Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting information

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

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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. 1,5,7-triazobicyclo[4.4.0]dec-5-ene (Aldrich, 98%) was transferred to a Schlenk flask, stored under nitrogen, and used as received. ε-Caprolactone (Aldrich, 97%) was dried over CaH_2, distilled and stored in a fridge under nitrogen over molecular sieves. 3/7-(prop-2-ynyl)oxepan-2-one was synthesized according to a procedure previously published in the literature,[1] and the resulting mixture of both isomers was separated by silica gel column chromatography using an 8:2 cyclohexane/ethyl acetate mixture as the mobile phase. Both isomers were dissolved in dry toluene and dried by azeotropic distillation immediately before use.

(Co)polymerization of 3/7-(prop-2-ynyl)oxepan-2-one initiated by benzyl alcohol and catalyzed by 1,5,7-triazobicyclo[4.4.0]dec-5-ene. In a typical (co)polymerization procedure, 7-(prop-2-ynyl)oxepan-2-one (0.22 g, 1.45 mmol, 25 eq.) was introduced to the flame-dried Schlenk flask equipped with a magnetic stirring bar. The monomer was dissolved in dry toluene, dried by azeotropic distillation, and dissolved in the desired volume of dry toluene (4.4 ml). Then, a solution of benzyl alcohol (6.0 µl, 57.8 µmol, 1 eq.) in toluene was added, and the whole mixture or aliquot (kinetic investigation) was transferred to the capped reaction vial designed for microwave synthesis (Biotage). These vials were heated, sealed, left standing 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, (16.1 mg, 115.6 µmol, 2.0 eq.) was dissolved in toluene, and polymerization was started by adding the catalyst solution to the reaction vial. The reaction mixture was magnetically stirred at a controlled reaction temperature (30 °C) for an allotted polymerization

time. Polymerization was quenched with a solution of benzoic acid in toluene, subsequently collecting a sample for ^{1}H NMR analysis (monomer conversion determination). Toluene was evaporated via a rotary evaporator, and the crude polymer was precipitated with hexane, extracted with cyclohexane/ethyl acetate, and dried *in vacuo* to constant weight. Other (co)polymerization kinetic experiments were performed using the same protocol.

Nuclear Magnetic Resonance Spectroscopy. ^{1}H, ^{13}C and DOSY NMR spectra were recorded on a Bruker Avance MSL 400 MHz spectrometer at room temperature in $CDCl_3$. Approximately 5-10 mg of sample was directly dissolved into the NMR tube in 0.6 ml of $CDCl_3$. The chemical shifts were calibrated using the residual resonances of the solvent.

Gas chromatography-mass spectrometry (GC-MS). GC-MS analysis was performed on a Perkin Elmer Clarus 680 Gas Chromatograph directly coupled with a Perkin Elmer Clarus SQ 8 T Mass spectrometer detector using a capillary column DB-35MS (30 m, 0.25 mm, 0.25 μm) and the following temperature program in the gas chromatograph: the initial temperature of 50 °C was increased to 150 °C at 20 °C·min^{-1} and then increased to 180 °C at 5 °C·min^{-1} and to 320 °C at 10 °C·min^{-1} and then held isothermally to complete the analysis. The temperature of the injector was 200 °C. The carrier gas was helium, at a flow rate of 1 ml·min^{-1}. For GC-MS detection, an electron ionization system was used with an ionization energy of 70 eV, at an ion source temperature of 190 °C, a scan mass range of 15-620 m/z, and an interface line temperature of 300 °C. The compounds were identified by comparison of the mass spectra with MS spectra found in NIST (version 14) and Wiley Libraries (version 9).

Pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS). Sample was directly applied into the ribbon filament using a pipette tip. The filament was inserted in a Pyroprobe 5000 Series (CDS Analytical). Pyrolysis was performed at 750 °C for 5s. The pyrolysate was transferred through a transfer line at 300°C into an injector, at the same temperature, connected to a GC-MS (Perkin Elmer Clarus 680 Gas Chromatograph directly coupled with a Perkin Elmer Clarus SQ 8 T Mass spectrometer detector) using a capillary column DB-35MS (30 m, 0.25 mm, 0.25 μm) and the following temperature program in the gas chromatograph: the initial temperature 50 °C was held for 5 min, increased to 340 °C at 10 °C·min^{-1}, and then held isothermally to complete the analysis. The temperature of the injector was 300 °C. The carrier gas was helium, at a flow rate of 1 ml·min^{-1} and a split of 50 ml·min^{-1}. For GC-MS detection, an electron ionization system was used, with an ionization energy of 70 eV, at an ion source temperature of 190 °C, a scan mass range of m/z 15-620, and an interface line temperature of 300 °C. The compounds were identified by comparing mass spectra with MS spectra found in NIST (version 14) and Wiley Libraries (version 9).

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.).

Matrix assisted laser desorption/ionization in combination with time-of-flight detector mass spectrometry (MALDI-TOF MS). MALDI-TOF MS mass spectra were acquired with the UltrafleXtreme TOF - TOF mass spectrometer (Bruker Daltonics, Bremen, Germany) equipped with a 2000 Hz smartbeam-II laser (355 nm) in positive ion reflectron mode. Panoramic pulsed ion extraction and external calibration were used for molecular weight assignment. Using the dried droplet method, the solutions of the sample (10 mg·ml^{-1}) and matrix 2,5-dihydroxybenzoic acid (DHB; 20 mg·ml^{-1}) in tetrahydrofuran were mixed in a volume ratio of 4:20. Lastly, 1 μl of the resulting mixture was deposited on the ground-steel target.

Differential scanning calorimetry (DSC). DSC measurements were performed on a module Discovery DSC 250 Auto (TA Instruments, USA) at a rate of 10 °C min^{-1} for both heating and cooling in a range from -80 to 100 °C. Glass transition and melting temperatures were obtained from the second heating run.

Quantum chemical calculations. The ground state molecular geometries of the reactants, intermediates, and products (Scheme 3) dissolved in toluene were determined by minimizating the total energy calculated using the hybrid Density Functional Theory (DFT) method B3LYP[2, 3] and the Pople basis set 6-311G(d). This method was successfully used for an extensive theoretical and experimental study of similar reactions conducted by Nifant'ev et al.[4] Solvation effects were described using the polarizable continuum model (PCM) with the integral equation formalism variant.[5, 6] For each reactant, different initial geometries were considered to find the lowest-energy

conformer. The resulting equilibrium structures were checked by normal mode analysis (no imaginary frequency was found).

The transition states on the TBD-catalyzed ring-opening polymerization (ROP) reaction path (Scheme 3) were found using the Berny algorithm with an initial guess obtained from the relaxed potential energy surface scans along the appropriate internal coordinates. All transition states were confirmed by 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 geometry optimizations, which proved that the reaction proceeds from the given transition state to the expected reaction intermediate. Thermodynamic parameters were calculated for room temperature (298.15 K) and 1 atm pressure.

Based on the optimized geometries of 3- and 7-isomer, single-point calculations were performed using the same method, but with the basis set supplemented by diffuse functions on heavy atoms (6-311G+(d)) for population analysis. Electrostatic potential (ESP)-derived atomic charges were fitted according to the Merz-Singh-Kollman scheme.[7, 8] In terms of atomic charges, this model is presumably more realistic than the standard Mulliken population analysis, among others, because the results are considerably less dependent on the quantum chemical method and basis set.[9] A very fine fitting point grid with 10 layers and 33 points per unit area (Gaussian 16 options IOP(6/41=10,6/42=33)) was used to increase the numerical accuracy.

All quantum chemical calculations were performed using the Gaussian 16 program package,[10] electrostatic potential maps were constructed in GaussView,[11] and condensed Fukui functions[12] were evaluated from the Gaussian 16 output using the frontier molecular orbital approach in the Multiwfn program.[13, 14]

RESULTS

Characterization of monomers

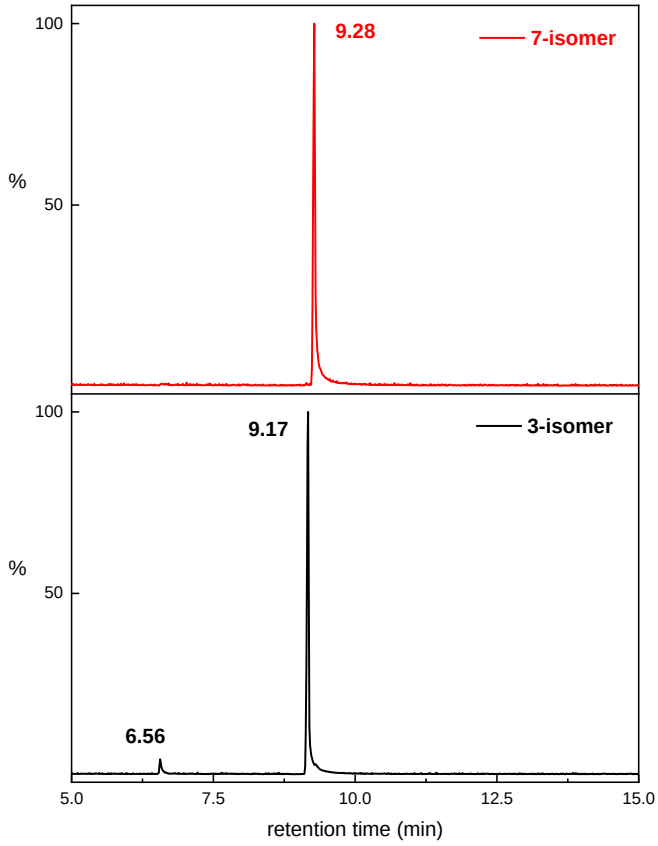


Figure S1. GC analysis of the separated isomers 3- and 7-(prop-2-ynyl)oxepan-2-one

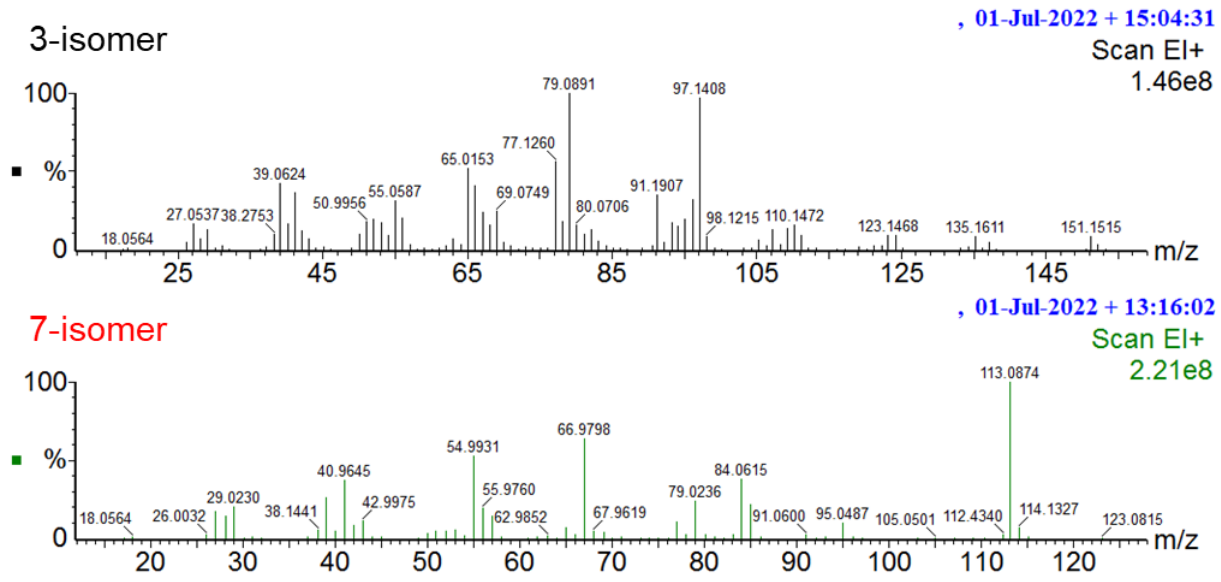


Figure S2. EI-MS analysis of the separated isomers 3- and 7-(prop-2-ynyl)oxepan-2-one

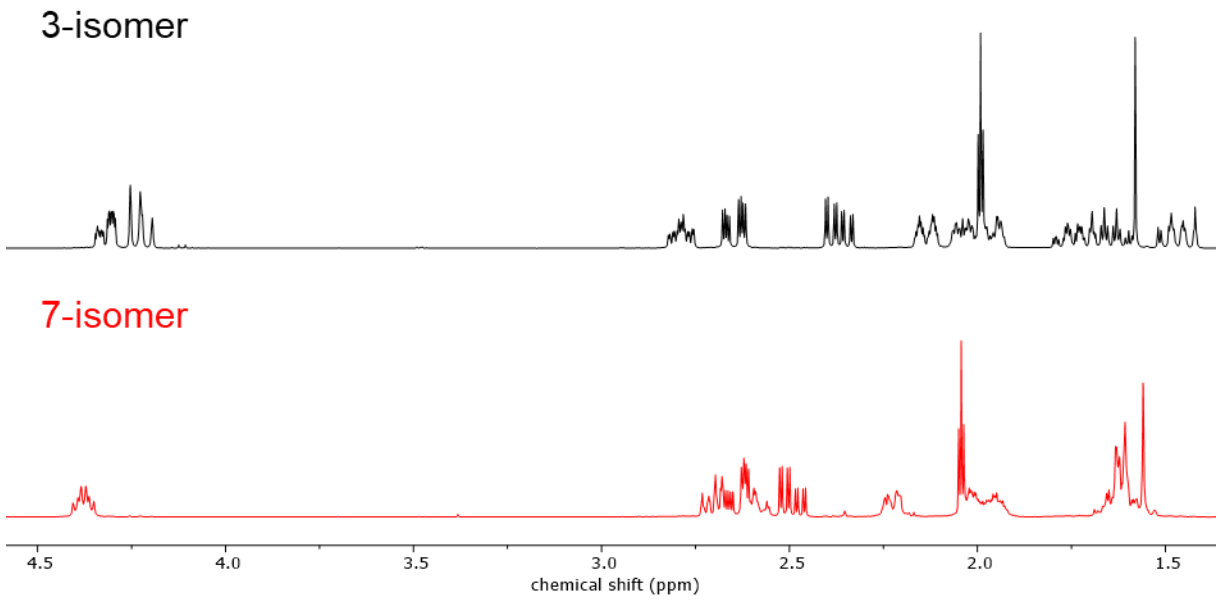
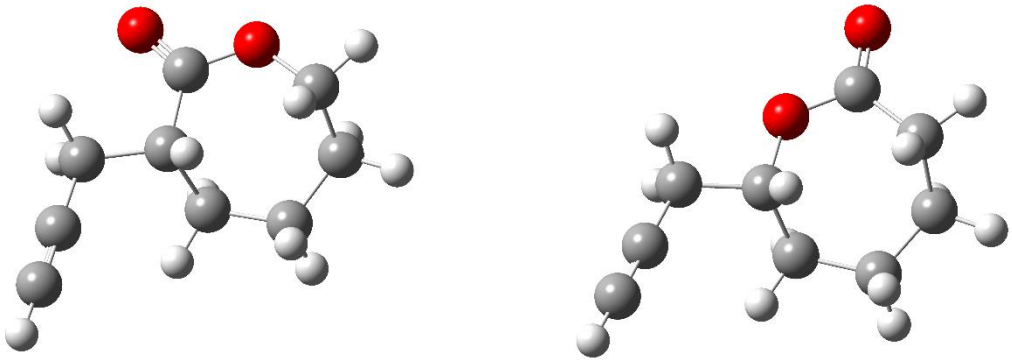


Figure S3. ^{1}H NMR spectra of the separated isomers 3- and 7-(prop-2-ynyl)oxepan-2-one

Quantum chemical calculations

Population analysis and reaction energies: Molecular conformations of the 3- and 7-isomer were calculated using quantum chemical methods to elucidate the influence of the monomer chemical structure on its reactivity. The resulting lowest-energy equilibrium conformations are shown in Figure S4, and Cartesian coordinates are shown in the Table S8.

For standalone isomers (Figure S4), the expected binding site (carbonyl carbon) of benzyl alcohol is rather well accessible since the propargyl groups are oriented to the opposite direction, although the proximity of this group to the binding site of 3-isomer may partially hinder its reactivity. There are also other conformers with the rotated propargyl groups, with only slightly higher energy. Therefore, these conformers may also be thermally accessible at room temperature.

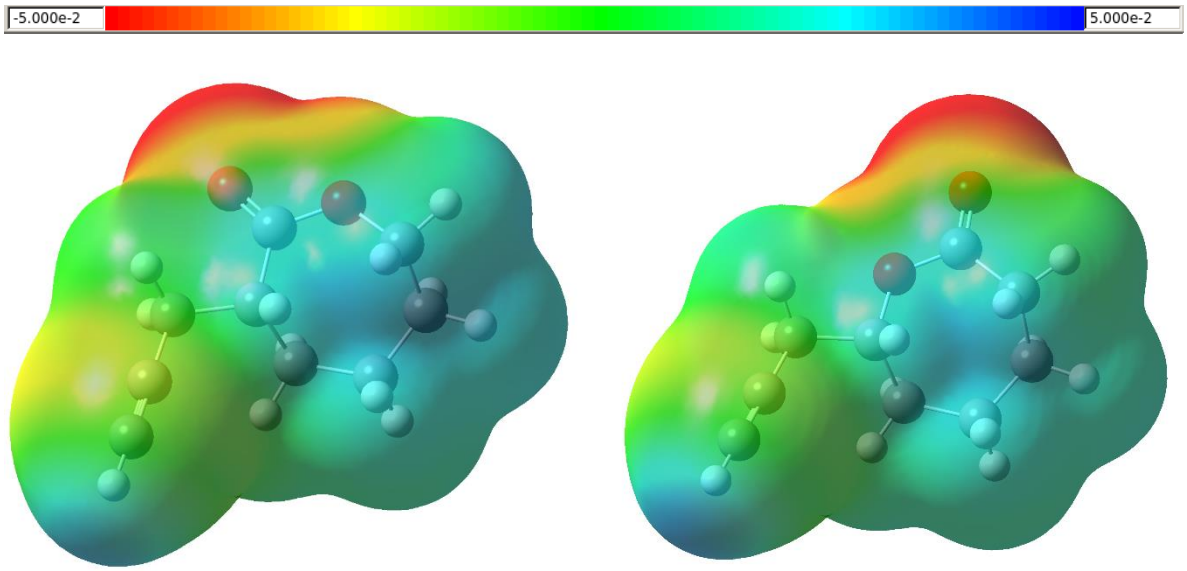


a) 3-isomer **b) 7-isomer**

Figure S4. Equilibrium molecular conformations of the studied isomers dissolved in toluene calculated using the PCM-B3LYP/6-311G(d) method

The calculated electrostatic potentials mapped onto the electron density surfaces with the isovalue 0.0004 a.u. for both studied isomers dissolved in toluene are shown in Figure S5, and the ESP-derived atomic charges together with the condensed Fukui functions are given in Table S1. Carbonyl carbon (3C, Figure S6) has the greatest positive charge due to two adjacent negatively

charged oxygen atoms and to the greatest nucleophilic Fukui function f^+ value of both isomers. Consequently, this is the most susceptible site for nucleophilic attack by the benzyl alcohol. When comparing the atomic charges and nucleophilic Fukui functions f^+ on the carbonyl carbons of both isomers, we found that the atomic charge value of 7-isomer is slightly higher than that of 3-isomer, but the 3-isomer has a slightly higher f^+ value than the 7-isomer. Thus, the population analysis unambiguously shows that the carbonyl carbon is the most susceptible site for the nucleophilic attack. Nevertheless, a more reliable comparison of the reactivity of both isomers is necessary to calculate the whole reaction path of the ROP (*vide infra*).



3-isomer **7-isomer**

Figure S5. Electrostatic potentials mapped onto the electron density surface (isovalue 0.0004 a.u.) for 3-isomer and 7-isomer in toluene. Color scale range from -0.05 a.u. (red) to 0.05 a.u. (blue). Computational method: PCM-B3LYP/6-311+G(d)//6-311G(d)

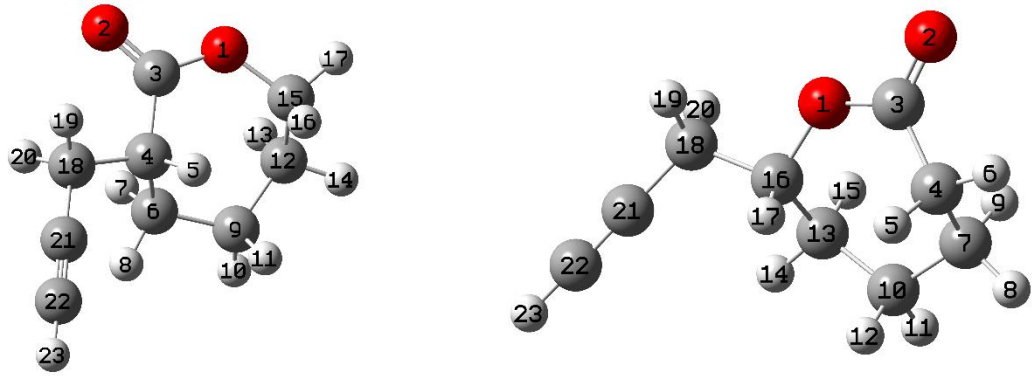
Table S1. Atomic charges derived from the electrostatic potential according to the Merz-Singh-Kollman scheme and condensed to atom Fukui functions for electrophilic (f^-) and nucleophilic (f^+) attack for 3-isomer (a) and 7-isomer (b) dissolved in toluene. Calculated using the PCM B3LYP/6-311+G(d)//6-311G(d) method. Numbering of atoms is shown in Figure S6.

a) 3-isomer

Atom		Charge	f^-	f^+
1	O	-0.490	0.047	0.096
2	O	-0.596	0.243	0.237
3	C	0.748	0.050	**0.349**
4	C	0.041	0.055	0.060
5	H	0.068	0.005	0.031
6	C	-0.062	0.012	0.046
7	H	0.043	0.002	0.017
8	H	0.043	0.007	0.031
9	C	-0.011	0.001	0.013
10	H	0.023	0.000	0.012
11	H	0.017	0.000	0.013
12	C	-0.072	0.001	0.007
13	H	0.058	0.000	0.003
14	H	0.025	0.000	0.001
15	C	0.179	0.006	0.012
16	H	0.015	0.001	0.006
17	H	0.069	0.003	0.003
18	C	-0.315	0.036	0.010
19	H	0.146	0.005	0.005
20	H	0.147	0.021	0.004
21	C	0.130	0.214	0.014
22	C	-0.540	0.272	0.023
23	H	0.332	0.018	0.008

b) 7-isomer

Atom		Charge	f^-	f^+
1	O	-0.535	0.064	0.084
2	O	-0.598	0.528	0.216
3	C	0.787	0.083	**0.314**
4	C	-0.227	0.074	0.070
5	H	0.072	0.014	0.053
6	H	0.066	0.007	0.025
7	C	0.102	0.019	0.052
8	H	0.010	0.008	0.062
9	H	0.004	0.004	0.021
10	C	-0.064	0.004	0.018
11	H	0.028	0.001	0.016
12	H	0.022	0.001	0.025
13	C	-0.133	0.002	0.006
14	H	0.052	0.002	0.001
15	H	0.076	0.000	0.004
16	C	0.401	0.020	0.010
17	H	0.026	0.003	0.006
18	C	-0.316	0.018	0.004
19	H	0.163	0.001	0.002
20	H	0.151	0.005	0.003
21	C	0.106	0.061	0.004
22	C	-0.526	0.078	0.006
23	H	0.334	0.005	0.002



3-isomer **7-isomer**

Figure S6. Numbering of atoms in 3- and 7-isomer

Investigation of the ROP mechanism:

The studied system consisted of polymerized isomers (3- and 7-isomer), BnOH, and TBD, which acted as a catalyst dissolved in toluene. This three-compound system may include three bimolecular and one trimolecular complex, of which the bimolecular complex of BnOH-TBD has the lowest Gibbs free energy. Thus, the energy of the most stable complex was taken as the ground state of the system.

Based on the previous DFT studies of six-membered and larger lactones,[15, 16] and experimental data,[15, 17] we used the so-called "donor-acceptor" mechanism to calculate the ROP reaction route rather than an alternative "amide" mechanism.[4] The energy profiles of the reactions of 3- and 7-isomer were calculated by initially performing a conformational analysis of the initial structure I1 and the first transition structure TS12 (Scheme 3). For both isomers, the free energy of the most stable structure I1 in vacuum is between 2 and 3 kcal·mol^{-1} above the ground state, corroborating the value of 2.8 kcal·mol^{-1} found by Nifant'ev *et al.*[4] for the complex of the unsubstituted ε-caprolactone with methanol and TBD. In toluene, this value increases to approximately 5

kcal·mol^{-1}. Since both isomers and BnOH are bound to the TBD molecule only by one relatively weak and flexible hydrogen bond, we did not explore transition states in the highly flat potential energy surface of the structure I1 (Scheme 3), but started the reaction route calculation with the lowest energy conformer of the transition state structure TS12 (Scheme 3). The energy profiles of the initial step of the ROP of both isomers are shown in Table S2a. The results demonstrate that the TS12 free energies of the 7-isomer are slightly above 21 kcal·mol^{-1}, in line with the value 21.3 kcal·mol^{-1} found by Nifant'ev et al.,[4] but the values of the 3-isomer are noticeably higher (23.0 kcal·mol^{-1} in vacuum and 26.6 kcal·mol^{-1} in toluene).

