-3.884194	1.828763	1.417639
C	-4.951051	2.541054	2.097975
C	-4.440590	3.931734	2.446121
C	-4.007943	4.634704	1.165636
C	-2.267717	3.500202	-1.974997
C	-1.629702	2.240016	-1.396040
N	-2.474106	1.616572	-0.388578
C	-2.579729	4.460451	-0.834810
H	-5.212298	1.975776	2.994128
H	-5.860728	2.611801	1.481166
H	-3.593831	3.838471	3.132391
H	-5.212379	4.525065	2.943626
H	-4.892870	4.991951	0.617937
H	-3.407300	5.520735	1.401873
H	-3.257366	5.251787	-1.175505
H	-1.662501	4.956528	-0.488160
H	-3.192386	3.228577	-2.495053
H	-1.611114	3.988880	-2.701116
H	-0.643603	2.493960	-0.974454
H	-1.442988	1.506969	-2.186620
H	-3.995306	0.823580	1.362108

O	5.600483	-2.735223	-1.175433
C	5.075781	-1.975892	-0.395485
O	-2.346886	-1.141139	-0.520470
C	-1.250073	-1.536206	0.285699
H	-1.185999	-0.904614	1.182840
H	-1.447003	-2.559095	0.628868
C	0.080145	-1.498981	-0.470568
H	0.257375	-0.475124	-0.821012
H	-0.016057	-2.121761	-1.368163
C	1.268753	-1.970680	0.373942
H	1.360167	-1.336005	1.264525
H	1.066006	-2.983575	0.740881
C	2.590227	-1.940728	-0.403326
H	2.730158	-0.934543	-0.813020
H	2.535500	-2.618722	-1.263122
C	3.841937	-2.292524	0.437451
H	3.860001	-1.647724	1.319767
C	3.866137	-3.771787	0.878187
H	3.975038	-4.401888	-0.009879
C	4.937910	-4.074353	1.824250
H	2.907479	-4.030045	1.335948
C	5.818806	-4.301774	2.610585
H	6.599942	-4.512958	3.302140
O	5.485607	-0.708401	-0.197891
C	6.623813	-0.273383	-0.997491
C	6.921656	1.155053	-0.642856
H	7.463764	-0.934694	-0.778365
H	6.369756	-0.388613	-2.052188
C	6.432706	2.201005	-1.429948
C	7.680078	1.459520	0.492267
C	6.697727	3.526996	-1.092983
H	5.842842	1.976041	-2.313755
C	7.944880	2.782983	0.833450
H	8.064080	0.653938	1.111145
H	6.315649	4.329841	-1.715205
C	7.454235	3.819890	0.040026
H	8.536712	3.006139	1.715262
H	7.663708	4.851791	0.302838
H	-2.434348	-0.151409	-0.466774

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure TS12, in toluene

O	-3.863895	1.693783	0.951006
O	-4.448050	1.385045	-1.165586
C	-3.525997	1.862200	-0.237699
C	-2.770385	3.135592	-0.628035
H	-2.021384	2.924450	-1.391527
H	-2.235210	3.444232	0.271574
C	-3.698732	4.266931	-1.112669
H	-4.615609	4.280426	-0.512445
H	-3.203008	5.226956	-0.931586
C	-4.033654	4.176809	-2.609130
H	-3.092227	4.212194	-3.173577
H	-4.598471	5.067026	-2.909621
C	-4.819185	2.928221	-3.031255
H	-5.844719	2.982326	-2.646967
H	-4.899029	2.908031	-4.125585
C	-4.224187	1.600223	-2.563515
H	-3.158702	1.513677	-2.788966
H	-4.734917	0.772719	-3.062778
N	-5.145783	-3.075505	0.658440
C	-4.540485	-1.867759	0.507222
N	-4.883366	-0.842052	1.294412
C	-5.864969	-0.959199	2.361632
C	-6.937199	-1.962493	1.957145
C	-6.270856	-3.278633	1.578254
C	-3.316456	-4.093821	-0.669178
C	-3.235423	-2.738384	-1.359801
N	-3.596832	-1.691250	-0.418093
C	-4.709597	-4.268075	-0.077656
H	-6.288125	0.032510	2.526435
H	-5.385578	-1.269626	3.299318
H	-7.500747	-1.568668	1.106300
H	-7.641869	-2.132527	2.774540
H	-5.913564	-3.801379	2.474985
H	-6.987493	-3.941647	1.083898
H	-4.726839	-5.113182	0.617627
H	-5.438644	-4.486751	-0.868352
H	-2.563016	-4.143117	0.122490
H	-3.115112	-4.906179	-1.371536
H	-3.895510	-2.719336	-2.237628
H	-2.224876	-2.527288	-1.712391
H	-4.485423	0.101364	1.108884
O	5.576302	2.522580	0.720196
C	5.092052	1.418432	0.802759
O	-2.186031	0.551836	-0.612162

C	-1.206389	0.457635	0.379560
H	-1.094021	-0.595341	0.705410
H	-1.520784	1.011048	1.281334
C	0.168835	0.959857	-0.082922
H	0.449130	0.415363	-0.993498
H	0.084025	2.014540	-0.369882
C	1.261843	0.800264	0.979256
H	1.357232	-0.259222	1.251218
H	0.948272	1.320749	1.891633
C	2.625174	1.322090	0.510250
H	2.882692	0.825265	-0.431727
H	2.560625	2.393026	0.284907
C	3.785656	1.087793	1.508689
H	3.807753	0.027918	1.774484
C	3.646441	1.938274	2.789843
H	3.749436	2.994738	2.523723
C	4.627066	1.597738	3.818420
H	2.641902	1.811181	3.201998
C	5.435839	1.297016	4.656102
H	6.152014	1.042145	5.401133
O	5.625155	0.325540	0.222523
C	6.846146	0.541251	-0.542923
C	7.278545	-0.780885	-1.108774
H	7.595909	0.966026	0.126585
H	6.639036	1.273024	-1.325229
C	6.924264	-1.148772	-2.409588
C	8.027714	-1.672177	-0.333908
C	7.312318	-2.382114	-2.929247
H	6.342684	-0.464371	-3.020304
C	8.415629	-2.906215	-0.848909
H	8.307597	-1.396283	0.678527
H	7.034111	-2.653558	-3.942474
C	8.058804	-3.263149	-2.149082
H	8.999218	-3.587701	-0.238413
H	8.364259	-4.223000	-2.553049
H	-3.093872	-0.752265	-0.499629

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I2, in toluene

O	3.885954	-1.634428	0.828294
O	4.237506	-1.337932	-1.368278
C	3.303104	-1.756820	-0.401493

C	2.817212	-3.204313	-0.580282
H	2.021000	-3.225499	-1.329261
H	2.363597	-3.496938	0.369320
C	3.920518	-4.202126	-0.968160
H	4.837748	-3.964811	-0.420330
H	3.616505	-5.201636	-0.639519
C	4.188841	-4.258365	-2.480681
H	3.246459	-4.502919	-2.989139
H	4.869042	-5.090449	-2.695004
C	4.772099	-2.978132	-3.092597
H	5.809964	-2.847659	-2.765702
H	4.799727	-3.078352	-4.184982
C	4.021718	-1.696140	-2.737959
H	2.951319	-1.768130	-2.955903
H	4.416004	-0.861061	-3.322377
N	5.075108	3.203183	0.828933
C	4.462121	1.982211	0.651303
N	4.729202	0.909540	1.339192
C	5.704413	1.008584	2.413846
C	6.827083	1.985877	2.072640
C	6.218075	3.340472	1.733792
C	3.428667	4.294030	-0.679292
C	3.322985	2.922371	-1.331929
N	3.464926	1.917788	-0.293931
C	4.766446	4.398146	0.042411
H	6.110759	0.010178	2.600177
H	5.217495	1.321702	3.351130
H	7.384567	1.603854	1.211155
H	7.532870	2.095226	2.901429
H	5.901000	3.859664	2.648847
H	6.960871	3.982631	1.246887
H	4.766746	5.261095	0.718189
H	5.572250	4.569796	-0.686925
H	2.604863	4.414927	0.030262
H	3.352856	5.092989	-1.421659
H	4.085888	2.819191	-2.119808
H	2.348441	2.785659	-1.805493
H	4.207030	-0.687320	0.960647
O	-5.655276	-2.557705	0.402845
C	-5.122591	-1.493922	0.614187
O	2.204789	-0.815675	-0.561057
C	1.197053	-0.798475	0.460177
H	1.144900	0.229521	0.835738
H	1.507673	-1.425378	1.298809

C	-0.161596	-1.223461	-0.089084
H	-0.395662	-0.605814	-0.963896
H	-0.104164	-2.257917	-0.445222
C	-1.277455	-1.094259	0.954248
H	-1.329816	-0.056905	1.307800
H	-1.020234	-1.701991	1.829084
C	-2.646279	-1.507002	0.400657
H	-2.850322	-0.915082	-0.498319
H	-2.623256	-2.555117	0.080521
C	-3.823650	-1.307180	1.385517
H	-3.799027	-0.279125	1.755248
C	-3.772760	-2.286547	2.578338
H	-3.926427	-3.303566	2.204712
C	-4.765720	-1.990980	3.608840
H	-2.776962	-2.260521	3.029010
C	-5.583110	-1.725506	4.449867
H	-6.307319	-1.502089	5.197314
O	-5.583576	-0.320661	0.141804
C	-6.796608	-0.388239	-0.663753
C	-7.152700	1.008518	-1.084815
H	-7.578929	-0.847117	-0.056790
H	-6.608998	-1.038030	-1.519693
C	-6.845252	1.466418	-2.368392
C	-7.785784	1.877275	-0.189465
C	-7.166259	2.766821	-2.754207
H	-6.353625	0.800622	-3.071720
C	-8.104511	3.177638	-0.569985
H	-8.028315	1.531285	0.810970
H	-6.925885	3.108593	-3.755733
C	-7.795850	3.624682	-1.854936
H	-8.597342	3.841376	0.133021
H	-8.048069	4.636986	-2.153860
H	3.143702	0.976333	-0.499939

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure TS2r, in toluene

O	3.968674	-1.614043	0.857838
O	4.280191	-1.261022	-1.336555
C	3.387248	-1.761914	-0.369677
C	3.008819	-3.239702	-0.567138
H	2.198233	-3.308079	-1.298017
H	2.603595	-3.585963	0.386021

C	4.175874	-4.142559	-0.998843
H	5.083074	-3.847296	-0.462622
H	3.954631	-5.168721	-0.686573
C	4.418901	-4.147689	-2.516620
H	3.486555	-4.446542	-3.014433
H	5.151233	-4.925441	-2.761109
C	4.900388	-2.817037	-3.108713
H	5.932169	-2.621083	-2.795629
H	4.915427	-2.890977	-4.203442
C	4.067788	-1.600228	-2.711659
H	3.001725	-1.743353	-2.914971
H	4.392003	-0.725514	-3.281044
N	4.860476	3.284406	0.869176
C	4.317182	2.029587	0.701196
N	4.666719	0.972184	1.375281
C	5.663738	1.124232	2.423278
C	6.715314	2.169717	2.058585
C	6.016395	3.486505	1.744890
C	3.109606	4.280736	-0.585503
C	3.068797	2.908447	-1.243974
N	3.299388	1.909145	-0.216663
C	4.458439	4.462283	0.099329
H	6.134803	0.151310	2.591190
H	5.184970	1.401978	3.375787
H	7.271389	1.826594	1.180016
H	7.435350	2.317693	2.868911
H	5.692724	3.980746	2.671404
H	6.705779	4.175103	1.243109
H	4.425638	5.320343	0.780501
H	5.231582	4.685858	-0.650950
H	2.300411	4.347772	0.147595
H	2.964499	5.077231	-1.320156
H	3.814478	2.855469	-2.053049
H	2.091544	2.715533	-1.691744
H	4.229699	-0.649803	0.997442
O	-5.663660	-2.606255	0.212285
C	-5.115740	-1.568506	0.500259
O	2.220579	-0.905178	-0.509757
C	1.218917	-0.983429	0.514305
H	1.188185	-0.010975	1.019093
H	1.506224	-1.720304	1.267134
C	-0.142237	-1.307552	-0.092002
H	-0.351257	-0.587750	-0.891795
H	-0.100037	-2.294642	-0.566389

C	-1.270058	-1.273394	0.945689
H	-1.311273	-0.279192	1.407898
H	-1.035082	-1.976006	1.753109
C	-2.636613	-1.602110	0.333067
H	-2.808139	-0.930849	-0.515534
H	-2.631314	-2.619461	-0.075082
C	-3.830107	-1.455620	1.307663
H	-3.798858	-0.456263	1.748842
C	-3.816424	-2.515891	2.430031
H	-3.975141	-3.502373	1.983802
C	-4.826938	-2.278273	3.458466
H	-2.830146	-2.534712	2.901437
C	-5.658128	-2.059724	4.299464
H	-6.394875	-1.878041	5.045970
O	-5.544321	-0.359228	0.092819
C	-6.740246	-0.352075	-0.740720
C	-7.055926	1.074695	-1.086532
H	-7.545995	-0.826837	-0.178273
H	-6.547598	-0.955664	-1.628776
C	-6.691817	1.605160	-2.326711
C	-7.706361	1.898926	-0.162111
C	-6.974045	2.933369	-2.641361
H	-6.186209	0.974453	-3.052116
C	-7.986787	3.226759	-0.471504
H	-7.992860	1.496395	0.805002
H	-6.689808	3.331762	-3.609941
C	-7.621462	3.746440	-1.713480
H	-8.493734	3.855476	0.253308
H	-7.843739	4.780356	-1.957100
H	3.035258	0.950521	-0.424474

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I2r, in toluene

O	3.896686	-1.323748	1.280443
O	4.679606	-1.575764	-0.806816
C	3.770918	-2.076812	0.146035
C	3.985197	-3.556913	0.507297
H	3.455409	-4.185571	-0.215314
H	3.501184	-3.711512	1.473602
C	5.458784	-3.987244	0.585669
H	6.045736	-3.198018	1.066020
H	5.526922	-4.862060	1.241119

C	6.066633	-4.363405	-0.775152
H	5.444394	-5.148019	-1.226413
H	7.051277	-4.817235	-0.615465
C	6.216028	-3.205539	-1.769839
H	7.009803	-2.527401	-1.436296
H	6.532553	-3.600797	-2.743353
C	4.955284	-2.367824	-1.968091
H	4.087435	-2.981046	-2.230627
H	5.106038	-1.653471	-2.781510
N	3.337747	3.250497	-0.578296
C	3.199066	1.913565	-0.277575
N	3.587890	1.355313	0.831680
C	4.165128	2.204381	1.862121
C	4.980095	3.348916	1.263674
C	4.097132	4.137965	0.305125
C	1.925012	2.984049	-2.606288
C	2.419255	1.543830	-2.593384
N	2.555894	1.128794	-1.208614
C	2.913509	3.855742	-1.841637
H	4.794893	1.582266	2.504730
H	3.375614	2.615530	2.510913
H	5.836305	2.933591	0.722082
H	5.370490	4.014760	2.039039
H	3.403022	4.782006	0.862504
H	4.707823	4.798152	-0.321120
H	2.466451	4.831563	-1.619783
H	3.799418	4.050276	-2.464515
H	0.938961	3.026084	-2.134443
H	1.824835	3.359202	-3.628254
H	3.367289	1.464436	-3.148419
H	1.703118	0.877184	-3.078407
H	3.791543	-0.346662	1.059752
O	-5.458886	-1.232044	-1.323931
C	-4.855781	-0.867408	-0.342121
O	2.477151	-1.874107	-0.481781
C	1.330055	-2.176466	0.317092
H	1.426405	-1.690693	1.292997
H	1.261500	-3.259647	0.482756
C	0.092092	-1.679833	-0.416509
H	0.187062	-0.600171	-0.573770
H	0.060592	-2.142278	-1.409964
C	-1.203593	-1.985682	0.343147
H	-1.157608	-1.536031	1.342550
H	-1.282508	-3.067813	0.496784

C	-2.442879	-1.458372	-0.389433
H	-2.315619	-0.382876	-0.555007
H	-2.517413	-1.915992	-1.382686
C	-3.776738	-1.675422	0.364915
H	-3.674519	-1.283442	1.379688
C	-4.187945	-3.163126	0.424175
H	-4.403842	-3.508047	-0.591778
C	-5.348261	-3.406930	1.278252
H	-3.347485	-3.758953	0.790308
C	-6.299083	-3.587979	1.991743
H	-7.143192	-3.756600	2.617952
O	-5.021436	0.338374	0.231864
C	-5.990709	1.222341	-0.405190
C	-6.030604	2.504652	0.374728
H	-6.957294	0.716413	-0.413598
H	-5.682985	1.380850	-1.439963
C	-5.203965	3.576021	0.024447
C	-6.880801	2.638061	1.476689
C	-5.226623	4.759423	0.759044
H	-4.540028	3.483068	-0.830123
C	-6.905944	3.819310	2.213820
H	-7.526148	1.811116	1.757962
H	-4.582463	5.585177	0.474642
C	-6.078312	4.882731	1.855615
H	-7.572412	3.911385	3.065256
H	-6.099330	5.804962	2.427252
H	2.617783	0.132912	-1.022375

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure TS23, in toluene

O	-3.874684	-0.695517	-1.620780
O	-4.845281	-0.621509	0.403487
C	-4.024791	-1.395890	-0.454907
C	-4.592495	-2.785891	-0.787036
H	-4.316340	-3.485367	0.008165
H	-4.074626	-3.116596	-1.689718
C	-6.112002	-2.824463	-1.012747
H	-6.419919	-1.939101	-1.577845
H	-6.345511	-3.687857	-1.644906
C	-6.926239	-2.950277	0.284634
H	-6.584127	-3.844861	0.822261
H	-7.976790	-3.135267	0.033435

C	-6.853057	-1.740736	1.224800
H	-7.395702	-0.894495	0.788195
H	-7.359622	-1.982641	2.167657
C	-5.439022	-1.260230	1.541199
H	-4.797471	-2.068326	1.906188
H	-5.473122	-0.495253	2.321295
N	-2.408140	3.814724	-0.056284
C	-2.715051	2.476676	-0.163170
N	-2.917793	1.845173	-1.282828
C	-2.752006	2.582407	-2.525856
C	-3.195243	4.037247	-2.386567
C	-2.430324	4.680969	-1.236798
C	-1.929389	3.552837	2.368563
C	-2.913849	2.393283	2.300307
N	-2.761335	1.752178	1.006645
C	-2.205658	4.510127	1.215636
H	-3.333311	2.078571	-3.303554
H	-1.702130	2.549227	-2.857529
H	-4.270009	4.066261	-2.178942
H	-3.021224	4.601632	-3.307489
H	-1.400333	4.912295	-1.541408
H	-2.897100	5.630525	-0.951501
H	-1.369285	5.207838	1.093818
H	-3.093650	5.119855	1.440106
H	-0.911395	3.158899	2.298011
H	-2.016864	4.090476	3.316394
H	-3.939746	2.757821	2.468344
H	-2.701270	1.651993	3.073531
H	-3.549804	0.237456	-1.428577
O	5.037999	-2.549910	1.756747
C	4.574455	-1.995084	0.788483
O	-2.790360	-1.498204	0.279926
C	-1.669622	-2.036808	-0.420119
H	-1.576334	-1.547273	-1.394150
H	-1.809650	-3.112921	-0.594284
C	-0.426344	-1.798432	0.424857
H	-0.331516	-0.722484	0.605588
H	-0.566895	-2.270169	1.404404
C	0.846229	-2.336227	-0.238363
H	0.980180	-1.855779	-1.215376
H	0.721930	-3.406613	-0.437787
C	2.095936	-2.095783	0.616656
H	2.161362	-1.026101	0.843683
H	1.998154	-2.609961	1.579833

C	3.423129	-2.527120	-0.053076
H	3.484584	-2.059077	-1.038652
C	3.543781	-4.059615	-0.200221
H	3.611961	-4.503516	0.797688
C	4.696551	-4.472868	-0.997406
H	2.634908	-4.453989	-0.662485
C	5.644001	-4.792873	-1.665167
H	6.483817	-5.085833	-2.249937
O	4.984586	-0.789978	0.350498
C	6.051085	-0.159636	1.117586
C	6.398661	1.140472	0.450789
H	6.898490	-0.846952	1.144409
H	5.703469	-0.013202	2.141335
C	5.969022	2.355914	0.988401
C	7.152778	1.150045	-0.727785
C	6.288830	3.561060	0.364688
H	5.382103	2.360509	1.902238
C	7.469832	2.350811	-1.355670
H	7.490482	0.210252	-1.154444
H	5.952305	4.498586	0.795389
C	7.039111	3.560093	-0.808944
H	8.056427	2.345191	-2.268657
H	7.290052	4.497030	-1.295676
H	-3.153528	0.825603	0.892606

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I3, in toluene

O	3.766563	-0.780881	1.620008
O	4.776659	-0.763746	-0.389480
C	3.918081	-1.506798	0.470686
C	4.468595	-2.896173	0.838119
H	4.187199	-3.610287	0.057865
H	3.941197	-3.199390	1.744909
C	5.986274	-2.951615	1.072214
H	6.305674	-2.056396	1.614895
H	6.203908	-3.801423	1.727999
C	6.803856	-3.125302	-0.217807
H	6.447459	-4.026843	-0.733983
H	7.849743	-3.323111	0.042817
C	6.757918	-1.939219	-1.189212
H	7.320078	-1.094777	-0.774210
H	7.258508	-2.216507	-2.125434

C	5.355148	-1.435591	-1.517739
H	4.693770	-2.234611	-1.864843
H	5.404652	-0.688532	-2.314438
N	2.615853	3.837010	0.145390
C	2.968103	2.507122	0.209671
N	2.814969	1.746922	1.256332
C	2.169676	2.316703	2.428391
C	2.530692	3.789107	2.613523
C	2.170807	4.550877	1.343928
C	2.998426	3.856031	-2.308406
C	3.991871	2.735499	-2.031183
N	3.479652	1.939657	-0.931580
C	2.804868	4.675613	-1.038712
H	2.473048	1.735156	3.303859
H	1.074981	2.215235	2.356890
H	3.605670	3.873120	2.804557
H	2.007746	4.228645	3.468102
H	1.086077	4.717473	1.289776
H	2.643240	5.539842	1.344959
H	1.929410	5.327436	-1.138241
H	3.671874	5.335043	-0.882795
H	2.047320	3.417833	-2.624543
H	3.352122	4.507640	-3.111794
H	4.986207	3.157731	-1.814691
H	4.098896	2.084299	-2.901559
H	3.443010	0.151403	1.414144
O	-5.116366	-2.472405	-1.844457
C	-4.661064	-1.927244	-0.866765
O	2.702563	-1.608182	-0.281163
C	1.568120	-2.133278	0.404532
H	1.476485	-1.654136	1.384090
H	1.683682	-3.214502	0.566771
C	0.337080	-1.857384	-0.446803
H	0.273954	-0.777975	-0.620515
H	0.472852	-2.324884	-1.428993
C	-0.954622	-2.365581	0.202379
H	-1.086487	-1.884557	1.179482
H	-0.858808	-3.439235	0.399991
C	-2.189258	-2.092593	-0.664652
H	-2.221485	-1.022382	-0.896655
H	-2.097671	-2.613093	-1.624946
C	-3.534772	-2.481665	-0.006064
H	-3.595243	-2.002769	0.974301
C	-3.699249	-4.008847	0.154610

H	-3.763991	-4.461672	-0.839538
C	-4.875327	-4.381230	0.937825
H	-2.808810	-4.422734	0.635366
C	-5.842009	-4.665753	1.593990
H	-6.698834	-4.927787	2.168663
O	-5.058050	-0.716132	-0.433631
C	-6.096620	-0.063947	-1.221646
C	-6.432925	1.239950	-0.557084
H	-6.956128	-0.734424	-1.269629
H	-5.722195	0.078658	-2.236535
C	-5.869281	2.436384	-1.007739
C	-7.304426	1.271857	0.536587
C	-6.171746	3.643969	-0.381154
H	-5.190967	2.423257	-1.855884
C	-7.606789	2.475756	1.166689
H	-7.746961	0.347237	0.895250
H	-5.730539	4.566739	-0.743847
C	-7.040926	3.665211	0.707731
H	-8.286281	2.487598	2.012740
H	-7.279467	4.604780	1.195653
H	3.857825	1.007386	-0.796667

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure TS3r, in toluene

O	4.031993	-1.372885	0.978038
O	4.410928	-0.736863	-1.144819
C	3.834858	-1.755766	-0.317241
C	4.466998	-3.138502	-0.533776
H	3.972066	-3.620482	-1.381147
H	4.197366	-3.720160	0.351439
C	5.988659	-3.141228	-0.738875
H	6.451202	-2.405369	-0.073277
H	6.380633	-4.117725	-0.434596
C	6.407326	-2.894338	-2.197306
H	5.921164	-3.650623	-2.827963
H	7.484744	-3.067656	-2.298594
C	6.083984	-1.499392	-2.748146
H	6.741176	-0.754205	-2.285284
H	6.297181	-1.476329	-3.824347
C	4.645638	-1.036230	-2.527379
H	3.911925	-1.761251	-2.891355
H	4.469291	-0.102400	-3.068437

N	3.173208	3.525034	1.291713
C	3.327473	2.232049	0.848282
N	3.327139	1.177043	1.614387
C	3.089218	1.362966	3.037544
C	3.698377	2.667200	3.547269
C	3.147906	3.825793	2.724950
C	2.930008	4.331666	-1.044489
C	3.784210	3.125658	-1.412016
N	3.448188	2.041931	-0.506669
C	3.182292	4.695776	0.413278
H	3.513323	0.507134	3.570505
H	2.009225	1.355260	3.254474
H	4.787127	2.620771	3.440194
H	3.477002	2.828633	4.606378
H	2.119706	4.061706	3.031792
H	3.743916	4.730107	2.891703
H	2.415437	5.393676	0.767814
H	4.148176	5.213744	0.508820
H	1.876056	4.080192	-1.194548
H	3.164493	5.189799	-1.679744
H	4.852308	3.391525	-1.367550
H	3.574757	2.794695	-2.431667
H	3.782518	-0.407307	1.125576
O	-5.477989	-2.932020	-0.281620
C	-4.891743	-1.947337	0.101635
O	2.452435	-1.839687	-0.695894
C	1.461426	-1.748166	0.326833
H	1.495620	-0.764562	0.807057
H	1.641526	-2.501792	1.102725
C	0.107524	-1.972591	-0.331724
H	-0.025270	-1.227368	-1.124128
H	0.110987	-2.952504	-0.822515
C	-1.052303	-1.889158	0.666474
H	-1.049989	-0.904563	1.150308
H	-0.890212	-2.622584	1.464356
C	-2.413650	-2.119043	-0.000107
H	-2.525315	-1.400573	-0.819601
H	-2.446107	-3.114703	-0.457357
C	-3.626856	-1.960334	0.948062
H	-3.551899	-0.993982	1.452724
C	-3.709067	-3.087792	2.000301
H	-3.913876	-4.032465	1.487299
C	-4.732617	-2.853800	3.016582
H	-2.739486	-3.197488	2.493433

C	-5.573515	-2.638352	3.848751
H	-6.319563	-2.459326	4.586589
O	-5.253838	-0.690841	-0.218601
C	-6.422720	-0.563499	-1.080265
C	-6.668041	0.899041	-1.315853
H	-7.264535	-1.046617	-0.581506
H	-6.227476	-1.100464	-2.009657
C	-6.199954	1.521804	-2.475832
C	-7.354693	1.663589	-0.366951
C	-6.415140	2.882349	-2.687444
H	-5.665728	0.937519	-3.219378
C	-7.569422	3.023464	-0.573680
H	-7.721953	1.189172	0.538298
H	-6.050176	3.352835	-3.594702
C	-7.100178	3.635429	-1.735937
H	-8.105975	3.605264	0.168809
H	-7.271050	4.694507	-1.900034
H	3.725725	1.098737	-0.763390

80 atoms
addition of another ε-CL unit to the 3-isomer chain end, structure I3r, in toluene

O	4.145795	-0.734632	1.724873
O	3.606156	-1.859716	-0.145857
C	3.492878	-1.858587	1.291332
C	4.118916	-3.091261	1.957223
H	3.368320	-3.884554	2.009296
H	4.321332	-2.788115	2.986568
C	5.396958	-3.612760	1.287074
H	6.020847	-2.767964	0.977460
H	5.978270	-4.162997	2.034595
C	5.132781	-4.557143	0.102625
H	4.489028	-5.375576	0.451360
H	6.075234	-5.026485	-0.201706
C	4.492659	-3.906251	-1.130477
H	5.222399	-3.258242	-1.629970
H	4.223359	-4.685699	-1.854414
C	3.253643	-3.063480	-0.838553
H	2.498892	-3.615525	-0.270597
H	2.784799	-2.746923	-1.774949
N	4.105880	2.969883	-1.614039
C	3.920354	1.768321	-0.970291
N	3.958093	1.598006	0.319829

C	4.154367	2.768811	1.160687
C	5.078302	3.791424	0.502482
C	4.517777	4.159864	-0.865809
C	3.394501	1.964873	-3.771945
C	3.901372	0.656613	-3.179398
N	3.629829	0.674520	-1.753197
C	4.079441	3.130311	-3.068684
H	4.568369	2.437839	2.117411
H	3.188284	3.244750	1.392309
H	6.075303	3.353147	0.388729
H	5.181718	4.692877	1.113582
H	3.662380	4.841200	-0.761151
H	5.272955	4.687985	-1.458655
H	3.562143	4.068484	-3.298991
H	5.109304	3.239200	-3.440145
H	2.311158	2.022512	-3.631787
H	3.597678	2.017330	-4.844742
H	4.973470	0.532309	-3.399860
H	3.379642	-0.198249	-3.615453
H	4.015798	0.059789	1.123589
O	-5.492799	0.436225	2.734331
C	-4.869822	0.515738	1.702093
O	2.120128	-1.898366	1.647649
C	1.356273	-0.724062	1.368932
H	1.446145	-0.457096	0.309861
H	1.741895	0.114776	1.957413
C	-0.092373	-1.015884	1.730130
H	-0.443240	-1.866604	1.134770
H	-0.135302	-1.331335	2.778771
C	-1.008693	0.191898	1.507148
H	-0.953247	0.506604	0.457561
H	-0.636709	1.035502	2.099061
C	-2.468640	-0.109831	1.864676
H	-2.794618	-0.982191	1.287771
H	-2.547728	-0.392353	2.920795
C	-3.450708	1.051937	1.578219
H	-3.307772	1.382914	0.546565
C	-3.252173	2.246020	2.536946
H	-3.533310	1.934683	3.547627
C	-4.027506	3.424922	2.156989
H	-2.192806	2.514398	2.570391
C	-4.665456	4.387314	1.821014
H	-5.232294	5.241991	1.535953
O	-5.333887	0.083804	0.514334

C	-6.664475	-0.511987	0.526445
C	-7.002264	-0.918356	-0.879007
H	-7.363244	0.227950	0.919874
H	-6.655115	-1.363852	1.208063
C	-6.776290	-2.226525	-1.315629
C	-7.530167	0.013692	-1.778228
C	-7.073682	-2.599118	-2.624990
H	-6.367072	-2.958588	-0.625508
C	-7.826952	-0.354384	-3.087804
H	-7.708907	1.033039	-1.448912
H	-6.897394	-3.619298	-2.950267
C	-7.599490	-1.662913	-3.513392
H	-8.239083	0.377349	-3.775107
H	-7.834352	-1.951980	-4.532719
H	3.664508	-0.203543	-1.244064

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure TS3r2, in toluene

O	3.453585	0.699855	-1.839154
O	3.215031	1.722764	0.150846
C	2.900060	1.811977	-1.248583
C	3.413342	3.099401	-1.913472
H	2.691524	3.905489	-1.752675
H	3.403549	2.884632	-2.983984
C	4.812576	3.538111	-1.461849
H	5.449873	2.656905	-1.329611
H	5.270298	4.126506	-2.263959
C	4.804606	4.395904	-0.186215
H	4.151660	5.261952	-0.357247
H	5.807335	4.804848	-0.017870
C	4.352372	3.670977	1.087821
H	5.123616	2.959816	1.405809
H	4.246143	4.398823	1.902044
C	3.043260	2.896032	0.955556
H	2.232800	3.511658	0.553870
H	2.719298	2.538031	1.936839
N	5.854367	-2.318008	1.321187
C	5.058463	-1.350126	0.752899
N	5.120603	-0.964868	-0.488473
C	6.059475	-1.638718	-1.371842
C	7.333047	-2.052451	-0.637614
C	6.958386	-2.911703	0.563987

C	4.458249	-2.310028	3.373937
C	4.142444	-0.867888	3.000525
N	4.094125	-0.778116	1.552162
C	5.776720	-2.716316	2.727152
H	6.295259	-0.963642	-2.199358
H	5.592783	-2.527292	-1.825129
H	7.861230	-1.154569	-0.299618
H	8.011722	-2.607960	-1.291500
H	6.680586	-3.924570	0.241678
H	7.814331	-3.017463	1.239882
H	5.905213	-3.803146	2.780710
H	6.618341	-2.271866	3.279420
H	3.648998	-2.954769	3.018978
H	4.532262	-2.429364	4.457990
H	4.895408	-0.192777	3.438073
H	3.169082	-0.566650	3.394395
H	4.034407	0.151403	-1.229065
O	-5.891308	-1.092381	-2.562277
C	-5.335942	-0.985634	-1.494493
O	1.498085	1.842085	-1.424043
C	0.792960	0.653246	-1.060234
H	0.851548	0.501549	0.024922
H	1.258300	-0.208619	-1.545944
C	-0.653315	0.815808	-1.502927
H	-1.072603	1.713162	-1.033410
H	-0.669256	0.993644	-2.583947
C	-1.513107	-0.405071	-1.158503
H	-1.495394	-0.573509	-0.074330
H	-1.065356	-1.295367	-1.613792
C	-2.966588	-0.243528	-1.618493
H	-3.367225	0.680903	-1.188235
H	-3.005051	-0.118373	-2.706693
C	-3.901367	-1.408174	-1.211346
H	-3.807264	-1.571509	-0.134849
C	-3.579555	-2.718288	-1.962750
H	-3.800012	-2.576853	-3.025224
C	-4.326270	-3.869165	-1.459489
H	-2.509540	-2.929099	-1.885742
C	-4.943352	-4.805360	-1.024949
H	-5.490006	-5.638937	-0.651661
O	-5.901942	-0.420619	-0.411421
C	-7.260047	0.079100	-0.587723
C	-7.711314	0.664735	0.719250
H	-7.888802	-0.755042	-0.903507

H	-7.254694	0.820090	-1.388403
C	-7.621758	2.039563	0.952561
C	-8.211167	-0.162350	1.730395
C	-8.025889	2.580536	2.171634
H	-7.235167	2.691141	0.174348
C	-8.613569	0.374097	2.950408
H	-8.284206	-1.232305	1.559190
H	-7.954980	3.650487	2.338454
C	-8.522233	1.748023	3.172830
H	-9.002161	-0.277842	3.726071
H	-8.839675	2.167722	4.121958
H	3.681630	0.049829	1.134546

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I3r2, in toluene

O	3.197672	-0.838746	-1.432382
O	2.775474	1.165658	-0.512112
C	2.659383	0.391494	-1.727563
C	3.320643	1.075127	-2.940801
H	2.598364	1.758713	-3.397210
H	3.481353	0.273216	-3.664553
C	4.633916	1.817104	-2.652753
H	5.239461	1.245727	-1.941225
H	5.213773	1.862130	-3.580963
C	4.429210	3.256015	-2.151460
H	3.814074	3.793705	-2.885257
H	5.395292	3.773403	-2.133353
C	3.781020	3.381777	-0.766897
H	4.489776	3.062679	0.006145
H	3.557048	4.436851	-0.564995
C	2.500701	2.569983	-0.582617
H	1.768772	2.768891	-1.371585
H	2.026661	2.828406	0.368444
N	6.754088	-0.768001	1.924444
C	5.688157	-0.494471	1.099175
N	5.608277	-0.839954	-0.156195
C	6.690642	-1.631556	-0.719060
C	8.043931	-1.246176	-0.125330
C	7.975906	-1.373933	1.391536
C	5.437874	-0.069283	3.908215
C	4.681496	0.829441	2.938834
N	4.617282	0.160714	1.653318

C	6.814825	-0.376439	3.333062
H	6.693340	-1.487793	-1.803470
H	6.511426	-2.705575	-0.553389
H	8.276328	-0.211700	-0.399548
H	8.848011	-1.878628	-0.512901
H	8.022949	-2.429841	1.691417
H	8.832993	-0.873667	1.856317
H	7.284283	-1.193359	3.892229
H	7.472341	0.499007	3.442093
H	4.873858	-0.995658	4.050828
H	5.548919	0.410445	4.884157
H	5.176643	1.811507	2.873830
H	3.659955	1.004686	3.283537
H	4.096545	-0.767328	-0.988467
O	-6.405764	-2.017155	-1.695406
C	-5.760707	-1.520156	-0.802864
O	1.308534	0.241647	-2.076735
C	0.510916	-0.555681	-1.193676
H	0.623510	-0.194790	-0.165633
H	0.855080	-1.592763	-1.225222
C	-0.934527	-0.444577	-1.654191
H	-1.241019	0.607259	-1.621305
H	-0.992559	-0.752847	-2.704285
C	-1.886614	-1.294491	-0.805889
H	-1.820540	-0.983537	0.244309
H	-1.555585	-2.338455	-0.837000
C	-3.342499	-1.181378	-1.272831
H	-3.625957	-0.123282	-1.275171
H	-3.433154	-1.526899	-2.309170
C	-4.358943	-1.949754	-0.393688
H	-4.210786	-1.654794	0.648198
C	-4.216721	-3.481752	-0.522363
H	-4.495167	-3.776450	-1.538756
C	-5.033630	-4.218802	0.439233
H	-3.169042	-3.762985	-0.385771
C	-5.705280	-4.806511	1.245187
H	-6.301538	-5.335841	1.950385
O	-6.179580	-0.467368	-0.075210
C	-7.487596	0.072301	-0.425738
C	-7.765275	1.238432	0.478619
H	-8.224656	-0.723836	-0.308074
H	-7.470903	0.364502	-1.476689
C	-7.507253	2.544852	0.055047
C	-8.269552	1.031653	1.766734

C	-7.749993	3.626118	0.899983
H	-7.116108	2.716985	-0.943476
C	-8.511159	2.109180	2.614540
H	-8.473056	0.020186	2.105779
H	-7.549252	4.635983	0.557147
C	-8.252085	3.409555	2.181748
H	-8.905030	1.935777	3.610766
H	-8.444067	4.250466	2.840361
H	3.918764	0.459468	0.980177

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure TS34, in toluene

O	3.367407	-0.200887	0.064220
O	2.823372	2.053610	-0.883373
C	4.122901	0.721234	-0.292750
C	4.934907	1.532980	0.708153
H	5.591857	2.218694	0.168544
H	5.592535	0.794244	1.182969
C	4.131505	2.280956	1.784448
H	3.171087	1.778979	1.935457
H	4.668607	2.201545	2.736678
C	3.922031	3.778810	1.498666
H	4.899988	4.220909	1.263294
H	3.594645	4.267890	2.425098
C	2.929960	4.139364	0.384409
H	1.908157	3.917762	0.720384
H	2.971923	5.225652	0.218856
C	3.144724	3.406310	-0.950407
H	4.189379	3.546967	-1.284138
H	2.526549	3.909706	-1.718584
N	-1.469147	0.357098	0.420330
C	-0.147902	0.577837	0.201974
N	0.775711	-0.081991	0.918817
C	0.433222	-1.149964	1.846056
C	-0.891131	-0.820795	2.520414
C	-1.950216	-0.566507	1.454984
C	-1.950026	1.479503	-1.728143
C	-0.656470	2.251420	-1.504867
N	0.266232	1.452179	-0.712689
C	-2.501484	1.021028	-0.384057
H	1.241780	-1.229376	2.574185
H	0.368241	-2.114562	1.324951

H	-0.770238	0.068021	3.146664
H	-1.212079	-1.641646	3.165705
H	-2.259260	-1.508731	0.984527
H	-2.843163	-0.122600	1.904454
H	-3.315583	0.305672	-0.530337
H	-2.912857	1.869896	0.176993
H	-1.753212	0.611065	-2.363889
H	-2.690490	2.102130	-2.235612
H	-0.866696	3.207931	-1.007840
H	-0.165703	2.481599	-2.452288
H	1.761897	-0.020798	0.609114
O	7.137273	-2.199204	-8.618156
C	6.094820	-1.630759	-8.393629
O	4.849722	0.606931	-1.457312
C	4.279402	-0.234604	-2.461008
H	3.291085	0.155497	-2.723717
H	4.148623	-1.245611	-2.063330
C	5.216595	-0.228034	-3.658213
H	5.335597	0.802369	-4.011167
H	6.208425	-0.561512	-3.331421
C	4.716433	-1.118812	-4.800366
H	3.727845	-0.774047	-5.128773
H	4.575314	-2.137561	-4.421991
C	5.673383	-1.122310	-5.998074
H	5.834122	-0.087078	-6.318185
H	6.654102	-1.505961	-5.693862
C	5.173396	-1.930649	-7.219923
H	4.171552	-1.582155	-7.483049
C	5.138072	-3.450944	-6.951574
H	6.163508	-3.807020	-6.813150
C	4.499011	-4.211730	-8.023142
H	4.606352	-3.642787	-6.015780
C	3.961372	-4.819457	-8.910713
H	3.493463	-5.366218	-9.695001
O	5.630338	-0.604451	-9.130888
C	6.472257	-0.187434	-10.245608
C	5.784962	0.949055	-10.945944
H	6.616150	-1.047582	-10.901429
H	7.447070	0.103817	-9.851684
C	6.117073	2.273624	-10.649391
C	4.787258	0.697134	-11.893234
C	5.467496	3.328248	-11.287888
H	6.890295	2.480815	-9.915382
C	4.134625	1.748163	-12.531731

H	4.521419	-0.328862	-12.130271
H	5.737480	4.352278	-11.051022
C	4.474588	3.066780	-12.230103
H	3.364093	1.539515	-13.266902
H	3.969278	3.886822	-12.730062
H	1.317450	1.677784	-0.776669

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I4, in toluene

O	4.213459	1.623981	-0.867730
O	3.679386	0.795118	2.171046
C	3.710497	2.441859	-0.123172
C	4.461098	3.432911	0.735615
H	3.984167	3.439404	1.717329
H	4.262950	4.418992	0.297531
C	5.972943	3.194540	0.832173
H	6.328629	2.777326	-0.114964
H	6.458160	4.171438	0.933212
C	6.470532	2.320944	1.997569
H	6.109228	2.746321	2.943601
H	7.559984	2.439025	2.024408
C	6.155730	0.809271	1.968103
H	6.089931	0.451121	0.935466
H	7.002451	0.277127	2.421837
C	4.906133	0.365507	2.736864
H	4.957936	0.763893	3.758868
H	4.917112	-0.730102	2.819844
N	3.019459	-3.382415	-0.533025
C	3.240474	-2.060061	-0.221716
N	4.115833	-1.366984	-1.024432
C	4.514577	-1.848494	-2.334941
C	4.844712	-3.329722	-2.215771
C	3.627173	-4.068335	-1.674785
C	1.065873	-3.269845	0.970879
C	1.865440	-2.192433	1.699318
N	2.709653	-1.431198	0.789958
C	2.029674	-4.168517	0.206391
H	5.385838	-1.274129	-2.655891
H	3.727987	-1.697627	-3.091394
H	5.693966	-3.452656	-1.537324
H	5.125281	-3.750381	-3.184883
H	2.875881	-4.187039	-2.469701