The free energies of the intermediate state I2 range from 15.8 to 22.7 kcal·mol^{-1}. Transformation of I2 into I3 consists of cleavage and formation of anew NH-O hydrogen bond upon rotation of the TBD molecule around the stronger N-HO bond with a low barrier (less than 3 kcal·mol^{-1}) and a low reaction energy (from -1 to 2 kcal·mol^{-1}). From state I3, the reaction proceeds exothermally to its relaxed conformer I3r (Table S3). Although barriers for this exothermic step are also rather low (1.5 kcal·mol^{-1} for 3-isomer and less than 4 kcal·mol^{-1} for the 7-isomer), free energies of this transition state with respect to the ground state are rather high in the case of 7-isomer (20.4 kcal·mol^{-1} in vacuum and 22.7 kcal·mol^{-1} in toluene). Nevertheless, these values are still considerably lower than the free energy of the TS12 state of the 3-isomer. With the 7-isomer, the reaction from the relaxed I3r state to the I4 state proceeds directly through the transition state TS34, which has a slightly higher energy than TS12. With the 3-isomer, this reaction, in turn, involves another conformer, I3r2 (Table S3), in which the alcohol moiety lies in the more distant position from the TBD molecule. The energy of the TS34 state of the 3-isomer is significantly lower than that of the TS12 state. The free energy of the state I4 ranges from 4.0 to 8.0 kcal·mol^{-1}

and, as such, is much lower than that of the transition state TS34, which hinders the reverse reaction.

The reaction from the I4 to the I5 state consists of the cleavage of the weak NH-O hydrogen bond and relaxation (straightening) of the released chain. As with the starting structure I1, the potential energy surface is very flat and complex at this step, so we did not look for a reaction pathway. The free energy of the final state I5 ranged from 0.1 to 2.9 kcal·mol^{-1} with respect to the ground state. In all cases, the free energy of I5 is lower than the one of I1, thus the entire reaction from I1 to I5 is exothermic. In the real system, the hydrogen bond cleaved in the reaction from I4 to I5 would be probably replaced by hydrogen bonds to surrounding molecules, which would make the reaction energy even more negative.

Table S2: Gibbs free energies in kcal·mol^{-1} of reaction intermediates and transition states for the TBD catalyzed ROP in vacuum and toluene, calculated by the PCM B3LYP/6 311G(d) method (the highest energy transition states of both isomers are 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						
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						
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

Calculations of the energy profiles of the next (co)polymerization step, i.e. addition of another 3- or 7-isomer unit to the chain ending with either a 3- or 7-isomer unit, were performed in the same way, but restricted only to the toluene solution (Table S2b).

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

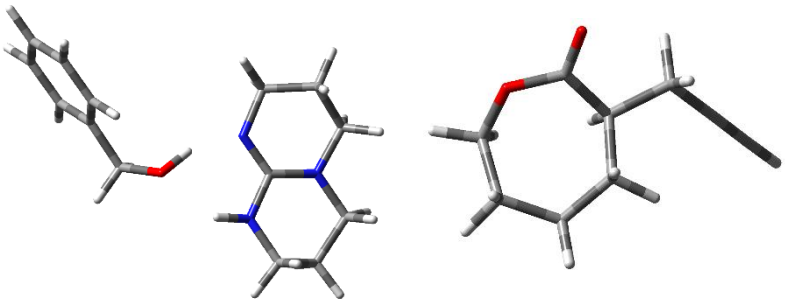
	I1	TS12	I2	TS23	I3	TSr	I3r	TSr2	I3r2	TS34	I4	I5
3-is 3-is	8.68	**27.68**	25.82	26.82	20.48	21.83	20.37	-	-	23.18	10.19	5.60
3-is 7-is	8.44	28.37	26.96	**29.70**	27.43	27.69	20.85	22.30	20.99	24.04	10.48	4.68
7-is 3-is	8.36	**25.44**	21.48	23.08	20.70	23.41	22.98	-	-	24.41	6.92	3.93
7-is 7-is	7.40	**25.96**	23.05	24.13	22.41	24.37	22.42	23.65	21.18	23.77	9.12	4.22

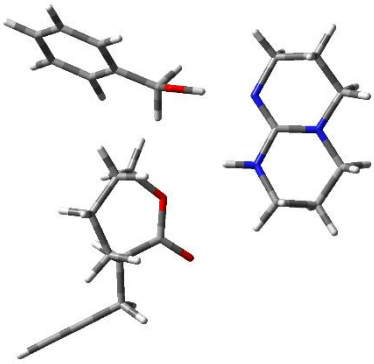
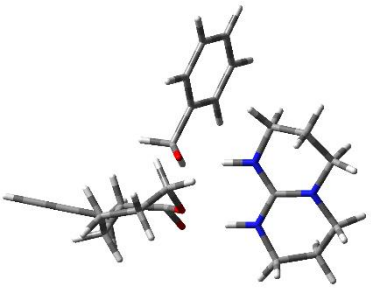
The results show that the energies of the first transition state TS12 for addition of the next 3-isomer unit are significantly higher than those of the addition of a 7-isomer unit. In particular, the addition of a 3-isomer unit to the 7-isomer chain end is strongly disfavored due to not only the highest value (ca 28.4 kcal·mol^{-1}) of the TS12 state energy but also the extremely high energy (ca 29.7 kcal·mol^{-1}) of the transition state TS23. Except for this strongly disfavored reaction, the first transition state TS12 is the highest state of the whole reaction path.

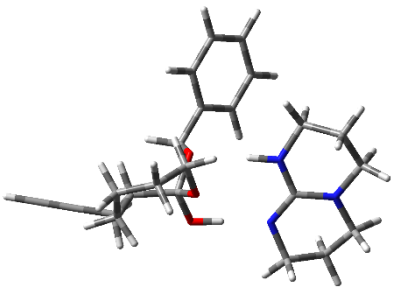
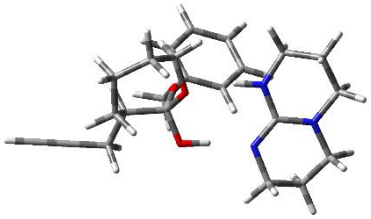
Table S3:

a) *initial step of the polymerization*

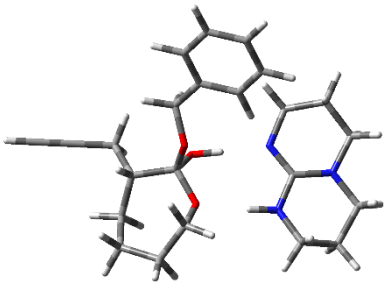
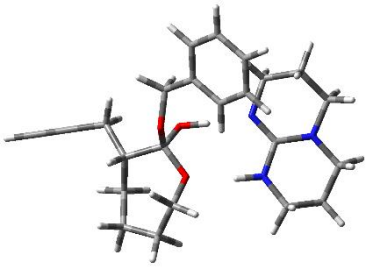
Optimized molecular conformations (in vacuum) and thermodynamic parameters (electronic energies (with the nuclear repulsion) E_{DFT}, sum of electronic and zero-point energies E_0, sum of electronic and thermal energies E_{298}, sum of electronic and thermal enthalpies H_{298}, and sum of electronic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

3-isomer		
State	**BnOH-TBD**	**3-isomer**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-493092.1104	-314186.7625
E_0 (kcal/mol)	-492878.1956	-314065.1060
E_{298} (kcal/mol)	-492867.4037	-314058.4544
H_{298} (kcal/mol)	-492866.8113	-314057.8621
G_{298} (kcal/mol)	-492908.9316	-314087.8238
Toluene		
E_{DFT} (kcal/mol)	-493094.9932	-314189.9527
E_0 (kcal/mol)	-492881.2691	-314068.3089
E_{298} (kcal/mol)	-492870.4509	-314061.6635
H_{298} (kcal/mol)	-492869.8579	-314061.0712
G_{298} (kcal/mol)	-492912.2512	-314091.0178

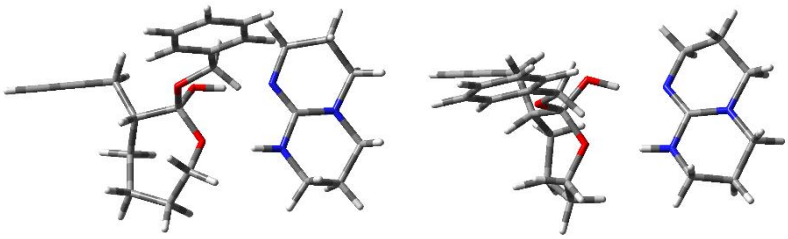
State	**I1**	**TS12**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807285.6334	-807270.8908
E_0 (kcal/mol)	-806949.9043	-806935.0009
E_{298} (kcal/mol)	-806930.8908	-806917.3943
H_{298} (kcal/mol)	-806930.2984	-806916.8019
G_{298} (kcal/mol)	-806994.3702	-806973.7321
Toluene		
E_{DFT} (kcal/mol)	-807289.8382	-807276.5790
E_0 (kcal/mol)	-806954.3019	-806939.9344
E_{298} (kcal/mol)	-806935.2858	-806922.6145
H_{298} (kcal/mol)	-806934.6935	-806922.0222
G_{298} (kcal/mol)	-806998.4785	-806976.6977

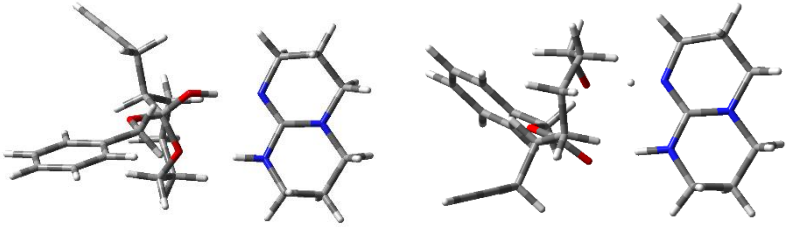
State	**I2**	**TS23**
Molecular geometry		

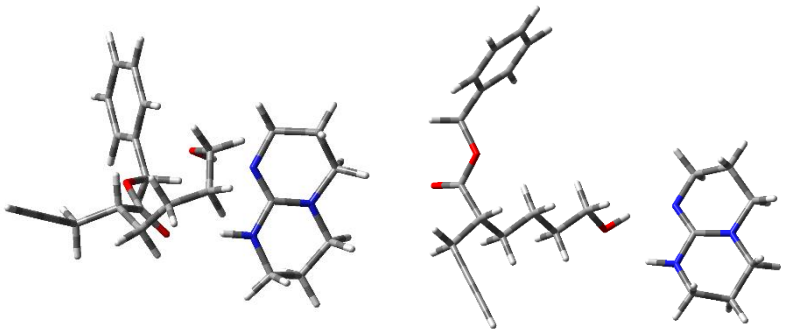
Vacuum		
E_{DFT} (kcal/mol)	-807273.9332	-807273.5304
E_0 (kcal/mol)	-806937.1175	-806936.8213
E_{298} (kcal/mol)	-806919.2680	-806919.4306
H_{298} (kcal/mol)	-806918.6757	-806918.8382
G_{298} (kcal/mol)	-806976.7435	-806975.1772
Toluene		
E_{DFT} (kcal/mol)	-807277.8554	-807277.4715
E_0 (kcal/mol)	-806941.1995	-806940.9541
E_{298} (kcal/mol)	-806923.3707	-806923.5721
H_{298} (kcal/mol)	-806922.7783	-806922.9797
G_{298} (kcal/mol)	-806980.6159	-806979.3175

State	**I3**	**TSr**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807274.7535	-807274.1819
E_0 (kcal/mol)	-806937.8843	-806937.5907
E_{298} (kcal/mol)	-806920.0443	-806920.2758
H_{298} (kcal/mol)	-806919.4519	-806919.6834
G_{298} (kcal/mol)	-806977.7061	-806976.2114
Toluene		
E_{DFT} (kcal/mol)	-807278.6930	-807277.9937

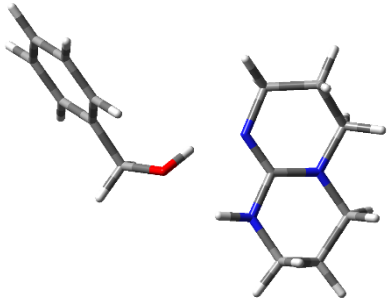
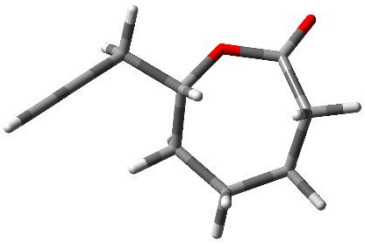
E_0 (kcal/mol)	-806942.0309	-806941.6551
E_{298} (kcal/mol)	-806924.2178	-806924.3471
H_{298} (kcal/mol)	-806923.6255	-806923.7547
G_{298} (kcal/mol)	-806981.5973	-806980.0009

State	**I3r**	**TSr2**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807278.0662	-807277.0733
E_0 (kcal/mol)	-806941.3576	-806940.6918
E_{298} (kcal/mol)	-806923.4209	-806923.2709
H_{298} (kcal/mol)	-806922.8285	-806922.6785
G_{298} (kcal/mol)	-806981.8088	-806980.0511
Toluene		
E_{DFT} (kcal/mol)	-807281.8306	-807281.0309
E_0 (kcal/mol)	-806945.2726	-806944.9049
E_{298} (kcal/mol)	-806927.3780	-806927.4840
H_{298} (kcal/mol)	-806926.7856	-806926.8916
G_{298} (kcal/mol)	-806985.1747	-806984.1136

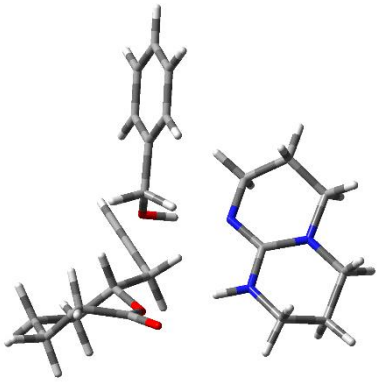
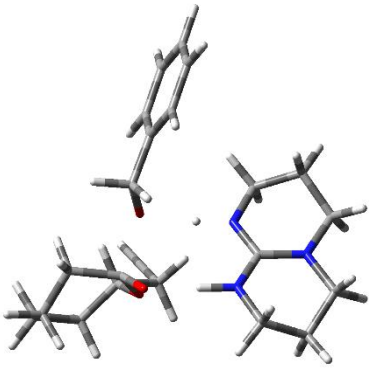
State	**I3r2**	**TS34**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807278.2373	-807270.9047
E_0 (kcal/mol)	-806941.3281	-806936.1035
E_{298} (kcal/mol)	-806923.4861	-806918.2659
H_{298} (kcal/mol)	-806922.8938	-806917.6735
G_{298} (kcal/mol)	-806981.3093	-806976.1461
Toluene		
E_{DFT} (kcal/mol)	-807282.1417	-807276.7632
E_0 (kcal/mol)	-806945.4590	-806941.6519
E_{298} (kcal/mol)	-806927.6359	-806923.8194
H_{298} (kcal/mol)	-806927.0435	-806923.2270
G_{298} (kcal/mol)	-806985.0630	-806981.0306

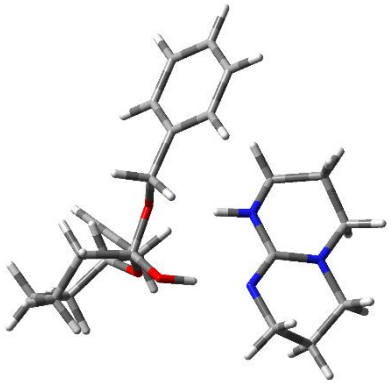
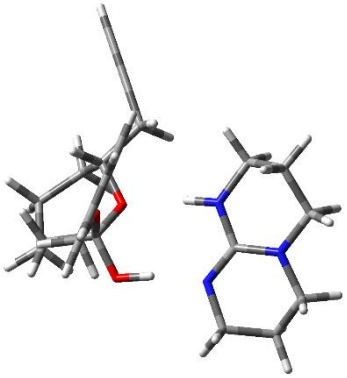
State	**I4**	**I5**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807285.9611	-807286.0669

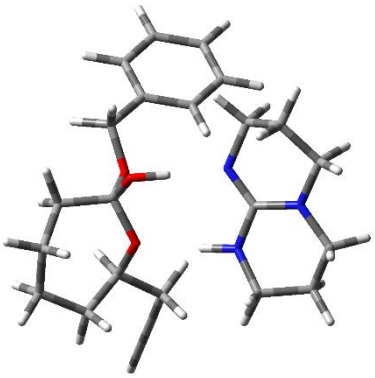
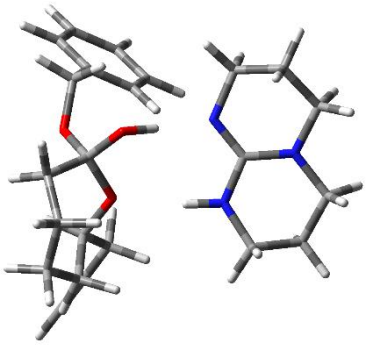
E_0 (kcal/mol)	-806949.7719	-806950.2425
E_{298} (kcal/mol)	-806930.9679	-806931.0853
H_{298} (kcal/mol)	-806930.3756	-806930.4929
G_{298} (kcal/mol)	-806991.3456	-806995.5424
Toluene		
E_{DFT} (kcal/mol)	-807289.5158	-807291.2244
E_0 (kcal/mol)	-806953.5269	-806955.5349
E_{298} (kcal/mol)	-806934.7010	-806936.3896
H_{298} (kcal/mol)	-806934.1086	-806935.7973
G_{298} (kcal/mol)	-806995.2406	-807000.3931

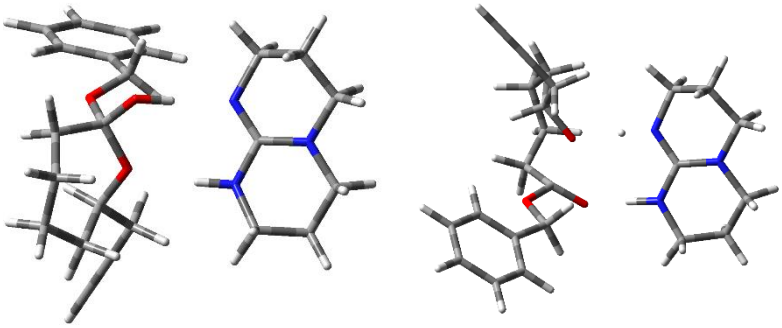
7-isomer		
State	**BnOH-TBD**	**7-isomer**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-493092.1104	-314188.7111
E_0 (kcal/mol)	-492878.1956	-314067.2182
E_{298} (kcal/mol)	-492867.4037	-314060.5466
H_{298} (kcal/mol)	-492866.8113	-314059.9542
G_{298} (kcal/mol)	-492908.9316	-314090.0564
Toluene		
E_{DFT} (kcal/mol)	-493094.9932	-314191.9501

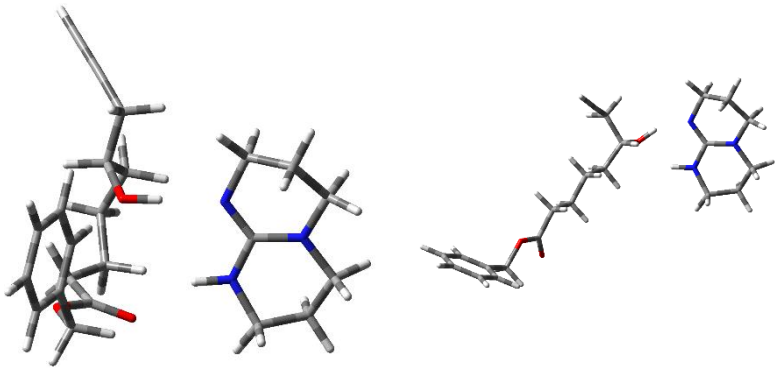
E_0 (kcal/mol)	-492881.2691	-314070.4229
E_{298} (kcal/mol)	-492870.4509	-314063.7789
H_{298} (kcal/mol)	-492869.8579	-314063.1865
G_{298} (kcal/mol)	-492912.2512	-314093.1902

State	**I1**	**TS12**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807289.3498	-807274.6460
E_0 (kcal/mol)	-806953.7001	-806938.9963
E_{298} (kcal/mol)	-806934.8121	-806921.3871
H_{298} (kcal/mol)	-806934.2197	-806920.7948
G_{298} (kcal/mol)	-806996.4529	-806977.7563
Toluene		
E_{DFT} (kcal/mol)	-807293.1010	-807280.3499
E_0 (kcal/mol)	-806957.6854	-806944.7449
E_{298} (kcal/mol)	-806938.7704	-806927.0498
H_{298} (kcal/mol)	-806938.1780	-806926.4574
G_{298} (kcal/mol)	-807000.3943	-806983.8569

State	**I2**	**TS23**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807279.6850	-807277.4943
E_0 (kcal/mol)	-806943.0237	-806941.2120
E_{298} (kcal/mol)	-806925.1227	-806923.7102
H_{298} (kcal/mol)	-806924.5303	-806923.1178
G_{298} (kcal/mol)	-806983.1573	-806980.5525
Toluene		
E_{DFT} (kcal/mol)	-807283.6038	-807282.2684
E_0 (kcal/mol)	-806947.1112	-806945.7960
E_{298} (kcal/mol)	-806929.2310	-806928.4341
H_{298} (kcal/mol)	-806928.6380	-806927.8417
G_{298} (kcal/mol)	-806987.1413	-806984.3113

State	**I3**	**TSr**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807279.2369	-807276.8155
E_0 (kcal/mol)	-806942.4376	-806940.1610
E_{298} (kcal/mol)	-806924.5805	-806922.8436
H_{298} (kcal/mol)	-806923.9882	-806922.2512
G_{298} (kcal/mol)	-806982.3039	-806978.5501
Toluene		
E_{DFT} (kcal/mol)	-807283.3111	-807280.7273
E_0 (kcal/mol)	-806946.6883	-806944.3251
E_{298} (kcal/mol)	-806928.8470	-806927.0027
H_{298} (kcal/mol)	-806928.2546	-806926.4103
G_{298} (kcal/mol)	-806986.6958	-806982.7412

State	**I3r**	**TS34**
Molecular geometry		
Vacuum		
E_{DFT} (kcal/mol)	-807280.0764	-807273.2289
E_0 (kcal/mol)	-806943.3311	-806937.9151
E_{298} (kcal/mol)	-806925.4415	-806920.1798
H_{298} (kcal/mol)	-806924.8491	-806919.5874
G_{298} (kcal/mol)	-806983.4309	-806977.6565
Toluene		
E_{DFT} (kcal/mol)	-807284.1383	-807279.6613
E_0 (kcal/mol)	-806947.6283	-806944.1996
E_{298} (kcal/mol)	-806929.7443	-806926.4455
H_{298} (kcal/mol)	-806929.1513	-806925.8531
G_{298} (kcal/mol)	-806987.5153	-806983.4917

State	**I4**	**I5**
Molecular geometry		

Vacuum		
E_{DFT} (kcal/mol)	-807289.4799	-807288.6470
E_0 (kcal/mol)	-806953.2477	-806953.1717
E_{298} (kcal/mol)	-806934.5749	-806934.0001
H_{298} (kcal/mol)	-806933.9819	-806933.4077
G_{298} (kcal/mol)	-806994.9463	-806998.8538
Toluene		
E_{DFT} (kcal/mol)	-807293.0598	-807293.8143
E_0 (kcal/mol)	-806957.0334	-806958.5231
E_{298} (kcal/mol)	-806938.3518	-806939.3527
H_{298} (kcal/mol)	-806937.7595	-806938.7604
G_{298} (kcal/mol)	-806998.7741	-807004.0370