H	3.907357	-5.078183	-1.354610
H	1.485068	-4.789813	-0.513405
H	2.543539	-4.854789	0.893518
H	0.370366	-2.793662	0.271474
H	0.472881	-3.870702	1.666609
H	2.473257	-2.663051	2.488596
H	1.196147	-1.494306	2.210098
H	4.105494	-0.363145	-0.882818
O	-5.445324	2.261646	-1.796993
C	-4.780832	1.358866	-1.346036
O	2.387076	2.635296	-0.029941
C	1.532448	1.758555	-0.801407
H	1.677601	0.735786	-0.445528
H	1.833002	1.805830	-1.851615
C	0.102491	2.228730	-0.601317
H	-0.130425	2.207195	0.468544
H	0.021155	3.274018	-0.919790
C	-0.900926	1.365108	-1.374179
H	-0.810931	0.320830	-1.051015
H	-0.641798	1.380901	-2.438772
C	-2.346631	1.832739	-1.169908
H	-2.559072	1.845524	-0.095503
H	-2.461512	2.865320	-1.519149
C	-3.409233	0.944828	-1.861372
H	-3.241533	-0.094077	-1.566765
C	-3.367859	1.059835	-3.400683
H	-3.670771	2.072273	-3.684593
C	-4.225819	0.087762	-4.074611
H	-2.340219	0.926229	-3.749473
C	-4.929863	-0.725910	-4.611483
H	-5.556908	-1.437544	-5.094695
O	-5.143802	0.623220	-0.279493
C	-6.415084	0.979533	0.340561
C	-6.634930	0.060081	1.506923
H	-7.198063	0.882309	-0.413066
H	-6.367593	2.025783	0.646078
C	-6.238814	0.436007	2.793469
C	-7.221338	-1.195465	1.318896
C	-6.425682	-0.424335	3.873322
H	-5.783013	1.409176	2.950984
C	-7.408570	-2.058532	2.395448
H	-7.532585	-1.497215	0.323097
H	-6.117030	-0.118860	4.867800
C	-7.011037	-1.673656	3.675527

H	-7.867749	-3.028983	2.237170
H	-7.160105	-2.343845	4.515969
H	3.333923	0.063750	1.602234

80 atoms
addition of another ε-CL unit to the 3-isomer chain end,
structure I5, in toluene

O	0.348644	-0.064222	-0.450000
O	7.776561	-1.940293	-1.572275
C	0.316107	-1.271376	-0.478435
C	1.497323	-2.183957	-0.731446
H	1.294750	-2.730159	-1.660749
H	1.508846	-2.947589	0.053725
C	2.834188	-1.448778	-0.811738
H	2.774130	-0.672908	-1.581433
H	3.014235	-0.920221	0.130512
C	4.007027	-2.387821	-1.110245
H	3.824851	-2.904984	-2.061913
H	4.049026	-3.173859	-0.344610
C	5.356192	-1.665508	-1.172472
H	5.320932	-0.873265	-1.930168
H	5.558301	-1.169629	-0.216257
C	6.521989	-2.601557	-1.498674
H	6.359771	-3.070206	-2.475230
H	6.560207	-3.414106	-0.757162
N	9.151351	1.721803	1.034962
C	8.649002	0.684916	0.282723
N	8.226473	0.987678	-0.993884
C	8.640925	2.197953	-1.679581
C	8.489427	3.362477	-0.709928
C	9.322158	3.087527	0.536307
C	10.038285	-0.005071	2.559817
C	8.860159	-0.846821	2.072314
N	8.507960	-0.542839	0.694949
C	9.710586	1.470276	2.364695
H	8.000409	2.330331	-2.554091
H	9.679793	2.138866	-2.041019
H	7.433795	3.468147	-0.443610
H	8.816621	4.300567	-1.165912
H	10.386737	3.265281	0.322596
H	9.043174	3.780382	1.338117
H	10.614704	2.079732	2.472770
H	9.002847	1.812600	3.132190

H	10.929676	-0.265084	1.979247
H	10.262534	-0.197480	3.613228
H	7.996656	-0.685162	2.737184
H	9.100169	-1.912071	2.139303
H	8.009321	0.167208	-1.548236
O	-7.751951	-1.493239	-1.423530
C	-7.453513	-1.036434	-0.344631
O	-0.813082	-1.987313	-0.291894
C	-2.027198	-1.233308	-0.065272
H	-2.200988	-0.579874	-0.924175
H	-1.888756	-0.597427	0.812680
C	-3.157481	-2.228229	0.127080
H	-3.218226	-2.872452	-0.756787
H	-2.917027	-2.879860	0.974366
C	-4.503130	-1.533561	0.362563
H	-4.722491	-0.875124	-0.486113
H	-4.434801	-0.881917	1.242052
C	-5.649666	-2.531610	0.557138
H	-5.745141	-3.164845	-0.331642
H	-5.408734	-3.198686	1.392631
C	-7.014749	-1.876326	0.847945
H	-6.926370	-1.218356	1.715228
C	-8.084705	-2.956605	1.138533
H	-8.225073	-3.564849	0.239429
C	-9.370412	-2.407241	1.562250
H	-7.704044	-3.626364	1.916670
C	-10.419926	-1.935892	1.911824
H	-11.353535	-1.528727	2.221294
O	-7.448786	0.277398	-0.063142
C	-7.859971	1.165362	-1.145236
C	-7.797507	2.576774	-0.636877
H	-8.868931	0.880126	-1.448062
H	-7.194874	1.006805	-1.995123
C	-6.724237	3.407014	-0.968960
C	-8.809658	3.075739	0.190115
C	-6.662178	4.713806	-0.487855
H	-5.932313	3.029857	-1.609434
C	-8.749182	4.378882	0.675097
H	-9.646894	2.437201	0.455889
H	-5.824571	5.349367	-0.756204
C	-7.674665	5.201386	0.335514
H	-9.541179	4.755221	1.314456
H	-7.629018	6.218893	0.710081
H	8.038771	-1.632635	-0.666554

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure I1, in toluene

O	-3.213170	-0.668834	-2.310576
O	-5.034498	-0.724753	-1.092115
C	-4.009604	-1.350114	-1.698946
C	-3.911554	-2.859537	-1.632468
H	-3.690581	-3.136135	-0.596338
H	-3.034616	-3.119735	-2.225213
C	-5.148374	-3.624837	-2.144113
H	-5.490039	-3.184511	-3.088203
H	-4.830068	-4.643480	-2.385985
C	-6.307901	-3.700800	-1.145486
H	-5.964532	-4.227701	-0.245988
H	-7.106774	-4.316774	-1.571938
C	-6.887245	-2.343727	-0.734812
H	-7.354201	-1.847506	-1.593618
H	-7.685559	-2.502572	-0.000685
C	-5.879701	-1.383652	-0.115200
H	-5.242799	-1.859394	0.633293
H	-6.391825	-0.550178	0.363877
N	-2.958948	3.796267	0.495831
C	-2.966688	2.439827	0.250438
N	-2.712804	2.038311	-1.032017
C	-2.422484	2.943300	-2.129645
C	-3.176806	4.251431	-1.925338
C	-2.826235	4.806912	-0.551932
C	-2.724556	3.216124	2.889546
C	-3.563834	2.005177	2.484252
N	-3.200426	1.530851	1.158203
C	-2.935578	4.322119	1.862385
H	-2.721765	2.449846	-3.055934
H	-1.344017	3.143312	-2.205048
H	-4.253383	4.066352	-1.992373
H	-2.912514	4.982026	-2.694690
H	-1.799820	5.203828	-0.557856
H	-3.485651	5.644995	-0.298115
H	-2.136119	5.070509	1.932125
H	-3.879444	4.849432	2.057486
H	-1.669881	2.923615	2.916698
H	-2.990524	3.584352	3.885023
H	-4.632383	2.273237	2.529738

H	-3.425317	1.183368	3.192568
H	-2.944834	1.080266	-1.262875
O	4.001989	0.614332	-1.795073
O	-2.791479	-1.193422	1.181527
C	4.340846	0.067868	-0.772331
C	3.413734	-0.497925	0.282170
H	3.560792	0.093971	1.194034
H	3.762396	-1.504623	0.535076
C	1.942208	-0.503617	-0.129576
H	1.641927	0.509322	-0.415485
H	1.819996	-1.115407	-1.030161
C	1.026087	-1.025939	0.982586
H	1.145650	-0.397005	1.874550
H	1.348342	-2.028515	1.280749
C	-0.448470	-1.042923	0.564547
H	-0.720880	-0.054355	0.179163
H	-0.596971	-1.740284	-0.269362
C	-1.467685	-1.382443	1.664074
H	-1.291036	-0.723389	2.527503
C	-1.416697	-2.844605	2.161274
H	-2.371710	-3.035414	2.660935
C	-0.334496	-3.170290	3.085970
H	-1.382273	-3.516932	1.295561
C	0.526492	-3.451745	3.877962
H	1.298165	-3.693779	4.569932
O	5.632880	-0.105422	-0.417695
C	6.625300	0.422266	-1.341991
C	7.985828	0.117547	-0.783118
H	6.459735	1.495664	-1.450850
H	6.470796	-0.042022	-2.317402
C	8.613588	1.013711	0.087082
C	8.635337	-1.077274	-1.106835
C	9.866123	0.723476	0.622839
H	8.117875	1.944929	0.345583
C	9.887989	-1.371365	-0.573301
H	8.156619	-1.780885	-1.781658
H	10.343939	1.429278	1.294598
C	10.505797	-0.470554	0.292950
H	10.382791	-2.300986	-0.835379
H	11.483136	-0.696750	0.706969
H	-2.951707	-0.213647	1.079130

80 atoms

addition of another ε-CL unit to the 7-isomer chain end,
structure TS12, in toluene

O	-4.119875	1.494545	1.387730
O	-4.310177	1.783416	-0.798792
C	-3.578381	1.990721	0.370583
C	-2.884882	3.350504	0.498037
H	-2.000858	3.406748	-0.140653
H	-2.540152	3.411630	1.531264
C	-3.818664	4.535986	0.183622
H	-4.818329	4.338529	0.586831
H	-3.446279	5.419549	0.713395
C	-3.896580	4.874502	-1.312663
H	-2.881827	5.100574	-1.666811
H	-4.473923	5.796872	-1.445687
C	-4.501608	3.780395	-2.201531
H	-5.577171	3.691758	-2.007729
H	-4.399289	4.074737	-3.253789
C	-3.886641	2.393087	-2.022654
H	-2.795497	2.406600	-2.074663
H	-4.245052	1.726657	-2.811747
N	-5.191813	-2.993490	-0.296161
C	-4.598143	-1.805990	-0.011562
N	-5.103937	-1.006500	0.930991
C	-6.268107	-1.366458	1.726720
C	-7.222641	-2.201006	0.882597
C	-6.468629	-3.393285	0.308214
C	-3.133829	-3.679076	-1.500294
C	-2.955732	-2.192011	-1.778038
N	-3.494581	-1.427685	-0.663927
C	-4.605690	-3.963671	-1.229500
H	-6.735099	-0.438616	2.059001
H	-5.967090	-1.920580	2.625101
H	-7.624042	-1.585218	0.072520
H	-8.065019	-2.556518	1.480586
H	-6.277887	-4.141227	1.088412
H	-7.063129	-3.883348	-0.468740
H	-4.728992	-4.960308	-0.794635
H	-5.178605	-3.947312	-2.165232
H	-2.529901	-3.960631	-0.632743
H	-2.797732	-4.279866	-2.348551
H	-3.452810	-1.916144	-2.717504
H	-1.902735	-1.927117	-1.879868
H	-4.713681	-0.044108	1.049860
O	4.898665	-1.424774	-1.754171

O	-2.156651	0.891424	-0.118974
C	5.088680	-0.744098	-0.773883
C	4.017477	-0.152510	0.117025
H	4.287617	0.886332	0.331649
H	4.077432	-0.670663	1.082248
C	2.608015	-0.254951	-0.464792
H	2.571977	0.278437	-1.421495
H	2.391186	-1.302174	-0.699524
C	1.538409	0.301587	0.481435
H	1.771353	1.346917	0.721867
H	1.579013	-0.237817	1.432624
C	0.129888	0.220821	-0.117938
H	0.124519	0.719698	-1.093827
H	-0.125895	-0.829714	-0.314092
C	-1.016765	0.855147	0.692967
H	-0.708010	1.878583	0.964615
C	-1.326695	0.103439	2.029693
H	-2.329135	0.421523	2.326839
C	-0.410705	0.353295	3.138219
H	-1.382877	-0.973873	1.827380
C	0.317589	0.587128	4.068949
H	0.967583	0.793384	4.885907
O	6.320732	-0.423138	-0.322942
C	7.439595	-0.960542	-1.082440
C	8.708920	-0.471391	-0.445460
H	7.346592	-0.626122	-2.117033
H	7.372087	-2.049964	-1.073835
C	9.277479	0.743943	-0.838299
C	9.329145	-1.212477	0.564541
C	10.443470	1.209795	-0.235506
H	8.803641	1.328018	-1.621868
C	10.495549	-0.750311	1.169806
H	8.895601	-2.157711	0.877983
H	10.876248	2.153343	-0.551941
C	11.054911	0.462492	0.770230
H	10.968781	-1.336910	1.950612
H	11.965156	0.822579	1.238792
H	-3.019632	-0.524948	-0.413111

80 atoms
addition of another ε-CL unit to the 7-is chain end, structure I2, in toluene

O	-3.598723	1.219401	1.642544

O	-3.988881	1.941889	-0.443749
C	-3.004616	1.797121	0.553897
C	-2.355772	3.122294	0.994955
H	-1.521273	3.359961	0.328422
H	-1.931799	2.947143	1.985086
C	-3.325098	4.314425	1.059193
H	-4.280331	3.986320	1.480957
H	-2.916510	5.048752	1.761494
C	-3.539556	5.016072	-0.291306
H	-2.559198	5.317344	-0.684320
H	-4.095045	5.946426	-0.127775
C	-4.273441	4.186286	-1.351763
H	-5.327753	4.073929	-1.074312
H	-4.258399	4.722589	-2.308899
C	-3.706187	2.786111	-1.567041
H	-2.631862	2.801667	-1.774602
H	-4.195729	2.311371	-2.421153
N	-5.877324	-2.657936	-0.485115
C	-4.974659	-1.681122	-0.131983
N	-4.934676	-1.088269	1.027791
C	-5.868855	-1.527751	2.053773
C	-7.216455	-1.928344	1.457764
C	-6.990432	-3.003089	0.401975
C	-4.617507	-3.122073	-2.577669
C	-4.178369	-1.667848	-2.473047
N	-4.020625	-1.347844	-1.065588
C	-5.912358	-3.307942	-1.796432
H	-5.994907	-0.713602	2.773169
H	-5.451091	-2.375436	2.618975
H	-7.681054	-1.049400	0.998950
H	-7.901381	-2.302486	2.224385
H	-6.792519	-3.973929	0.876566
H	-7.887799	-3.128790	-0.214349
H	-6.113322	-4.374340	-1.643139
H	-6.758801	-2.908144	-2.374303
H	-3.831199	-3.761456	-2.166067
H	-4.776556	-3.413610	-3.619174
H	-4.912277	-1.013793	-2.969649
H	-3.217068	-1.510497	-2.966599
H	-4.107961	0.398393	1.358793
O	5.216250	0.664688	-2.147778
O	-2.037519	0.908754	-0.068471
C	5.316002	0.273028	-1.009143
C	4.171831	0.068850	-0.038678

H	4.383970	0.664300	0.856501
H	4.202850	-0.973888	0.297072
C	2.805299	0.419463	-0.624485
H	2.811690	1.462563	-0.957964
H	2.634448	-0.179426	-1.525265
C	1.662961	0.196392	0.372562
H	1.836418	0.802084	1.270803
H	1.671443	-0.844384	0.709507
C	0.299510	0.548895	-0.231187
H	0.332730	1.571866	-0.622332
H	0.098463	-0.097375	-1.094776
C	-0.907926	0.469554	0.708737
H	-0.761541	1.141840	1.557821
C	-1.206061	-0.948623	1.259512
H	-2.249151	-0.963513	1.582185
C	-0.368664	-1.360018	2.382970
H	-1.126922	-1.676713	0.443801
C	0.288498	-1.694090	3.334053
H	0.875918	-1.989648	4.170956
O	6.495201	-0.044877	-0.434241
C	7.676055	0.105942	-1.272316
C	8.872501	-0.311353	-0.465942
H	7.742067	1.147256	-1.592189
H	7.547575	-0.511922	-2.162780
C	9.593182	0.628610	0.276186
C	9.270581	-1.651170	-0.428787
C	10.691515	0.239270	1.039652
H	9.292676	1.672106	0.254849
C	10.367515	-2.044656	0.333713
H	8.717679	-2.389835	-1.001797
H	11.244561	0.979702	1.608478
C	11.080518	-1.098942	1.069521
H	10.668040	-3.087278	0.351334
H	11.937642	-1.403443	1.661429
H	-3.479052	-0.524955	-0.828244

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure TS23, in toluene

O	-3.591050	1.214361	1.645715
O	-3.989372	1.944872	-0.436418
C	-3.001278	1.796342	0.556972
C	-2.350836	3.119879	1.000533

H	-1.519643	3.360493	0.330952
H	-1.921938	2.940647	1.987818
C	-3.320154	4.311462	1.074428
H	-4.273416	3.981356	1.499116
H	-2.908568	5.042880	1.778016
C	-3.540834	5.018871	-0.272057
H	-2.562356	5.322519	-0.667905
H	-4.096229	5.948132	-0.102107
C	-4.278667	4.193271	-1.333055
H	-5.331725	4.079005	-1.051669
H	-4.267981	4.733802	-2.287868
C	-3.711535	2.794388	-1.556953
H	-2.638059	2.811424	-1.768748
H	-4.204271	2.323300	-2.411248
N	-5.880565	-2.655560	-0.485396
C	-4.977321	-1.678594	-0.134253
N	-4.930028	-1.091076	1.027970
C	-5.855652	-1.537313	2.058783
C	-7.206706	-1.938325	1.470929
C	-6.986072	-3.007592	0.408458
C	-4.634778	-3.107688	-2.588880
C	-4.197408	-1.653171	-2.480852
N	-4.030767	-1.339007	-1.073125
C	-5.923865	-3.299322	-1.799539
H	-5.978253	-0.726718	2.782776
H	-5.431813	-2.386562	2.617056
H	-7.676797	-1.058374	1.019723
H	-7.884999	-2.317677	2.240881
H	-6.782176	-3.980119	0.877028
H	-7.887762	-3.132654	-0.201640
H	-6.122078	-4.366750	-1.649913
H	-6.774952	-2.898128	-2.369570
H	-3.844557	-3.747525	-2.185557
H	-4.800508	-3.394852	-3.630554
H	-4.935739	-0.998232	-2.969672
H	-3.239704	-1.492034	-2.980147
H	-4.101715	0.394695	1.360835
O	5.221703	0.679878	-2.145536
O	-2.036369	0.910624	-0.072258
C	5.319230	0.280687	-1.009329
C	4.173228	0.069307	-0.042570
H	4.385084	0.655473	0.858750
H	4.202015	-0.976774	0.282922
C	2.808003	0.427658	-0.626751

H	2.815820	1.474360	-0.948759
H	2.638016	-0.161202	-1.534264
C	1.664014	0.194667	0.366128
H	1.836363	0.790653	1.271040
H	1.671625	-0.849611	0.692043
C	0.301500	0.553867	-0.235787
H	0.335472	1.580833	-0.616276
H	0.101425	-0.083376	-1.106270
C	-0.907117	0.464854	0.701743
H	-0.762409	1.128877	1.557578
C	-1.205320	-0.958689	1.238320
H	-2.248589	-0.976883	1.560355
C	-0.368525	-1.381295	2.358057
H	-1.125774	-1.678659	0.415484
C	0.287986	-1.725013	3.306148
H	0.874931	-2.028918	4.140388
O	6.497347	-0.040707	-0.434109
C	7.679892	0.115302	-1.268801
C	8.874424	-0.309061	-0.463257
H	7.747507	1.158884	-1.580828
H	7.552513	-0.495829	-2.164065
C	9.598563	0.625725	0.281977
C	9.267163	-1.650593	-0.430075
C	10.695126	0.229680	1.044600
H	9.302211	1.670467	0.263780
C	10.362195	-2.050768	0.331618
H	8.711527	-2.385277	-1.005552
H	11.250910	0.966169	1.615868
C	11.078743	-1.110137	1.070546
H	10.658546	-3.094632	0.346191
H	11.934427	-1.419878	1.661820
H	-3.488923	-0.516411	-0.835607

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure I3, in toluene

O	-3.272341	1.154463	1.212207
O	-3.900678	1.805823	-0.848485
C	-2.804404	1.707108	0.051906
C	-2.159212	3.063874	0.383466
H	-1.450367	3.324584	-0.407156
H	-1.571338	2.905954	1.290433
C	-3.152405	4.217487	0.594916

H	-4.029095	3.851298	1.138259
H	-2.682771	4.966731	1.241035
C	-3.570409	4.910900	-0.711590
H	-2.663544	5.265252	-1.219550
H	-4.150680	5.809478	-0.473479
C	-4.384249	4.046794	-1.683417
H	-5.390763	3.880616	-1.282716
H	-4.511397	4.587086	-2.629861
C	-3.782848	2.676294	-1.983864
H	-2.741162	2.737200	-2.311184
H	-4.345034	2.190575	-2.785650
N	-6.306245	-2.587512	-0.058205
C	-5.416009	-1.539623	-0.075060
N	-4.705688	-1.149225	0.946756
C	-4.812775	-1.903515	2.187302
C	-6.226387	-2.438068	2.404738
C	-6.632674	-3.270823	1.195370
C	-6.522792	-2.485523	-2.530240
C	-6.178772	-1.011060	-2.367419
N	-5.236635	-0.886270	-1.270086
C	-7.090621	-3.012908	-1.218467
H	-4.518658	-1.248473	3.012288
H	-4.098937	-2.741662	2.192688
H	-6.915955	-1.595668	2.523044
H	-6.290758	-3.047607	3.310866
H	-6.137341	-4.251161	1.218699
H	-7.711938	-3.460106	1.205885
H	-7.115519	-4.108401	-1.229597
H	-8.130479	-2.675213	-1.096671
H	-5.615557	-3.034899	-2.797838
H	-7.253734	-2.634472	-3.329268
H	-7.096391	-0.425275	-2.198993
H	-5.704111	-0.618551	-3.269462
H	-3.818119	0.327463	1.029950
O	5.611796	1.345551	-1.675310
O	-1.874560	0.854472	-0.638047
C	5.580527	0.631859	-0.700941
C	4.331073	0.142493	0.000145
H	4.388072	0.467949	1.045222
H	4.376866	-0.951647	0.038303
C	3.036109	0.618951	-0.655365
H	3.031102	1.713376	-0.692824
H	3.015548	0.285571	-1.698379
C	1.787234	0.115591	0.076549

H	1.809393	0.460475	1.118098
H	1.808166	-0.977156	0.124758
C	0.495420	0.593726	-0.595100
H	0.531755	1.683409	-0.703820
H	0.433212	0.191300	-1.613842
C	-0.813833	0.260195	0.127929
H	-0.808601	0.679933	1.136955
C	-1.132277	-1.252688	0.235359
H	-2.204402	-1.340724	0.433762
C	-0.407208	-1.976061	1.276448
H	-0.959017	-1.722890	-0.740092
C	0.152129	-2.577224	2.156435
H	0.657224	-3.104130	2.931052
O	6.689072	0.163147	-0.088958
C	7.959769	0.571313	-0.670154
C	9.061037	-0.032062	0.153892
H	8.002383	1.661821	-0.673890
H	7.991256	0.230092	-1.706355
C	9.559456	0.640189	1.273937
C	9.589396	-1.284130	-0.173342
C	10.566557	0.073806	2.051544
H	9.156194	1.613651	1.537374
C	10.597140	-1.853932	0.601497
H	9.209417	-1.815211	-1.041201
H	10.946878	0.607509	2.916537
C	11.087577	-1.175176	1.715939
H	11.001047	-2.825134	0.334446
H	11.874734	-1.616253	2.318917
H	-4.712898	-0.020327	-1.188292

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure TS3r, in toluene

O	-2.858353	0.876531	1.487632
O	-4.049746	1.833686	-0.158592
C	-2.796229	1.843637	0.529333
C	-2.486945	3.193663	1.195723
H	-2.013414	3.848840	0.460084
H	-1.725578	2.974870	1.948791
C	-3.691620	3.900716	1.833229
H	-4.335653	3.163409	2.323548
H	-3.327430	4.563072	2.625900
C	-4.497076	4.750834	0.836697

H	-3.813443	5.470867	0.367655
H	-5.232956	5.350055	1.384799
C	-5.227908	3.965850	-0.260716
H	-6.077067	3.423972	0.171955
H	-5.647935	4.668850	-0.991047
C	-4.366880	2.947899	-1.005014
H	-3.451758	3.388704	-1.409302
H	-4.922337	2.531820	-1.849937
N	-5.730703	-2.924978	0.101644
C	-5.029551	-1.743408	0.116992
N	-3.995436	-1.498286	0.871729
C	-3.495740	-2.568418	1.723510
C	-4.627606	-3.449843	2.246839
C	-5.428117	-3.984867	1.065946
C	-6.981118	-2.193705	-1.917223
C	-6.732131	-0.783851	-1.397802
N	-5.427098	-0.763761	-0.761823
C	-6.888960	-3.177569	-0.757119
H	-2.948014	-2.115634	2.555006
H	-2.767972	-3.185380	1.175834
H	-5.278302	-2.854006	2.895499
H	-4.244470	-4.284826	2.840786
H	-4.879400	-4.792505	0.562549
H	-6.377650	-4.411098	1.408482
H	-6.815242	-4.203166	-1.135823
H	-7.805654	-3.130477	-0.150979
H	-6.228639	-2.430871	-2.674786
H	-7.965841	-2.274095	-2.384888
H	-7.537888	-0.487019	-0.707901
H	-6.723651	-0.061172	-2.216751
H	-3.320410	0.036234	1.165862
O	5.730626	2.192867	-0.971619
O	-1.785635	1.619237	-0.477069
C	5.627817	1.057802	-0.570873
C	4.330970	0.307436	-0.353953
H	4.336252	-0.080711	0.670580
H	4.351953	-0.580353	-0.996738
C	3.084419	1.149306	-0.620690
H	3.098146	2.031553	0.028249
H	3.120439	1.533301	-1.645516
C	1.787621	0.361805	-0.403639
H	1.759493	-0.019555	0.625117
H	1.784643	-0.520699	-1.049275
C	0.543648	1.218707	-0.663865

H	0.613304	2.136359	-0.069661
H	0.522422	1.539560	-1.712895
C	-0.809130	0.583066	-0.320004
H	-0.811242	0.240374	0.716570
C	-1.235449	-0.592469	-1.236662
H	-2.298283	-0.773427	-1.055184
C	-0.525301	-1.852885	-1.034950
H	-1.142332	-0.273083	-2.281404
C	0.022512	-2.911257	-0.865866
H	0.522438	-3.838626	-0.714782
O	6.688465	0.283159	-0.256746
C	7.998665	0.892248	-0.432405
C	9.035069	-0.111662	-0.015085
H	8.041920	1.799305	0.172714
H	8.107360	1.180990	-1.479378
C	9.485301	-0.159426	1.307476
C	9.548867	-1.028021	-0.937486
C	10.431223	-1.102920	1.701719
H	9.092794	0.547733	2.032410
C	10.494664	-1.973152	-0.547329
H	9.206025	-0.999967	-1.967715
H	10.774817	-1.126984	2.730827
C	10.937803	-2.011850	0.774017
H	10.887910	-2.676724	-1.274008
H	11.677172	-2.745500	1.078739
H	-4.987626	0.135360	-0.588485

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure I3r, in toluene

O	-3.052956	0.971910	1.601990
O	-4.483393	0.752893	-0.116584
C	-3.735010	1.702505	0.663414
C	-4.607193	2.744027	1.376677
H	-4.788986	3.581250	0.697603
H	-3.983821	3.131065	2.185034
C	-5.934447	2.207727	1.929562
H	-5.777956	1.214102	2.362148
H	-6.249390	2.853333	2.756152
C	-7.069178	2.176214	0.892732
H	-7.183434	3.185296	0.474981
H	-8.014979	1.952861	1.399202
C	-6.883158	1.176661	-0.255941

H	-7.004054	0.152909	0.117195
H	-7.672548	1.329858	-1.002488
C	-5.529952	1.254455	-0.958070
H	-5.293111	2.270823	-1.286988
H	-5.529436	0.618076	-1.847587
N	-2.144363	-3.728237	0.237579
C	-2.559990	-2.417754	0.247886
N	-2.027219	-1.470429	0.967699
C	-0.872392	-1.801034	1.788712
C	-0.958367	-3.221725	2.342586
C	-1.129893	-4.196676	1.184299
C	-3.585280	-4.201917	-1.728879
C	-4.458445	-3.071341	-1.200278
N	-3.590723	-2.078845	-0.594033
C	-2.759796	-4.772866	-0.582387
H	-0.813043	-1.074670	2.604203
H	0.058633	-1.690647	1.210355
H	-1.817873	-3.292750	3.017289
H	-0.065147	-3.484542	2.916897
H	-0.176411	-4.341749	0.658154
H	-1.440805	-5.179993	1.554644
H	-1.961442	-5.413683	-0.973212
H	-3.391591	-5.409417	0.054693
H	-2.927339	-3.807833	-2.508782
H	-4.192841	-4.996093	-2.170516
H	-5.200420	-3.467944	-0.489290
H	-5.010817	-2.592286	-2.011762
H	-2.739365	0.077863	1.265223
O	4.489383	2.324400	1.603731
O	-2.895034	2.456759	-0.202162
C	4.472040	1.541899	0.683714
C	3.263363	1.181091	-0.153312
H	3.148588	0.091734	-0.119653
H	3.503729	1.410984	-1.197762
C	1.979719	1.884535	0.284049
H	1.776253	1.648566	1.333729
H	2.130284	2.968660	0.246641
C	0.775792	1.494890	-0.580635
H	0.629396	0.408434	-0.535717
H	0.991615	1.724966	-1.628489
C	-0.509293	2.198037	-0.130668
H	-0.667083	2.015238	0.935801
H	-0.404373	3.284384	-0.244722
C	-1.800681	1.765558	-0.833279

H	-1.936419	0.686331	-0.732698
C	-1.888229	2.140164	-2.331800
H	-2.943064	2.086352	-2.616778
C	-1.123537	1.292163	-3.242772
H	-1.591752	3.188135	-2.457706
C	-0.534822	0.585232	-4.018032
H	0.000533	-0.039394	-4.693361
O	5.563702	0.864343	0.265792
C	6.797892	1.133816	0.988383
C	7.883858	0.294198	0.378371
H	6.641496	0.896784	2.042081
H	7.015369	2.200782	0.912875
C	8.179057	-0.971234	0.893222
C	8.601544	0.757779	-0.728529
C	9.172857	-1.758626	0.315769
H	7.627911	-1.341436	1.752798
C	9.595014	-0.026459	-1.309302
H	8.380304	1.739694	-1.136615
H	9.394813	-2.737730	0.727869
C	9.882704	-1.287059	-0.787241
H	10.146891	0.346576	-2.166031
H	10.659278	-1.897751	-1.236416
H	-3.950137	-1.142563	-0.439350

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure TS3r2, in toluene

O	-2.784439	-0.999326	-1.472372
O	-4.162971	-1.149071	0.295966
C	-3.360542	-1.909805	-0.620124
C	-4.147002	-2.965177	-1.410955
H	-4.248019	-3.872537	-0.808727
H	-3.499859	-3.223024	-2.251730
C	-5.519840	-2.497254	-1.911475
H	-5.454604	-1.454555	-2.240792
H	-5.783477	-3.080203	-2.800112
C	-6.643794	-2.669197	-0.877671
H	-6.674978	-3.723693	-0.573057
H	-7.609230	-2.466081	-1.354699
C	-6.521875	-1.789877	0.373103
H	-6.722934	-0.743504	0.116035
H	-7.288910	-2.084246	1.100328
C	-5.159896	-1.838989	1.061363

H	-4.836144	-2.864169	1.266050
H	-5.206935	-1.317229	2.021168
N	-3.403964	3.759953	-0.138154
C	-3.396841	2.385167	-0.179623
N	-3.184084	1.670132	-1.246123
C	-2.879927	2.360799	-2.489781
C	-3.619275	3.692902	-2.595627
C	-3.295222	4.541254	-1.371879
C	-3.441290	3.718512	2.342054
C	-4.127372	2.367729	2.189278
N	-3.588543	1.717759	1.008546
C	-3.659474	4.536613	1.075401
H	-3.151943	1.703919	-3.320954
H	-1.796160	2.534994	-2.579450
H	-4.697163	3.503989	-2.639209
H	-3.342227	4.234841	-3.504632
H	-2.284205	4.963629	-1.452520
H	-3.987772	5.387144	-1.298931
H	-2.993710	5.406701	1.068209
H	-4.688277	4.926340	1.051483
H	-2.372106	3.557907	2.507903
H	-3.836923	4.265066	3.202063
H	-5.218977	2.505316	2.129672
H	-3.926264	1.728594	3.051893
H	-3.009048	-0.038300	-1.272062
O	4.972887	-2.117615	-1.695353
O	-2.383812	-2.647101	0.100495
C	4.915463	-1.333922	-0.777926
C	3.687704	-1.027286	0.053005
H	3.526992	0.056223	0.023634
H	3.931663	-1.252350	1.097781
C	2.438373	-1.783343	-0.395620
H	2.224651	-1.542008	-1.442026
H	2.639483	-2.859558	-0.373412
C	1.216412	-1.464286	0.472682
H	1.020717	-0.384913	0.446427
H	1.441805	-1.702246	1.517076
C	-0.032390	-2.220823	0.008167
H	-0.210876	-2.010821	-1.050347
H	0.134143	-3.302817	0.085058
C	-1.339102	-1.887907	0.733913
H	-1.554710	-0.821933	0.637322
C	-1.375102	-2.273560	2.232805
H	-2.427195	-2.328502	2.526789

C	-0.693320	-1.349331	3.135593
H	-0.970628	-3.285022	2.356476
C	-0.170628	-0.580010	3.898930
H	0.309026	0.098195	4.564403
O	5.973270	-0.606690	-0.356649
C	7.220649	-0.818434	-1.075749
C	8.258724	0.088140	-0.478311
H	7.050351	-0.604937	-2.132442
H	7.497642	-1.870270	-0.986039
C	8.400323	1.402370	-0.934237
C	9.083780	-0.360470	0.556923
C	9.347876	2.251622	-0.368190
H	7.764458	1.761294	-1.738315
C	10.033461	0.485614	1.125380
H	8.982292	-1.379386	0.919036
H	9.449934	3.268387	-0.733591
C	10.166925	1.793902	0.663310
H	10.670203	0.123477	1.926086
H	10.908267	2.453404	1.102919
H	-3.762468	0.726697	0.880213

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure I3r2, in toluene

O	-2.331792	-0.568242	-1.093684
O	-3.643243	-1.442436	0.502134
C	-2.923778	-1.749575	-0.711416
C	-3.813988	-2.369070	-1.805131
H	-3.883192	-3.448023	-1.637352
H	-3.252412	-2.239591	-2.732602
C	-5.220006	-1.764916	-1.934448
H	-5.176412	-0.679299	-1.795738
H	-5.571549	-1.928764	-2.958689
C	-6.246405	-2.386862	-0.974194
H	-6.261480	-3.472569	-1.138274
H	-7.249084	-2.030007	-1.235837
C	-6.000723	-2.108412	0.513780
H	-6.212315	-1.056082	0.735926
H	-6.703105	-2.699373	1.114892
C	-4.582572	-2.406053	0.996241
H	-4.261492	-3.417139	0.726170
H	-4.534016	-2.332217	2.086026
N	-4.709213	3.483559	0.250380

C	-4.231722	2.202592	0.101548
N	-3.889704	1.660824	-1.034986
C	-3.950323	2.483976	-2.232497
C	-5.115540	3.469986	-2.184568
C	-5.001874	4.313073	-0.920362
C	-4.451981	3.326798	2.712767
C	-4.650302	1.829421	2.518521
N	-4.073028	1.455030	1.241374
C	-5.078708	4.069444	1.539443
H	-4.043055	1.822994	-3.099152
H	-3.008293	3.037785	-2.369662
H	-6.058657	2.913378	-2.174657
H	-5.126695	4.122109	-3.062802
H	-4.219075	5.075351	-1.034918
H	-5.939748	4.847337	-0.731264
H	-4.757642	5.116909	1.540023
H	-6.174423	4.075034	1.639280
H	-3.380754	3.541721	2.765941
H	-4.909743	3.665775	3.645716
H	-5.722172	1.582424	2.579584
H	-4.142294	1.262312	3.301632
H	-2.971415	0.209153	-1.068846
O	5.232816	-0.949530	-2.293718
O	-1.929233	-2.711281	-0.455060
C	5.223844	-0.651303	-1.123187
C	4.072085	-0.857189	-0.162621
H	3.871069	0.100655	0.329642
H	4.424660	-1.521121	0.635567
C	2.812671	-1.414779	-0.823742
H	2.488037	-0.734024	-1.617728
H	3.053299	-2.359993	-1.321419
C	1.671244	-1.628071	0.176613
H	1.437969	-0.677004	0.671993
H	2.004333	-2.305026	0.969424
C	0.408062	-2.172018	-0.499435
H	0.125672	-1.509337	-1.321482
H	0.614085	-3.152827	-0.946960
C	-0.833123	-2.299814	0.388195
H	-1.073912	-1.335700	0.837661
C	-0.738499	-3.370097	1.501036
H	-1.760181	-3.599538	1.817420
C	0.030574	-2.980710	2.680348
H	-0.333762	-4.297328	1.078647
C	0.626059	-2.663761	3.676490

```
H      1.165789    -2.378545     4.548430
O      6.275914    -0.081366    -0.495680
C      7.452950     0.160775    -1.316386
C      8.496427     0.807124    -0.450498
H      7.164015     0.798827    -2.153436
H      7.793974    -0.792763    -1.723245
C      8.513397     2.194393    -0.276086
C      9.452913     0.031368     0.210424
C      9.467363     2.795204     0.541431
H      7.774638     2.806698    -0.784982
C     10.409690     0.628561     1.028348
H      9.448789    -1.047167     0.082456
H      9.471531     3.873286     0.665773
C     10.418279     2.012391     1.195159
H     11.149006     0.014838     1.532799
H     11.164649     2.479542     1.829578
H     -3.852822     0.479392     1.070514
```

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure TS34, in toluene

```
O     -2.767093     0.768035     1.339768
O     -3.766209     1.398827    -0.841532
C     -2.695847     1.825535     0.684234
C     -3.359837     3.110908     1.165289
H     -3.089289     3.931179     0.496629
H     -2.863446     3.324444     2.119636
C     -4.881785     3.051910     1.369647
H     -5.183354     2.018691     1.567599
H     -5.133489     3.619138     2.273019
C     -5.702125     3.643216     0.210205
H     -5.314845     4.648755    -0.003986
H     -6.734598     3.792249     0.550927
C     -5.732830     2.832125    -1.091971
H     -6.335558     1.926270    -0.944456
H     -6.249331     3.424367    -1.860712
C     -4.360107     2.392151    -1.624107
H     -3.697464     3.271178    -1.714285
H     -4.495190     2.022641    -2.656972
N     -5.793046    -2.868917     0.261491
C     -5.131889    -1.685353     0.262452
N     -4.705041    -1.145319     1.414190
C     -4.788049    -1.849368     2.685717
```

C	-6.063846	-2.678977	2.715290
C	-6.097380	-3.596861	1.499779
C	-5.386071	-3.027272	-2.170341
C	-5.345941	-1.505214	-2.171303
N	-4.902259	-1.023295	-0.871200
C	-6.218823	-3.508828	-0.989102
H	-4.781621	-1.101922	3.480407
H	-3.909461	-2.490987	2.834075
H	-6.932128	-2.013545	2.705121
H	-6.114746	-3.278561	3.626879
H	-5.384223	-4.422406	1.618780
H	-7.090047	-4.041503	1.385665
H	-6.107609	-4.588842	-0.859920
H	-7.284945	-3.310115	-1.157420
H	-4.367965	-3.419521	-2.091483
H	-5.817119	-3.403055	-3.101075
H	-6.335763	-1.098502	-2.416872
H	-4.646387	-1.130233	-2.920285
H	-4.042741	-0.350297	1.353633
O	6.065650	2.408910	0.370526
O	-1.497456	2.176976	0.069046
C	5.885230	1.230706	0.174146
C	4.546020	0.563354	-0.055731
H	4.468213	-0.281561	0.637135
H	4.571371	0.112866	-1.055080
C	3.355438	1.510099	0.087260
H	3.354531	1.942193	1.093762
H	3.480600	2.354163	-0.598785
C	2.017191	0.813711	-0.181666
H	1.896501	-0.029506	0.510131
H	2.030462	0.376235	-1.185191
C	0.827388	1.767629	-0.036184
H	0.853064	2.232172	0.955835
H	0.917423	2.588395	-0.758895
C	-0.552532	1.128955	-0.196872
H	-0.701410	0.340971	0.543729
C	-0.852798	0.559770	-1.606925
H	-1.943746	0.566846	-1.701081
C	-0.348846	-0.787376	-1.852239
H	-0.466276	1.248748	-2.367974
C	0.035218	-1.910602	-2.055715
H	0.389849	-2.898307	-2.232200
O	6.887187	0.325643	0.125706
C	8.230772	0.851838	0.314731

C	9.195565	-0.295295	0.217754
H	8.276952	1.342533	1.288370
H	8.415951	1.607208	-0.451097
C	9.602962	-0.981272	1.365304
C	9.684830	-0.707570	-1.025608
C	10.483419	-2.057236	1.274474
H	9.228800	-0.669924	2.336237
C	10.564173	-1.783201	-1.120897
H	9.374891	-0.181525	-1.923872
H	10.794564	-2.578847	2.173827
C	10.965613	-2.460032	0.030272
H	10.939052	-2.091066	-2.091691
H	11.653802	-3.296065	-0.042171
H	-4.448167	-0.064079	-0.822739

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure I4, in toluene

O	-2.752751	1.136893	1.410946
O	-4.237288	1.474253	-1.290605
C	-2.560130	2.175076	0.815132
C	-3.438137	3.404145	0.861644
H	-3.449307	3.827107	-0.143417
H	-2.901940	4.136184	1.477820
C	-4.860460	3.171768	1.406776
H	-4.965049	2.128075	1.712675
H	-4.984088	3.761127	2.320595
C	-6.002071	3.546689	0.442423
H	-5.772842	4.507792	-0.037800
H	-6.898847	3.730399	1.045843
C	-6.387300	2.518315	-0.634217
H	-6.661166	1.570225	-0.155362
H	-7.298186	2.881505	-1.129393
C	-5.358758	2.221071	-1.731390
H	-4.973618	3.157627	-2.151081
H	-5.867160	1.693582	-2.552278
N	-5.466551	-3.133468	0.337180
C	-5.050422	-1.826030	0.219304
N	-4.633871	-1.195797	1.371847
C	-4.254086	-1.945608	2.557533
C	-5.322255	-2.999146	2.812293
C	-5.435355	-3.896054	1.586275
C	-5.270964	-3.268812	-2.118228