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

Thermodynamic parameters of DFT-optimized structures in the second step of the TBD catalyzed ROP of 3-/7-isomer in toluene solution calculated using 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 3-isomer unit to the 3-isomer chain end		
State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1121486.1973	-1121472.1263
E_0 (kcal/mol)	-1121028.5438	-1121014.3144
E_{298} (kcal/mol)	-1121001.3080	-1120988.4397
H_{298} (kcal/mol)	-1121000.7157	-1120987.8473
G_{298} (kcal/mol)	-1121085.6114	-1121066.6023
State	**I2**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1121473.6316	-1121473.4990
E_0 (kcal/mol)	-1121015.0085	-1121015.2136
E_{298} (kcal/mol)	-1120988.9128	-1120989.5046
H_{298} (kcal/mol)	-1120988.3205	-1120988.9122
G_{298} (kcal/mol)	-1121068.4691	-1121067.4626

State	**I3**	**TSr**
Toluene		
E_{DFT} (kcal/mol)	-1121479.3482	-1121478.4541
E_0 (kcal/mol)	-1121020.7583	-1121020.1879
E_{298} (kcal/mol)	-1120994.5786	-1120994.5008
H_{298} (kcal/mol)	-1120993.9863	-1120993.9084
G_{298} (kcal/mol)	-1121073.8036	-1121072.4588

State	**I3r**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1121479.6087	-1121473.9951
E_0 (kcal/mol)	-1121020.8562	-1121017.0956
E_{298} (kcal/mol)	-1120994.7430	-1120990.9209
H_{298} (kcal/mol)	-1120994.1507	-1120990.3285
G_{298} (kcal/mol)	-1121073.9216	-1121071.1084

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1121486.8835	-1121488.7838
E_0 (kcal/mol)	-1121028.8946	-1121030.9666
E_{298} (kcal/mol)	-1121001.7548	-1121003.5859
H_{298} (kcal/mol)	-1121001.1625	-1121002.9935
G_{298} (kcal/mol)	-1121084.0954	-1121088.6875

Addition of another 3-isomer unit to the 7-isomer chain end		
State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1121488.2355	-1121473.1855
E_0 (kcal/mol)	-1121030.9830	-1121015.6096
E_{298} (kcal/mol)	-1121003.7202	-1120989.6464
H_{298} (kcal/mol)	-1121003.1278	-1120989.0534
G_{298} (kcal/mol)	-1121088.0167	-1121068.0863
State	**I2**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1121473.8659	-1121473.5781
E_0 (kcal/mol)	-1121015.7414	-1121015.3398
E_{298} (kcal/mol)	-1120989.5121	-1120989.7135
H_{298} (kcal/mol)	-1120988.9197	-1120989.1212
G_{298} (kcal/mol)	-1121069.5033	-1121066.7629
State	**I3**	**TSr**
Toluene		
E_{DFT} (kcal/mol)	-1121474.1647	-1121473.9682
E_0 (kcal/mol)	-1121015.8769	-1121015.8512
E_{298} (kcal/mol)	-1120989.7462	-1120990.1948
H_{298} (kcal/mol)	-1120989.1532	-1120989.6025

G_{298} (kcal/mol)	-1121069.0295	-1121068.7741

State	**I3r**	**TSr2**
Toluene		
E_{DFT} (kcal/mol)	-1121480.5141	-1121479.7308
E_0 (kcal/mol)	-1121022.3227	-1121021.8125
E_{298} (kcal/mol)	-1120996.1261	-1120996.1279
H_{298} (kcal/mol)	-1120995.5331	-1120995.5350
G_{298} (kcal/mol)	-1121075.6077	-1121074.1638

State	**I3r2**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1121480.9234	-1121475.3679
E_0 (kcal/mol)	-1121022.4576	-1121018.8902
E_{298} (kcal/mol)	-1120996.3564	-1120992.6553
H_{298} (kcal/mol)	-1120995.7640	-1120992.0629
G_{298} (kcal/mol)	-1121075.4665	-1121072.4212

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1121487.1399	-1121491.2999
E_0 (kcal/mol)	-1121029.6470	-1121033.8450
E_{298} (kcal/mol)	-1121002.4143	-1121006.4674

H_{298} (kcal/mol)	-1121001.8220	-1121005.8744
G_{298} (kcal/mol)	-1121085.9810	-1121091.7773

Addition of another 7-isomer unit to the 3-isomer chain end		
State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1121489.0395	-1121475.2553
E_0 (kcal/mol)	-1121031.6199	-1121017.9427
E_{298} (kcal/mol)	-1121004.3841	-1120991.9676
H_{298} (kcal/mol)	-1121003.7917	-1120991.3752
G_{298} (kcal/mol)	-1121088.1001	-1121071.0143
State	**I2**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1121481.0183	-1121479.6231
E_0 (kcal/mol)	-1121022.2844	-1121021.1850
E_{298} (kcal/mol)	-1120996.2020	-1120995.5199
H_{298} (kcal/mol)	-1120995.6090	-1120994.9275
G_{298} (kcal/mol)	-1121074.9814	-1121073.3781
State	**I3**	**TSr**
Toluene		
E_{DFT} (kcal/mol)	-1121480.2879	-1121478.6957

E_0 (kcal/mol)	-1121021.6996	-1121020.3755
E_{298} (kcal/mol)	-1120995.5362	-1120994.6520
H_{298} (kcal/mol)	-1120994.9438	-1120994.0597
G_{298} (kcal/mol)	-1121075.7558	-1121073.0462

State	**I3r**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1121481.3998	-1121477.1732
E_0 (kcal/mol)	-1121021.9631	-1121019.5322
E_{298} (kcal/mol)	-1120996.0878	-1120993.5345
H_{298} (kcal/mol)	-1120995.4954	-1120992.9421
G_{298} (kcal/mol)	-1121073.4785	-1121072.0516

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1121491.9345	-1121492.1624
E_0 (kcal/mol)	-1121033.9774	-1121034.8095
E_{298} (kcal/mol)	-1121006.9104	-1121007.3999
H_{298} (kcal/mol)	-1121006.3181	-1121006.8075
G_{298} (kcal/mol)	-1121089.5390	-1121092.5260

Addition of another 7-isomer unit to the 7-isomer chain end		
State	**I1**	**TS12**
Toluene		
E_{DFT} (kcal/mol)	-1121491.4008	-1121477.6955
E_0 (kcal/mol)	-1121034.4462	-1121020.2726
E_{298} (kcal/mol)	-1121007.1646	-1120994.3220
H_{298} (kcal/mol)	-1121006.5722	-1120993.7290
G_{298} (kcal/mol)	-1121091.2352	-1121072.6734
State	**I2**	**TS23**
Toluene		
E_{DFT} (kcal/mol)	-1121480.8986	-1121480.3703
E_0 (kcal/mol)	-1121022.5317	-1121022.2825
E_{298} (kcal/mol)	-1120996.4022	-1120996.5685
H_{298} (kcal/mol)	-1120995.8098	-1120995.9761
G_{298} (kcal/mol)	-1121075.5788	-1121074.5014
State	**I3**	**TSr**
Toluene		
E_{DFT} (kcal/mol)	-1121480.9189	-1121479.8985
E_0 (kcal/mol)	-1121022.6459	-1121021.9638
E_{298} (kcal/mol)	-1120996.4681	-1120996.2817
H_{298} (kcal/mol)	-1120995.8757	-1120995.6893

G_{298} (kcal/mol)	-1121076.2245	-1121074.2598

State	**I3r**	**TSr2**
Toluene		
E_{DFT} (kcal/mol)	-1121480.8417	-1121480.3160
E_0 (kcal/mol)	-1121022.7739	-1121022.3647
E_{298} (kcal/mol)	-1120996.5641	-1120996.6482
H_{298} (kcal/mol)	-1120995.9717	-1120996.0558
G_{298} (kcal/mol)	-1121076.2164	-1121074.9814

State	**I3r2**	**TS34**
Toluene		
E_{DFT} (kcal/mol)	-1121481.7890	-1121477.8792
E_0 (kcal/mol)	-1121023.6028	-1121020.8531
E_{298} (kcal/mol)	-1120997.4150	-1120994.6979
H_{298} (kcal/mol)	-1120996.8226	-1120994.1055
G_{298} (kcal/mol)	-1121077.4513	-1121074.8591

State	**I4**	**I5**
Toluene		
E_{DFT} (kcal/mol)	-1121491.9912	-1121493.5180
E_0 (kcal/mol)	-1121034.3194	-1121036.5854
E_{298} (kcal/mol)	-1121007.3033	-1121009.1299

H_{298} (kcal/mol)	-1121006.7103	-1121008.5376
G_{298} (kcal/mol)	-1121089.5076	-1121094.4072

A note on artefact intermediate states. In all standard quantum chemical methods, geometry optimization 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 geometry optimization and IRC calculations do not need to be local minima of G. Intermediate states should be considered either thermally unstable at the given temperature, or even artefacts of the method if they occur at zero temperature due to zero-point energy corrections. Such artefact intermediate states (not shown in Table S3) were found for both isomers between TS12 and I2 and between I3 and TS34.

Kinetic data

Table S4. Copolymerization of 3- and 7-(prop-2-ynyl)oxepan-2-one in toluene catalyzed by BnOH/TBD at 30 °C [a]

entry	time (h)	conv. 3-is. [b] (%)	conv. 7-is. [b] (%)	M_n [c] (kg.mol^{-1})	$Đ$ [c]
1	1	8.4	15.8	0.5	1.13
2	2	19.5	46.5	1.3	1.18
3	3	24.3	60.6	1.5	1.18
4	4	28.7	66.7	1.5	1.28
5	5	36.1	72.5	1.6	1.19

[a]n_{BnOH} = 10.8 µmol (1 eq.), 3-is/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

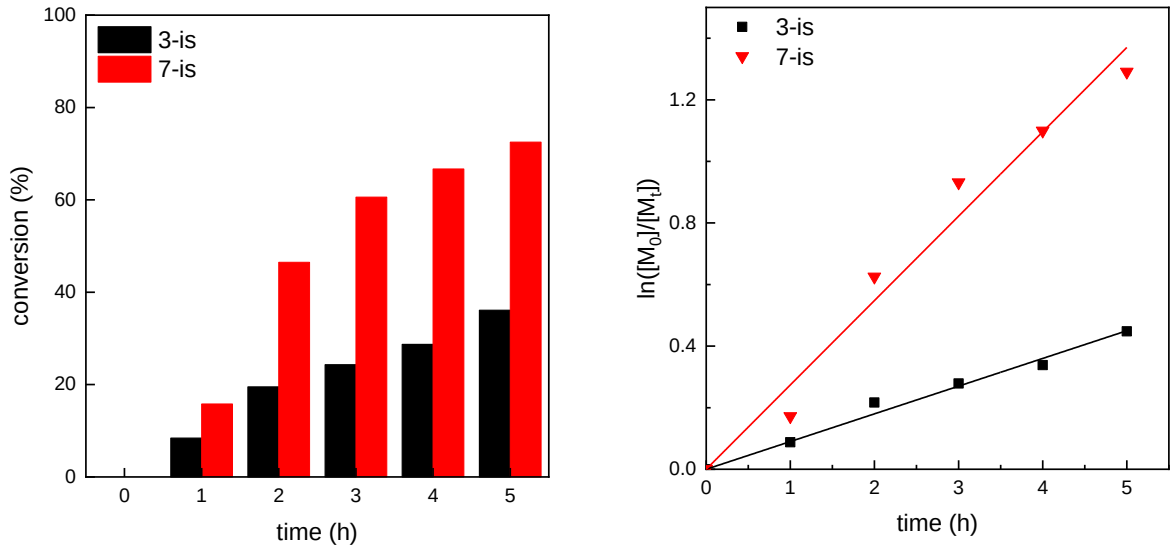


Figure S7. Kinetic plots of 3- and 7-(prop-2-ynyl)oxepan-2-one copolymerization in toluene catalyzed by BnOH/TBD at 30 °C

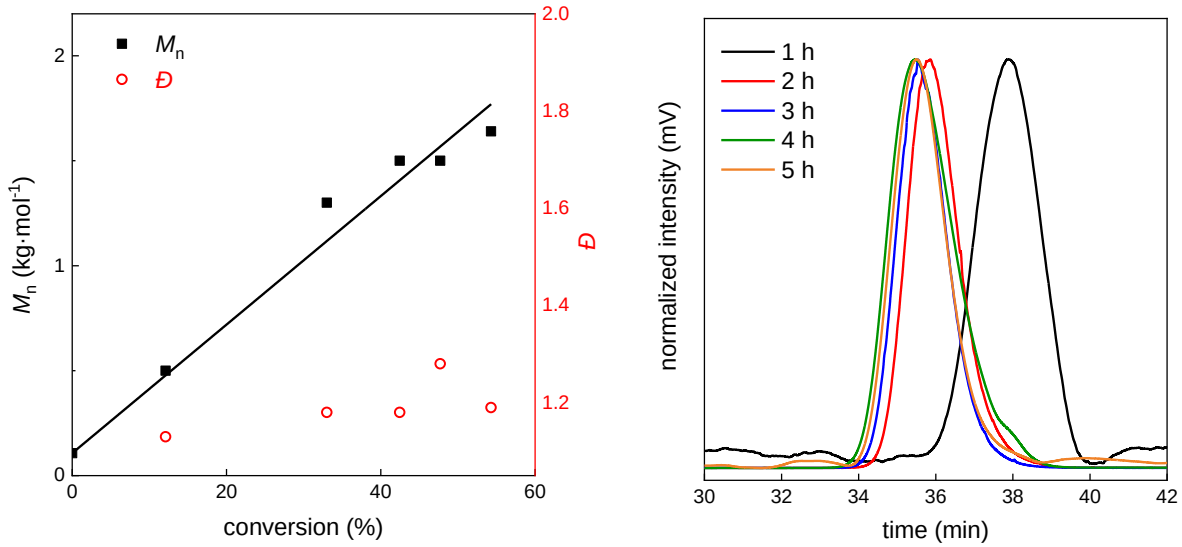


Figure S8: Kinetics of 3- and 7-(prop-2-ynyl)oxepan-2-one copolymerization in toluene catalyzed by BnOH/TBD at 30 °C: The apparent number-average molecular weights (M_n) and dispersities ($Đ$) determined by SEC-ELS with PS calibration plotted vs. total monomer conversion (left). Corresponding SEC-ELS chromatograms (right).

Table S5. Polymerization of 7-(prop-2-ynyl)oxepan-2-one in toluene catalyzed by BnOH/TBD at 30 °C [a]

entry	time (h)	conv. 7-is. [b] (%)	M_n [c] (kg.mol^{-1})	$Đ$ [c]
6	1	12.7	1.0	1.20
7	2	36.0	1.7	1.19
8	3	53.2	2.1	1.19
9	4	63.3	2.5	1.19
10	5	72.5	2.7	1.21

[a]n_{BnOH} = 10.8 µmol (1 eq.), 7-is/BnOH/TBD = 25/1/2, 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

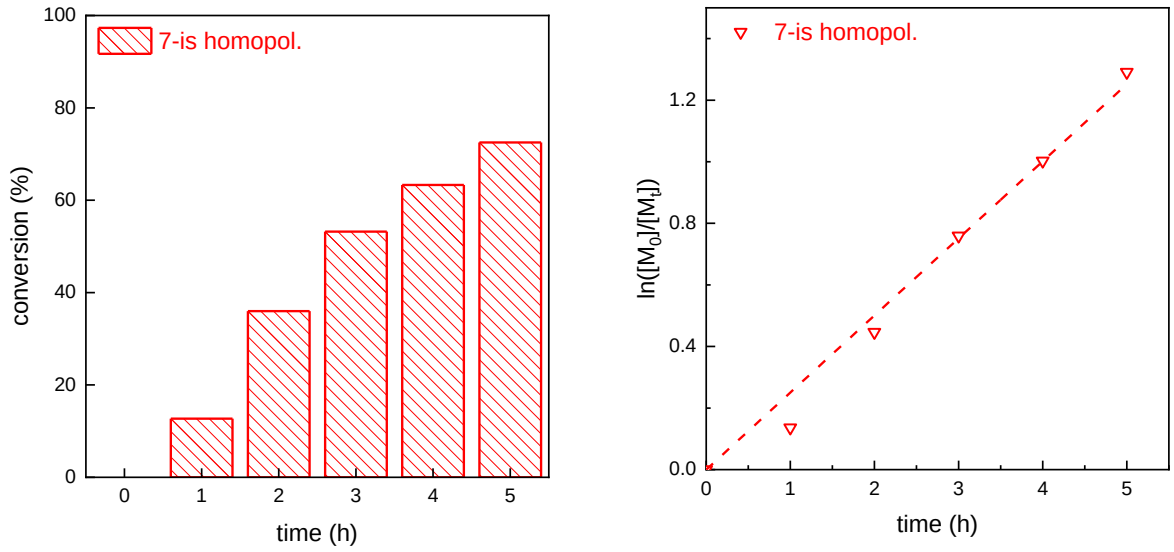


Figure S9. Kinetic plots of 7-(prop-2-ynyl)oxepan-2-one homopolymerization (in toluene catalyzed by BnOH/TBD at 30 °C)

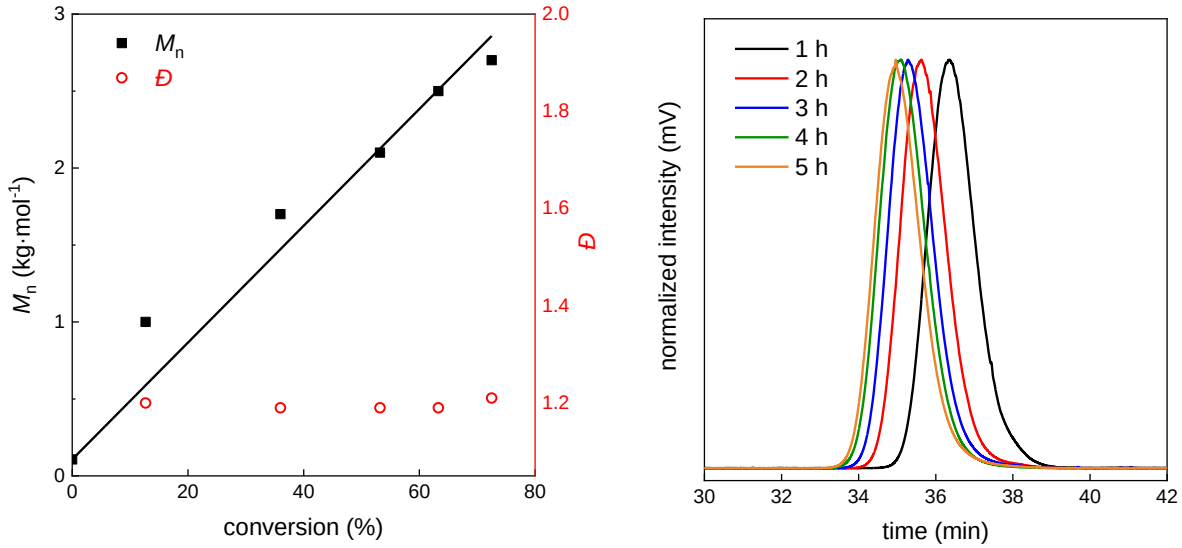


Figure S10. Kinetics of 7-(prop-2-ynyl)oxepan-2-one homopolymerization in toluene catalyzed by BnOH/TBD at 30 °C: The apparent number-average molecular weights (M_n) and dispersities ($Đ$) determined by SEC-ELS with PS calibration plotted vs. monomer conversion (left). Corresponding SEC-ELS chromatograms (right).

Table S6. Polymerization of 3-(prop-2-ynyl)oxepan-2-one in toluene catalyzed by BnOH/TBD at 30 °C [a]

entry	time (h)	conv. 3-is. [b] (%)	M_n [c] (kg.mol^{-1})	$Đ$ [c]
11	1	32.0	1.0	1.27
12	2	50.7	1.4	1.31
13	3	68.7	1.7	1.36
14	4	71.9	1.9	1.36
15	5	83.1	1.6	1.50

[a]n_{BnOH} = 4.3 µmol (1 eq.), 3-is/BnOH/TBD = 25/1/2, 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

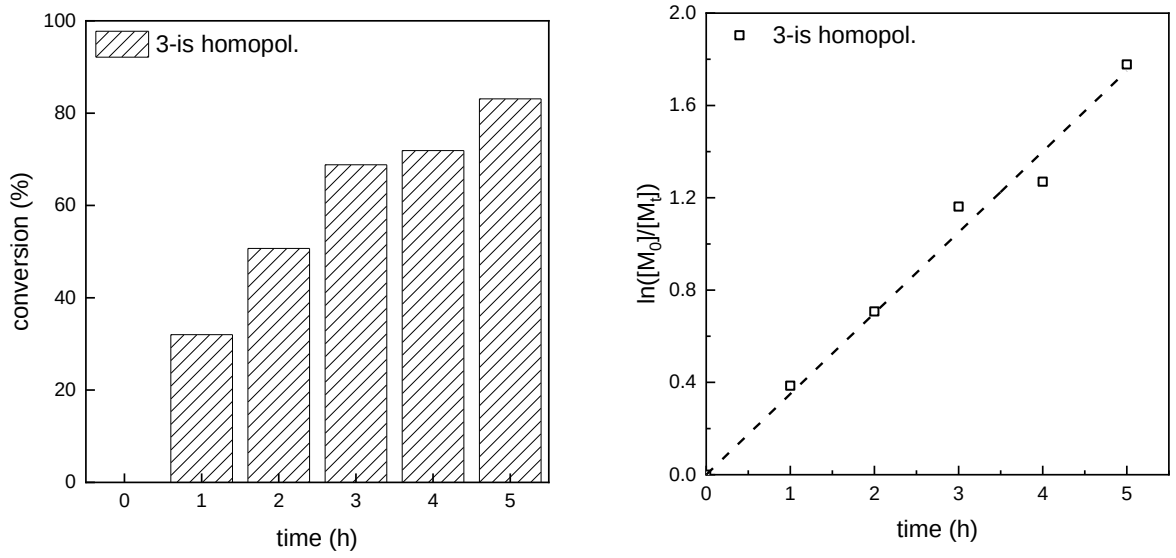


Figure S11. Kinetic plots of 3-(prop-2-ynyl)oxepan-2-one homopolymerization (in toluene catalyzed by BnOH/TBD at 30 °C)

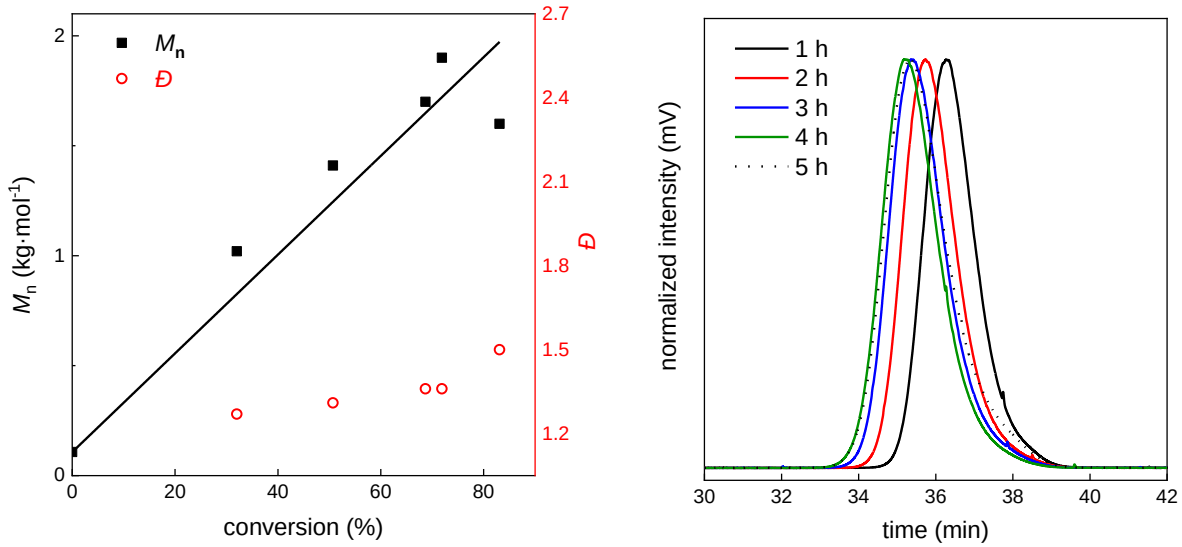


Figure S12. Kinetics of 3-(prop-2-ynyl)oxepan-2-one homopolymerization in toluene catalyzed by BnOH/TBD at 30 °C: The apparent number-average molecular weights (M_n) and dispersities ($Đ$) determined by SEC-ELS with PS calibration plotted vs. monomer conversion (left). Corresponding SEC-ELS chromatograms (right).