C	-5.575142	-1.773099	-2.088542
N	-5.062625	-1.136531	-0.884860
C	-5.824291	-3.909513	-0.851868
H	-4.182323	-1.244360	3.391192
H	-3.268470	-2.424759	2.448459
H	-6.276504	-2.500532	3.006261
H	-5.076889	-3.607037	3.687083
H	-4.592022	-4.602241	1.559681
H	-6.348668	-4.499523	1.639397
H	-5.422405	-4.921349	-0.728151
H	-6.917005	-4.007072	-0.914551
H	-4.186578	-3.413652	-2.163271
H	-5.706742	-3.750962	-2.998335
H	-6.662988	-1.620635	-2.174381
H	-5.127586	-1.275352	-2.953968
H	-4.122217	-0.336800	1.208643
O	6.098459	2.474135	0.346805
O	-1.463858	2.411687	0.068129
C	5.900806	1.298253	0.152709
C	4.548627	0.650332	-0.058115
H	4.454873	-0.171058	0.660763
H	4.562656	0.169498	-1.043068
C	3.379626	1.626650	0.060068
H	3.397102	2.094696	1.049994
H	3.516151	2.442293	-0.657423
C	2.025445	0.948489	-0.172752
H	1.892207	0.135480	0.551708
H	2.019249	0.474260	-1.158922
C	0.860026	1.936357	-0.053634
H	0.911301	2.439858	0.918241
H	0.957631	2.723056	-0.811306
C	-0.532333	1.319817	-0.169501
H	-0.692934	0.566970	0.602099
C	-0.892711	0.729174	-1.552189
H	-1.983517	0.734773	-1.645054
C	-0.400579	-0.627584	-1.773399
H	-0.517524	1.395877	-2.337522
C	-0.021700	-1.754652	-1.956278
H	0.319191	-2.749877	-2.117920
O	6.887676	0.379347	0.092288
C	8.241847	0.884574	0.268515
C	9.187653	-0.276958	0.159249
H	8.304786	1.372357	1.242657
H	8.430048	1.638587	-0.497774

C	9.588897	-0.977307	1.300314
C	9.665060	-0.687975	-1.089092
C	10.451767	-2.066341	1.198110
H	9.223940	-0.666944	2.275067
C	10.526914	-1.776646	-1.195677
H	9.359965	-0.150660	-1.982333
H	10.758521	-2.599131	2.092377
C	10.922342	-2.467798	-0.051002
H	10.892951	-2.083435	-2.170151
H	11.596967	-3.313982	-0.132251
H	-4.531445	0.544963	-1.091268

80 atoms
addition of another ε-CL unit to the 7-isomer chain end,
structure I5, in toluene

O	-0.792081	-3.121395	0.841273
O	-6.451487	0.729648	-2.763854
C	-0.298969	-2.878369	-0.233604
C	-0.957266	-2.099511	-1.351851
H	-0.917275	-2.716891	-2.256319
H	-0.323313	-1.231803	-1.568893
C	-2.389082	-1.668146	-1.038453
H	-2.992820	-2.553377	-0.812835
H	-2.393848	-1.063880	-0.125640
C	-3.032364	-0.881617	-2.184860
H	-3.026293	-1.495103	-3.095798
H	-2.417680	-0.000455	-2.411864
C	-4.465831	-0.437607	-1.878704
H	-5.085545	-1.312375	-1.646785
H	-4.477831	0.195405	-0.984153
C	-5.116335	0.328010	-3.033136
H	-5.155547	-0.307580	-3.924365
H	-4.497817	1.201200	-3.290650
N	-8.068512	2.133291	1.424115
C	-7.529030	1.663654	0.248804
N	-7.811590	0.357687	-0.089645
C	-8.916578	-0.374199	0.502027
C	-8.883010	-0.140447	2.006577
C	-8.964385	1.355989	2.282143
C	-7.487642	4.393355	0.619763
C	-6.368250	3.687138	-0.143500
N	-6.746917	2.341363	-0.542565
C	-7.896918	3.535163	1.810512

H	-8.788701	-1.432942	0.266966
H	-9.890684	-0.063490	0.092324
H	-7.951602	-0.548930	2.409199
H	-9.714611	-0.647296	2.503036
H	-9.997390	1.707593	2.141443
H	-8.701455	1.563343	3.325494
H	-8.845604	3.889717	2.228614
H	-7.149387	3.607052	2.612480
H	-8.345023	4.531933	-0.047256
H	-7.176257	5.382940	0.967220
H	-5.459857	3.664779	0.479467
H	-6.106009	4.251949	-1.043016
H	-7.516986	0.115040	-1.028679
O	7.781107	-1.144100	-0.415209
O	0.943658	-3.277120	-0.596408
C	6.962818	-0.314241	-0.097253
C	5.497497	-0.577139	0.180655
H	4.910157	0.096727	-0.452793
H	5.293603	-0.255990	1.208687
C	5.089409	-2.033790	-0.031697
H	5.308930	-2.323860	-1.064614
H	5.711366	-2.678606	0.597571
C	3.608452	-2.278437	0.272684
H	2.990604	-1.630541	-0.358327
H	3.395357	-1.991194	1.310456
C	3.197320	-3.738110	0.058359
H	3.396112	-4.035363	-0.978273
H	3.806542	-4.390332	0.692255
C	1.734163	-4.018296	0.373672
H	1.470216	-3.656284	1.368889
C	1.348877	-5.507300	0.262187
H	0.265991	-5.593421	0.389916
C	2.014372	-6.348254	1.252291
H	1.581952	-5.860117	-0.748693
C	2.559602	-7.033191	2.076499
H	3.039010	-7.644308	2.804531
O	7.252983	0.993969	0.060802
C	8.639968	1.374306	-0.168706
C	8.752509	2.857789	0.036987
H	8.915189	1.080322	-1.182842
H	9.269433	0.815737	0.526360
C	8.580636	3.738375	-1.034974
C	9.008702	3.381342	1.307799
C	8.664156	5.115497	-0.842610

H	8.381256	3.342463	-2.026535
C	9.092593	4.757610	1.504408
H	9.144038	2.706136	2.147685
H	8.532341	5.788146	-1.683935
C	8.920527	5.627432	0.428415
H	9.295301	5.151166	2.495215
H	8.989063	6.699918	0.579419
H	-6.444873	1.446130	-2.077744

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure I1, in toluene

N	-0.927880	5.274291	1.766960
C	-1.140553	3.936642	2.022932
N	-2.426410	3.550946	2.284900
C	-3.562313	4.453814	2.333050
C	-3.103504	5.830511	2.797365
C	-1.965595	6.294793	1.898842
C	1.229160	4.590953	0.769963
C	1.162680	3.497719	1.835544
N	-0.200794	3.030621	2.029862
C	0.336316	5.748492	1.200373
H	-4.297225	4.025466	3.016675
H	-4.045598	4.536389	1.348633
H	-2.761197	5.771011	3.835146
H	-3.923682	6.552278	2.754479
H	-2.355720	6.562888	0.905175
H	-1.499497	7.198609	2.307778
H	0.110972	6.399576	0.346372
H	0.850444	6.371230	1.945314
H	0.878715	4.179784	-0.182333
H	2.250769	4.951843	0.617544
H	1.586514	3.883465	2.777412
H	1.782455	2.643003	1.549971
H	-2.546951	2.633332	2.690743
O	-3.578225	1.081190	3.672243
C	-2.693622	0.503430	4.269741
O	-1.787787	1.252431	4.919236
C	-0.563122	0.705542	5.473129
H	-0.066802	0.111256	4.703898
H	0.040917	1.594217	5.651932
C	-0.789133	-0.057158	6.771272
H	-1.433391	0.549527	7.418350

H	0.176814	-0.133627	7.283651
C	-1.375179	-1.460766	6.593176
H	-0.641674	-2.091626	6.075803
H	-1.522480	-1.913266	7.579563
C	-2.697335	-1.517671	5.819785
H	-3.478145	-0.962677	6.354015
H	-3.029549	-2.558939	5.790533
C	-2.604953	-1.013990	4.358752
H	-1.631773	-1.293798	3.944668
C	-3.695603	-1.632898	3.455625
H	-3.665587	-1.147652	2.477384
C	-3.543952	-3.075944	3.287243
H	-4.684803	-1.409566	3.868599
C	-3.409861	-4.263088	3.145433
H	-3.296466	-5.313086	3.012303
O	4.156431	-1.714264	-3.560124
O	-0.542181	0.296191	2.227338
C	3.067176	-1.983254	-4.008193
C	1.744735	-1.799827	-3.293970
H	1.099889	-1.190594	-3.937260
H	1.256380	-2.779963	-3.244598
C	1.881976	-1.182363	-1.903408
H	2.382935	-0.212164	-1.986696
H	2.543308	-1.806912	-1.294136
C	0.534305	-1.010608	-1.195556
H	-0.125405	-0.386955	-1.813421
H	0.037467	-1.986720	-1.116517
C	0.663314	-0.391388	0.199324
H	1.153456	0.587205	0.125821
H	1.309482	-1.014320	0.829239
C	-0.678945	-0.216573	0.912785
H	-1.336088	0.430916	0.313655
H	-1.177366	-1.189265	0.996653
O	2.879207	-2.499928	-5.241445
C	4.082588	-2.731536	-6.027076
C	3.668028	-3.309739	-7.349904
H	4.608345	-1.782349	-6.143273
H	4.731847	-3.409372	-5.469993
C	3.473612	-4.687179	-7.492106
C	3.450256	-2.479234	-8.452719
C	3.070494	-5.224637	-8.711846
H	3.640134	-5.341774	-6.641557
C	3.048160	-3.013091	-9.675208
H	3.597816	-1.407756	-8.353581

H	2.926117	-6.295746	-8.809716
C	2.857450	-4.387534	-9.806558
H	2.886190	-2.357403	-10.524640
H	2.546953	-4.805415	-10.758774
H	-0.420577	1.283632	2.175966

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure TS12, in toluene

N	-5.243822	-3.330346	0.141522
C	-4.538116	-2.172457	0.221357
N	-4.441787	-1.522814	1.386589
C	-5.036159	-2.018803	2.618857
C	-6.324857	-2.764057	2.297061
C	-6.031439	-3.847046	1.267139
C	-4.117152	-3.802152	-2.015052
C	-4.043304	-2.288258	-2.167248
N	-3.926653	-1.673553	-0.854320
C	-5.262851	-4.152818	-1.074263
H	-5.223166	-1.157334	3.261056
H	-4.336255	-2.676783	3.150075
H	-7.062685	-2.060023	1.901471
H	-6.746831	-3.220226	3.195591
H	-5.491827	-4.683122	1.730340
H	-6.963741	-4.251189	0.861251
H	-5.198327	-5.201152	-0.767158
H	-6.228670	-4.023426	-1.579062
H	-3.171192	-4.173134	-1.609640
H	-4.278102	-4.286233	-2.981144
H	-4.931331	-1.915543	-2.695141
H	-3.171712	-1.986159	-2.749568
H	-3.988524	-0.587934	1.415233
O	-3.222692	0.947038	1.626972
C	-3.232925	1.521635	0.519149
O	-4.446673	1.418170	-0.160911
C	-4.587297	1.988272	-1.469824
H	-3.632481	1.946977	-1.997336
H	-5.284673	1.330648	-1.996167
C	-5.156892	3.400803	-1.397736
H	-6.053459	3.367035	-0.767354
H	-5.491193	3.698272	-2.399715
C	-4.174391	4.444411	-0.856445
H	-3.397084	4.632249	-1.608555

H	-4.703688	5.395509	-0.726946
C	-3.486108	4.071988	0.464716
H	-4.231435	3.869124	1.242742
H	-2.921055	4.946678	0.801732
C	-2.504627	2.879694	0.362660
H	-2.022170	2.907970	-0.615239
C	-1.403382	2.985145	1.444590
H	-0.821254	2.062690	1.470713
C	-0.497385	4.113854	1.240237
H	-1.876779	3.058862	2.428428
C	0.253356	5.037590	1.059794
H	0.920762	5.851836	0.903945
O	5.327229	0.941735	-2.012610
O	-2.272301	0.426589	-0.678344
C	5.270565	0.216628	-1.048085
C	4.004529	-0.286844	-0.388410
H	3.987618	-1.377351	-0.506460
H	4.095000	-0.116545	0.689651
C	2.728246	0.342135	-0.945626
H	2.687548	0.180134	-2.027488
H	2.769768	1.427886	-0.808111
C	1.460854	-0.212970	-0.287888
H	1.421139	-1.300819	-0.437497
H	1.519367	-0.062901	0.798511
C	0.172753	0.423208	-0.818595
H	0.103954	0.281282	-1.904491
H	0.204252	1.506922	-0.656992
C	-1.099194	-0.147163	-0.177216
H	-1.110549	-1.240079	-0.355405
H	-1.056125	-0.035532	0.919915
O	6.364871	-0.263302	-0.417098
C	7.648203	0.142364	-0.970083
C	8.730421	-0.464725	-0.123592
H	7.702340	-0.196669	-2.006149
H	7.693388	1.232783	-0.970861
C	9.181458	0.189168	1.027191
C	9.288381	-1.701087	-0.460590
C	10.170899	-0.379891	1.824981
H	8.754581	1.150272	1.298586
C	10.279253	-2.273406	0.334243
H	8.945253	-2.217960	-1.352089
H	10.514216	0.139538	2.713825
C	10.722227	-1.613121	1.479071
H	10.706725	-3.232217	0.059096

H 11.496005 -2.056013 2.097862
H -3.335641 -0.795769 -0.764420

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure I2, in toluene
N -5.295034 -3.432729 0.248575
C -4.542080 -2.280622 0.270269
N -4.307751 -1.566133 1.334134
C -4.825283 -2.041866 2.607995
C -6.177382 -2.732689 2.446667
C -6.037889 -3.863133 1.435147
C -4.572461 -3.907583 -2.081568
C -4.418592 -2.397147 -2.197488
N -3.962965 -1.891940 -0.914931
C -5.551349 -4.222165 -0.957223
H -4.911576 -1.185752 3.283351
H -4.112368 -2.735890 3.080560
H -6.911729 -2.003323 2.089532
H -6.542667 -3.131507 3.397614
H -5.532914 -4.726595 1.889634
H -7.025478 -4.209065 1.109593
H -5.492875 -5.283086 -0.688741
H -6.581889 -4.039824 -1.296332
H -3.594893 -4.349454 -1.867728
H -4.939954 -4.340825 -3.015516
H -5.372206 -1.942899 -2.509556
H -3.672608 -2.133885 -2.950278
H -3.659021 0.000056 1.354640
O -3.229247 0.913845 1.447615
C -3.050025 1.467913 0.218104
O -4.301358 1.476206 -0.432737
C -4.408005 2.122668 -1.709616
H -3.435600 2.147368 -2.208969
H -5.067622 1.490599 -2.310280
C -5.009148 3.513204 -1.549826
H -5.952999 3.405190 -1.003340
H -5.264533 3.907759 -2.541235
C -4.094937 4.502229 -0.819591
H -3.266273 4.788911 -1.480298
H -4.656525 5.423371 -0.627849
C -3.505232 3.997569 0.507296
H -4.299406 3.646926 1.174416

H	-3.037785	4.852876	1.004522
C	-2.434668	2.893319	0.363732
H	-1.862230	3.084111	-0.548403
C	-1.449204	2.953001	1.561010
H	-0.803909	2.073189	1.579592
C	-0.604236	4.145801	1.544275
H	-2.021889	2.914534	2.491585
C	0.099900	5.121376	1.515863
H	0.723038	5.984115	1.497333
O	5.360661	1.060500	-1.947552
O	-2.240581	0.618436	-0.647579
C	5.296767	0.281660	-1.026266
C	4.023681	-0.234623	-0.389398
H	3.978618	-1.313929	-0.579512
H	4.125067	-0.137648	0.696563
C	2.761687	0.461962	-0.895840
H	2.710614	0.371213	-1.985312
H	2.832056	1.534958	-0.688224
C	1.485319	-0.103790	-0.265760
H	1.413279	-1.176539	-0.488434
H	1.552808	-0.027703	0.827332
C	0.214839	0.604607	-0.747786
H	0.140645	0.537006	-1.839317
H	0.275957	1.671917	-0.509785
C	-1.049143	0.005277	-0.136857
H	-1.117673	-1.056135	-0.398755
H	-1.043949	0.057606	0.953951
O	6.382663	-0.255039	-0.430649
C	7.673172	0.153576	-0.966727
C	8.744329	-0.526397	-0.162979
H	7.713935	-0.126012	-2.020924
H	7.742911	1.240797	-0.904209
C	9.236178	0.062661	1.005798
C	9.250120	-1.767913	-0.558740
C	10.214862	-0.575103	1.764110
H	8.850232	1.027196	1.322591
C	10.229606	-2.408840	0.196575
H	8.875003	-2.234538	-1.464974
H	10.590446	-0.105630	2.667551
C	10.713686	-1.812843	1.360034
H	10.616611	-3.370787	-0.123703
H	11.478859	-2.309290	1.948067
H	-3.543416	-0.967994	-0.891242

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure TS23, in toluene

N	-4.615838	-3.782253	0.250202
C	-4.120325	-2.498637	0.251365
N	-3.967315	-1.761330	1.314000
C	-4.284582	-2.346266	2.607991
C	-5.466647	-3.308742	2.519902
C	-5.161382	-4.373575	1.474104
C	-3.974713	-4.070010	-2.133608
C	-4.145827	-2.559727	-2.221847
N	-3.715103	-1.985065	-0.959524
C	-4.786350	-4.594607	-0.955753
H	-4.504244	-1.533697	3.306496
H	-3.409814	-2.875537	3.017510
H	-6.362896	-2.750427	2.230390
H	-5.670724	-3.785319	3.483194
H	-4.451722	-5.111997	1.871806
H	-6.072682	-4.920987	1.208390
H	-4.489813	-5.622611	-0.718655
H	-5.853377	-4.627978	-1.221185
H	-2.914295	-4.300449	-1.995752
H	-4.308180	-4.559878	-3.052125
H	-5.192335	-2.310577	-2.457925
H	-3.524515	-2.139040	-3.015196
H	-3.609054	-0.103144	1.330682
O	-3.347871	0.872229	1.422248
C	-3.235235	1.443256	0.192040
O	-4.436116	1.176452	-0.509476
C	-4.669207	1.838591	-1.760886
H	-3.722131	2.107381	-2.237254
H	-5.157407	1.099401	-2.401854
C	-5.580843	3.043982	-1.561961
H	-6.476917	2.694589	-1.036328
H	-5.914196	3.403721	-2.543433
C	-4.935787	4.195682	-0.783075
H	-4.201380	4.701424	-1.423474
H	-5.705399	4.943822	-0.562457
C	-4.239355	3.796623	0.528203
H	-4.928386	3.253489	1.182987
H	-3.974059	4.718930	1.053598
C	-2.952534	2.965581	0.335607
H	-2.468667	3.280627	-0.593312

C	-1.948479	3.224640	1.487564
H	-1.100621	2.539854	1.414260
C	-1.431847	4.592069	1.501546
H	-2.433913	2.998841	2.440861
C	-0.998110	5.714563	1.500476
H	-0.612701	6.706712	1.505309
O	5.336336	1.254928	-1.928792
O	-2.218068	0.810160	-0.628472
C	5.290632	0.511487	-0.977682
C	4.030821	0.035584	-0.285273
H	3.993138	-1.055624	-0.386953
H	4.146006	0.220275	0.788197
C	2.756530	0.680504	-0.827692
H	2.693988	0.505230	-1.906325
H	2.819961	1.766936	-0.705518
C	1.491426	0.154699	-0.142557
H	1.432558	-0.933860	-0.272837
H	1.563210	0.324579	0.939665
C	0.210238	0.802011	-0.678362
H	0.139607	0.645820	-1.761023
H	0.249020	1.887020	-0.527337
C	-1.048175	0.242547	-0.023931
H	-1.096906	-0.842822	-0.169426
H	-1.058361	0.415670	1.053384
O	6.387797	-0.014803	-0.393377
C	7.665762	0.360190	-0.981732
C	8.753190	-0.316988	-0.197807
H	7.666233	0.054390	-2.029411
H	7.754567	1.447296	-0.948857
C	9.328369	0.313074	0.909646
C	9.191911	-1.596568	-0.551011
C	10.323471	-0.321316	1.649627
H	8.995008	1.307139	1.193051
C	10.186584	-2.234450	0.186374
H	8.752080	-2.095157	-1.409906
H	10.764172	0.180355	2.505061
C	10.754440	-1.597034	1.288649
H	10.520746	-3.226317	-0.100406
H	11.531988	-2.091249	1.862150
H	-3.520264	-0.990991	-0.939358

80 atoms

addition of another 3-isomer unit to the ε-CL chain end, structure I3, in toluene

N	-2.746074	-4.264437	0.380183
C	-2.925817	-2.908540	0.238026
N	-2.787969	-2.033098	1.192901
C	-2.353164	-2.504880	2.498627
C	-2.914698	-3.889262	2.815896
C	-2.520335	-4.852352	1.702782
C	-2.885592	-4.575774	-2.081243
C	-3.744058	-3.317776	-2.059542
N	-3.233052	-2.443957	-1.018862
C	-2.923333	-5.230172	-0.705590
H	-2.676049	-1.778313	3.249625
H	-1.253384	-2.534859	2.552510
H	-4.005804	-3.827019	2.883202
H	-2.545489	-4.263602	3.775185
H	-1.464897	-5.141437	1.799412
H	-3.108859	-5.774258	1.768431
H	-2.132959	-5.984654	-0.623233
H	-3.878475	-5.758265	-0.567804
H	-1.859233	-4.301129	-2.341476
H	-3.243913	-5.285639	-2.831287
H	-4.800904	-3.583984	-1.900275
H	-3.683878	-2.786512	-3.011957
H	-3.330705	-0.413341	1.113308
O	-3.694779	0.518049	1.249864
C	-3.556821	1.328180	0.157032
O	-3.808599	0.499248	-0.990904
C	-3.977656	1.138162	-2.263599
H	-3.434165	2.086918	-2.283012
H	-3.503265	0.479847	-2.997181
C	-5.459863	1.307065	-2.583348
H	-5.933211	0.323106	-2.484006
H	-5.562594	1.595793	-3.636819
C	-6.190904	2.326349	-1.700117
H	-5.893056	3.340473	-1.995920
H	-7.264778	2.258229	-1.907076
C	-5.962332	2.181020	-0.186017
H	-6.217978	1.171360	0.151986
H	-6.654074	2.861468	0.319540
C	-4.530618	2.526769	0.261956
H	-4.134338	3.306367	-0.394766
C	-4.481190	3.089149	1.703890
H	-3.435792	3.183206	2.009937