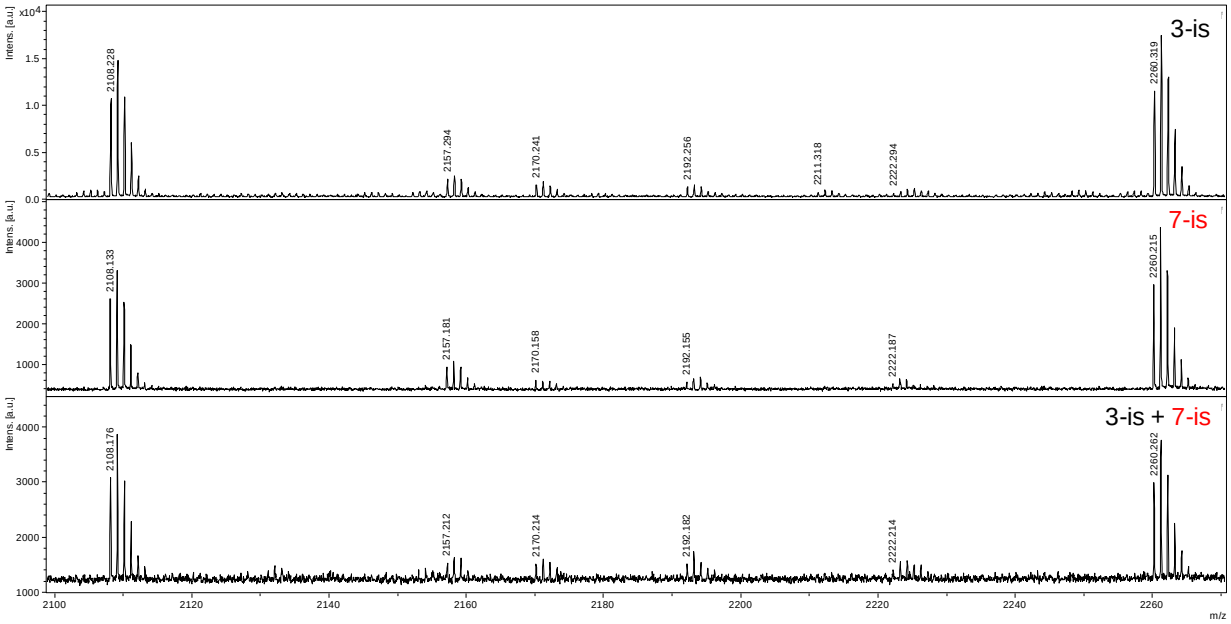


Figure S13: High resolution MALDI-TOF MS spectra of (co)polymers obtained after 4 hours of (co)polymerization during kinetic measurements

Copolymerization parameters

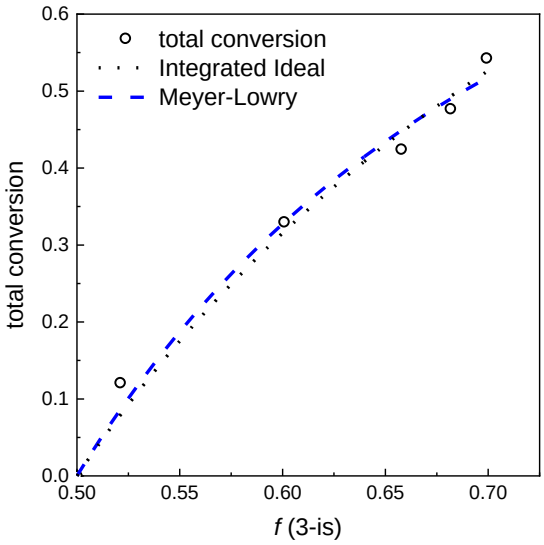


Figure S14. Overlay of the Integrated Ideal Model (black) and the Meyer-Lowry evaluation (blue) for the copolymerization of 3- and 7-(prop-2-ynyl)oxepan-2-one in toluene catalyzed by BnOH/TBD at 30 °C

Table S7. Data of the determined copolymerization parameters (Integrated Ideal Model[18]) used to construct simulated copolymer composition profiles

f (3-is)	total conversion [a]	F (3-is) [b]	f (3-is)	total conversion [a]	F (3-is) [b]
0.500	0.000	0.248	0.775	0.649	0.532
0.525	0.093	0.267	0.800	0.684	0.569
0.550	0.176	0.287	0.825	0.718	0.609
0.575	0.251	0.309	0.850	0.750	0.652
0.600	0.318	0.331	0.875	0.781	0.698
0.625	0.378	0.355	0.900	0.812	0.748
0.650	0.433	0.380	0.925	0.843	0.803
0.675	0.483	0.407	0.950	0.877	0.862
0.700	0.529	0.435	0.975	0.916	0.928
0.725	0.572	0.465	1.000	1.000	1.000
0.750	0.612	0.497			

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

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

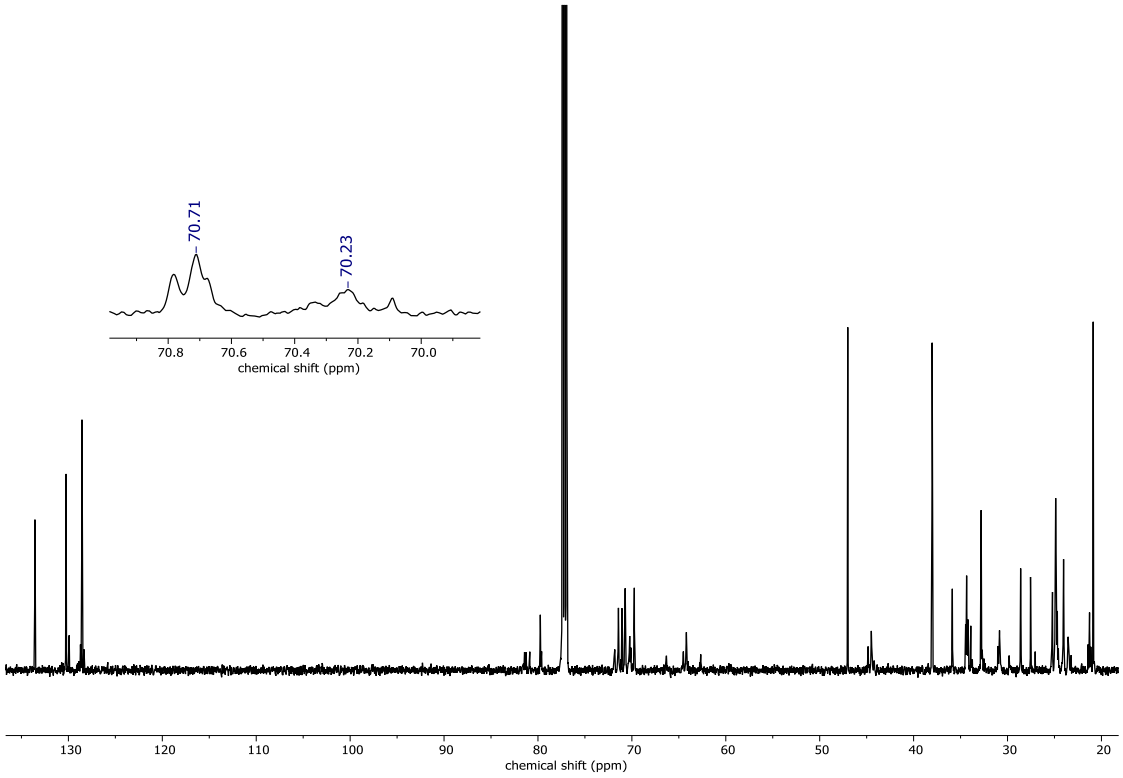


Figure S15. ^{13}C NMR spectrum of copolymer obtained after 4 hours showing the higher content of 7-isomer dyads (70.71 ppm) than 3-isomer dyads (70.23 ppm)

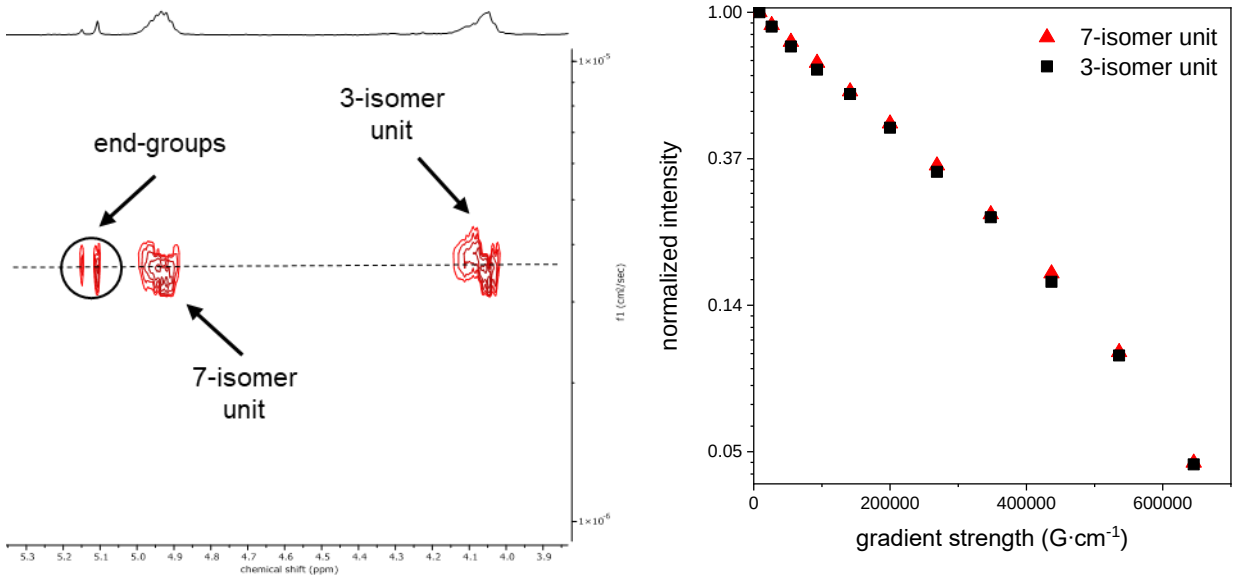


Figure S16. Representative DOSY NMR spectrum of copolymer obtained after 4 hours (left). Experimental signal intensity decay of 3- and 7-isomer characteristic peaks (right).

Table S8: Cartesian coordinates (in Angstroms) of all intermediates and transition states of the initial step of the TBD catalyzed ROP of 3-/7-isomer (**Scheme 3**) 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
```

23 atoms
3-isomer in vacuum

O	-0.297327	2.409772	0.513662
C	-0.566583	1.331103	0.055163
O	-1.851252	1.086777	-0.304139
C	-2.291386	-0.161647	-0.876237
H	-1.709372	-0.388153	-1.776278
H	-3.311245	0.058389	-1.190932
C	-2.277957	-1.322672	0.111957
H	-2.714992	-0.971321	1.053592
H	-2.953476	-2.096395	-0.270966
C	-0.896525	-1.939778	0.351692
H	-0.545559	-2.400609	-0.580699
H	-0.991500	-2.757611	1.073626
C	0.175992	-0.964490	0.847908
H	-0.092243	-0.569101	1.834991
H	1.108083	-1.519828	0.982175
C	0.465812	0.215854	-0.111625
H	0.420258	-0.158606	-1.141237
C	1.876279	0.808420	0.110632
H	1.984008	1.719253	-0.484157
C	2.942333	-0.129435	-0.229471
H	1.973643	1.128147	1.152637
C	3.810416	-0.909164	-0.519108
H	4.590739	-1.585706	-0.774398

62 atoms
3-isomer, structure I1 in vacuum

N	4.301753	1.785642	0.140116
C	3.169400	1.002352	0.046441
N	1.970761	1.633804	0.246130
C	1.825437	3.077730	0.239423
C	2.963553	3.665515	1.062461
C	4.291741	3.211033	0.469072
C	5.500473	-0.062978	-0.974194
C	4.457211	-0.949169	-0.297065
N	3.172627	-0.278039	-0.188134
C	5.616935	1.242122	-0.196536
H	0.848762	3.314796	0.658994
H	1.853018	3.487261	-0.783627
H	2.870635	3.319581	2.096102
H	2.923067	4.758304	1.069863
H	4.514057	3.793223	-0.438373
H	5.110961	3.404972	1.172376
H	6.155464	1.993444	-0.787075

H	6.197890	1.088933	0.724336
H	5.181851	0.143166	-2.001320
H	6.478110	-0.552206	-1.023196
H	4.825317	-1.252329	0.696549
H	4.311709	-1.873228	-0.863988
H	1.144745	1.072270	0.100363
O	-1.500531	2.895334	0.821610
C	-2.014694	1.944761	0.282487
O	-1.217968	0.961291	-0.185287
C	-1.723326	-0.235674	-0.848363
H	-2.443399	-0.732595	-0.190964
H	-0.837604	-0.865997	-0.916120
C	-2.310536	0.052281	-2.222657
H	-1.623139	0.718475	-2.756970
H	-2.313033	-0.891243	-2.779585
C	-3.728936	0.630884	-2.209769
H	-4.414658	-0.118492	-1.794089
H	-4.058467	0.800369	-3.240384
C	-3.894545	1.933620	-1.420052
H	-3.308970	2.738939	-1.880140
H	-4.941517	2.242689	-1.480429
C	-3.524115	1.829457	0.080901
H	-3.855413	0.852190	0.450040
C	-4.225219	2.917076	0.927178
H	-3.828754	2.895642	1.945806
C	-5.675874	2.755693	0.963122
H	-3.966105	3.904733	0.533542
C	-6.868610	2.607809	0.990437
H	-7.924922	2.486554	1.026816
O	1.017529	-1.931523	-0.497493
C	0.820535	-2.558625	0.750743
C	-0.023661	-3.806096	0.605484
H	0.335450	-1.878991	1.469891
H	1.788810	-2.833962	1.196815
C	-0.115005	-4.472707	-0.618326
C	-0.703198	-4.330998	1.709351
C	-0.865445	-5.641928	-0.733394
H	0.402586	-4.056444	-1.474184
C	-1.448941	-5.501709	1.597988
H	-0.649475	-3.817469	2.666491
H	-0.928393	-6.148326	-1.692162
C	-1.532877	-6.162607	0.373181
H	-1.970143	-5.895104	2.465639
H	-2.117137	-7.073144	0.282531
H	1.788646	-1.303713	-0.418454

62 atoms
3-isomer, structure TS12 in vacuum

N	3.539018	-1.604023	-0.035473
C	2.236957	-1.232483	-0.195187
N	1.434925	-1.930345	-1.001348
C	1.842944	-3.177815	-1.621248
C	3.311974	-3.084993	-2.012559
C	4.134190	-2.715700	-0.783554
C	3.666151	-0.123879	1.946150
C	2.597894	0.707208	1.248466
N	1.757108	-0.164926	0.442786
C	4.436642	-0.924129	0.903534
H	1.205832	-3.335083	-2.492860
H	1.678374	-4.025912	-0.942193
H	3.431692	-2.321581	-2.786985
H	3.672264	-4.032674	-2.420769
H	4.238210	-3.583181	-0.117743
H	5.145657	-2.416497	-1.077813
H	5.053778	-1.688746	1.386910
H	5.117411	-0.269147	0.343275
H	3.191423	-0.802110	2.661700
H	4.358544	0.514273	2.501033
H	3.056506	1.486947	0.627433
H	1.950237	1.214213	1.963569
H	0.423616	-1.655826	-1.080568
O	-1.156278	-1.251896	-1.294457
C	-1.646210	-0.859888	-0.212124
O	-1.183561	-1.569047	0.899220
C	-1.586892	-1.179370	2.217474
H	-1.749868	-0.100467	2.249525
H	-0.729564	-1.403919	2.858999
C	-2.805977	-1.968911	2.679943
H	-2.595613	-3.033530	2.522486
H	-2.927675	-1.831216	3.762225
C	-4.103711	-1.580448	1.965208
H	-4.417217	-0.582929	2.300265
H	-4.899769	-2.265806	2.278963
C	-4.028703	-1.574993	0.431717
H	-3.690422	-2.550256	0.062323
H	-5.045392	-1.436431	0.051193
C	-3.144236	-0.460640	-0.175561
H	-3.255667	0.441070	0.430676
C	-3.610736	-0.135792	-1.616481
H	-2.880673	0.507590	-2.109154
C	-4.925040	0.500537	-1.665884
H	-3.619361	-1.060759	-2.201241
C	-6.003499	1.033056	-1.696999

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H     -6.954834     1.506977    -1.733789
O     -0.801305     0.726679     0.237887
C     -0.831979     1.710520    -0.757385
C      0.125982     2.848395    -0.446351
H     -1.844641     2.142030    -0.848357
H     -0.580750     1.288865    -1.744845
C      0.087544     3.476052     0.805088
C      1.058530     3.297556    -1.384274
C      0.949735     4.526586     1.105105
H     -0.627143     3.125944     1.542848
C      1.926041     4.350764    -1.089230
H      1.105970     2.817906    -2.358379
H      0.898577     5.007349     2.077875
C      1.874672     4.968936     0.157455
H      2.640956     4.687465    -1.834495
H      2.545441     5.790659     0.389419
H      0.742260     0.110525     0.335702


62 atoms
3-isomer, structure I2 in vacuum
N      3.737652    -1.491780    -0.023222
C      2.391541    -1.192187    -0.098775
N      1.558890    -1.737965    -0.937189
C      2.052352    -2.793592    -1.804724
C      3.490287    -2.533374    -2.248533
C      4.367022    -2.364814    -1.013569
C      3.935104    -0.222786     2.100745
C      2.769192     0.600748     1.569032
N      1.910356    -0.276164     0.799165
C      4.658673    -0.873215     0.927978
H      1.390490    -2.860937    -2.673057
H      1.994729    -3.770602    -1.298939
H      3.518714    -1.619252    -2.850997
H      3.877051    -3.348662    -2.867643
H      4.580413    -3.342670    -0.558672
H      5.334546    -1.927421    -1.288680
H      5.346946    -1.646716     1.289345
H      5.275354    -0.123872     0.407379
H      3.550318    -0.990721     2.778278
H      4.637221     0.400573     2.661636
H      3.141258     1.447729     0.972081
H      2.179249     1.021624     2.385838
H     -0.135536    -1.494946    -0.967569
O     -1.122500    -1.323082    -1.102959
C     -1.636612    -0.678011    -0.023824
O     -1.274084    -1.402912     1.122585
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C     -1.717160    -0.937626     2.403234
H     -1.906784     0.138918     2.373278
H     -0.878400    -1.104457     3.084357
C     -2.940590    -1.720752     2.859968
H     -2.685936    -2.786311     2.830439
H     -3.149947    -1.476982     3.909410
C     -4.187195    -1.460947     2.008822
H     -4.562853    -0.448407     2.208377
H     -4.981715    -2.142159     2.333745
C     -3.992782    -1.621777     0.492470
H     -3.535065    -2.590472     0.266074
H     -4.985754    -1.631019     0.032893
C     -3.178900    -0.504332    -0.195509
H     -3.449841     0.449770     0.268674
C     -3.569326    -0.431167    -1.697326
H     -2.861971     0.182790    -2.256400
C     -4.917878     0.091162    -1.906309
H     -3.483089    -1.431611    -2.130527
C     -6.023372     0.536810    -2.067820
H     -7.000946     0.926811    -2.221334
O     -0.975149     0.612895     0.188627
C     -1.000173     1.552043    -0.889915
C     -0.069965     2.692869    -0.559986
H     -2.019132     1.935332    -1.027855
H     -0.689620     1.059129    -1.815183
C     -0.379051     3.581021     0.476134
C      1.115255     2.880649    -1.273980
C      0.474881     4.634689     0.787797
H     -1.297485     3.443313     1.038800
C      1.971121     3.938970    -0.969153
H      1.370380     2.192266    -2.074195
H      0.219537     5.318524     1.591359
C      1.652797     4.818021     0.062956
H      2.884593     4.076685    -1.539440
H      2.315747     5.644121     0.300400
H      0.941772    -0.008622     0.662561


62 atoms
3-isomer, structure TS23 in vacuum
N      3.737314    -1.455242    -0.255076
C      2.376817    -1.229061    -0.210202
N      1.561602    -1.399747    -1.210623
C      2.096103    -1.956248    -2.442170
C      3.516275    -1.464650    -2.715600
C      4.397025    -1.794252    -1.516051
C      3.899162    -1.179338     2.209301
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C	2.675216	-0.284217	2.058696
N	1.857591	-0.821051	0.990129
C	4.637577	-1.243897	0.877354
H	1.429438	-1.674751	-3.262230
H	2.088554	-3.057094	-2.405112
H	3.496408	-0.381279	-2.874661
H	3.935515	-1.921358	-3.617304
H	4.661534	-2.861176	-1.516196
H	5.339374	-1.235866	-1.569245
H	5.369037	-2.060684	0.890079
H	5.208195	-0.315222	0.721391
H	3.572902	-2.179762	2.508013
H	4.574780	-0.800662	2.981400
H	2.982102	0.755309	1.865268
H	2.079348	-0.277861	2.973847
H	-0.162410	-1.196168	-1.154167
O	-1.151479	-1.032780	-1.249915
C	-1.674726	-0.560649	-0.085333
O	-1.253531	-1.424252	0.951436
C	-1.750785	-1.196781	2.277791
H	-2.026484	-0.146355	2.405107
H	-0.910152	-1.398981	2.947870
C	-2.905388	-2.141206	2.584159
H	-2.559247	-3.162747	2.390029
H	-3.135817	-2.086149	3.655758
C	-4.168849	-1.855725	1.767148
H	-4.635809	-0.929217	2.126775
H	-4.897869	-2.650882	1.959769
C	-3.956162	-1.738743	0.249671
H	-3.423216	-2.615593	-0.132568
H	-4.943539	-1.744039	-0.221606
C	-3.226153	-0.459876	-0.215304
H	-3.546483	0.371264	0.421490
C	-3.641332	-0.125718	-1.674085
H	-2.995404	0.644127	-2.098511
C	-5.029909	0.317031	-1.779760
H	-3.481163	-1.011193	-2.295349
C	-6.169306	0.694976	-1.854858
H	-7.176816	1.027072	-1.931968
O	-1.081538	0.702325	0.307885
C	-1.117208	1.782470	-0.627267
C	-0.069951	2.793673	-0.234023
H	-2.108553	2.252794	-0.629741
H	-0.912666	1.397903	-1.630577
C	-0.414678	3.962049	0.447391
C	1.276284	2.560585	-0.535612
C	0.561583	4.886451	0.817406

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H     -1.456531     4.151446     0.690172
C      2.253727     3.481293    -0.168940
H      1.549708     1.650052    -1.060377
H      0.277351     5.792334     1.343770
C      1.898276     4.648055     0.508990
H      3.293872     3.294641    -0.418870
H      2.659804     5.368490     0.791068
H      0.869483    -0.605793     0.968191


62 atoms
3-isomer, structure I3 in vacuum
N      4.083296    -0.772998    -0.562211
C      2.710363    -0.874979    -0.492290
N      1.874691    -0.135629    -1.163065
C      2.411046     0.830594    -2.106836
C      3.729208     1.428840    -1.620037
C      4.712777     0.301424    -1.330319
C      4.335711    -2.894340     0.698814
C      2.989593    -2.540798     1.318142
N      2.196546    -1.853964     0.319473
C      5.002427    -1.619783     0.195445
H      1.666958     1.618949    -2.250734
H      2.560354     0.364398    -3.093502
H      3.545841     2.005107    -0.707353
H      4.157859     2.112100    -2.359333
H      5.118887    -0.105232    -2.267381
H      5.565692     0.677440    -0.753014
H      5.850581    -1.868497    -0.453126
H      5.412710    -1.050596     1.043949
H      4.173586    -3.587708    -0.131541
H      4.988538    -3.385603     1.425613
H      3.141641    -1.932155     2.224635
H      2.450998    -3.441720     1.621538
H      0.198752    -0.485218    -1.214608
O     -0.782707    -0.693740    -1.332772
C     -1.442717    -0.660946    -0.144377
O     -0.751547    -1.526189     0.750779
C     -1.272102    -1.682874     2.080343
H     -1.875763    -0.813356     2.348109
H     -0.405005    -1.690272     2.747167
C     -2.047281    -2.989122     2.187735
H     -1.383176    -3.802878     1.872815
H     -2.289397    -3.174556     3.241888
C     -3.330323    -3.015601     1.349684
H     -4.082807    -2.365011     1.814306
H     -3.749035    -4.027596     1.386063
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C	-3.169878	-2.600803	-0.122615
H	-2.367680	-3.173683	-0.599414
H	-4.095127	-2.870451	-0.640548
C	-2.929608	-1.094052	-0.355773
H	-3.525041	-0.536615	0.374639
C	-3.425674	-0.691265	-1.770590
H	-3.097501	0.318471	-2.023019
C	-4.879338	-0.758926	-1.902896
H	-2.950367	-1.342216	-2.509587
C	-6.077485	-0.803550	-1.998530
H	-7.136179	-0.842214	-2.093323
O	-1.355286	0.615882	0.508416
C	-1.732342	1.774516	-0.223493
C	-1.061442	2.986832	0.379979
H	-2.822329	1.908281	-0.208773
H	-1.421726	1.660553	-1.268326
C	-1.747727	4.197647	0.488755
C	0.270248	2.923374	0.803009
C	-1.116234	5.331484	0.998450
H	-2.787063	4.256630	0.176521
C	0.899432	4.053023	1.318810
H	0.798613	1.979333	0.730453
H	-1.664710	6.265019	1.078289
C	0.210134	5.261883	1.416131
H	1.932059	3.990513	1.649442
H	0.702318	6.141116	1.820147
H	1.189376	-1.807286	0.442009

62 atoms
3-isomer, structure TSr in vacuum

N	3.577624	-1.555975	-0.741693
C	2.220922	-1.347831	-0.625257
N	1.558255	-0.407205	-1.231842
C	2.275506	0.475208	-2.137508
C	3.706833	0.726683	-1.669267
C	4.413383	-0.610517	-1.483058
C	3.375754	-3.730815	0.434770
C	2.164169	-3.106400	1.114456
N	1.516249	-2.225489	0.163263
C	4.300897	-2.621447	-0.050742
H	1.728363	1.419834	-2.200409
H	2.285924	0.054938	-3.155386
H	3.680454	1.270178	-0.719815
H	4.260761	1.340193	-2.386147
H	4.684757	-1.043501	-2.456292
H	5.347310	-0.474571	-0.925336

H	5.049485	-3.028963	-0.740216
H	4.856166	-2.196976	0.799974
H	3.035707	-4.335427	-0.410984
H	3.919626	-4.386271	1.120502
H	2.478068	-2.579292	2.030522
H	1.446147	-3.873714	1.413888
H	-0.115655	-0.294927	-1.186454
O	-1.124771	-0.205628	-1.272216
C	-1.748093	-0.077598	-0.075290
O	-1.149990	-1.019427	0.816717
C	-1.767116	-1.244626	2.091842
H	-2.324373	-0.357727	2.402820
H	-0.947085	-1.372863	2.804143
C	-2.632679	-2.500260	2.047900
H	-2.004444	-3.322358	1.684231
H	-2.925173	-2.764439	3.072101
C	-3.885966	-2.380793	1.171053
H	-4.627600	-1.754345	1.683208
H	-4.344035	-3.372336	1.082542
C	-3.661340	-1.804171	-0.237067
H	-2.904860	-2.380459	-0.779740
H	-4.596903	-1.917992	-0.792538
C	-3.273248	-0.312787	-0.240610
H	-3.754388	0.177189	0.610564
C	-3.769617	0.411531	-1.516285
H	-3.376887	1.432330	-1.537511
C	-5.226071	0.471593	-1.611833
H	-3.355818	-0.088829	-2.395932
C	-6.425723	0.524284	-1.678767
H	-7.485952	0.575939	-1.745925
O	-1.564269	1.208547	0.559391
C	-1.097531	2.322403	-0.184187
C	0.105522	2.974009	0.468510
H	-1.907870	3.058960	-0.259996
H	-0.845453	2.006555	-1.200136
C	0.394168	4.316199	0.202962
C	0.953537	2.258336	1.315105
C	1.514164	4.929166	0.759199
H	-0.266546	4.890718	-0.441894
C	2.071287	2.872014	1.878390
H	0.724456	1.221734	1.528878
H	1.721569	5.972994	0.543945
C	2.358033	4.207510	1.601832
H	2.718380	2.305033	2.541381
H	3.226402	4.684980	2.045143
H	0.566069	-1.923962	0.354740

62 atoms
3-isomer, structure I3r in vacuum

N	4.365022	0.062539	-0.394384
C	3.029423	-0.270205	-0.322035
N	2.142273	0.009147	-1.232047
C	2.593903	0.650765	-2.455495
C	3.731964	1.634595	-2.190557
C	4.866499	0.904790	-1.480919
C	4.862491	-1.384818	1.558710
C	3.424535	-1.104471	1.977432
N	2.620470	-0.977673	0.779483
C	5.342213	-0.266096	0.641592
H	1.741321	1.163709	-2.909371
H	2.922105	-0.102712	-3.188548
H	3.362821	2.448709	-1.557944
H	4.103582	2.080942	-3.117805
H	5.430906	0.286927	-2.193438
H	5.575987	1.624073	-1.054882
H	6.277276	-0.557138	0.148927
H	5.567000	0.634213	1.234185
H	4.898994	-2.343709	1.033675
H	5.521616	-1.451516	2.428641
H	3.385803	-0.200168	2.606532
H	3.024239	-1.928332	2.573077
H	0.525615	-0.590230	-1.213856
O	-0.401384	-0.954820	-1.357774
C	-1.206144	-0.871826	-0.260310
O	-0.367969	-1.126756	0.880737
C	-1.001778	-1.338470	2.148883
H	-1.960322	-0.813267	2.180269
H	-0.353189	-0.866288	2.892833
C	-1.139185	-2.831028	2.435616
H	-0.145163	-3.281345	2.326601
H	-1.425216	-2.963496	3.486766
C	-2.141138	-3.565810	1.535570
H	-3.162012	-3.298349	1.837232
H	-2.048679	-4.642029	1.720043
C	-2.000975	-3.301292	0.026933
H	-0.985573	-3.524542	-0.316756
H	-2.665781	-3.996558	-0.493788
C	-2.381482	-1.868959	-0.389337
H	-3.172582	-1.507848	0.274085
C	-2.940749	-1.800892	-1.831867
H	-3.065897	-0.751714	-2.113458
C	-4.216951	-2.494634	-1.983079
H	-2.202859	-2.216449	-2.523200

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C     -5.270930    -3.063253    -2.095479
H     -6.204122    -3.561275    -2.206373
O     -1.823507     0.399522    -0.093221
C     -0.963451     1.526493    -0.203669
C     -1.686299     2.778079     0.236425
H     -0.632290     1.631033    -1.243834
H     -0.066079     1.378088     0.406163
C     -0.949293     3.945454     0.463713
C     -3.072368     2.817493     0.395567
C     -1.581875     5.127473     0.836716
H      0.131918     3.927992     0.349335
C     -3.707177     4.000443     0.773306
H     -3.648382     1.916082     0.227732
H     -0.993533     6.023411     1.010309
C     -2.967136     5.158959     0.993587
H     -4.786079     4.014243     0.894910
H     -3.463210     6.078642     1.287526
H      1.615743    -1.109509     0.837282


62 atoms
3-isomer, structure TSr2 in vacuum
N      4.471153     0.738897    -0.364831
C      3.185587     0.273578    -0.189328
N      2.451766    -0.257887    -1.120438
C      3.040206    -0.444946    -2.436237
C      3.999581     0.690328    -2.789654
C      5.062230     0.803832    -1.702325
C      4.742677     1.005313     2.089510
C      3.229952     1.190422     2.110037
N      2.661556     0.348472     1.077490
C      5.269747     1.343496     0.699595
H      2.229088    -0.504317    -3.166969
H      3.572433    -1.407720    -2.487992
H      3.435697     1.626662    -2.855468
H      4.480265     0.526480    -3.758811
H      5.810223     0.005981    -1.811115
H      5.599758     1.755354    -1.791719
H      6.303630     0.994540     0.593082
H      5.292558     2.435977     0.564325
H      4.975515    -0.034067     2.338358
H      5.230066     1.646188     2.829430
H      2.978439     2.254516     1.971467
H      2.812873     0.883934     3.072195
H      0.775743    -0.578061    -1.020562
O     -0.196399    -0.758039    -1.211113
C     -0.988132    -0.896741    -0.103860
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O     -0.137398    -0.708787     1.036325
C     -0.640287    -1.074789     2.328676
H     -1.728770    -0.972811     2.351085
H     -0.236608    -0.334824     3.026219
C     -0.170375    -2.474938     2.712007
H      0.918416    -2.499616     2.586804
H     -0.364625    -2.631852     3.780583
C     -0.814304    -3.607334     1.902227
H     -1.852483    -3.742836     2.231631
H     -0.300015    -4.544220     2.143939
C     -0.815459    -3.413151     0.377090
H      0.202555    -3.256989     0.003567
H     -1.172436    -4.342666    -0.075574
C     -1.719021    -2.262479    -0.101575
H     -2.572858    -2.173387     0.576649
C     -2.294885    -2.515532    -1.516566
H     -2.813115    -1.613463    -1.853293
C     -3.216795    -3.646899    -1.564747
H     -1.469005    -2.672933    -2.215368
C     -3.978837    -4.577158    -1.593055
H     -4.656969    -5.395686    -1.629201
O     -2.023073     0.072684    -0.077292
C     -1.609808     1.411630    -0.318269
C     -2.776449     2.357337    -0.152367
H     -1.195163     1.489190    -1.328163
H     -0.809955     1.683939     0.382128
C     -2.575820     3.723857    -0.379383
C     -4.047733     1.918174     0.218140
C     -3.620068     4.631582    -0.236629
H     -1.591214     4.080256    -0.673137
C     -5.096282     2.827575     0.360254
H     -4.211088     0.861979     0.390704
H     -3.445840     5.687921    -0.417606
C     -4.888271     4.185107     0.135145
H     -6.080420     2.469443     0.647089
H     -5.705580     4.890881     0.245559
H      1.687798     0.069384     1.129152


62 atoms
3-isomer, structure I3r2 in vacuum
N      4.493247     1.065880    -0.436678
C      3.194593     0.653620    -0.233531
N      2.596066    -0.283904    -0.910384
C      3.364974    -1.000667    -1.914572
C      4.364054    -0.084703    -2.619256
C      5.264849     0.565335    -1.575604
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C	4.421113	2.424926	1.642673
C	2.923149	2.511032	1.376519
N	2.500020	1.258117	0.784063
C	5.143795	2.124296	0.334642
H	2.666433	-1.431936	-2.637017
H	3.900271	-1.848803	-1.459690
H	3.815264	0.687486	-3.168172
H	4.974705	-0.633072	-3.342825
H	6.019748	-0.149752	-1.219870
H	5.810560	1.409130	-2.014201
H	6.176937	1.816807	0.535177
H	5.201986	3.036737	-0.278346
H	4.606922	1.628225	2.368747
H	4.803803	3.359065	2.062973
H	2.703139	3.375431	0.729687
H	2.367781	2.654828	2.305982
H	0.876281	-0.319654	-0.987944
O	-0.115135	-0.267162	-1.144758
C	-0.844401	-0.607806	-0.033978
O	-0.257507	0.128483	1.057144
C	-0.679858	-0.175904	2.393586
H	-1.709764	-0.544634	2.386194
H	-0.686276	0.779132	2.926582
C	0.285918	-1.149625	3.063395
H	1.295566	-0.736124	2.958617
H	0.069780	-1.175095	4.139007
C	0.247545	-2.575383	2.499876
H	-0.674485	-3.071068	2.830297
H	1.069760	-3.147778	2.943983
C	0.331456	-2.683892	0.968427
H	1.234589	-2.189160	0.595149
H	0.431916	-3.743927	0.717003
C	-0.909803	-2.135133	0.240019
H	-1.788082	-2.303619	0.870546
C	-1.179246	-2.863657	-1.099760
H	-1.978652	-2.340223	-1.630996
C	-1.552342	-4.264682	-0.924425
H	-0.293076	-2.792432	-1.737092
C	-1.862679	-5.416576	-0.770777
H	-2.143373	-6.434675	-0.644810
O	-2.180274	-0.209621	-0.213762
C	-2.370425	1.122912	-0.683943
C	-3.821860	1.519880	-0.545877
H	-2.053978	1.189385	-1.729002
H	-1.737219	1.807343	-0.109139
C	-4.211342	2.801146	-0.953374
C	-4.789951	0.655835	-0.033400

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C     -5.536217     3.211421    -0.848038
H     -3.468399     3.484433    -1.358103
C     -6.119459     1.065884     0.071736
H     -4.497478    -0.338674     0.278797
H     -5.819466     4.209344    -1.168762
C     -6.498257     2.342336    -0.333129
H     -6.861091     0.380679     0.471231
H     -7.533190     2.659294    -0.250824
H      1.523440     0.985481     0.841568


62 atoms
3-isomer, structure TS34 in vacuum
N     -4.275586    -1.205401    -0.305032
C     -3.012054    -0.708972    -0.192196
N     -2.536111     0.124966    -1.127104
C     -3.323475     0.571080    -2.263673
C     -4.270698    -0.543399    -2.693098
C     -5.103308    -0.981711    -1.493934
C     -4.150866    -1.854453     2.084501
C     -2.653578    -1.998026     1.831268
N     -2.231657    -1.031970     0.831929
C     -4.898298    -1.993694     0.763102
H     -2.626911     0.834253    -3.060666
H     -3.890331     1.478103    -2.014220
H     -3.687777    -1.387536    -3.073303
H     -4.934280    -0.208900    -3.494524
H     -5.869836    -0.229045    -1.264599
H     -5.629894    -1.915959    -1.715759
H     -5.934142    -1.654609     0.871890
H     -4.937100    -3.046783     0.453982
H     -4.348622    -0.873185     2.525970
H     -4.509053    -2.612253     2.786128
H     -2.418341    -3.021774     1.508988
H     -2.077678    -1.808891     2.738294
H     -1.522445     0.339478    -1.119514
O      0.132944     0.571848    -1.332671
C      0.947151     0.878236    -0.446652
O      0.006324     0.214690     1.162617
C      0.276894     0.711873     2.436042
H      1.354472     0.925538     2.550451
H      0.053322    -0.054407     3.202756
C     -0.537084     1.973173     2.762824
H     -1.593781     1.741321     2.572727
H     -0.457787     2.195881     3.836464
C     -0.141044     3.228500     1.973439
H      0.821430     3.601398     2.347632
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H     -0.867402     4.019603     2.198251
C     -0.037733     3.088679     0.443818
H     -0.933580     2.610408     0.037479
H     -0.012736     4.101712     0.029492
C      1.210644     2.332848    -0.051819
H      1.976807     2.334264     0.726278
C      1.834614     3.003675    -1.310906
H      2.649646     2.373776    -1.681232
C      2.347072     4.347654    -1.063823
H      1.079618     3.031009    -2.103871
C      2.770815     5.452635    -0.848479
H      3.153692     6.427277    -0.662759
O      2.108261     0.161449    -0.295530
C      2.036091    -1.204265    -0.707475
C      3.354027    -1.884846    -0.436525
H      1.776393    -1.260019    -1.767726
H      1.227683    -1.678573    -0.140728
C      3.785961    -2.920260    -1.269919
C      4.143669    -1.534344     0.662568
C      4.972719    -3.601597    -1.007540
H      3.190203    -3.193689    -2.137046
C      5.334565    -2.208146     0.921854
H      3.822418    -0.721937     1.303533
H      5.293468    -4.401745    -1.667831
C      5.752466    -3.246358     0.090710
H      5.939764    -1.920273     1.776275
H      6.681593    -3.769867     0.293860
H     -1.276854    -0.501329     0.964920


62 atoms
3-isomer, structure I4 in vacuum
N      4.201035    -0.267519    -0.179511
C      2.825835    -0.372847    -0.154875
N      2.251462    -1.209886    -1.070342
C      2.991991    -2.078174    -1.961407
C      4.268112    -1.367590    -2.397916
C      5.046958    -0.946151    -1.158149
C      4.016816     0.741952     2.070448
C      2.674613     1.250863     1.545996
N      2.047723     0.281201     0.661714
C      4.923823     0.428551     0.886068
H      2.354249    -2.308189    -2.817423
H      3.243557    -3.036253    -1.480940
H      4.005598    -0.487823    -2.993280
H      4.890835    -2.019228    -3.017320
H      5.518353    -1.826621    -0.694406
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H	5.860932	-0.265292	-1.434155
H	5.763880	-0.202746	1.202305
H	5.358602	1.353404	0.481674
H	3.848022	-0.164335	2.661264
H	4.504072	1.473737	2.722061
H	2.823275	2.212694	1.030061
H	1.988012	1.451801	2.372628
H	1.240545	-1.185994	-1.123306
O	-0.691336	-1.190460	-1.398931
C	-1.668465	-0.748248	-0.830072
O	-0.470283	-0.403912	1.616329
C	-0.288924	-1.473642	2.526244
H	-1.047743	-1.365798	3.310704
H	0.691789	-1.385926	3.015733
C	-0.397132	-2.871030	1.903740
H	0.286945	-2.937215	1.049663
H	-0.011475	-3.574460	2.654147
C	-1.807063	-3.350602	1.501205
H	-2.534697	-2.998379	2.244518
H	-1.816717	-4.443612	1.585555
C	-2.334392	-3.031790	0.089950
H	-1.592998	-3.327065	-0.658534
H	-3.204982	-3.675309	-0.068742
C	-2.769136	-1.582844	-0.189558
H	-3.038637	-1.074422	0.738245
C	-4.009469	-1.516823	-1.133278
H	-4.209931	-0.471980	-1.386584
C	-5.210493	-2.103525	-0.547681
H	-3.775192	-2.030100	-2.073897
C	-6.197044	-2.582213	-0.055076
H	-7.074700	-2.999627	0.377274
O	-1.968367	0.554423	-0.772853
C	-0.968509	1.497976	-1.237463
C	-1.289389	2.842829	-0.645854
H	-0.984927	1.519405	-2.329981
H	0.011256	1.145064	-0.911389
C	-1.356286	2.990794	0.745353
C	-1.500455	3.955768	-1.460022
C	-1.629018	4.235349	1.303374
H	-1.199667	2.122161	1.377713
C	-1.765921	5.205355	-0.899761
H	-1.459311	3.847943	-2.540549
H	-1.682354	4.341094	2.382538
C	-1.831890	5.346518	0.483201
H	-1.928094	6.063659	-1.544332
H	-2.043066	6.316682	0.922218
H	0.405567	-0.197108	1.200348

62 atoms
3-isomer, structure I5 in vacuum

N	-6.255014	-0.734718	0.492527
C	-5.156697	-0.293894	-0.217897
N	-4.848735	1.042183	-0.117758
C	-5.387923	1.900419	0.915632
C	-6.876147	1.602405	1.051339
C	-7.062368	0.121240	1.358901
C	-5.417461	-3.020940	0.080721
C	-4.817201	-2.417707	-1.188906
N	-4.421709	-1.034771	-0.993848
C	-6.588430	-2.158298	0.537380
H	-5.222639	2.938633	0.618651
H	-4.885900	1.756814	1.886712
H	-7.375909	1.857894	0.112484
H	-7.328683	2.199813	1.847763
H	-6.808094	-0.076673	2.412063
H	-8.114649	-0.160662	1.234116
H	-6.869862	-2.411265	1.566768
H	-7.472281	-2.348650	-0.087982
H	-4.649945	-3.045226	0.861537
H	-5.757190	-4.048777	-0.080016
H	-5.544065	-2.500452	-2.012888
H	-3.937613	-2.987702	-1.502015
H	-3.984216	1.298035	-0.584978
O	4.707977	1.631360	-1.757516
C	4.199790	1.345699	-0.699992
O	-2.417954	0.698501	-1.754880
C	-1.191372	0.349334	-1.136355
H	-0.700891	-0.468133	-1.687684
H	-1.357141	-0.011129	-0.108853
C	-0.280555	1.568648	-1.121387
H	-0.177811	1.929696	-2.150917
H	-0.778266	2.370517	-0.562752
C	1.099049	1.286990	-0.519444
H	1.585368	0.485170	-1.088102
H	0.986195	0.901716	0.502068
C	1.995867	2.529328	-0.493202
H	2.142181	2.905407	-1.512239
H	1.494457	3.326282	0.064945
C	3.380264	2.304263	0.149844
H	3.249635	1.858506	1.138943
C	4.173330	3.629107	0.291125
H	5.184717	3.411495	0.652750
C	3.545445	4.585077	1.197529

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H      4.297663     4.073511    -0.701171
C      3.029253     5.361788     1.955955
H      2.579437     6.058371     2.622286
O      4.285449     0.122702    -0.137274
C      5.028407    -0.872139    -0.898233
C      5.029519    -2.153248    -0.115061
H      6.037427    -0.489877    -1.064278
H      4.552562    -0.987818    -1.873458
C      4.108898    -3.164157    -0.400978
C      5.943534    -2.346485     0.925330
C      4.101543    -4.347068     0.334879
H      3.393147    -3.024596    -1.205919
C      5.937923    -3.525547     1.664529
H      6.662999    -1.566394     1.156953
H      3.383023    -5.125658     0.099636
C      5.016302    -4.529361     1.369408
H      6.654327    -3.663897     2.467969
H      5.013609    -5.451066     1.942465
H     -3.042982    -0.065984    -1.680637


23 atoms
7-isomer in vacuum
O     -2.545691    -1.851020    -0.160074
O     -0.449796    -1.182862    -0.256280
C     -1.748339    -0.996768     0.115407
C     -2.124443     0.291654     0.827498
H     -1.551181     0.395762     1.756302
H     -3.169924     0.167286     1.108667
C     -1.952593     1.555968    -0.039195
H     -2.365524     1.367116    -1.036747
H     -2.567380     2.349824     0.395949
C     -0.509383     2.058238    -0.148642
H     -0.162514     2.362519     0.847426
H     -0.494533     2.965820    -0.761270
C      0.488781     1.051746    -0.731315
H      0.223204     0.794638    -1.763664
H      1.476764     1.520451    -0.768647
C      0.611612    -0.252403     0.058524
H      0.605753    -0.051361     1.135384
C      1.888946    -1.042156    -0.278956
H      1.817273    -2.021942     0.202449
C      3.109999    -0.366682     0.145945
H      1.913497    -1.229179    -1.358181
C      4.108647     0.194894     0.508596
H      4.999101     0.683177     0.825993
```

62 atoms
7-isomer, structure I1 in vacuum

O	-1.840999	1.105294	-2.307489
O	-2.529787	0.775785	-0.251622
C	-2.451240	0.391984	-1.542808
C	-3.174902	-0.861491	-1.984928
H	-2.655393	-1.721580	-1.550281
H	-3.031898	-0.913778	-3.064525
C	-4.676054	-0.902808	-1.637333
H	-5.138033	0.059983	-1.886377
H	-5.149289	-1.640257	-2.293458
C	-4.986737	-1.277042	-0.183592
H	-4.593747	-2.282624	0.013506
H	-6.072887	-1.348163	-0.059910
C	-4.430513	-0.313985	0.870628
H	-4.895610	0.674781	0.774341
H	-4.693212	-0.688550	1.864813
C	-2.915862	-0.131694	0.817100
H	-2.398966	-1.079738	0.656220
C	-2.328439	0.536035	2.072049
H	-1.271505	0.738665	1.871594
C	-2.464414	-0.280676	3.272968
H	-2.815688	1.506865	2.220006
C	-2.575063	-0.962888	4.256622
H	-2.664742	-1.562772	5.130511
O	-0.218011	-1.276432	-0.522111
C	0.642315	-1.826988	-1.495664
C	1.731641	-2.727382	-0.934054
H	1.102631	-1.036539	-2.104407
H	0.015056	-2.416349	-2.175917
C	1.578767	-3.347563	0.307869
C	2.890714	-2.982637	-1.673184
C	2.561524	-4.205682	0.798924
H	0.684697	-3.140925	0.885159
C	3.872812	-3.842996	-1.187531
H	3.028529	-2.500190	-2.638090
H	2.428098	-4.678989	1.767269
C	3.710927	-4.458641	0.052766
H	4.767903	-4.027885	-1.774023
H	4.476490	-5.126522	0.435428
H	0.234230	-0.490434	-0.105186
N	2.344889	2.877754	0.431485
C	1.321332	2.023347	0.072176
N	0.458905	2.469058	-0.887389
C	0.676621	3.660018	-1.680469
C	1.245791	4.746133	-0.776483

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C      2.515754     4.220818    -0.118895
C      3.433586     0.912304     1.461043
C      1.997693     0.450103     1.697514
N      1.121936     0.848023     0.605017
C      3.440793     2.425977     1.289996
H     -0.283115     3.955403    -2.108051
H      1.362072     3.474775    -2.522595
H      0.504254     5.003455    -0.014267
H      1.476077     5.653538    -1.341950
H      3.339716     4.215810    -0.849325
H      2.826142     4.885999     0.696093
H      4.386179     2.757865     0.842367
H      3.363075     2.922958     2.267443
H      3.817293     0.429067     0.557007
H      4.091911     0.631782     2.288880
H      1.636299     0.855572     2.656483
H      1.957824    -0.638206     1.788137
H     -0.306401     1.860484    -1.149202
```

62 atoms
7-isomer, structure TS12 in vacuum