C	-5.137364	4.387712	1.837297
H	-4.938014	2.368826	2.387730
C	-5.673394	5.460524	1.938741
H	-6.143456	6.410452	2.035952
O	5.276569	2.822037	-0.793981
O	-2.269911	1.913358	0.033820
C	5.200400	1.675808	-0.420609
C	3.920567	0.923255	-0.123452
H	3.894919	0.044131	-0.777870
H	3.998057	0.521769	0.893108
C	2.659501	1.769554	-0.289038
H	2.621231	2.167740	-1.308111
H	2.719451	2.642156	0.369667
C	1.381022	0.980972	0.010600
H	1.325808	0.109309	-0.654540
H	1.431618	0.578634	1.030612
C	0.109603	1.821592	-0.141640
H	0.046094	2.223952	-1.159118
H	0.149891	2.685582	0.531308
C	-1.153197	1.028463	0.157525
H	-1.261126	0.190186	-0.539492
H	-1.121206	0.616043	1.171194
O	6.277880	0.888705	-0.214712
C	7.573904	1.501549	-0.468490
C	8.635264	0.483732	-0.162773
H	7.605940	1.824638	-1.510379
H	7.663943	2.388272	0.161347
C	9.116041	0.330851	1.141384
C	9.143785	-0.339498	-1.171291
C	10.085840	-0.625126	1.432535
H	8.728254	0.965829	1.932633
C	10.115029	-1.296358	-0.884392
H	8.777897	-0.229300	-2.187975
H	10.452974	-0.731305	2.448229
C	10.587638	-1.440725	0.418869
H	10.504359	-1.926442	-1.677555
H	11.346365	-2.183414	0.643579
H	-3.494370	-1.463003	-1.034997

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure TS3r, in toluene

N	-4.308161	4.003688	-0.396760

C	-3.938566	2.685990	-0.261920
N	-4.120862	1.762510	-1.160790
C	-4.710653	2.145931	-2.434281
C	-5.734511	3.267088	-2.271248
C	-5.075001	4.444775	-1.563886
C	-3.067737	4.599015	1.670136
C	-3.330731	3.158837	2.089181
N	-3.288298	2.328834	0.898218
C	-4.108951	5.017846	0.639521
H	-5.177900	1.260563	-2.874666
H	-3.928392	2.463375	-3.141323
H	-6.576594	2.901795	-1.673947
H	-6.131591	3.591761	-3.237440
H	-4.415219	4.988484	-2.253796
H	-5.832771	5.157895	-1.220905
H	-3.803077	5.949109	0.149994
H	-5.068366	5.223673	1.137098
H	-2.063537	4.667117	1.241751
H	-3.113316	5.273799	2.528863
H	-4.297109	3.090079	2.613873
H	-2.561027	2.806021	2.779370
H	-3.527684	0.166759	-1.058135
O	-3.189492	-0.770942	-1.215011
C	-3.058724	-1.530364	-0.079497
O	-3.373172	-0.666541	1.021211
C	-3.581006	-1.253995	2.313360
H	-3.005464	-2.179556	2.403330
H	-3.163715	-0.544688	3.033699
C	-5.069142	-1.460393	2.579008
H	-5.570162	-0.501996	2.399684
H	-5.207781	-1.689554	3.642901
C	-5.723423	-2.556817	1.729282
H	-5.405576	-3.539807	2.099656
H	-6.807659	-2.515694	1.882064
C	-5.425022	-2.491462	0.222356
H	-5.707277	-1.515165	-0.187062
H	-6.060520	-3.230353	-0.274708
C	-3.957762	-2.793004	-0.132278
H	-3.554530	-3.504665	0.594039
C	-3.810921	-3.445967	-1.528473
H	-2.748124	-3.511848	-1.776886
C	-4.403794	-4.778856	-1.605934
H	-4.261697	-2.791908	-2.279630
C	-4.888236	-5.879227	-1.662146

H	-5.311738	-6.854040	-1.718194
O	5.848401	-2.420659	0.823357
O	-1.742423	-2.025760	0.065009
C	5.699572	-1.299923	0.397876
C	4.372346	-0.630841	0.108433
H	4.298084	0.246789	0.761687
H	4.413495	-0.228410	-0.909468
C	3.169654	-1.554730	0.292468
H	3.174242	-1.956628	1.310637
H	3.273835	-2.420499	-0.369956
C	1.837966	-0.849796	0.017237
H	1.736804	0.012668	0.689184
H	1.844874	-0.439455	-1.000730
C	0.628152	-1.774324	0.184863
H	0.611301	-2.188591	1.199491
H	0.714335	-2.628106	-0.496652
C	-0.690761	-1.066575	-0.084358
H	-0.838330	-0.239824	0.620692
H	-0.717053	-0.650860	-1.095545
O	6.726395	-0.468130	0.121519
C	8.060314	-0.995305	0.371754
C	9.055185	0.064660	-0.005871
H	8.132013	-1.266210	1.426556
H	8.187932	-1.904394	-0.218226
C	9.554777	0.137143	-1.309542
C	9.480291	1.007919	0.934304
C	10.462100	1.131433	-1.667692
H	9.231545	-0.590821	-2.047927
C	10.387567	2.003759	0.580232
H	9.099010	0.960853	1.950237
H	10.844931	1.174319	-2.682222
C	10.880280	2.066933	-0.722391
H	10.712293	2.727727	1.320591
H	11.589855	2.840112	-0.998880
H	-3.224338	1.322722	1.014572

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure I3r, in toluene

N	-5.831963	3.220074	-0.517634
C	-4.963319	2.167029	-0.354598
N	-4.897570	1.125355	-1.137809
C	-5.756581	1.093830	-2.311284

C	-7.105484	1.758520	-2.045412
C	-6.870271	3.179821	-1.549508
C	-4.604755	4.537424	1.190006
C	-4.221107	3.186959	1.780179
N	-4.077894	2.238777	0.691495
C	-5.880915	4.380600	0.372710
H	-5.897139	0.049951	-2.606717
H	-5.265832	1.589742	-3.163382
H	-7.646002	1.185652	-1.284552
H	-7.726884	1.779940	-2.945402
H	-6.585272	3.836513	-2.382862
H	-7.790167	3.592479	-1.120424
H	-6.048191	5.272205	-0.241526
H	-6.748862	4.291442	1.042813
H	-3.790173	4.893213	0.552462
H	-4.764486	5.279155	1.976870
H	-4.979354	2.868686	2.513267
H	-3.266549	3.247324	2.307630
H	-3.571013	0.050644	-1.055141
O	-2.741900	-0.522008	-1.103322
C	-2.582458	-1.322338	0.000865
O	-2.820367	-0.467179	1.136246
C	-2.921163	-1.067286	2.434899
H	-2.332061	-1.988398	2.469671
H	-2.453826	-0.360429	3.126073
C	-4.379636	-1.296296	2.821354
H	-4.908503	-0.344449	2.694412
H	-4.425784	-1.536280	3.890918
C	-5.087417	-2.395193	2.019536
H	-4.719979	-3.375875	2.348163
H	-6.154439	-2.376653	2.268531
C	-4.926930	-2.307043	0.492794
H	-5.265944	-1.332591	0.124632
H	-5.589769	-3.054906	0.046874
C	-3.492648	-2.582806	0.004299
H	-3.024397	-3.303756	0.681025
C	-3.461574	-3.214048	-1.409355
H	-2.424842	-3.253841	-1.753951
C	-4.034311	-4.557381	-1.453426
H	-3.990859	-2.562553	-2.110687
C	-4.502793	-5.665623	-1.483749
H	-4.911307	-6.647891	-1.516114
O	6.322607	-2.103646	0.854754
O	-1.270133	-1.819778	0.038027

C	6.164592	-1.007373	0.372587
C	4.833274	-0.374350	0.026548
H	4.745679	0.548532	0.611954
H	4.878975	-0.047869	-1.018199
C	3.637449	-1.293753	0.268401
H	3.636698	-1.619706	1.313456
H	3.754607	-2.204736	-0.327784
C	2.302348	-0.622616	-0.068024
H	2.189978	0.287547	0.535730
H	2.313521	-0.290515	-1.114114
C	1.097708	-1.540605	0.161643
H	1.078026	-1.879204	1.203909
H	1.192852	-2.441641	-0.454989
C	-0.223004	-0.860966	-0.164817
H	-0.388000	0.006111	0.483150
H	-0.242171	-0.513309	-1.201287
O	7.183584	-0.173799	0.073404
C	8.520789	-0.667721	0.369338
C	9.505551	0.390862	-0.037528
H	8.578017	-0.891003	1.436085
H	8.672991	-1.599526	-0.177871
C	10.022208	0.418334	-1.336278
C	9.903544	1.377610	0.869248
C	10.919782	1.411053	-1.722181
H	9.719906	-0.343556	-2.048861
C	10.801116	2.372002	0.487389
H	9.508550	1.365896	1.880938
H	11.316016	1.418964	-2.732427
C	11.310989	2.390122	-0.809993
H	11.104711	3.130090	1.202124
H	12.012893	3.162271	-1.108095
H	-3.559875	1.381555	0.854593

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure TS34, in toluene

N	-4.577252	3.826574	-0.324017
C	-4.186024	2.533885	-0.189045
N	-4.400614	1.657815	-1.186459
C	-4.912955	2.057492	-2.488675
C	-5.919003	3.184427	-2.303476
C	-5.266867	4.318617	-1.522911
C	-3.148193	4.393324	1.610202

C	-3.365634	2.957766	2.069894
N	-3.595925	2.096831	0.919287
C	-4.311159	4.819690	0.723174
H	-5.375985	1.182353	-2.946771
H	-4.096384	2.378386	-3.149325
H	-6.790847	2.809101	-1.759710
H	-6.264496	3.557774	-3.270112
H	-4.552611	4.861612	-2.155202
H	-6.022068	5.039564	-1.197010
H	-4.085163	5.768051	0.227846
H	-5.218958	4.974203	1.320322
H	-2.210759	4.460647	1.049841
H	-3.072764	5.067873	2.466262
H	-4.212593	2.907172	2.767209
H	-2.490426	2.576062	2.598960
H	-3.942489	0.737694	-1.123282
O	-3.048258	-0.753654	-1.314009
C	-2.877067	-1.602881	-0.429215
O	-3.164116	-0.456126	1.221950
C	-3.554065	-0.997651	2.441618
H	-3.059480	-1.971654	2.618085
H	-3.222359	-0.352483	3.279398
C	-5.077063	-1.174630	2.558047
H	-5.540302	-0.207820	2.319290
H	-5.344231	-1.396357	3.601457
C	-5.681466	-2.262770	1.660219
H	-5.407028	-3.250194	2.054616
H	-6.774389	-2.208874	1.742934
C	-5.309520	-2.221976	0.166786
H	-5.439013	-1.213717	-0.235978
H	-6.025814	-2.860020	-0.361506
C	-3.886871	-2.718797	-0.157975
H	-3.504457	-3.317601	0.671043
C	-3.865492	-3.622210	-1.427176
H	-2.827048	-3.857232	-1.681743
C	-4.607167	-4.870066	-1.271285
H	-4.269403	-3.052258	-2.270803
C	-5.215392	-5.899432	-1.133314
H	-5.747873	-6.813000	-1.012652
O	5.951061	-2.329000	0.940469
O	-1.622520	-2.049188	-0.115166
C	5.808543	-1.257424	0.401716
C	4.491351	-0.651367	-0.034424
H	4.390905	0.317998	0.467326

H	4.571479	-0.414875	-1.101495
C	3.282882	-1.543456	0.244083
H	3.238247	-1.770511	1.314118
H	3.419292	-2.506113	-0.259432
C	1.966263	-0.903896	-0.207042
H	1.835466	0.059692	0.302701
H	2.022148	-0.672692	-1.278901
C	0.746012	-1.790562	0.059906
H	0.675627	-2.019766	1.128927
H	0.862314	-2.750105	-0.457207
C	-0.550871	-1.139608	-0.391589
H	-0.745595	-0.211368	0.152382
H	-0.531748	-0.910428	-1.461315
O	6.835855	-0.431294	0.108313
C	8.161625	-0.904310	0.479443
C	9.158700	0.137716	0.059821
H	8.178480	-1.075435	1.557143
H	8.337256	-1.860842	-0.015697
C	9.705666	0.118921	-1.226755
C	9.538340	1.154476	0.940760
C	10.614808	1.095638	-1.625766
H	9.417886	-0.666788	-1.919196
C	10.447818	2.133000	0.545787
H	9.119829	1.178767	1.942717
H	11.034688	1.067502	-2.626065
C	10.987730	2.104979	-0.739095
H	10.737121	2.914608	1.240854
H	11.698915	2.864593	-1.047263
H	-3.414594	1.028660	1.030843

80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure I4, in toluene

N	-2.019999	4.115389	-0.066782
C	-2.498047	2.826020	-0.012397
N	-3.226293	2.383650	-1.091890
C	-3.202421	3.062341	-2.375499
C	-3.338405	4.557519	-2.124169
C	-2.209306	5.012440	-1.208277
C	-0.555609	3.508374	1.824615
C	-1.659839	2.515246	2.178238
N	-2.340293	2.011738	0.993998
C	-1.153337	4.635949	0.992628

H	-4.034393	2.684923	-2.973256
H	-2.277484	2.857348	-2.937641
H	-4.307391	4.754188	-1.656245
H	-3.297154	5.120077	-3.060479
H	-1.269475	5.081595	-1.776041
H	-2.416414	6.016204	-0.820630
H	-0.359840	5.226251	0.520839
H	-1.724682	5.324023	1.630737
H	0.221691	2.995285	1.248140
H	-0.082970	3.920727	2.720911
H	-2.377389	2.998690	2.860259
H	-1.250700	1.661813	2.726337
H	-3.394346	1.384156	-1.099465
O	-3.789292	-0.548407	-1.412716
C	-3.650009	-1.515484	-0.690981
O	-3.921367	-0.167971	1.741466
C	-5.165860	0.398734	2.115894
H	-5.525229	-0.146430	2.998383
H	-5.024148	1.444589	2.421830
C	-6.243347	0.350030	1.027442
H	-5.866943	0.842996	0.124494
H	-7.074826	0.970313	1.388045
C	-6.807670	-1.045647	0.687048
H	-6.812848	-1.664898	1.593873
H	-7.862537	-0.922052	0.415904
C	-6.167882	-1.844558	-0.462787
H	-6.137876	-1.228799	-1.366668
H	-6.845772	-2.675712	-0.679946
C	-4.768787	-2.436183	-0.221033
H	-4.597646	-2.595511	0.845426
C	-4.588479	-3.809884	-0.937333
H	-3.549120	-4.133376	-0.838306
C	-5.461881	-4.853679	-0.408866
H	-4.778402	-3.687259	-2.010538
C	-6.176981	-5.712146	0.036597
H	-6.805826	-6.475209	0.430703
O	5.049192	-2.939092	0.766967
O	-2.456371	-1.957991	-0.277267
C	5.011882	-1.840702	0.265978
C	3.764936	-1.129343	-0.216598
H	3.755934	-0.128162	0.227626
H	3.877716	-0.965123	-1.294877
C	2.473628	-1.885709	0.090297
H	2.388102	-2.033560	1.171862

```
H      2.529268    -2.888700    -0.344291
C      1.230205    -1.159825    -0.432349
H      1.184254    -0.153038     0.001913
H      1.320057    -1.018345    -1.517317
C     -0.069224    -1.908990    -0.118614
H     -0.173920    -2.039483     0.963601
H     -0.035480    -2.913922    -0.554200
C     -1.291414    -1.177539    -0.643537
H     -1.392568    -0.184068    -0.200578
H     -1.267745    -1.071284    -1.731383
O      6.107514    -1.080903     0.057079
C      7.378140    -1.665605     0.462896
C      8.463980    -0.677842     0.145068
H      7.330071    -1.891129     1.529413
H      7.510606    -2.606369    -0.074406
C      9.039341    -0.642284    -1.128896
C      8.900810     0.234319     1.109702
C     10.031907     0.285735    -1.433414
H      8.707809    -1.347274    -1.885702
C      9.894523     1.163598     0.809427
H      8.461120     0.215447     2.102647
H     10.472859     0.300554    -2.424888
C     10.461612     1.190825    -0.463501
H     10.227582     1.863628     1.568830
H     11.237946     1.911924    -0.698114
H     -3.348005     0.560198     1.396219


80 atoms
addition of another 3-isomer unit to the ε-CL chain end,
structure I5, in toluene
N     -9.428564    -1.437964    -0.107887
C     -8.073859    -1.642601     0.019758
N     -7.547765    -1.565323     1.292074
C     -8.376786    -1.681232     2.478259
C     -9.598864    -0.793326     2.285680
C    -10.334235    -1.222386     1.021955
C     -9.212460    -2.389843    -2.375360
C     -7.784509    -1.849706    -2.318735
N     -7.251148    -1.862484    -0.966201
C    -10.083194    -1.597116    -1.408198
H     -7.787735    -1.356407     3.338509
H     -8.689910    -2.719754     2.669643
H     -9.272311     0.247018     2.198358
```

H	-10.275677	-0.862460	3.141283
H	-10.901395	-2.145502	1.213621
H	-11.065258	-0.459463	0.731639
H	-11.037985	-2.109525	-1.246174
H	-10.319863	-0.608250	-1.824416
H	-9.208368	-3.446331	-2.087172
H	-9.628168	-2.324682	-3.385245
H	-7.764143	-0.829007	-2.732939
H	-7.125554	-2.448636	-2.954257
H	-6.584987	-1.879118	1.344544
O	-0.659790	2.992152	1.826490
C	-0.712727	2.792770	0.635037
O	-4.878595	-2.522093	0.282021
C	-3.769478	-1.691146	-0.026210
H	-2.943096	-2.027934	0.608568
H	-3.453930	-1.844059	-1.069550
C	-4.037139	-0.203625	0.214306
H	-4.336930	-0.066336	1.260226
H	-4.894452	0.102969	-0.395958
C	-2.826196	0.679844	-0.101883
H	-1.971757	0.350436	0.502260
H	-2.529005	0.537085	-1.148530
C	-3.096224	2.167259	0.149099
H	-3.345291	2.325731	1.204200
H	-3.975230	2.475320	-0.428697
C	-1.927679	3.099682	-0.229780
H	-1.654175	2.934210	-1.274294
C	-2.333083	4.581764	-0.041647
H	-2.523309	4.762237	1.021031
C	-1.332578	5.529529	-0.526788
H	-3.278778	4.755202	-0.565691
C	-0.498347	6.293358	-0.934990
H	0.236260	6.975805	-1.292381
O	7.044608	-0.656064	-2.149894
O	0.291207	2.255603	-0.078195
C	7.209064	-0.476696	-0.966649
C	6.179174	0.076130	-0.003640
H	6.028385	-0.670477	0.784491
H	6.624279	0.940855	0.501031
C	4.856770	0.445889	-0.672812
H	4.448410	-0.434281	-1.179595
H	5.042476	1.184070	-1.459782
C	3.830444	0.995992	0.322200
H	3.646970	0.251160	1.107071

H	4.248423	1.874455	0.830201
C	2.503711	1.374759	-0.344673
H	2.073077	0.500647	-0.845138
H	2.676540	2.127195	-1.121671
C	1.498006	1.919998	0.652334
H	1.246921	1.188091	1.424194
H	1.862415	2.820425	1.152241
O	8.363118	-0.754110	-0.325363
C	9.436819	-1.297387	-1.145907
C	10.623159	-1.535195	-0.256142
H	9.083035	-2.218869	-1.611188
H	9.657951	-0.582539	-1.940356
C	11.551485	-0.515861	-0.023831
C	10.804904	-2.771048	0.371150
C	12.640799	-0.726677	0.817948
H	11.419990	0.448205	-0.506485
C	11.893483	-2.986159	1.213360
H	10.089838	-3.569939	0.197758
H	13.355996	0.071715	0.987416
C	12.813536	-1.963367	1.438263
H	12.024980	-3.951425	1.691502
H	13.663738	-2.130230	2.091742
H	-5.618401	-2.332748	-0.350997

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I1, in toluene

O	3.109445	0.768452	-2.509298
O	4.242105	1.689554	-0.875111
C	3.188288	1.681417	-1.714345
C	2.203687	2.828604	-1.674875
H	1.640170	2.757663	-0.739280
H	1.499974	2.639961	-2.485963
C	2.832509	4.228594	-1.822696
H	3.564860	4.219496	-2.638556
H	2.040578	4.914905	-2.137798
C	3.472448	4.780111	-0.543804
H	2.699015	4.864978	0.229842
H	3.822906	5.800041	-0.734507
C	4.637603	3.953427	0.010074
H	5.478790	3.949959	-0.693689
H	4.999841	4.426033	0.928252
C	4.283310	2.504292	0.331365

H	3.311794	2.423854	0.823057
C	5.332128	1.786690	1.197836
H	5.052574	0.729029	1.241276
C	5.436643	2.334524	2.546080
H	6.304948	1.838583	0.695445
C	5.514502	2.784705	3.658684
H	5.582829	3.177258	4.645778
N	4.969988	-3.483407	0.084762
C	4.384694	-2.253501	-0.128238
N	4.493130	-1.728703	-1.386345
C	4.930995	-2.493861	-2.536786
C	6.112567	-3.357956	-2.116396
C	5.690590	-4.234322	-0.944073
C	3.637549	-3.604680	2.162618
C	3.773437	-2.083834	2.147288
N	3.771529	-1.556054	0.790620
C	4.771292	-4.206626	1.342416
H	5.212953	-1.789098	-3.321225
H	4.126605	-3.126903	-2.942902
H	6.944152	-2.709888	-1.824232
H	6.452824	-3.990933	-2.940314
H	5.057682	-5.059975	-1.302541
H	6.569345	-4.693536	-0.476671
H	4.556937	-5.254940	1.102686
H	5.707166	-4.198793	1.918086
H	2.672809	-3.883484	1.725876
H	3.667110	-4.004617	3.180616
H	4.695341	-1.796952	2.678429
H	2.950101	-1.615892	2.694368
H	4.027165	-0.845155	-1.553125
O	-5.694828	2.004393	0.888158
O	1.784168	0.367932	0.618200
C	-5.699832	0.879180	0.448424
C	-4.475955	0.050388	0.120130
H	-4.497983	-0.153331	-0.957210
H	-4.592768	-0.927515	0.599467
C	-3.160864	0.714778	0.524156
H	-3.092191	1.698688	0.049223
H	-3.167596	0.904730	1.602778
C	-1.936035	-0.127551	0.154668
H	-1.931680	-0.307523	-0.928460
H	-2.018960	-1.116938	0.623617
C	-0.613613	0.523361	0.569540
H	-0.530829	1.516149	0.110769

H	-0.595622	0.682610	1.654033
C	0.609569	-0.298205	0.184466
H	0.627770	-0.449962	-0.906400
H	0.540740	-1.295632	0.644224
O	-6.830885	0.193701	0.176578
C	-8.080253	0.895371	0.433744
C	-9.210972	-0.026181	0.076028
H	-8.092116	1.808367	-0.164225
H	-8.104988	1.182371	1.486274
C	-9.769951	-0.871683	1.038641
C	-9.707300	-0.067772	-1.230375
C	-10.805855	-1.741027	0.704387
H	-9.391795	-0.847669	2.056534
C	-10.742488	-0.935866	-1.568814
H	-9.280404	0.584952	-1.986276
H	-11.233433	-2.389593	1.462169
C	-11.293990	-1.774351	-0.600917
H	-11.120947	-0.955979	-2.585700
H	-12.103063	-2.448759	-0.862309
H	2.536600	-0.279824	0.601765

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure TS12, in toluene

O	3.115029	0.476441	-2.279345
O	4.170217	1.458345	-0.594960
C	3.020338	1.317056	-1.368140
C	2.198903	2.586963	-1.594529
H	1.660070	2.869145	-0.690127
H	1.453434	2.324740	-2.346908
C	3.053437	3.775138	-2.078167
H	3.810941	3.426896	-2.789698
H	2.408337	4.464063	-2.634215
C	3.709214	4.555920	-0.930020
H	2.915519	4.927921	-0.268917
H	4.205185	5.445900	-1.334311
C	4.726865	3.772665	-0.090601
H	5.622130	3.559419	-0.687686
H	5.049338	4.400223	0.747121
C	4.220381	2.435324	0.456671
H	3.229701	2.529374	0.906938
C	5.174448	1.828607	1.504194
H	4.816972	0.820660	1.731878

C	5.275111	2.605140	2.735965
H	6.166675	1.713596	1.052298
C	5.345959	3.242243	3.753990
H	5.408991	3.807725	4.653609
N	4.735926	-3.472467	0.240680
C	4.133690	-2.313962	-0.136127
N	4.243791	-1.880898	-1.397523
C	4.943667	-2.627901	-2.431201
C	6.121539	-3.367095	-1.810174
C	5.620427	-4.225543	-0.656137
C	3.287263	-3.500312	2.249389
C	3.307892	-1.981499	2.135803
N	3.428847	-1.594763	0.738277
C	4.526306	-4.065476	1.566943
H	5.274562	-1.912273	-3.184928
H	4.266443	-3.335401	-2.927520
H	6.855118	-2.641358	-1.447136
H	6.617489	-4.001783	-2.548208
H	5.084298	-5.105165	-1.035126
H	6.461260	-4.593634	-0.060390
H	4.430770	-5.147595	1.435121
H	5.418068	-3.893309	2.183080
H	2.384177	-3.889662	1.769925
H	3.271398	-3.815246	3.295440
H	4.136951	-1.571019	2.728003
H	2.389075	-1.536350	2.520073
H	3.827573	-0.967172	-1.663728
O	-5.546088	2.029257	0.945183
O	1.966751	0.482900	0.027046
C	-5.560631	0.958012	0.386921
C	-4.349738	0.209670	-0.128550
H	-4.433347	0.170223	-1.221647
H	-4.428063	-0.831108	0.202976
C	-3.018916	0.831733	0.292370
H	-2.992102	1.877700	-0.029048
H	-2.960521	0.855545	1.386199
C	-1.807874	0.083059	-0.273346
H	-1.868981	0.070122	-1.369936
H	-1.850518	-0.968894	0.040728
C	-0.467861	0.688903	0.154270
H	-0.425516	1.740984	-0.151424
H	-0.388744	0.686270	1.248784
C	0.751737	-0.045787	-0.419135
H	0.706842	-0.036193	-1.522318

```
H      0.671948    -1.114311    -0.135575
O     -6.695691     0.270623     0.132720
C     -7.934630     0.906363     0.555407
C     -9.070345    -0.011217     0.202637
H     -8.016318     1.870621     0.050112
H     -7.880280     1.093547     1.628991
C     -9.572802    -0.915388     1.142398
C     -9.629086     0.011924    -1.079064
C    -10.614921    -1.778766     0.810689
H     -9.145993    -0.942265     2.140801
C    -10.669575    -0.850269    -1.415121
H     -9.246129     0.710617    -1.817169
H    -10.998327    -2.473255     1.551247
C    -11.165036    -1.747532    -0.469493
H    -11.096378    -0.820071    -2.412441
H    -11.978614    -2.417319    -0.728827
H      2.890283    -0.723384     0.411723
```

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I2, in toluene

```
O     -3.100006    -0.445046    -2.156934
O     -4.023030    -1.474047    -0.389726
C     -2.826660    -1.281708    -1.113074
C     -2.219416    -2.582799    -1.662006
H     -1.627290    -3.063479    -0.878769
H     -1.522419    -2.292788    -2.451227
C     -3.255309    -3.576341    -2.212233
H     -4.031736    -3.031157    -2.757845
H     -2.760613    -4.222014    -2.945589
C     -3.878305    -4.474713    -1.131843
H     -3.068635    -5.005604    -0.613761
H     -4.481838    -5.250765    -1.615835
C     -4.753834    -3.761135    -0.093280
H     -5.681051    -3.411644    -0.562911
H     -5.042554    -4.477703     0.682903
C     -4.099355    -2.544174     0.563377
H     -3.098934    -2.785700     0.935042
C     -4.926094    -1.982122     1.736857
H     -4.460237    -1.045501     2.056620
C     -5.033008    -2.890663     2.874205
H     -5.924679    -1.721543     1.368065
C     -5.104451    -3.637383     3.814578
```

H	-5.172661	-4.298780	4.645888
N	-4.800523	3.605375	0.206575
C	-4.135036	2.459341	-0.168793
N	-4.194986	1.918064	-1.350964
C	-4.980945	2.587991	-2.375318
C	-6.214670	3.270491	-1.788938
C	-5.775020	4.229774	-0.690225
C	-3.510470	3.707745	2.326374
C	-3.413241	2.194837	2.185124
N	-3.316367	1.877718	0.771937
C	-4.718077	4.202202	1.540221
H	-5.274639	1.843897	-3.121460
H	-4.368352	3.332347	-2.908352
H	-6.881111	2.508813	-1.371078
H	-6.774910	3.816467	-2.553732
H	-5.342316	5.141288	-1.125322
H	-6.636159	4.543600	-0.089399
H	-4.674795	5.291107	1.423944
H	-5.642121	3.981442	2.095197
H	-2.594049	4.161966	1.938245
H	-3.613371	4.000773	3.374499
H	-4.283645	1.717028	2.662460
H	-2.520527	1.809236	2.682265
H	-3.519527	0.406151	-1.812997
O	5.575286	-2.052140	0.920525
O	-1.941220	-0.651542	-0.148447
C	5.581585	-0.989315	0.346181
C	4.367418	-0.278715	-0.214179
H	4.479479	-0.254312	-1.305032
H	4.410571	0.768370	0.103015
C	3.042592	-0.928623	0.182163
H	3.050632	-1.979993	-0.121578
H	2.953994	-0.934117	1.273977
C	1.832482	-0.217713	-0.431292
H	1.922769	-0.224354	-1.525424
H	1.840603	0.839512	-0.135607
C	0.496658	-0.849084	-0.024933
H	0.480477	-1.904364	-0.318647
H	0.392083	-0.829632	1.066100
C	-0.697287	-0.129157	-0.643350
H	-0.680443	-0.182154	-1.733924
H	-0.673081	0.933941	-0.379010
O	6.704215	-0.277949	0.111686
C	7.948582	-0.873223	0.578133

C	9.067365	0.070671	0.241728
H	8.069830	-1.842036	0.089932
H	7.868729	-1.045603	1.652522
C	9.515551	1.005489	1.178972
C	9.663017	0.042156	-1.023102
C	10.540485	1.894181	0.861035
H	9.059931	1.036596	2.164423
C	10.686529	0.929586	-1.345322
H	9.322460	-0.680485	-1.758947
H	10.881696	2.612624	1.599336
C	11.127507	1.857686	-0.402515
H	11.142464	0.895201	-2.329500
H	11.927634	2.547452	-0.650991
H	-2.962030	0.961913	0.511561

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure TS2r, in toluene

O	-3.187862	-0.468550	-2.185846
O	-4.059719	-1.474222	-0.379308
C	-2.889702	-1.307049	-1.150423
C	-2.330885	-2.622986	-1.718848
H	-1.698399	-3.102073	-0.966323
H	-1.680071	-2.352213	-2.552657
C	-3.407793	-3.610646	-2.196105
H	-4.204334	-3.063559	-2.709909
H	-2.960188	-4.274296	-2.943593
C	-3.986198	-4.484049	-1.071489
H	-3.157459	-5.013568	-0.582980
H	-4.618601	-5.262573	-1.512785
C	-4.805218	-3.744337	-0.005933
H	-5.749493	-3.392085	-0.438088
H	-5.065038	-4.444385	0.795126
C	-4.106202	-2.524879	0.597477
H	-3.092747	-2.773498	0.926599
C	-4.869512	-1.930158	1.797539
H	-4.374261	-0.996781	2.080645
C	-4.939336	-2.818506	2.953599
H	-5.879511	-1.658481	1.470045
C	-4.980173	-3.548862	3.908543
H	-5.021159	-4.195580	4.753081
N	-4.707360	3.634483	0.211729
C	-4.081342	2.472733	-0.182639

N	-4.213147	1.917119	-1.352079
C	-5.042540	2.585890	-2.342243
C	-6.231911	3.296396	-1.700174
C	-5.718584	4.263006	-0.640495
C	-3.302466	3.744011	2.256400
C	-3.237076	2.227902	2.132535
N	-3.222291	1.889712	0.720855
C	-4.543617	4.247356	1.530505
H	-5.387614	1.836652	-3.060715
H	-4.447863	3.312754	-2.917982
H	-6.886617	2.551408	-1.236187
H	-6.824075	3.841148	-2.441414
H	-5.295474	5.161251	-1.111165
H	-6.541014	4.599126	0.001097
H	-4.490282	5.333803	1.396816
H	-5.439307	4.048571	2.137837
H	-2.401837	4.177498	1.811659
H	-3.342493	4.053260	3.304135
H	-4.087602	1.771304	2.663408
H	-2.324785	1.834514	2.586153
H	-3.577852	0.391388	-1.830180
O	5.524520	-1.960057	1.097428
O	-1.954080	-0.693148	-0.224732
C	5.547473	-0.968925	0.407031
C	4.347366	-0.321982	-0.252204
H	4.474916	-0.429398	-1.336357
H	4.394338	0.755206	-0.061962
C	3.012577	-0.912578	0.199586
H	3.019721	-1.993249	0.027338
H	2.907721	-0.783988	1.282379
C	1.815259	-0.278122	-0.514477
H	1.921134	-0.419248	-1.598074
H	1.824096	0.807302	-0.350404
C	0.471491	-0.851584	-0.052710
H	0.452808	-1.935058	-0.215690
H	0.353475	-0.699789	1.026556
C	-0.713458	-0.213854	-0.769013
H	-0.677908	-0.399964	-1.844220
H	-0.696859	0.873927	-0.636382
O	6.678430	-0.293378	0.114084
C	7.910136	-0.835518	0.670777
C	9.038547	0.067723	0.262732
H	8.041874	-1.850717	0.292254
H	7.802782	-0.892054	1.755199

```
C      9.394313     1.162240     1.056486
C      9.735120    -0.158763    -0.927900
C     10.426272     2.013837     0.669490
H      8.859860     1.347433     1.983728
C     10.767886     0.690462    -1.318457
H      9.467093    -1.006318    -1.551959
H     10.694855     2.857941     1.296413
C     11.115207     1.778879    -0.519601
H     11.302993     0.501580    -2.243460
H     11.921650     2.439650    -0.820856
H     -2.901014     0.962968     0.456399


80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I2r, in toluene
O     -3.358586    -0.647817    -2.224143
O     -4.354843    -1.298481    -0.322660
C     -3.254067    -1.520277    -1.178571
C     -3.179444    -2.952521    -1.734560
H     -2.652233    -3.594153    -1.021622
H     -2.561396    -2.904286    -2.633120
C     -4.547163    -3.566624    -2.072120
H     -5.180937    -2.808377    -2.542448
H     -4.396528    -4.349642    -2.822927
C     -5.258953    -4.197302    -0.864598
H     -4.588833    -4.944324    -0.418642
H     -6.134390    -4.754423    -1.216721
C     -5.716159    -3.219961     0.225946
H     -6.546544    -2.607516    -0.145190
H     -6.099479    -3.789515     1.079159
C     -4.629947    -2.257817     0.708845
H     -3.713677    -2.795876     0.969838
C     -5.065563    -1.428854     1.933208
H     -4.289292    -0.682734     2.125984
C     -5.290775    -2.224189     3.136240
H     -5.973692    -0.872525     1.674567
C     -5.458601    -2.883357     4.128383
H     -5.612743    -3.465031     5.006483
N     -3.550933     3.769289     0.075791
C     -3.264456     2.479208    -0.311031
N     -3.582728     1.958481    -1.460346
C     -4.248478     2.805052    -2.437977
C     -5.186766     3.809784    -1.773020
```

C	-4.399180	4.625644	-0.755678
C	-2.091225	3.537397	2.072308
C	-2.423784	2.054365	1.979643
N	-2.549905	1.706650	0.575809
C	-3.184475	4.336485	1.374297
H	-4.803715	2.160540	-3.125613
H	-3.508713	3.343626	-3.051186
H	-5.993266	3.267376	-1.268740
H	-5.646469	4.478673	-2.506593
H	-3.777569	5.376668	-1.262495
H	-5.080516	5.172532	-0.094114
H	-2.855251	5.369422	1.214078
H	-4.078334	4.386698	2.013855
H	-1.125114	3.717251	1.591874
H	-2.013383	3.859722	3.113899
H	-3.342885	1.839698	2.547715
H	-1.627060	1.444627	2.410873
H	-3.452484	0.296808	-1.883299
O	4.977335	0.763746	1.754483
O	-2.105855	-1.214764	-0.345363
C	5.181038	0.169831	0.722226
C	4.120133	-0.400690	-0.195424
H	4.387448	-1.439668	-0.415617
H	4.198878	0.126213	-1.153916
C	2.704765	-0.296953	0.370094
H	2.656113	-0.831543	1.324820
H	2.484343	0.749627	0.602438
C	1.645401	-0.850715	-0.587590
H	1.878094	-1.896916	-0.824831
H	1.694364	-0.306461	-1.539432
C	0.225723	-0.757850	-0.019216
H	0.161375	-1.323644	0.917459
H	-0.008313	0.284124	0.224046
C	-0.825967	-1.286376	-0.984030
H	-0.599115	-2.325690	-1.253205
H	-0.844843	-0.695138	-1.905125
O	6.416118	-0.064350	0.231460
C	7.525484	0.452856	1.020256
C	8.803032	0.072239	0.328463
H	7.461210	0.028190	2.023416
H	7.413450	1.535106	1.105222
C	9.390793	0.932247	-0.603584
C	9.412496	-1.158391	0.591290
C	10.565469	0.571659	-1.259952

H	8.926015	1.890757	-0.815438
C	10.586438	-1.522977	-0.063310
H	8.964590	-1.834070	1.314153
H	11.013532	1.250089	-1.978713
C	11.165331	-0.657452	-0.990599
H	11.051175	-2.479677	0.152143
H	12.082025	-0.938643	-1.498853
H	-2.480811	0.727731	0.317190

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure TS23, in toluene

O	-3.244473	-0.451222	-2.188026
O	-4.361403	-1.126478	-0.349465
C	-3.281203	-1.427149	-1.231249
C	-3.423426	-2.784346	-1.940327
H	-3.061688	-3.579086	-1.280740
H	-2.742220	-2.751682	-2.793114
C	-4.847623	-3.103735	-2.420942
H	-5.307007	-2.195029	-2.822159
H	-4.782137	-3.808900	-3.256456
C	-5.739895	-3.730921	-1.339089
H	-5.251147	-4.643346	-0.972313
H	-6.680532	-4.058935	-1.795624
C	-6.071194	-2.828655	-0.143652
H	-6.744127	-2.021326	-0.456005
H	-6.608485	-3.416780	0.607548
C	-4.852892	-2.171200	0.507603
H	-4.060546	-2.903073	0.689022
C	-5.182201	-1.491356	1.850849
H	-4.277780	-0.982848	2.198016
C	-5.639918	-2.413473	2.885638
H	-5.937699	-0.716155	1.678358
C	-6.002374	-3.177329	3.741043
H	-6.325632	-3.851980	4.498378
N	-3.038201	3.960345	0.143707
C	-3.111680	2.620116	-0.158503
N	-2.929052	2.111226	-1.341911
C	-2.562913	3.007902	-2.427121
C	-3.230862	4.373758	-2.283285
C	-2.882081	4.955738	-0.919048
C	-3.128865	3.455998	2.573036
C	-3.894776	2.208422	2.153760

N	-3.355693	1.755594	0.883902
C	-3.256109	4.511343	1.481907
H	-2.851138	2.537913	-3.371858
H	-1.469875	3.137426	-2.469591
H	-4.315880	4.253349	-2.368394
H	-2.912303	5.062934	-3.070918
H	-1.852039	5.337945	-0.915176
H	-3.535768	5.803988	-0.686886
H	-2.526443	5.312801	1.643424
H	-4.251495	4.977983	1.524843
H	-2.078026	3.193621	2.725370
H	-3.515049	3.856401	3.513934
H	-4.972695	2.427624	2.096546
H	-3.764519	1.409084	2.886060
H	-3.165279	0.465972	-1.779611
O	4.957771	-0.064229	2.118661
O	-2.140268	-1.395316	-0.365985
C	5.152661	-0.373333	0.967177
C	4.090940	-0.775528	-0.034616
H	4.340700	-1.779541	-0.396723
H	4.192909	-0.122156	-0.908389
C	2.671009	-0.729952	0.527086
H	2.606701	-1.383440	1.403176
H	2.457927	0.279974	0.892561
C	1.616721	-1.139819	-0.505784
H	1.834574	-2.153901	-0.865805
H	1.692578	-0.485170	-1.383662
C	0.189216	-1.086561	0.046399
H	0.098149	-1.750653	0.913791
H	-0.040634	-0.076339	0.401740
C	-0.857226	-1.479935	-0.985931
H	-0.673214	-2.502353	-1.344941
H	-0.822640	-0.807855	-1.848750
O	6.379195	-0.403046	0.403922
C	7.489400	-0.038128	1.272223
C	8.754702	-0.123212	0.467538
H	7.499512	-0.720970	2.123601
H	7.314029	0.969843	1.651710
C	9.239416	0.996368	-0.214772
C	9.455692	-1.329128	0.371784
C	10.402557	0.914548	-0.976976
H	8.702873	1.938301	-0.147190
C	10.618654	-1.415288	-0.389652
H	9.088171	-2.205164	0.898238

H	10.770114	1.792171	-1.498865
C	11.094360	-0.292416	-1.065593
H	11.155211	-2.356441	-0.453020
H	12.002357	-0.357156	-1.656427
H	-3.556299	0.808749	0.586547

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I3, in toluene

O	-2.962158	-0.240139	-2.036146
O	-3.947962	-1.365177	-0.356175
C	-2.851909	-1.366957	-1.269338
C	-2.863613	-2.597392	-2.197881
H	-2.303440	-3.411139	-1.726761
H	-2.309661	-2.313169	-3.094842
C	-4.267039	-3.094017	-2.581291
H	-4.914874	-2.237035	-2.791281
H	-4.187847	-3.654878	-3.518813
C	-4.910935	-4.018436	-1.533402
H	-4.224388	-4.853759	-1.342138
H	-5.814143	-4.467538	-1.961575
C	-5.286010	-3.364937	-0.195830
H	-6.141111	-2.692119	-0.334955
H	-5.607267	-4.141937	0.505916
C	-4.160589	-2.546258	0.435428
H	-3.232556	-3.121471	0.479495
C	-4.479111	-2.056542	1.861423
H	-3.687273	-1.363097	2.158789
C	-4.589098	-3.134802	2.839051
H	-5.410834	-1.478960	1.842889
C	-4.665719	-4.029593	3.639245
H	-4.734339	-4.817693	4.351514
N	-4.617073	3.696589	0.288891
C	-4.241888	2.415120	-0.044575
N	-3.139456	2.096713	-0.661374
C	-2.193889	3.160458	-0.958748
C	-2.905517	4.463071	-1.320679
C	-3.845773	4.847876	-0.184766
C	-6.491628	2.826140	1.670138
C	-6.461873	1.633399	0.722368
N	-5.083528	1.400666	0.336719
C	-5.864744	4.030099	0.977330
H	-1.556014	2.831302	-1.784194