```
O      1.081019    -0.749856    -2.231721
O      2.071422    -0.790400    -0.246855
C      1.743305    -0.087063    -1.408559
C      2.803352     0.890684    -1.922368
H      2.812739     1.806190    -1.327279
H      2.484442     1.161187    -2.929757
C      4.217683     0.281081    -1.961411
H      4.163353    -0.757163    -2.307849
H      4.806451     0.821342    -2.711017
C      4.962069     0.364376    -0.620648
H      5.025482     1.420304    -0.325774
H      5.996743     0.030317    -0.761214
C      4.345221    -0.436755     0.533006
H      4.450045    -1.511923     0.341845
H      4.902547    -0.222825     1.451343
C      2.858957    -0.163457     0.774769
H      2.643356     0.907135     0.789294
C      2.349481    -0.777598     2.093353
H      1.262814    -0.655515     2.113001
C      2.934795    -0.185328     3.291506
H      2.542280    -1.856861     2.075396
C      3.411814     0.315954     4.274892
H      3.835971     0.757330     5.144775
O      0.543931     1.108105    -0.574158
C     -0.123975     1.913567    -1.500041
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C     -1.180821     2.789754    -0.847052
H     -0.595446     1.310891    -2.294683
H      0.587835     2.583605    -2.016068
C     -0.935549     3.386818     0.395261
C     -2.404988     3.040963    -1.473293
C     -1.883291     4.218024     0.988292
H      0.007474     3.182785     0.890732
C     -3.357030     3.873027    -0.883923
H     -2.615202     2.579049    -2.434684
H     -1.671730     4.678034     1.949434
C     -3.099444     4.465310     0.350534
H     -4.301643     4.055720    -1.388187
H     -3.838177     5.113793     0.811716
H     -0.517941     0.029920     0.032704
N     -2.590361    -2.514146     0.451059
C     -1.576202    -1.763368    -0.065040
N     -0.886465    -2.203400    -1.118811
C     -1.196110    -3.447602    -1.800443
C     -1.704024    -4.466649    -0.788385
C     -2.881155    -3.868242    -0.028150
C     -3.411069    -0.492245     1.619243
C     -1.950777    -0.061324     1.647918
N     -1.263015    -0.586118     0.477865
C     -3.481202    -2.009225     1.500830
H     -0.281472    -3.788371    -2.288081
H     -1.944032    -3.287385    -2.589265
H     -0.898149    -4.719179    -0.092894
H     -2.019068    -5.389137    -1.282642
H     -3.775902    -3.843393    -0.665144
H     -3.126637    -4.484812     0.842965
H     -4.499651    -2.328204     1.254851
H     -3.218765    -2.482640     2.456548
H     -3.908603    -0.022675     0.765795
H     -3.931789    -0.171231     2.524865
H     -1.469724    -0.412338     2.571493
H     -1.856155     1.024351     1.621327
H     -0.089766    -1.629652    -1.494220


62 atoms
7-isomer, structure I2 in vacuum
O      0.897725    -0.855392    -2.168141
O      1.848989    -0.996364    -0.144423
C      1.640419    -0.165745    -1.260451
C      2.938089     0.311056    -1.935049
H      3.298638     1.218488    -1.439772
H      2.672551     0.589030    -2.956742
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C	4.053000	-0.746784	-1.955992
H	3.619608	-1.724631	-2.187248
H	4.735288	-0.510206	-2.779584
C	4.877233	-0.808824	-0.659762
H	5.282738	0.191816	-0.457804
H	5.747686	-1.454750	-0.821288
C	4.130627	-1.307713	0.584187
H	3.907425	-2.376362	0.481737
H	4.778937	-1.200835	1.460281
C	2.803114	-0.596115	0.848357
H	2.928844	0.490801	0.828817
C	2.169354	-0.980841	2.199240
H	1.173268	-0.530169	2.238294
C	2.948739	-0.561017	3.359051
H	2.019073	-2.066358	2.217453
C	3.590339	-0.197562	4.308693
H	4.157036	0.116995	5.152173
O	0.889485	0.961636	-0.707953
C	0.428101	1.928796	-1.656861
C	-0.409317	2.959120	-0.939272
H	-0.151385	1.432337	-2.439758
H	1.286768	2.417407	-2.135462
C	0.100566	3.640620	0.171856
C	-1.700699	3.259987	-1.376578
C	-0.662151	4.604513	0.824707
H	1.098501	3.405819	0.527301
C	-2.465268	4.230493	-0.729271
H	-2.114169	2.726927	-2.227533
H	-0.252538	5.125713	1.684483
C	-1.947965	4.904926	0.373598
H	-3.466160	4.454838	-1.084843
H	-2.541275	5.659837	0.879973
H	-0.807977	0.129271	0.068282
N	-3.211587	-2.020908	0.389545
C	-2.073372	-1.438378	-0.132380
N	-1.360425	-1.941480	-1.096220
C	-1.801558	-3.185354	-1.702264
C	-2.454571	-4.112738	-0.679122
C	-3.603169	-3.374389	-0.002530
C	-3.773068	0.075496	1.586459
C	-2.272292	0.333753	1.597770
N	-1.703138	-0.225015	0.388388
C	-4.018977	-1.421883	1.449550
H	-0.933080	-3.669761	-2.157851
H	-2.509394	-2.988491	-2.523607
H	-1.708216	-4.401243	0.068334
H	-2.828111	-5.030033	-1.144582

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H     -4.475404    -3.327010    -0.670344
H     -3.924398    -3.911202     0.898370
H     -5.074707    -1.613233     1.222918
H     -3.807465    -1.925413     2.405910
H     -4.220404     0.610184     0.743431
H     -4.242494     0.441013     2.504032
H     -1.825980    -0.100060     2.507613
H     -2.057051     1.404095     1.609146
H      0.087254    -1.260514    -1.723598


62 atoms
7-isomer, structure TS23 in vacuum
O      0.702198    -0.407076    -2.222313
O      1.788368    -0.862458    -0.299440
C      1.546461     0.125820    -1.296178
C      2.811389     0.604935    -2.025542
H      3.321541     1.357706    -1.416621
H      2.460938     1.112887    -2.926207
C      3.783459    -0.520221    -2.411071
H      3.210614    -1.387714    -2.752801
H      4.378103    -0.187673    -3.268697
C      4.750426    -0.913770    -1.285120
H      5.314532    -0.021456    -0.982145
H      5.493625    -1.616412    -1.678738
C      4.103268    -1.539550    -0.043915
H      3.709789    -2.533898    -0.285976
H      4.869749    -1.679133     0.725415
C      2.944100    -0.731663     0.544391
H      3.211244     0.324406     0.647548
C      2.505782    -1.246845     1.929374
H      1.622136    -0.678230     2.234901
C      3.532583    -1.126747     2.958979
H      2.190843    -2.292251     1.830896
C      4.375891    -1.010971     3.807683
H      5.122141    -0.912361     4.559409
O      0.941417     1.196154    -0.543962
C      0.351685     2.241578    -1.300927
C     -0.449302     3.156577    -0.402191
H     -0.293520     1.815896    -2.075797
H      1.128971     2.830420    -1.810120
C     -0.429967     3.036766     0.987400
C     -1.223111     4.168997    -0.980200
C     -1.168714     3.912581     1.783237
H      0.165099     2.252763     1.437827
C     -1.959671     5.043847    -0.187860
H     -1.251441     4.271482    -2.062383
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H     -1.141768     3.807966     2.863888
C     -1.934802     4.918574     1.201060
H     -2.555432     5.822744    -0.653983
H     -2.508498     5.599844     1.821657
H     -0.282885    -0.950627     0.607288
N     -3.331026    -1.969441     0.264858
C     -2.078132    -1.523821    -0.101221
N     -1.666738    -1.387904    -1.325878
C     -2.603727    -1.665741    -2.400946
C     -3.545974    -2.814013    -2.044514
C     -4.261577    -2.482986    -0.740171
C     -2.930947    -1.258309     2.605645
C     -1.459198    -1.507056     2.300378
N     -1.222063    -1.172277     0.911924
C     -3.784206    -2.081969     1.649069
H     -2.030580    -1.905630    -3.300999
H     -3.194191    -0.767691    -2.642490
H     -2.961206    -3.731875    -1.923696
H     -4.282119    -2.992963    -2.834130
H     -5.057718    -1.745425    -0.915161
H     -4.744630    -3.378604    -0.331197
H     -4.828554    -1.751123     1.695033
H     -3.776458    -3.139800     1.954836
H     -3.144076    -0.193065     2.479334
H     -3.170802    -1.531503     3.636951
H     -1.198126    -2.552802     2.530881
H     -0.822928    -0.872008     2.921065
H     -0.125765    -0.795549    -1.800566


62 atoms
7-isomer, structure I3 in vacuum
O      0.297662    -0.112483    -2.068415
O      0.789404    -1.531851    -0.389467
C      1.317745    -0.543706    -1.271365
C      2.441690    -1.095271    -2.169988
H      3.402665    -0.979544    -1.658860
H      2.472733    -0.450797    -3.051041
C      2.254987    -2.560535    -2.594896
H      1.204128    -2.735935    -2.845166
H      2.821554    -2.726257    -3.517659
C      2.745723    -3.579651    -1.551902
H      3.797302    -3.360527    -1.323621
H      2.741657    -4.579446    -2.000698
C      1.952898    -3.637800    -0.238307
H      0.966365    -4.083100    -0.417124
H      2.472794    -4.294285     0.467273
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C	1.724484	-2.274243	0.412945
H	2.657944	-1.711589	0.489830
C	1.112833	-2.357445	1.824353
H	0.868213	-1.338950	2.139321
C	1.990746	-2.985533	2.806005
H	0.165382	-2.907570	1.772488
C	2.726138	-3.495816	3.608415
H	3.373830	-3.943806	4.323522
O	1.795766	0.474146	-0.385551
C	2.276382	1.669468	-0.992869
C	2.167158	2.812751	-0.011472
H	1.678735	1.883785	-1.886038
H	3.320538	1.548559	-1.310650
C	1.041675	2.938311	0.809615
C	3.169292	3.781922	0.063552
C	0.924320	4.016670	1.682212
H	0.268249	2.179878	0.761102
C	3.049302	4.866060	0.931962
H	4.055451	3.688328	-0.558863
H	0.048213	4.100686	2.318390
C	1.925547	4.985854	1.745264
H	3.838855	5.609795	0.979715
H	1.832491	5.824747	2.428047
H	-1.213096	-1.373215	0.018995
N	-4.036986	0.202032	0.127070
C	-2.704390	-0.025138	-0.142775
N	-1.917050	0.805742	-0.760735
C	-2.453396	2.099894	-1.148795
C	-3.920992	2.001230	-1.561239
C	-4.717341	1.375800	-0.422019
C	-4.118097	-1.807600	1.586548
C	-2.998011	-2.331635	0.696017
N	-2.171340	-1.207173	0.307700
C	-4.903659	-0.745487	0.825957
H	-1.848807	2.487055	-1.973558
H	-2.348769	2.825267	-0.327163
H	-3.999896	1.374549	-2.455674
H	-4.338442	2.982231	-1.807583
H	-4.884893	2.110166	0.378416
H	-5.706896	1.061550	-0.774711
H	-5.543450	-0.181976	1.515590
H	-5.575327	-1.227238	0.098836
H	-3.678624	-1.377891	2.491245
H	-4.793720	-2.612176	1.889780
H	-3.421218	-2.861314	-0.172655
H	-2.373256	-3.047141	1.235631
H	-0.475920	0.224853	-1.521211

62 atoms
7-isomer, structure TSr in vacuum

O	0.182482	-0.214194	-2.217424
O	0.952800	-1.192564	-0.347713
C	1.334383	-0.533935	-1.565108
C	2.194408	-1.433466	-2.468569
H	3.246263	-1.286163	-2.210157
H	2.064490	-1.039830	-3.479698
C	1.841102	-2.926946	-2.418520
H	0.752909	-3.047039	-2.398958
H	2.181997	-3.395301	-3.348380
C	2.495596	-3.679105	-1.246044
H	3.580965	-3.522506	-1.300875
H	2.344068	-4.756113	-1.381827
C	2.010564	-3.299119	0.160957
H	0.989502	-3.670611	0.316453
H	2.641333	-3.796945	0.904649
C	1.997532	-1.794902	0.435082
H	2.954292	-1.339228	0.169462
C	1.698032	-1.430907	1.902283
H	1.625743	-0.341047	1.963406
C	2.702098	-1.913962	2.844420
H	0.711677	-1.824150	2.176342
C	3.539839	-2.307516	3.611582
H	4.279958	-2.649250	4.294925
O	2.142811	0.588378	-1.178015
C	1.799280	1.916883	-1.571675
C	1.731003	2.835058	-0.371943
H	0.848928	1.905821	-2.107552
H	2.567746	2.273859	-2.266952
C	0.758070	2.641555	0.616969
C	2.634568	3.888519	-0.227072
C	0.695004	3.487311	1.720215
H	0.045442	1.829499	0.510100
C	2.571275	4.740309	0.876201
H	3.400203	4.043703	-0.982515
H	-0.065568	3.327561	2.478838
C	1.601528	4.540419	1.853874
H	3.283655	5.553956	0.973017
H	1.551083	5.198423	2.715948
H	-0.977572	-1.342929	0.189096
N	-3.949431	-0.077080	0.310260
C	-2.615791	-0.190679	-0.013763
N	-1.954213	0.648668	-0.758253
C	-2.649274	1.832429	-1.238941

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C     -4.115743     1.538825    -1.549863
C     -4.781199     0.956161    -0.308755
C     -3.735452    -1.917089     1.968021
C     -2.608271    -2.412403     1.069940
N     -1.933008    -1.254374     0.519668
C     -4.670230    -1.030946     1.152516
H     -2.134720     2.191601    -2.134604
H     -2.582693     2.646279    -0.500798
H     -4.170184     0.817991    -2.372220
H     -4.649527     2.440358    -1.865244
H     -4.987853     1.747992     0.424801
H     -5.746427     0.505419    -0.568103
H     -5.333927    -0.467183     1.818757
H     -5.318801    -1.655143     0.519112
H     -3.303808    -1.349438     2.797328
H     -4.302146    -2.751369     2.390471
H     -3.011363    -3.073777     0.286407
H     -1.881248    -2.995111     1.640222
H     -0.542508     0.108256    -1.598793


62 atoms
7-isomer, structure I3r in vacuum
O     -0.178689     0.015081    -2.171796
O      0.250803    -1.279986    -0.382386
C      0.825065    -0.692916    -1.572825
C      1.365284    -1.735798    -2.558744
H      2.409451    -1.948835    -2.314337
H      1.367673    -1.237954    -3.530394
C      0.556205    -3.038229    -2.619563
H     -0.513562    -2.806696    -2.589972
H      0.737625    -3.510814    -3.590865
C      0.926505    -4.053387    -1.524913
H      2.006328    -4.243795    -1.582008
H      0.443959    -5.012130    -1.746798
C      0.567810    -3.657043    -0.085797
H     -0.520777    -3.691298     0.049983
H      0.992718    -4.392456     0.605039
C      1.035518    -2.258094     0.318315
H      2.091397    -2.111496     0.074875
C      0.852341    -1.959993     1.820155
H      1.132926    -0.916547     1.992562
C      1.636730    -2.827265     2.692820
H     -0.211349    -2.039356     2.074086
C      2.294743    -3.538912     3.403817
H      2.878068    -4.163309     4.037433
O      1.942791     0.092935    -1.193146
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C      1.646009     1.331717    -0.554305
C      2.906604     1.917671     0.034800
H      0.891829     1.190493     0.226179
H      1.220038     2.022238    -1.292337
C      2.816721     2.823787     1.095882
C      4.167624     1.611984    -0.482946
C      3.959413     3.419185     1.624512
H      1.842964     3.064027     1.515169
C      5.312301     2.201949     0.049131
H      4.244541     0.901928    -1.297460
H      3.870902     4.118514     2.450342
C      5.213464     3.109179     1.101966
H      6.285813     1.950810    -0.361056
H      6.106470     3.567121     1.515721
H     -1.658242    -0.881431     0.154991
N     -4.070882     1.247520     0.462598
C     -2.842385     0.744296     0.092743
N     -1.948848     1.389369    -0.598513
C     -2.230685     2.767849    -0.963376
C     -3.714031     2.981801    -1.260176
C     -4.532447     2.537173    -0.053633
C     -4.462173    -0.707350     1.947079
C     -3.546436    -1.451869     0.982856
N     -2.533983    -0.523302     0.521587
C     -5.062218     0.498930     1.233901
H     -1.626120     3.020424    -1.838923
H     -1.913528     3.453433    -0.161620
H     -3.991910     2.386813    -2.136250
H     -3.933928     4.028936    -1.489077
H     -4.481269     3.290621     0.744873
H     -5.589860     2.436371    -0.325550
H     -5.517527     1.180884     1.961860
H     -5.871312     0.171328     0.563188
H     -3.876546    -0.382836     2.811982
H     -5.267047    -1.353127     2.308804
H     -4.135028    -1.876990     0.154060
H     -3.046709    -2.284826     1.482834
H     -0.763006     0.502623    -1.518606


62 atoms
7-isomer, structure TS34 in vacuum
O     -0.150590    -0.619741     2.063823
O      0.092091     1.090228     0.289278
C      0.768210     0.188424     1.817719
C      1.058994     1.341369     2.771776
H      2.022013     1.791358     2.519457
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H	1.194479	0.854787	3.744166
C	-0.033422	2.418276	2.875366
H	-1.005389	1.966726	2.656509
H	-0.082587	2.760046	3.915666
C	0.211127	3.660485	1.998400
H	1.231191	4.018131	2.192680
H	-0.450299	4.466276	2.340689
C	0.023278	3.500626	0.482307
H	-1.048682	3.417672	0.254455
H	0.375792	4.414382	-0.010437
C	0.716048	2.267007	-0.120097
H	1.771500	2.261387	0.197872
C	0.739710	2.313300	-1.675974
H	1.149311	1.357877	-2.018523
C	1.509113	3.413023	-2.248254
H	-0.292870	2.357730	-2.046715
C	2.156675	4.322487	-2.697097
H	2.731257	5.122708	-3.097819
O	1.969000	-0.260060	1.289141
C	1.881714	-1.445467	0.510323
C	3.229551	-1.775706	-0.083916
H	1.144396	-1.284732	-0.285169
H	1.522771	-2.273452	1.130221
C	4.199990	-0.794535	-0.300418
C	3.508550	-3.091244	-0.467597
C	5.417945	-1.122505	-0.893257
H	3.997484	0.223221	0.009510
C	4.722017	-3.419828	-1.066226
H	2.769435	-3.869204	-0.291713
H	6.162747	-0.348378	-1.051442
C	5.683309	-2.433840	-1.281380
H	4.921235	-4.447455	-1.355221
H	6.632941	-2.687303	-1.742356
H	-1.445892	0.745781	-0.049269
N	-4.010214	-1.222717	-0.705679
C	-2.829703	-0.791553	-0.183515
N	-2.045178	-1.632498	0.494738
C	-2.381706	-3.031338	0.699471
C	-3.894866	-3.181552	0.806997
C	-4.547156	-2.557100	-0.420644
C	-4.039093	0.799182	-2.138622
C	-3.278366	1.458055	-0.993390
N	-2.435224	0.472100	-0.338793
C	-4.823474	-0.390117	-1.597868
H	-1.881957	-3.356341	1.612927
H	-1.994710	-3.649147	-0.121891
H	-4.244956	-2.679532	1.713768

```
H     -4.182208    -4.233665     0.876890
H     -4.403645    -3.199303    -1.299952
H     -5.627231    -2.457201    -0.270675
H     -5.176003    -1.022391    -2.419773
H     -5.713051    -0.047017    -1.053203
H     -3.327219     0.466376    -2.899638
H     -4.726970     1.503832    -2.612636
H     -3.979570     1.908928    -0.278248
H     -2.632820     2.258696    -1.356158
H     -1.250861    -1.227116     1.041618


62 atoms
7-isomer, structure I4 in vacuum
O      0.492603    -1.208584     2.122782
O      0.444646     1.242043    -0.075810
C      1.400361    -0.414118     2.237858
C      1.297944     0.982196     2.806117
H      1.832496     1.631543     2.112710
H      1.893496     0.995342     3.726436
C     -0.137688     1.472671     3.065625
H     -0.849359     0.775335     2.620221
H     -0.331112     1.441262     4.142713
C     -0.430331     2.895858     2.555715
H      0.417880     3.553591     2.787581
H     -1.273105     3.296175     3.130992
C     -0.794338     3.040791     1.067509
H     -1.694842     2.452904     0.850326
H     -1.061286     4.089433     0.895260
C      0.283248     2.645741     0.045231
H      1.255089     3.027724     0.376854
C      0.008541     3.263088    -1.352600
H      0.724413     2.817821    -2.050963
C      0.119511     4.717004    -1.396818
H     -0.989105     2.958295    -1.689486
C      0.228559     5.914721    -1.408752
H      0.322560     6.974023    -1.429790
O      2.672904    -0.679103     1.886071
C      2.963904    -1.938853     1.235676
C      3.677865    -1.698377    -0.070210
H      2.023541    -2.472440     1.092719
H      3.588678    -2.513362     1.922938
C      3.194375    -0.757220    -0.986996
C      4.812666    -2.444573    -0.393830
C      3.841677    -0.578016    -2.206351
H      2.322649    -0.156272    -0.744817
C      5.453918    -2.269303    -1.619191
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H      5.202514    -3.168063     0.317433
H      3.462494     0.157079    -2.909577
C      4.969135    -1.333608    -2.528693
H      6.335886    -2.856072    -1.856501
H      5.469333    -1.189035    -3.481262
H     -0.397542     0.815226    -0.385084
N     -3.761160    -1.480923    -0.844577
C     -2.597613    -0.905717    -0.374383
N     -2.199177    -1.264245     0.892505
C     -2.722783    -2.439844     1.562954
C     -4.235127    -2.446195     1.393324
C     -4.563667    -2.446429    -0.094365
C     -3.058348    -0.735221    -3.083797
C     -2.340540     0.386483    -2.337173
N     -1.882496    -0.033034    -1.022346
C     -4.201985    -1.248366    -2.219288
H     -2.437707    -2.380266     2.614785
H     -2.294074    -3.372813     1.163133
H     -4.651606    -1.555577     1.873066
H     -4.683937    -3.324025     1.866287
H     -4.407371    -3.453099    -0.511754
H     -5.621921    -2.204691    -0.249958
H     -4.587467    -2.194684    -2.616468
H     -5.040083    -0.536789    -2.226278
H     -2.350443    -1.547279    -3.280095
H     -3.445218    -0.393045    -4.048447
H     -3.013443     1.255686    -2.256244
H     -1.472207     0.725158    -2.910385
H     -1.246275    -1.012779     1.124870


62 atoms
7-isomer, structure I5 in vacuum
O     -3.906464     1.784699     1.492022
O      3.157589    -0.873693     1.643580
C     -4.028387     0.825000     0.771756
C     -2.922673    -0.126240     0.363749
H     -2.807004    -0.046875    -0.724132
H     -3.273737    -1.148838     0.538782
C     -1.597099     0.138958     1.075484
H     -1.301797     1.180171     0.910802
H     -1.742670     0.042406     2.156939
C     -0.481879    -0.804808     0.612887
H     -0.330261    -0.689866    -0.468047
H     -0.798051    -1.842611     0.756665
C      0.836382    -0.544843     1.347630
H      1.094846     0.517031     1.262281
```

H	0.713998	-0.736590	2.420892
C	2.058644	-1.331817	0.869929
H	2.237193	-1.124213	-0.195382
C	1.937839	-2.871916	1.043846
H	2.954324	-3.279326	1.023947
C	1.147314	-3.565608	0.030966
H	1.547957	-3.085097	2.045968
C	0.530666	-4.146207	-0.822957
H	-0.024930	-4.656761	-1.572619
O	-5.203553	0.463201	0.207276
C	-6.339910	1.314325	0.515475
C	-7.543919	0.754391	-0.186786
H	-6.111887	2.330794	0.188635
H	-6.471431	1.336798	1.599107
C	-7.889744	1.194667	-1.467012
C	-8.325188	-0.232532	0.420917
C	-8.994597	0.662667	-2.127131
H	-7.288555	1.959828	-1.949734
C	-9.430116	-0.767819	-0.235448
H	-8.064354	-0.583655	1.415161
H	-9.253748	1.016339	-3.119973
C	-9.767221	-0.320143	-1.511677
H	-10.029785	-1.531611	0.249291
H	-10.630359	-0.733920	-2.023315
H	4.001320	-1.082816	1.162135
N	6.673364	0.996265	-0.808436
C	5.669655	0.461767	-0.028253
N	4.886067	1.349939	0.669679
C	4.845492	2.767175	0.374702
C	6.275490	3.247219	0.159562
C	6.913476	2.430252	-0.957808
C	6.826871	-1.226502	-1.873945
C	6.335823	-1.748587	-0.524297
N	5.435706	-0.809416	0.121148
C	7.480643	0.135890	-1.673940
H	4.384075	3.279592	1.221882
H	4.234524	2.993977	-0.514255
H	6.837004	3.117366	1.089231
H	6.301040	4.308119	-0.104254
H	6.529989	2.767129	-1.933498
H	7.997226	2.595362	-0.974685
H	7.607046	0.643570	-2.637687
H	8.485104	0.020697	-1.242676
H	5.972302	-1.130932	-2.551925
H	7.540785	-1.913643	-2.338234
H	7.201011	-1.962736	0.123279
H	5.809883	-2.698911	-0.653325