H	-1.523659	3.334403	-0.102165
H	-3.477886	4.313662	-2.242110
H	-2.195117	5.275340	-1.501146
H	-3.280465	5.277585	0.653517
H	-4.552230	5.617002	-0.517552
H	-5.651555	4.818719	1.707892
H	-6.574659	4.456029	0.252681
H	-5.930165	2.575143	2.574627
H	-7.515253	3.070197	1.966350
H	-7.111359	1.823527	-0.146412
H	-6.837162	0.733680	1.214805
H	-3.002234	0.588149	-1.460503
O	5.321741	0.177256	2.141081
O	-1.702489	-1.346596	-0.421582
C	5.529863	-0.035733	0.970381
C	4.480676	-0.366033	-0.070348
H	4.787353	-1.289743	-0.573433
H	4.526807	0.410501	-0.842891
C	3.069682	-0.488112	0.502452
H	3.057934	-1.265066	1.274005
H	2.804309	0.442851	1.013518
C	2.023892	-0.807593	-0.570319
H	2.299090	-1.739409	-1.081571
H	2.040396	-0.024882	-1.339897
C	0.607869	-0.933979	-0.000634
H	0.579605	-1.723760	0.758775
H	0.320096	-0.006282	0.505509
C	-0.433753	-1.242660	-1.066150
H	-0.185849	-2.182934	-1.578446
H	-0.466241	-0.448804	-1.819738
O	6.760961	-0.002896	0.417199
C	7.857962	0.315655	1.319979
C	9.133395	0.288205	0.527331
H	7.863235	-0.417262	2.128457
H	7.670249	1.297676	1.757606
C	9.599867	1.442714	-0.108180
C	9.862535	-0.897332	0.395796
C	10.772456	1.414796	-0.859437
H	9.041442	2.369344	-0.012370
C	11.035600	-0.929485	-0.354536
H	9.509469	-1.800137	0.885673
H	11.125562	2.318915	-1.344803
C	11.492705	0.227615	-0.983681
H	11.594201	-1.855414	-0.445647

H 12.408344 0.205041 -1.565779
H -4.801324 0.478354 0.025555

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure TS3r, in toluene
O -3.055835 -0.218428 -2.070274
O -4.042252 -1.184770 -0.292028
C -3.064727 -1.362722 -1.328718
C -3.400253 -2.551131 -2.245575
H -2.964646 -3.458297 -1.818425
H -2.867452 -2.362480 -3.180984
C -4.898635 -2.761544 -2.510505
H -5.386885 -1.792036 -2.653317
H -5.012169 -3.302895 -3.456011
C -5.610088 -3.574059 -1.414553
H -5.086798 -4.532871 -1.303546
H -6.621725 -3.824301 -1.753601
C -5.716797 -2.903544 -0.037181
H -6.433528 -2.074134 -0.079450
H -6.114216 -3.626890 0.682742
C -4.398160 -2.336555 0.490306
H -3.598491 -3.078725 0.427112
C -4.477040 -1.858739 1.953737
H -3.542170 -1.339865 2.184501
C -4.694397 -2.938817 2.911258
H -5.278957 -1.117041 2.048076
C -4.862920 -3.836704 3.693637
H -5.010613 -4.628895 4.389179
N -3.958768 3.906813 0.356390
C -3.781384 2.583244 0.028038
N -2.823684 2.123854 -0.728863
C -1.827982 3.065694 -1.216451
C -2.442567 4.429987 -1.522419
C -3.144587 4.948790 -0.273580
C -5.690729 3.293789 2.030627
C -5.935267 2.083921 1.137680
N -4.663112 1.681814 0.567993
C -5.044650 4.399995 1.205450
H -1.368382 2.643382 -2.114660
H -1.015635 3.186985 -0.482338
H -3.165647 4.322586 -2.337577
H -1.685226 5.150416 -1.845220

H	-2.411018	5.327189	0.451329
H	-3.802938	5.787851	-0.525452
H	-4.637590	5.175573	1.863997
H	-5.802446	4.888066	0.574858
H	-5.032201	3.000974	2.853406
H	-6.625186	3.661443	2.462463
H	-6.679461	2.328100	0.363760
H	-6.332904	1.246325	1.714816
H	-2.969630	0.609676	-1.498651
O	5.511627	-2.149625	1.348332
O	-1.828450	-1.637661	-0.657717
C	5.531363	-1.213767	0.584836
C	4.338894	-0.653557	-0.161528
H	4.567843	-0.697227	-1.232558
H	4.270614	0.414546	0.073912
C	3.028795	-1.373842	0.152232
H	3.135455	-2.437813	-0.082514
H	2.837680	-1.324414	1.229174
C	1.837338	-0.789776	-0.612996
H	2.035504	-0.842321	-1.691576
H	1.739715	0.277618	-0.375795
C	0.519424	-1.504466	-0.299027
H	0.601386	-2.568868	-0.546402
H	0.311926	-1.450640	0.775570
C	-0.663694	-0.913329	-1.052028
H	-0.510559	-0.992768	-2.134827
H	-0.776516	0.148855	-0.809276
O	6.652039	-0.522773	0.285657
C	7.873108	-0.971300	0.939464
C	8.998413	-0.094577	0.469240
H	8.036365	-2.019329	0.682304
H	7.730341	-0.908437	2.019535
C	9.356878	1.049734	1.187286
C	9.690382	-0.398966	-0.707089
C	10.387646	1.873994	0.740998
H	8.826014	1.295928	2.102298
C	10.720566	0.422865	-1.157168
H	9.420193	-1.285960	-1.272691
H	10.658570	2.757470	1.310016
C	11.071344	1.561564	-0.432807
H	11.251821	0.173580	-2.070036
H	11.876472	2.200873	-0.780363
H	-4.546628	0.730367	0.236855

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I3r, in toluene

O	-3.424780	-0.225714	-2.160050
O	-3.700549	-1.168170	-0.137823
C	-3.283696	-1.417629	-1.499325
C	-4.129537	-2.488399	-2.200491
H	-3.678356	-3.468194	-2.022083
H	-4.022649	-2.287695	-3.268546
C	-5.610470	-2.504585	-1.798922
H	-5.981698	-1.477444	-1.718599
H	-6.181145	-2.971129	-2.608958
C	-5.896751	-3.289584	-0.507702
H	-5.494092	-4.304203	-0.624562
H	-6.980069	-3.410168	-0.394279
C	-5.343661	-2.681019	0.788388
H	-5.903961	-1.772827	1.044066
H	-5.501020	-3.387377	1.610176
C	-3.863134	-2.302484	0.727020
H	-3.262229	-3.133240	0.346729
C	-3.284927	-1.882648	2.093983
H	-2.263843	-1.524115	1.932770
C	-3.275169	-2.954816	3.084387
H	-3.853757	-1.027055	2.475977
C	-3.257745	-3.846516	3.891404
H	-3.241245	-4.633885	4.607652
N	-3.813313	3.877586	0.394763
C	-3.659017	2.552415	0.060295
N	-2.850879	2.101062	-0.857421
C	-1.995226	3.058230	-1.541533
C	-2.697179	4.399386	-1.746776
C	-3.166277	4.926931	-0.396323
C	-5.195095	3.255719	2.367343
C	-5.556123	2.018767	1.554380
N	-4.390101	1.638348	0.778972
C	-4.740009	4.360011	1.420541
H	-1.702763	2.629384	-2.504253
H	-1.061846	3.215861	-0.978262
H	-3.557805	4.255222	-2.408077
H	-2.036774	5.132525	-2.219203
H	-2.321167	5.341988	0.169663
H	-3.886410	5.741530	-0.533293
H	-4.242655	5.159217	1.981717

H	-5.613246	4.815758	0.930823
H	-4.392559	3.000288	3.065277
H	-6.049007	3.608346	2.951674
H	-6.430876	2.225615	0.918288
H	-5.821264	1.184076	2.207002
H	-3.160568	0.569717	-1.603539
O	5.507327	-2.640285	-0.035012
O	-1.959920	-1.919729	-1.491919
C	5.380701	-1.441196	-0.107212
C	4.079785	-0.698803	-0.329111
H	4.224263	-0.013650	-1.171606
H	3.917246	-0.052914	0.541879
C	2.882131	-1.618435	-0.560787
H	3.075415	-2.252717	-1.432312
H	2.780454	-2.301720	0.288352
C	1.576909	-0.842965	-0.763804
H	1.689508	-0.154047	-1.610930
H	1.387645	-0.212111	0.114575
C	0.371522	-1.756113	-1.007592
H	0.544268	-2.374559	-1.895649
H	0.250711	-2.448849	-0.166853
C	-0.922044	-0.979817	-1.200994
H	-0.827623	-0.272713	-2.032377
H	-1.172324	-0.404874	-0.303071
O	6.411680	-0.577142	0.008564
C	7.721047	-1.171698	0.235832
C	8.726302	-0.058809	0.318600
H	7.936199	-1.856573	-0.586072
H	7.680131	-1.754819	1.157491
C	9.024601	0.539488	1.546293
C	9.363020	0.410121	-0.834294
C	9.941988	1.584928	1.622103
H	8.535745	0.182975	2.448266
C	10.280871	1.455352	-0.762866
H	9.138865	-0.047595	-1.793407
H	10.167368	2.038222	2.582017
C	10.572102	2.044652	0.466628
H	10.770884	1.807489	-1.664845
H	11.289694	2.856737	0.524417
H	-4.306999	0.685957	0.440913

80 atoms

addition of another 7-isomer unit to the ε-CL chain end,
structure TS34, in toluene

O	-3.241752	-0.171360	-2.247617
O	-3.563282	-1.081162	0.047184
C	-3.100405	-1.327558	-1.802417
C	-4.055552	-2.442814	-2.215016
H	-3.643561	-3.406511	-1.906723
H	-4.021433	-2.433312	-3.310878
C	-5.510904	-2.300527	-1.739955
H	-5.746920	-1.240399	-1.610975
H	-6.170125	-2.666945	-2.535465
C	-5.845004	-3.099384	-0.466394
H	-5.497213	-4.131014	-0.611762
H	-6.936161	-3.169243	-0.373873
C	-5.286791	-2.569760	0.862786
H	-5.835371	-1.663385	1.153683
H	-5.482680	-3.315883	1.642559
C	-3.792225	-2.206278	0.830250
H	-3.225317	-3.065513	0.432620
C	-3.232759	-1.950767	2.262773
H	-2.208874	-1.582051	2.145175
C	-3.237751	-3.113061	3.145608
H	-3.803328	-1.135686	2.726149
C	-3.242212	-4.088816	3.851375
H	-3.243431	-4.950426	4.476138
N	-4.182656	3.687181	0.479955
C	-3.939104	2.426168	0.045730
N	-3.097595	2.210460	-0.971955
C	-2.395178	3.288664	-1.652780
C	-3.265339	4.539839	-1.658405
C	-3.677540	4.869222	-0.229414
C	-5.118006	2.722041	2.562731
C	-5.509505	1.539421	1.684495
N	-4.529115	1.376337	0.621598
C	-4.964602	3.962297	1.691832
H	-2.178057	2.949757	-2.666285
H	-1.434618	3.494216	-1.163380
H	-4.152135	4.362646	-2.273803
H	-2.726893	5.388715	-2.086164
H	-2.830626	5.286900	0.329468
H	-4.470433	5.623205	-0.223746
H	-4.455300	4.758240	2.243913
H	-5.947898	4.350911	1.398824
H	-4.175122	2.499158	3.070570

H	-5.873317	2.907962	3.329805
H	-6.513527	1.689081	1.267068
H	-5.534741	0.612208	2.258135
H	-3.092768	1.265249	-1.402290
O	5.677616	-2.573025	-0.397508
O	-1.838519	-1.868228	-1.636023
C	5.523187	-1.376105	-0.351112
C	4.216010	-0.641262	-0.560820
H	4.351449	0.033564	-1.414274
H	4.059611	0.015267	0.302335
C	3.019670	-1.566363	-0.777087
H	3.217001	-2.220432	-1.632336
H	2.913288	-2.230052	0.087293
C	1.715398	-0.795456	-1.001992
H	1.829142	-0.133962	-1.871055
H	1.529285	-0.136470	-0.143558
C	0.505144	-1.710436	-1.212584
H	0.674735	-2.362156	-2.077447
H	0.380163	-2.370422	-0.346907
C	-0.782274	-0.930947	-1.429864
H	-0.700422	-0.271509	-2.300770
H	-1.021938	-0.312367	-0.559141
O	6.526398	-0.506700	-0.102821
C	7.842060	-1.092673	0.109245
C	8.810092	0.026740	0.366103
H	8.110574	-1.669672	-0.777308
H	7.780639	-1.781924	0.953221
C	9.019318	0.500793	1.664604
C	9.499736	0.626490	-0.691632
C	9.900650	1.552706	1.902677
H	8.489074	0.041715	2.493896
C	10.382336	1.678538	-0.457795
H	9.344928	0.265905	-1.704383
H	10.056845	1.908741	2.915877
C	10.584238	2.143524	0.840827
H	10.914392	2.132784	-1.287416
H	11.274156	2.960716	1.025182
H	-4.197337	0.402944	0.372527

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I4, in toluene

O	-1.780931	0.206810	-0.743422

O	-4.930799	-1.437934	1.204223
C	-1.576170	-0.991128	-0.757078
C	-2.651255	-2.044617	-0.810316
H	-3.125422	-2.036963	0.176566
H	-2.196767	-3.024670	-0.968327
C	-3.719430	-1.745016	-1.874349
H	-4.035323	-0.702171	-1.788689
H	-3.258347	-1.841797	-2.864257
C	-4.954904	-2.660880	-1.811926
H	-4.641625	-3.694917	-1.616368
H	-5.404495	-2.678211	-2.811200
C	-6.073980	-2.272450	-0.827743
H	-6.378213	-1.233456	-1.005222
H	-6.945115	-2.891899	-1.068364
C	-5.782137	-2.437968	0.672008
H	-5.255580	-3.386462	0.829333
C	-7.088812	-2.498268	1.510860
H	-6.795994	-2.464141	2.564821
C	-7.906923	-3.681873	1.267031
H	-7.680344	-1.594990	1.320932
C	-8.559585	-4.671369	1.058619
H	-9.142566	-5.543697	0.879361
N	-5.967592	3.413966	0.027159
C	-5.393589	2.165325	0.132441
N	-4.244288	1.952316	-0.594851
C	-3.458195	3.046092	-1.139775
C	-4.410927	4.024720	-1.809611
C	-5.423959	4.507948	-0.780191
C	-7.271847	2.833269	2.034441
C	-7.128302	1.395127	1.544003
N	-5.877714	1.177787	0.830636
C	-7.125517	3.773800	0.846684
H	-2.747921	2.622713	-1.850506
H	-2.872804	3.561512	-0.362239
H	-4.920477	3.520363	-2.635995
H	-3.871977	4.882366	-2.220757
H	-4.958131	5.251349	-0.116297
H	-6.261203	5.011711	-1.276718
H	-6.989540	4.805814	1.188964
H	-8.034740	3.760867	0.229628
H	-6.489557	3.043004	2.771502
H	-8.237690	2.996567	2.521499
H	-7.989746	1.143306	0.904584
H	-7.163444	0.702602	2.390449

H	-3.725966	1.118451	-0.352906
O	7.220696	-2.425212	-0.188356
O	-0.340955	-1.517075	-0.693546
C	7.115089	-1.226676	-0.081011
C	5.819363	-0.444436	-0.136544
H	5.896444	0.262800	-0.970591
H	5.764378	0.177288	0.763761
C	4.581603	-1.328440	-0.277568
H	4.681808	-1.952001	-1.171581
H	4.534376	-2.023460	0.567142
C	3.285129	-0.516302	-0.353321
H	3.337238	0.175966	-1.203495
H	3.193001	0.110657	0.542706
C	2.041251	-1.400948	-0.488627
H	2.122555	-2.026582	-1.384174
H	1.973151	-2.084015	0.364911
C	0.762934	-0.586848	-0.570648
H	0.757408	0.079842	-1.436672
H	0.607786	0.024534	0.321699
O	8.165731	-0.400790	0.103646
C	9.475393	-1.035613	0.162562
C	10.502525	0.040938	0.366532
H	9.634510	-1.582101	-0.768663
H	9.472290	-1.757909	0.980481
C	10.907958	0.401844	1.654582
C	11.052695	0.713466	-0.728940
C	11.846053	1.413863	1.845914
H	10.487226	-0.114098	2.512722
C	11.990056	1.726293	-0.541902
H	10.745129	0.440545	-1.734210
H	12.155167	1.681777	2.851056
C	12.388630	2.078134	0.747127
H	12.412011	2.238265	-1.400687
H	13.121778	2.864616	0.894311
H	-5.274917	-0.526177	1.010987

80 atoms
addition of another 7-isomer unit to the ε-CL chain end,
structure I5, in toluene

O	0.526390	2.220651	1.442283
O	-6.139304	0.271070	-0.048392
C	0.420831	1.449301	0.518540
C	-0.872260	1.050037	-0.159851

H	-0.991703	-0.032260	-0.030481
H	-0.745319	1.197216	-1.238074
C	-2.096986	1.799507	0.361797
H	-2.173700	1.654156	1.444246
H	-1.951981	2.875605	0.215687
C	-3.393897	1.348874	-0.316466
H	-3.543011	0.275849	-0.161557
H	-3.308992	1.493364	-1.401923
C	-4.625590	2.099789	0.196131
H	-4.706467	1.976352	1.283916
H	-4.512497	3.173007	0.008317
C	-5.933098	1.622840	-0.429346
H	-5.852937	1.692053	-1.524646
C	-7.148815	2.481751	0.008311
H	-8.056606	1.993114	-0.360181
C	-7.110713	3.859786	-0.471016
H	-7.210501	2.467032	1.102935
C	-7.070182	4.988112	-0.887574
H	-7.036505	5.988802	-1.248741
N	-10.234012	-2.040435	0.046252
C	-9.090551	-1.278202	0.062402
N	-8.612018	-0.894637	1.297612
C	-9.011070	-1.564268	2.523049
C	-10.524451	-1.730869	2.494703
C	-10.918521	-2.516502	1.250002
C	-9.696704	-2.540167	-2.310748
C	-9.002075	-1.179709	-2.301124
N	-8.450503	-0.860802	-0.993449
C	-10.757358	-2.565616	-1.217055
H	-8.700540	-0.944206	3.366529
H	-8.523781	-2.544826	2.640320
H	-10.991079	-0.741667	2.481069
H	-10.879389	-2.257466	3.384334
H	-10.696884	-3.584260	1.394171
H	-11.998128	-2.439780	1.079953
H	-11.099791	-3.591129	-1.040538
H	-11.638212	-1.983457	-1.520200
H	-8.955110	-3.323996	-2.124090
H	-10.160096	-2.748043	-3.279618
H	-9.715177	-0.402960	-2.618883
H	-8.187808	-1.162331	-3.031247
H	-7.690226	-0.477077	1.256680
O	8.520892	-1.641952	-1.657571
O	1.473350	0.818376	-0.044180

C	8.733536	-0.876331	-0.747652
C	7.687017	-0.073285	-0.003553
H	7.963232	0.984431	-0.080495
H	7.775920	-0.316684	1.061224
C	6.264823	-0.310813	-0.507990
H	6.214659	-0.073734	-1.575615
H	6.024510	-1.375856	-0.427356
C	5.225506	0.514615	0.256634
H	5.475060	1.580444	0.177598
H	5.278746	0.269801	1.325170
C	3.797929	0.285010	-0.250751
H	3.732851	0.542362	-1.313576
H	3.537616	-0.776032	-0.169710
C	2.776091	1.103161	0.517806
H	2.967241	2.176358	0.436153
H	2.764916	0.848580	1.580744
O	9.965791	-0.626149	-0.258537
C	11.063938	-1.340594	-0.894883
C	12.340061	-0.919613	-0.224192
H	11.061829	-1.098207	-1.958906
H	10.882758	-2.411971	-0.793318
C	12.823756	-1.618443	0.885690
C	13.052052	0.191107	-0.686778
C	13.996592	-1.217097	1.521084
H	12.278636	-2.482904	1.253380
C	14.224988	0.595851	-0.054089
H	12.685358	0.741159	-1.548532
H	14.363266	-1.770401	2.379600
C	14.699451	-0.108464	1.051647
H	14.770071	1.457718	-0.425194
H	15.615049	0.203620	1.543576
H	-6.892301	-0.115235	-0.572818

REFERENCES

(1) Jazkewitsch, O.; Mondrzyk, A.; Staffel, R.; Ritter, H., Cyclodextrin-Modified Polyesters from Lactones and from Bacteria: An Approach to New Drug Carrier Systems. *Macromolecules* **2011,** *44*, 1365-1371.

(2) Bruckner, R., In *Advanced Organic Chemistry*, Bruckner, R., Ed. Academic Press: San Diego, 2002; pp 1-42.

(3) Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993,** *98* (7), 5648-5652.

(4) Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988,** *37* (2), 785-789.

(5) Nifant'ev, I.; Shlyakhtin, A.; Bagrov, V.; Lozhkin, B.; Zakirova, G.; Ivchenko, P.; Legon'kova, O., Theoretical and experimental studies of 1,5,7-triazabicyclo[4.4.0]dec-5-ene-catalyzed ring opening/ring closure reaction mechanism for 5-, 6- and 7-membered cyclic esters and carbonates. *Reac. Kinet. Mech. Cat.* **2016,** *117* (2), 447-476.
(6) Tomasi, J.; Mennucci, B.; Cammi, R., Quantum Mechanical Continuum Solvation Models. *Chem. Rev.* **2005,** *105* (8), 2999-3094.
(7) Scalmani, G.; Frisch, M. J., Continuous surface charge polarizable continuum models of solvation. I. General formalism. *J. Chem. Phys.* **2010,** *132* (11), 114110.
(8) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H. *Computer Program Gaussian 16, Revision B.01*, Gaussian, Inc.: Wallingford CT, 2016.
(9) Blankenburg, J.; Kersten, E.; Maciol, K.; Wagner, M.; Zarbakhsh, S.; Frey, H., The poly(propylene oxide-co-ethylene oxide) gradient is controlled by the polymerization method: determination of reactivity ratios by direct comparison of different copolymerization models. *Polym. Chem.* **2019,** *10*, 2863-2871.
(10) Mundil, R.; Kanizsová, L.; Toman, P.; Kočková, O.; Uchman, M., Unveiling the reverse reactivity and composition profile of copolymers from synthesized and separated 3-/7-(prop-2-ynyl)oxepan-2-one isomers: implications for precise polymer structure prediction. *Polym. Chem.* **2024,** *15* (17), 1695-1703.