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H      4.107021     0.916314     1.153091


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


23 atoms
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3-isomer in toluene

O	-0.299084	2.412793	0.512490
C	-0.565963	1.329551	0.054411
O	-1.846674	1.088362	-0.306105
C	-2.291295	-0.163828	-0.879974
H	-1.707708	-0.387130	-1.778651
H	-3.309952	0.060090	-1.194030
C	-2.279475	-1.321910	0.110013
H	-2.719498	-0.971325	1.050451
H	-2.953649	-2.094768	-0.275841
C	-0.898992	-1.939170	0.353447
H	-0.545859	-2.400749	-0.577403
H	-0.996220	-2.755162	1.076782
C	0.171710	-0.963491	0.852452
H	-0.098972	-0.567334	1.838315
H	1.103232	-1.518730	0.990241
C	0.465774	0.215710	-0.108361
H	0.418224	-0.157816	-1.137828
C	1.877364	0.805536	0.114568
H	1.987999	1.717068	-0.478524
C	2.942957	-0.132101	-0.230148
H	1.978354	1.118962	1.158094
C	3.814023	-0.908087	-0.523269
H	4.593495	-1.585604	-0.781510

62 atoms

3-isomer, structure I1 in toluene

N	4.253836	1.863148	0.150900
C	3.131805	1.069832	0.062593
N	1.925826	1.682927	0.284801
C	1.761459	3.126189	0.280336
C	2.904044	3.729532	1.085172
C	4.228623	3.291555	0.472705
C	5.465428	0.036971	-0.987825
C	4.438061	-0.866416	-0.310004
N	3.145367	-0.210365	-0.182978
C	5.573835	1.336083	-0.199761
H	0.789415	3.349134	0.718352
H	1.765654	3.535739	-0.742459
H	2.831630	3.385428	2.121057
H	2.849392	4.821342	1.090126
H	4.428207	3.870596	-0.441129
H	5.055348	3.499047	1.161990
H	6.098542	2.098301	-0.787391
H	6.161423	1.181843	0.715865
H	5.137835	0.248256	-2.011128

H	6.447501	-0.441378	-1.047173
H	4.818277	-1.173415	0.677534
H	4.297439	-1.787420	-0.883066
H	1.107323	1.114439	0.123505
O	-1.578327	2.805664	0.942546
C	-2.066300	1.881421	0.334569
O	-1.242106	0.937192	-0.163798
C	-1.711919	-0.226926	-0.909177
H	-2.444420	-0.767431	-0.302741
H	-0.816486	-0.842022	-0.984404
C	-2.260347	0.132016	-2.282506
H	-1.567263	0.836123	-2.757270
H	-2.234189	-0.778223	-2.891432
C	-3.686482	0.690929	-2.278788
H	-4.372749	-0.089550	-1.926808
H	-3.987114	0.915640	-3.307362
C	-3.892783	1.944575	-1.422234
H	-3.305934	2.781999	-1.818176
H	-4.941734	2.243376	-1.497173
C	-3.566397	1.759070	0.081590
H	-3.891801	0.757750	0.384620
C	-4.308896	2.786606	0.966820
H	-3.940944	2.714723	1.993739
C	-5.757477	2.599609	0.955636
H	-4.060550	3.799064	0.634045
C	-6.948796	2.434116	0.946815
H	-8.004178	2.294379	0.948293
O	1.071920	-1.944403	-0.533278
C	0.826111	-2.530338	0.726565
C	0.046235	-3.820138	0.589684
H	0.269209	-1.844966	1.385167
H	1.776046	-2.742731	1.240944
C	0.009031	-4.517574	-0.619681
C	-0.630186	-4.351962	1.693142
C	-0.686076	-5.722528	-0.722575
H	0.524296	-4.099874	-1.476066
C	-1.320864	-5.557284	1.594407
H	-0.617993	-3.816193	2.639299
H	-0.707462	-6.251533	-1.670779
C	-1.351646	-6.248392	0.382921
H	-1.840458	-5.954870	2.460978
H	-1.893173	-7.185745	0.302071
H	1.803030	-1.271108	-0.428273

62 atoms
3-isomer, structure TS12 in toluene

N	3.603373	-1.532712	-0.032809
C	2.297675	-1.192015	-0.185317
N	1.521056	-1.868188	-1.038989
C	1.974219	-3.060272	-1.738671
C	3.446463	-2.903433	-2.092433
C	4.235273	-2.593690	-0.826840
C	3.668324	-0.169290	2.032291
C	2.575721	0.667760	1.381816
N	1.775228	-0.175563	0.504624
C	4.473585	-0.871268	0.946957
H	1.359279	-3.171558	-2.632770
H	1.820100	-3.956364	-1.123020
H	3.561985	-2.090116	-2.814822
H	3.836666	-3.814717	-2.551418
H	4.338035	-3.493499	-0.206912
H	5.245981	-2.259904	-1.079584
H	5.119474	-1.637969	1.384931
H	5.125428	-0.157897	0.426781
H	3.215285	-0.909314	2.698810
H	4.332699	0.457011	2.632179
H	3.013211	1.504698	0.823236
H	1.903930	1.097517	2.125085
H	0.507768	-1.637470	-1.093206
O	-1.153767	-1.313310	-1.310706
C	-1.651852	-0.937736	-0.229861
O	-1.186364	-1.639614	0.879263
C	-1.596015	-1.256883	2.200266
H	-1.760623	-0.178766	2.234585
H	-0.739734	-1.483003	2.841506
C	-2.815069	-2.049606	2.656090
H	-2.605949	-3.113678	2.493070
H	-2.935928	-1.917985	3.738814
C	-4.112986	-1.655338	1.945120
H	-4.423931	-0.659142	2.286096
H	-4.909646	-2.341451	2.255012
C	-4.038896	-1.641186	0.411789
H	-3.709407	-2.617118	0.036074
H	-5.055083	-1.493922	0.032711
C	-3.146729	-0.529159	-0.189342
H	-3.248913	0.368515	0.423649
C	-3.614262	-0.189320	-1.626530
H	-2.874119	0.441014	-2.120734
C	-4.915050	0.476239	-1.665726
H	-3.650651	-1.110971	-2.215884
C	-5.981527	1.034108	-1.690659
H	-6.922737	1.530066	-1.719798
O	-0.806175	0.687134	0.238799

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C     -0.831713     1.662130    -0.760772
C      0.075144     2.838588    -0.435718
H     -1.853687     2.063890    -0.891265
H     -0.536867     1.246914    -1.740028
C      0.019640     3.439450     0.827936
C      0.966861     3.357333    -1.378135
C      0.824572     4.532590     1.136343
H     -0.662438     3.034614     1.568215
C      1.777043     4.453302    -1.074938
H      1.029094     2.898409    -2.361418
H      0.762318     4.990130     2.119535
C      1.707867     5.045152     0.184089
H      2.462485     4.842341    -1.822238
H      2.335234     5.898443     0.423124
H      0.763839     0.088097     0.374519
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62 atoms
3-isomer, structure I2 in toluene
N      3.772422    -1.451071    -0.031981
C      2.428100    -1.158994    -0.100072
N      1.597629    -1.682204    -0.958956
C      2.101172    -2.701461    -1.866388
C      3.541067    -2.421805    -2.290147
C      4.408276    -2.296356    -1.043994
C      3.959859    -0.249184     2.132356
C      2.786583     0.580742     1.628896
N      1.934887    -0.277727     0.827432
C      4.689422    -0.853626     0.939443
H      1.445199    -2.735426    -2.741341
H      2.043192    -3.698153    -1.401020
H      3.573020    -1.487082    -2.859970
H      3.932692    -3.214556    -2.934400
H      4.613950    -3.287896    -0.617549
H      5.378387    -1.852852    -1.296068
H      5.383525    -1.632581     1.274655
H      5.297211    -0.083152     0.441569
H      3.583767    -1.042064     2.785545
H      4.655459     0.362948     2.712564
H      3.151616     1.449441     1.060036
H      2.192758     0.967591     2.459438
H     -0.089688    -1.487577    -0.961464
O     -1.087779    -1.361959    -1.088202
C     -1.616906    -0.709768    -0.017582
O     -1.253449    -1.423531     1.137232
C     -1.704034    -0.948802     2.414529
H     -1.901017     0.125606     2.372560
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H     -0.865979    -1.102621     3.099155
C     -2.923104    -1.735408     2.875388
H     -2.661945    -2.799786     2.861292
H     -3.137796    -1.479218     3.920449
C     -4.168200    -1.494700     2.016676
H     -4.550633    -0.482103     2.201775
H     -4.959061    -2.177299     2.347106
C     -3.967159    -1.673994     0.503239
H     -3.501814    -2.642353     0.291376
H     -4.958745    -1.699056     0.040970
C     -3.161698    -0.558416    -0.197781
H     -3.444490     0.398527     0.252840
C     -3.548060    -0.509307    -1.701930
H     -2.840871     0.097408    -2.268909
C     -4.897280     0.007490    -1.923922
H     -3.462120    -1.516191    -2.120332
C     -6.003029     0.449088    -2.099187
H     -6.981317     0.835399    -2.262430
O     -0.972706     0.586702     0.184331
C     -1.029076     1.527619    -0.894579
C     -0.137099     2.697320    -0.562491
H     -2.059562     1.876897    -1.031016
H     -0.701753     1.046239    -1.819887
C     -0.519678     3.624568     0.413210
C      1.086849     2.871798    -1.212798
C      0.301474     4.703246     0.729928
H     -1.470103     3.500314     0.923795
C      1.910286     3.954177    -0.902706
H      1.396905     2.155566    -1.967743
H     -0.010234     5.417012     1.485979
C      1.519379     4.871747     0.070104
H      2.854690     4.080990    -1.422618
H      2.157209     5.716206     0.311224
H      0.971584     0.001301     0.678908


62 atoms
3-isomer, structure TS23 in toluene
N      3.774412    -1.425888    -0.259793
C      2.418268    -1.197316    -0.205705
N      1.592992    -1.371807    -1.200360
C      2.119762    -1.926522    -2.437936
C      3.539566    -1.439415    -2.718547
C      4.424883    -1.774425    -1.524532
C      3.955418    -1.148691     2.202847
C      2.731038    -0.253249     2.064361
N      1.904831    -0.784137     0.996737
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C	4.684378	-1.209324	0.866172
H	1.449097	-1.640699	-3.253457
H	2.109952	-3.027326	-2.404268
H	3.523774	-0.355822	-2.876692
H	3.950962	-1.897857	-3.622612
H	4.679780	-2.843065	-1.522821
H	5.370411	-1.223439	-1.582960
H	5.417762	-2.023436	0.871883
H	5.248428	-0.278649	0.703855
H	3.632883	-2.150095	2.502285
H	4.635410	-0.770648	2.970787
H	3.038248	0.786231	1.872708
H	2.140626	-0.250850	2.982784
H	-0.113357	-1.210078	-1.131947
O	-1.112009	-1.086393	-1.230544
C	-1.651153	-0.601278	-0.076862
O	-1.229606	-1.445041	0.974316
C	-1.733716	-1.199224	2.296844
H	-2.021900	-0.150146	2.403215
H	-0.893172	-1.379256	2.972482
C	-2.880590	-2.148506	2.614774
H	-2.525473	-3.171013	2.442862
H	-3.116906	-2.074383	3.683612
C	-4.142219	-1.888740	1.786424
H	-4.618156	-0.959747	2.127083
H	-4.865286	-2.686633	1.989173
C	-3.923533	-1.797132	0.267908
H	-3.382520	-2.676718	-0.096620
H	-4.908873	-1.820870	-0.207474
C	-3.203542	-0.520383	-0.218905
H	-3.535927	0.319410	0.399863
C	-3.615135	-0.220258	-1.686372
H	-2.967877	0.538115	-2.128645
C	-5.003442	0.221906	-1.805361
H	-3.458148	-1.120707	-2.286778
C	-6.142516	0.600277	-1.893045
H	-7.150180	0.932165	-1.979051
O	-1.074445	0.674186	0.298175
C	-1.141159	1.745784	-0.647531
C	-0.143900	2.803433	-0.246870
H	-2.150482	2.174164	-0.668055
H	-0.905922	1.362376	-1.644527
C	-0.552274	3.968290	0.405932
C	1.217791	2.620705	-0.513166
C	0.377131	4.938012	0.782260
H	-1.606325	4.119835	0.620627
C	2.148632	3.586375	-0.139647

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H      1.541489     1.714761    -1.016679
H      0.043969     5.840008     1.285877
C      1.729851     4.749007     0.509376
H      3.201120     3.437313    -0.360473
H      2.454778     5.503919     0.797135
H      0.923422    -0.542011     0.970662


62 atoms
3-isomer, structure I3 in toluene
N      4.113078    -0.696204    -0.555071
C      2.747060    -0.837655    -0.486668
N      1.889559    -0.139314    -1.179233
C      2.401940     0.819070    -2.146200
C      3.701670     1.465583    -1.672833
C      4.714487     0.372881    -1.354764
C      4.427818    -2.766443     0.777865
C      3.065413    -2.439686     1.374612
N      2.257337    -1.813371     0.344895
C      5.055356    -1.487762     0.237256
H      1.635806     1.581818    -2.312414
H      2.568344     0.333433    -3.120541
H      3.502616     2.059406    -0.774637
H      4.112205     2.140722    -2.429290
H      5.128974    -0.049602    -2.280376
H      5.557290     0.785334    -0.789064
H      5.914940    -1.727783    -0.398193
H      5.437877    -0.876002     1.067802
H      4.298624    -3.493608    -0.029029
H      5.089808    -3.209035     1.526706
H      3.186619    -1.794468     2.259191
H      2.554674    -3.347529     1.703289
H      0.233499    -0.504166    -1.211401
O     -0.749211    -0.723754    -1.333704
C     -1.417418    -0.695735    -0.147989
O     -0.715106    -1.541157     0.753971
C     -1.241014    -1.709587     2.081971
H     -1.865865    -0.853968     2.345733
H     -0.377507    -1.698723     2.752531
C     -1.989165    -3.031201     2.185609
H     -1.307594    -3.831395     1.873786
H     -2.231168    -3.220382     3.238792
C     -3.268736    -3.082845     1.343890
H     -4.034590    -2.446039     1.805597
H     -3.667901    -4.102616     1.378837
C     -3.111091    -2.666265    -0.128105
H     -2.298898    -3.227131    -0.602474
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H	-4.029882	-2.952961	-0.648747
C	-2.896149	-1.155660	-0.363313
H	-3.502740	-0.607582	0.364800
C	-3.396752	-0.765671	-1.780468
H	-3.074776	0.243298	-2.042959
C	-4.850866	-0.840892	-1.910287
H	-2.923151	-1.421788	-2.516053
C	-6.049441	-0.889339	-2.007085
H	-7.108816	-0.933297	-2.100445
O	-1.355376	0.588796	0.495205
C	-1.767805	1.733703	-0.242935
C	-1.146096	2.968061	0.367930
H	-2.861299	1.828684	-0.238057
H	-1.442651	1.630498	-1.284196
C	-1.898988	4.130264	0.546881
C	0.205344	2.974810	0.731244
C	-1.314566	5.285273	1.067139
H	-2.952525	4.134584	0.280864
C	0.788460	4.124705	1.256696
H	0.789031	2.069464	0.604198
H	-1.914237	6.180151	1.201415
C	0.031434	5.285171	1.424475
H	1.837219	4.116714	1.538028
H	0.487461	6.180478	1.835246
H	1.250975	-1.780046	0.473613

62 atoms
3-isomer, structure TSr in toluene

N	3.628777	-1.518479	-0.733585
C	2.274469	-1.329892	-0.598095
N	1.581834	-0.420437	-1.225638
C	2.267658	0.438438	-2.179124
C	3.705012	0.726526	-1.753114
C	4.433721	-0.593126	-1.533949
C	3.491062	-3.650539	0.529805
C	2.277579	-3.026266	1.205372
N	1.597986	-2.189947	0.232766
C	4.385582	-2.542796	-0.012233
H	1.704804	1.372196	-2.266335
H	2.264536	-0.018563	-3.181011
H	3.694433	1.304076	-0.823395
H	4.233303	1.319817	-2.505066
H	4.684349	-1.060944	-2.495870
H	5.378961	-0.425102	-1.006303
H	5.130569	-2.960271	-0.698463
H	4.943338	-2.072273	0.811003

H	3.152217	-4.295313	-0.286291
H	4.058573	-4.266927	1.231755
H	2.592542	-2.459305	2.095869
H	1.578516	-3.795398	1.541478
H	-0.075664	-0.345418	-1.176355
O	-1.090541	-0.280633	-1.272234
C	-1.726840	-0.132374	-0.083136
O	-1.111255	-1.029458	0.838566
C	-1.733967	-1.247461	2.114211
H	-2.319415	-0.371411	2.403148
H	-0.916130	-1.338630	2.833823
C	-2.563745	-2.527206	2.089730
H	-1.911113	-3.338898	1.746814
H	-2.854976	-2.777350	3.117469
C	-3.814732	-2.459667	1.204734
H	-4.574584	-1.840613	1.698769
H	-4.246560	-3.464279	1.135520
C	-3.595544	-1.909570	-0.214688
H	-2.820884	-2.479348	-0.738311
H	-4.523417	-2.061157	-0.774354
C	-3.244966	-0.409229	-0.250181
H	-3.742158	0.086388	0.588315
C	-3.752994	0.274598	-1.543647
H	-3.378702	1.301226	-1.591382
C	-5.210657	0.307479	-1.642839
H	-3.332423	-0.240629	-2.411423
C	-6.411228	0.340605	-1.717422
H	-7.472749	0.372537	-1.788340
O	-1.580538	1.179624	0.511456
C	-1.129819	2.281329	-0.262503
C	0.001651	3.018621	0.424712
H	-1.967072	2.973075	-0.420364
H	-0.805649	1.931364	-1.245916
C	0.198897	4.379496	0.170306
C	0.877580	2.362256	1.292209
C	1.257516	5.069315	0.757724
H	-0.484345	4.907458	-0.490244
C	1.933340	3.052085	1.886326
H	0.718841	1.310981	1.499374
H	1.394431	6.126221	0.550539
C	2.129531	4.406689	1.620333
H	2.603315	2.530098	2.563081
H	2.949881	4.943330	2.086556
H	0.647089	-1.897031	0.431617

62 atoms

3-isomer, structure I3r in toluene

N	4.341950	0.226712	-0.496382
C	3.040793	-0.208077	-0.403935
N	2.116131	0.010842	-1.296572
C	2.495527	0.701981	-2.519393
C	3.556748	1.768847	-2.258799
C	4.757132	1.120614	-1.579851
C	4.985824	-1.191466	1.436939
C	3.537864	-1.029380	1.881279
N	2.705853	-0.957985	0.695210
C	5.360624	-0.032100	0.522050
H	1.597145	1.151397	-2.952174
H	2.870719	-0.013534	-3.267695
H	3.136292	2.543307	-1.608746
H	3.875630	2.254045	-3.185875
H	5.354526	0.557399	-2.309643
H	5.415474	1.886333	-1.154296
H	6.305954	-0.244543	0.010544
H	5.521842	0.879362	1.116830
H	5.091119	-2.141275	0.904706
H	5.661465	-1.210641	2.296002
H	3.436931	-0.134982	2.516435
H	3.213287	-1.886547	2.475446
H	0.520259	-0.570583	-1.215218
O	-0.432078	-0.886080	-1.340764
C	-1.169195	-0.912107	-0.191242
O	-0.273570	-1.313442	0.857190
C	-0.834945	-1.666177	2.129866
H	-1.778090	-1.134512	2.283556
H	-0.130257	-1.298158	2.881239
C	-0.988944	-3.179416	2.246323
H	-0.014555	-3.628785	2.021256
H	-1.212788	-3.430697	3.290549
C	-2.062708	-3.784257	1.332967
H	-3.055899	-3.536143	1.728685
H	-1.985450	-4.876108	1.382298
C	-2.007992	-3.344138	-0.139734
H	-1.020954	-3.543488	-0.569838
H	-2.719175	-3.961740	-0.696242
C	-2.377208	-1.865680	-0.359353
H	-3.114107	-1.570416	0.392617
C	-3.025888	-1.616676	-1.743314
H	-3.145631	-0.539564	-1.888025
C	-4.326160	-2.265600	-1.893891
H	-2.345088	-1.958458	-2.527387
C	-5.400168	-2.796316	-2.009292
H	-6.351286	-3.261419	-2.118018

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O     -1.746049     0.344119     0.149828
C     -0.842103     1.453504     0.216231
C     -1.639359     2.705686     0.475463
H     -0.293637     1.532647    -0.727042
H     -0.110001     1.293184     1.013903
C     -2.550254     3.173737    -0.478877
C     -1.488639     3.420805     1.665131
C     -3.289273     4.330017    -0.248709
H     -2.678182     2.624630    -1.406517
C     -2.223932     4.583377     1.898595
H     -0.790904     3.065152     2.418081
H     -3.991681     4.680629    -0.998435
C     -3.126872     5.039958     0.942095
H     -2.093614     5.127984     2.828568
H     -3.702154     5.942780     1.121247
H      1.713613    -1.153846     0.774069
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62 atoms
3-isomer, structure TSr2 in toluene
N     -4.463051    -0.731745    -0.377105
C     -3.181951    -0.269553    -0.187200
N     -2.449912     0.299371    -1.102334
C     -3.046659     0.531157    -2.409051
C     -4.000786    -0.595571    -2.800425
C     -5.059116    -0.752304    -1.715012
C     -4.733007    -1.081057     2.068155
C     -3.220110    -1.261742     2.082907
N     -2.653825    -0.386924     1.074059
C     -5.259182    -1.375927     0.668540
H     -2.240034     0.622680    -3.141760
H     -3.586166     1.491141    -2.423530
H     -3.433058    -1.526361    -2.902406
H     -4.485235    -0.397930    -3.761079
H     -5.810404     0.045399    -1.792031
H     -5.592021    -1.702369    -1.834774
H     -6.293569    -1.027532     0.572409
H     -5.275360    -2.462296     0.495430
H     -4.971056    -0.051827     2.351962
H     -5.216852    -1.748314     2.786154
H     -2.964521    -2.319024     1.910074
H     -2.802308    -0.982468     3.052588
H     -0.787503     0.591648    -1.002926
O      0.191729     0.759614    -1.193412
C      0.982680     0.900418    -0.084382
O      0.131163     0.725192     1.051407
C      0.626697     1.098892     2.346633
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H      1.714201     0.989995     2.379278
H      0.210136     0.367842     3.044903
C      0.164076     2.504894     2.714747
H     -0.923490     2.536830     2.582118
H      0.352526     2.667699     3.783115
C      0.822821     3.626154     1.901929
H      1.860493     3.753629     2.236010
H      0.315663     4.569119     2.134209
C      0.829433     3.422239     0.378092
H     -0.188472     3.273251     0.001279
H      1.195353     4.346251    -0.079162
C      1.724979     2.260692    -0.090061
H      2.575044     2.169261     0.592422
C      2.306760     2.500940    -1.505140
H      2.805717     1.588716    -1.843486
C      3.254213     3.611788    -1.554772
H      1.485665     2.678777    -2.204780
C      4.039246     4.523505    -1.587210
H      4.735767     5.327429    -1.624069
O      2.013235    -0.077746    -0.054836
C      1.585712    -1.418675    -0.259321
C      2.756088    -2.366661    -0.137101
H      1.124515    -1.509874    -1.247487
H      0.818905    -1.679769     0.480847
C      4.036741    -1.934199     0.209985
C      2.548138    -3.730285    -0.377816
C      5.087708    -2.846650     0.315505
H      4.207284    -0.880828     0.392992
C      3.594520    -4.641190    -0.270963
H      1.556933    -4.081570    -0.654164
H      6.078659    -2.493379     0.584027
C      4.872303    -4.201263     0.077292
H      3.414552    -5.694610    -0.462323
H      5.690825    -4.909383     0.159002
H     -1.681521    -0.107135     1.135564


62 atoms
3-isomer, structure I3r2 in toluene
N      4.496077     1.060666    -0.438596
C      3.199572     0.657640    -0.227404
N      2.582140    -0.263141    -0.915988
C      3.333935    -0.966897    -1.944163
C      4.333745    -0.046689    -2.641481
C      5.251925     0.572844    -1.595055
C      4.462755     2.383534     1.666261
C      2.962180     2.485402     1.424045
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N	2.521399	1.246299	0.810502
C	5.164756	2.102892	0.343076
H	2.623331	-1.377684	-2.666980
H	3.867440	-1.828246	-1.512864
H	3.787667	0.741690	-3.169778
H	4.931019	-0.587462	-3.381345
H	6.001236	-0.156813	-1.259395
H	5.801961	1.419062	-2.021659
H	6.197794	1.784434	0.522096
H	5.218211	3.024050	-0.255536
H	4.654711	1.573441	2.375758
H	4.856818	3.307618	2.097112
H	2.738582	3.362357	0.796964
H	2.420665	2.612741	2.363689
H	0.888587	-0.301268	-0.978051
O	-0.108052	-0.256014	-1.140241
C	-0.842439	-0.603746	-0.033997
O	-0.263991	0.123817	1.061889
C	-0.680399	-0.196277	2.398547
H	-1.708606	-0.569511	2.392374
H	-0.686884	0.753544	2.939619
C	0.291020	-1.172683	3.055102
H	1.298901	-0.755119	2.951143
H	0.077974	-1.208030	4.130708
C	0.254801	-2.593542	2.479698
H	-0.665239	-3.094066	2.808238
H	1.079997	-3.167457	2.915884
C	0.335089	-2.687601	0.947148
H	1.235997	-2.187227	0.576087
H	0.438387	-3.744903	0.685031
C	-0.908695	-2.133661	0.226793
H	-1.784890	-2.307095	0.858837
C	-1.180801	-2.850269	-1.118920
H	-1.977775	-2.319382	-1.646419
C	-1.562577	-4.251178	-0.957024
H	-0.293669	-2.779750	-1.754910
C	-1.882714	-5.402971	-0.817930
H	-2.169974	-6.421230	-0.702018
O	-2.181153	-0.206651	-0.221185
C	-2.371946	1.136052	-0.661341
C	-3.826837	1.524150	-0.532065
H	-2.044437	1.233417	-1.700236
H	-1.749716	1.808677	-0.060859
C	-4.769222	0.705429	0.092036
C	-4.244051	2.756144	-1.050528
C	-6.100142	1.111867	0.199376
H	-4.457850	-0.253464	0.486805

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C     -5.569828     3.164240    -0.940883
H     -3.523081     3.401587    -1.546221
H     -6.821303     0.461511     0.685065
C     -6.505785     2.340946    -0.313551
H     -5.874632     4.123015    -1.348953
H     -7.541271     2.655344    -0.229792
H      1.542230     0.986496     0.868046


62 atoms
3-isomer, structure TS34 in toluene
N     -4.273819    -1.217822    -0.235078
C     -3.015300    -0.717458    -0.156483
N     -2.577394     0.148429    -1.084359
C     -3.408122     0.615261    -2.184766
C     -4.364012    -0.495045    -2.603939
C     -5.149011    -0.966820    -1.386399
C     -4.059143    -1.930285     2.130479
C     -2.570656    -2.054967     1.823900
N     -2.191721    -1.063464     0.828938
C     -4.850318    -2.044089     0.833037
H     -2.743037     0.899174    -3.000958
H     -3.969337     1.512166    -1.893193
H     -3.792431    -1.326183    -3.027240
H     -5.058619    -0.143505    -3.370372
H     -5.906907    -0.224326    -1.105743
H     -5.678635    -1.897813    -1.610279
H     -5.884348    -1.719238     0.984998
H     -4.886357    -3.087154     0.494401
H     -4.250779    -0.962836     2.603812
H     -4.385189    -2.709531     2.823518
H     -2.337971    -3.068237     1.470694
H     -1.965582    -1.878490     2.714091
H     -1.570983     0.362788    -1.107203
O      0.129671     0.613443    -1.409116
C      0.976781     0.909070    -0.555805
O      0.060032     0.228740     1.121155
C      0.301889     0.767620     2.380178
H      1.375811     0.999726     2.514208
H      0.069470     0.026275     3.170289
C     -0.525140     2.032542     2.663082
H     -1.575723     1.792712     2.451471
H     -0.472172     2.274685     3.734374
C     -0.114579     3.276939     1.864411
H      0.845149     3.649954     2.245998
H     -0.840564     4.073576     2.070475
C      0.003883     3.117838     0.338332
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H     -0.888662     2.635304    -0.069434
H      0.032341     4.125063    -0.090301
C      1.254534     2.352354    -0.137421
H      2.003772     2.331210     0.656426
C      1.914678     3.032118    -1.374189
H      2.726176     2.395404    -1.740339
C      2.446541     4.362736    -1.094889
H      1.176102     3.088974    -2.181158
C      2.888547     5.455955    -0.854121
H      3.285598     6.420877    -0.644392
O      2.128123     0.175763    -0.432687
C      2.032430    -1.185444    -0.876451
C      3.289304    -1.914232    -0.478726
H      1.884073    -1.214736    -1.958746
H      1.153297    -1.628921    -0.401549
C      3.705398    -1.928165     0.858028
C      4.045503    -2.608773    -1.424802
C      4.849613    -2.623291     1.236838
H      3.125704    -1.384142     1.596187
C      5.190291    -3.312037    -1.047624
H      3.739926    -2.597862    -2.467358
H      5.161739    -2.623365     2.276706
C      5.595513    -3.320143     0.284379
H      5.767475    -3.845953    -1.796202
H      6.488072    -3.862443     0.580373
H     -1.255028    -0.526600     0.942260


62 atoms
3-isomer, structure I4 in toluene
N      4.188444    -0.273379    -0.170125
C      2.816783    -0.383689    -0.149820
N      2.244956    -1.209168    -1.078232
C      2.988579    -2.050550    -1.995821
C      4.263534    -1.326223    -2.411054
C      5.038624    -0.933832    -1.160072
C      4.000678     0.695947     2.096753
C      2.656730     1.208954     1.581620
N      2.032175     0.254734     0.677005
C      4.908760     0.409717     0.907011
H      2.351943    -2.256716    -2.858490
H      3.240714    -3.020357    -1.541611
H      4.001883    -0.432974    -2.986425
H      4.888213    -1.962361    -3.043744
H      5.505243    -1.823822    -0.711876
H      5.853387    -0.247676    -1.417150
H      5.752202    -0.222192     1.210344
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H	5.336376	1.343646	0.517563
H	3.836706	-0.221843	2.671037
H	4.483776	1.418414	2.761309
H	2.803373	2.181408	1.085381
H	1.969710	1.391228	2.412463
H	1.235004	-1.183555	-1.132820
O	-0.724726	-1.182659	-1.422188
C	-1.683671	-0.734677	-0.826982
O	-0.459211	-0.483471	1.640017
C	-0.248023	-1.604086	2.481953
H	-0.970410	-1.536362	3.304570
H	0.754028	-1.549727	2.930556
C	-0.397012	-2.963935	1.789623
H	0.253126	-2.990855	0.907587
H	0.007860	-3.710447	2.485975
C	-1.828430	-3.403562	1.417102
H	-2.525701	-3.059747	2.192708
H	-1.859075	-4.498127	1.467267
C	-2.390373	-3.029416	0.033238
H	-1.681161	-3.323063	-0.746358
H	-3.282720	-3.644631	-0.116940
C	-2.793163	-1.561994	-0.191634
H	-3.030854	-1.078411	0.757839
C	-4.050060	-1.435998	-1.107246
H	-4.226046	-0.380425	-1.331945
C	-5.255849	-2.001007	-0.508789
H	-3.851886	-1.932622	-2.064619
C	-6.246848	-2.459903	-0.004797
H	-7.127561	-2.861459	0.438091
O	-1.950584	0.572882	-0.729687
C	-0.940317	1.503316	-1.203953
C	-1.248259	2.855114	-0.621508
H	-0.958106	1.516786	-2.296009
H	0.035308	1.142350	-0.874007
C	-1.292016	3.019526	0.769031
C	-1.471846	3.959793	-1.444386
C	-1.554897	4.270088	1.319179
H	-1.125216	2.158901	1.409574
C	-1.727396	5.215853	-0.892907
H	-1.447397	3.840523	-2.523954
H	-1.589546	4.387575	2.397730
C	-1.770669	5.372514	0.489829
H	-1.898836	6.067216	-1.544017
H	-1.973493	6.347542	0.921554
H	0.407144	-0.249231	1.214523

62 atoms
3-isomer, structure I5 in toluene

N	-6.217702	-0.791762	0.455402
C	-5.174447	-0.185642	-0.206427
N	-4.896088	1.119116	0.131120
C	-5.384476	1.735134	1.349958
C	-6.853963	1.366292	1.508407
C	-6.991333	-0.151385	1.519963
C	-5.351355	-2.926927	-0.432700
C	-4.826393	-2.072970	-1.585989
N	-4.460613	-0.736572	-1.146877
C	-6.519743	-2.206601	0.229614
H	-5.259500	2.816222	1.259543
H	-4.816752	1.413869	2.237815
H	-7.418915	1.789992	0.673096
H	-7.265419	1.775646	2.434763
H	-6.669879	-0.549715	2.494060
H	-8.042016	-0.436612	1.395793
H	-6.750337	-2.663601	1.198599
H	-7.425107	-2.294535	-0.386523
H	-4.548340	-3.077049	0.296758
H	-5.673900	-3.914327	-0.776194
H	-5.587856	-2.024286	-2.380571
H	-3.946579	-2.541122	-2.037053
H	-4.052792	1.478248	-0.302255
O	4.636334	1.472347	-1.852731
C	4.181656	1.235929	-0.757335
O	-2.483806	1.098025	-1.661578
C	-1.256913	0.644929	-1.110588
H	-0.839421	-0.171814	-1.719290
H	-1.406943	0.243866	-0.095879
C	-0.271080	1.803774	-1.071275
H	-0.168828	2.201250	-2.087565
H	-0.701878	2.610618	-0.466248
C	1.102537	1.411574	-0.519413
H	1.515176	0.595311	-1.125025
H	0.992497	1.007832	0.495057
C	2.083448	2.588679	-0.491718
H	2.231276	2.973562	-1.507086
H	1.651259	3.406861	0.092862
C	3.462119	2.254614	0.113172
H	3.325462	1.818640	1.105519
C	4.361666	3.512584	0.233916
H	5.362178	3.214770	0.566913
C	3.837345	4.511915	1.160037
H	4.490829	3.952423	-0.759838
C	3.408723	5.326651	1.933919

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H      3.034081     6.054570     2.614325
O      4.248440     0.027899    -0.167348
C      4.901325    -1.025110    -0.938632
C      4.898620    -2.276819    -0.109715
H      5.912607    -0.694023    -1.179352
H      4.355417    -1.151269    -1.874826
C      3.842402    -3.187913    -0.201514
C      5.943774    -2.539958     0.780900
C      3.830237    -4.340764     0.580215
H      3.025844    -2.993866    -0.890736
C      5.934971    -3.691265     1.564464
H      6.769900    -1.839284     0.859457
H      3.006187    -5.041908     0.496841
C      4.877282    -4.594194     1.464956
H      6.753994    -3.885738     2.249287
H      4.870886    -5.493598     2.072201
H     -3.128464     0.342266    -1.663986


23 atoms
7-isomer in toluene
O     -2.538391    -1.860653    -0.158087
O     -0.450908    -1.179967    -0.258733
C     -1.744714    -0.997166     0.115996
C     -2.127448     0.287854     0.825570
H     -1.553887     0.392865     1.753633
H     -3.172547     0.162404     1.107353
C     -1.957522     1.552773    -0.041390
H     -2.366709     1.364231    -1.040393
H     -2.576114     2.342763     0.394441
C     -0.515754     2.059339    -0.144636
H     -0.172915     2.360776     0.853434
H     -0.501905     2.967939    -0.755251
C      0.486299     1.057544    -0.728373
H      0.225217     0.803304    -1.762439
H      1.472725     1.529610    -0.761814
C      0.613349    -0.246752     0.058753
H      0.603532    -0.051738     1.135907
C      1.889242    -1.036808    -0.282573
H      1.818923    -2.018212     0.195552
C      3.111789    -0.364844     0.145257
H      1.915381    -1.218360    -1.362586
C      4.114184     0.190254     0.509426
H      5.006132     0.676213     0.828549


62 atoms
```

7-isomer, structure I1 in toluene

O	-1.848767	0.997608	-2.351170
O	-2.516405	0.725293	-0.281523
C	-2.440662	0.297467	-1.557688
C	-3.143166	-0.982795	-1.951176
H	-2.613881	-1.819066	-1.483197
H	-2.999428	-1.076526	-3.027731
C	-4.644579	-1.031146	-1.603504
H	-5.119392	-0.085761	-1.891182
H	-5.104605	-1.801044	-2.230501
C	-4.951933	-1.352149	-0.136668
H	-4.547626	-2.344486	0.099820
H	-6.037108	-1.429792	-0.011035
C	-4.408029	-0.342093	0.879272
H	-4.883392	0.637045	0.744817
H	-4.668645	-0.680795	1.886730
C	-2.895487	-0.147028	0.820614
H	-2.369960	-1.095147	0.692710
C	-2.313695	0.571217	2.050104
H	-1.259760	0.780821	1.840995
C	-2.433100	-0.206403	3.279042
H	-2.813958	1.539239	2.168316
C	-2.526476	-0.854346	4.288033
H	-2.604017	-1.425079	5.183250
O	-0.144020	-1.266615	-0.488853
C	0.718865	-1.827290	-1.454010
C	1.769526	-2.771009	-0.887707
H	1.216819	-1.041282	-2.038027
H	0.091470	-2.385742	-2.159848
C	1.613270	-3.349582	0.373536
C	2.896724	-3.107357	-1.645049
C	2.561450	-4.245556	0.867432
H	0.744591	-3.082784	0.964505
C	3.843807	-4.004802	-1.156738
H	3.037287	-2.659452	-2.626009
H	2.425743	-4.684782	1.851316
C	3.678923	-4.578360	0.104140
H	4.714155	-4.252071	-1.757162
H	4.417482	-5.274901	0.488536
H	0.295143	-0.460793	-0.093020
N	2.284505	2.985149	0.387765
C	1.299171	2.087424	0.039326
N	0.411441	2.488583	-0.918604
C	0.582427	3.675669	-1.732243
C	1.116776	4.794317	-0.847648
C	2.406470	4.325482	-0.186792
C	3.456656	1.080193	1.439043

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C      2.043083     0.554080     1.675607
N      1.149415     0.906660     0.581002
C      3.394452     2.591125     1.258474
H     -0.389522     3.932165    -2.157232
H      1.269256     3.501232    -2.574858
H      0.369379     5.039274    -0.087141
H      1.313298     5.698720    -1.429607
H      3.227602     4.335014    -0.919109
H      2.694976     5.013322     0.616348
H      4.325272     2.963948     0.814442
H      3.285691     3.090176     2.231242
H      3.865842     0.610781     0.538662
H      4.124220     0.835814     2.270632
H      1.663672     0.947361     2.632516
H      2.051655    -0.534700     1.772514
H     -0.313077     1.833907    -1.182853
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62 atoms
7-isomer, structure TS12 in toluene

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O      1.055035    -0.797891    -2.261053
O      2.024100    -0.915613    -0.270847
C      1.735632    -0.180012    -1.420295
C      2.828752     0.779415    -1.896653
H      2.858022     1.677407    -1.276807
H      2.530814     1.087947    -2.899459
C      4.225977     0.130761    -1.938552
H      4.148168    -0.895819    -2.314721
H      4.837039     0.675233    -2.666671
C      4.957740     0.155684    -0.588812
H      5.050068     1.200900    -0.265461
H      5.982629    -0.207263    -0.727861
C      4.303077    -0.655783     0.536234
H      4.375798    -1.728489     0.318547
H      4.858139    -0.484328     1.464778
C      2.824566    -0.339738     0.772852
H      2.644012     0.736543     0.809527
C      2.283258    -0.967897     2.072024
H      1.199906    -0.819168     2.083515
C      2.869821    -0.413053     3.287986
H      2.449669    -2.050980     2.036836
C      3.347897     0.057068     4.286883
H      3.772755     0.471128     5.170692
O      0.559655     1.060215    -0.559094
C     -0.083284     1.892853    -1.472591
C     -1.009970     2.901742    -0.809264
H     -0.663945     1.317153    -2.215095
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H      0.653628     2.469763    -2.062449
C     -0.730324     3.395821     0.469116
C     -2.140888     3.386064    -1.475568
C     -1.552787     4.353456     1.061557
H      0.139014     3.013150     0.991716
C     -2.965645     4.344574    -0.888191
H     -2.379047     3.006687    -2.466376
H     -1.316548     4.727990     2.053516
C     -2.674212     4.833104     0.385078
H     -3.839370     4.706414    -1.422441
H     -3.315571     5.578242     0.845715
H     -0.559190     0.004192     0.049585
N     -2.740097    -2.444185     0.419783
C     -1.699489    -1.730860    -0.082524
N     -1.035532    -2.174885    -1.154434
C     -1.407082    -3.387598    -1.867238
C     -1.960753    -4.404919    -0.878475
C     -3.102342    -3.769877    -0.095482
C     -3.457436    -0.421015     1.652430
C     -1.980295    -0.052285     1.674750
N     -1.325338    -0.581650     0.486067
C     -3.593216    -1.929726     1.498073
H     -0.511770    -3.761688    -2.365527
H     -2.148179    -3.169371    -2.647315
H     -1.165677    -4.718021    -0.195479
H     -2.324823    -5.295043    -1.396693
H     -3.997308    -3.679146    -0.724287
H     -3.373060    -4.395019     0.760819
H     -4.626439    -2.199391     1.258991
H     -3.334953    -2.439172     2.435158
H     -3.946203     0.088802     0.817179
H     -3.952478    -0.101898     2.572494
H     -1.506171    -0.442704     2.585189
H     -1.839490     1.028869     1.670058
H     -0.216988    -1.638264    -1.509679


62 atoms
7-isomer, structure I2 in toluene
O      0.819027    -0.919218    -2.166604
O      1.739037    -1.119978    -0.132544
C      1.604397    -0.278377    -1.254079
C      2.942066     0.091432    -1.917455
H      3.369249     0.967817    -1.419792
H      2.710305     0.390067    -2.941446
C      3.970712    -1.050837    -1.928088
H      3.465369    -1.993254    -2.161135
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H	4.675228	-0.869706	-2.746759
C	4.778190	-1.174673	-0.625881
H	5.261088	-0.209178	-0.424283
H	5.594223	-1.889694	-0.779165
C	3.984736	-1.606815	0.614069
H	3.679198	-2.655315	0.515960
H	4.633935	-1.546993	1.493950
C	2.716710	-0.790301	0.865484
H	2.928001	0.282808	0.838603
C	2.046563	-1.113809	2.215072
H	1.088921	-0.586063	2.246651
C	2.849862	-0.745718	3.376866
H	1.812729	-2.184175	2.242818
C	3.510714	-0.424953	4.329463
H	4.094992	-0.147242	5.174832
O	0.935646	0.900886	-0.716145
C	0.581343	1.910322	-1.672088
C	-0.145211	3.022632	-0.957881
H	-0.045586	1.474266	-2.454066
H	1.487946	2.303468	-2.147368
C	0.500216	3.764382	0.038681
C	-1.468593	3.334612	-1.276612
C	-0.161613	4.796747	0.697024
H	1.527250	3.527849	0.298910
C	-2.133636	4.372953	-0.623587
H	-1.984576	2.758954	-2.038923
H	0.352463	5.364623	1.466157
C	-1.481815	5.105802	0.365277
H	-3.160715	4.605792	-0.886529
H	-1.996923	5.913898	0.874929
H	-0.852579	0.195675	0.049568
N	-3.350789	-1.834793	0.379063
C	-2.198925	-1.299607	-0.153648
N	-1.518704	-1.826202	-1.131654
C	-2.019820	-3.047879	-1.740532
C	-2.709122	-3.950043	-0.719211
C	-3.814867	-3.162208	-0.028233
C	-3.785627	0.259749	1.635199
C	-2.274856	0.446585	1.609076
N	-1.769346	-0.102868	0.364890
C	-4.106928	-1.220036	1.470389
H	-1.176492	-3.569013	-2.203130
H	-2.722348	-2.815294	-2.556692
H	-1.973071	-4.282110	0.020341
H	-3.130631	-4.843026	-1.190208
H	-4.686100	-3.060126	-0.690101
H	-4.158265	-3.691128	0.868099

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H     -5.174199    -1.355490     1.261834
H     -3.898636    -1.756272     2.408450
H     -4.231214     0.836534     0.819400
H     -4.210405     0.622943     2.574718
H     -1.822611    -0.035247     2.490497
H     -2.007987     1.504588     1.643930
H     -0.033361    -1.246194    -1.729626


62 atoms
7-isomer, structure TS23 in toluene
O      0.622025    -0.526791    -2.186056
O      1.435315    -1.231456    -0.209402
C      1.561457    -0.254099    -1.231393
C      2.940939    -0.230938    -1.909352
H      3.634151     0.363830    -1.306678
H      2.806302     0.303522    -2.851992
C      3.535712    -1.621489    -2.179390
H      2.742112    -2.295364    -2.516928
H      4.243204    -1.540052    -3.011408
C      4.281858    -2.219111    -0.977097
H      5.073168    -1.519563    -0.676662
H      4.796035    -3.133796    -1.292821
C      3.416732    -2.548767     0.245703
H      2.760221    -3.398511     0.023979
H      4.068410    -2.858369     1.069254
C      2.521721    -1.401293     0.717772
H      3.085626    -0.467701     0.800056
C      1.862326    -1.679758     2.082596
H      1.178333    -0.854383     2.300757
C      2.812434    -1.817186     3.182158
H      1.250078    -2.585033     1.999342
C      3.595798    -1.914142     4.089629
H      4.288512    -2.002522     4.893091
O      1.293712     0.979209    -0.536312
C      1.215628     2.153216    -1.347770
C      0.610305     3.279129    -0.544952
H      0.600342     1.936942    -2.227969
H      2.212518     2.445631    -1.699334
C      1.229389     4.529963    -0.496343
C     -0.596833     3.097179     0.140437
C      0.653990     5.585734     0.211379
H      2.172375     4.682400    -1.014114
C     -1.169406     4.147637     0.852110
H     -1.079170     2.125759     0.121941
H      1.149378     6.551322     0.238325
C     -0.547863     5.396873     0.888439
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H     -2.106098     3.993076     1.379238
H     -0.996710     6.214772     1.443351
H     -0.662416    -0.403276     0.606560
N     -3.732444    -1.259443     0.166785
C     -2.442405    -0.913837    -0.159709
N     -1.936302    -0.954050    -1.355872
C     -2.798106    -1.354288    -2.457906
C     -3.832161    -2.391181    -2.024558
C     -4.620329    -1.844411    -0.840782
C     -3.440165    -0.353939     2.459543
C     -1.963828    -0.666890     2.259428
N     -1.641694    -0.439731     0.860387
C     -4.268591    -1.229875     1.528457
H     -2.167410    -1.754288    -3.257062
H     -3.311447    -0.477222    -2.881486
H     -3.317283    -3.312211    -1.731730
H     -4.516516    -2.640724    -2.840632
H     -5.344899    -1.089427    -1.174997
H     -5.193912    -2.645008    -0.361119
H     -5.299320    -0.861718     1.480050
H     -4.317995    -2.255743     1.922745
H     -3.614171     0.703068     2.238212
H     -3.742203    -0.534178     3.494371
H     -1.750628    -1.700198     2.574843
H     -1.339513    -0.005843     2.864271
H     -0.288013    -0.671509    -1.780794


62 atoms
7-isomer, structure I3 in toluene
O      0.281730    -0.124845    -2.068506
O      0.817766    -1.527243    -0.390441
C      1.317298    -0.525402    -1.271827
C      2.459401    -1.039284    -2.168435
H      3.413888    -0.902102    -1.650927
H      2.480670    -0.386674    -3.043760
C      2.316196    -2.505721    -2.606396
H      1.271952    -2.711504    -2.861691
H      2.890304    -2.646687    -3.528350
C      2.832787    -3.517797    -1.569609
H      3.877358    -3.271492    -1.337855
H      2.855511    -4.514390    -2.024498
C      2.038188    -3.604945    -0.259091
H      1.063902    -4.074188    -0.442391
H      2.573645    -4.253517     0.442242
C      1.773181    -2.253848     0.404118
H      2.691243    -1.667205     0.487427
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C	1.161059	-2.370999	1.813298
H	0.871798	-1.366834	2.135763
C	2.063350	-2.965878	2.794344
H	0.239170	-2.962017	1.756045
C	2.816143	-3.447964	3.599019
H	3.480165	-3.871798	4.314962
O	1.761528	0.510149	-0.386892
C	2.219882	1.713849	-0.998296
C	2.108293	2.851792	-0.010985
H	1.607583	1.923236	-1.882477
H	3.260634	1.607577	-1.330001
C	3.116314	3.813976	0.080691
C	0.975647	2.979102	0.800862
C	2.995145	4.892625	0.956768
H	4.007013	3.719740	-0.534716
C	0.856735	4.051634	1.681036
H	0.196126	2.227644	0.739208
H	3.788756	5.630931	1.017113
C	1.864390	5.013717	1.760861
H	-0.025070	4.137129	2.308824
H	1.770237	5.848109	2.448823
H	-1.205336	-1.395272	0.057966
N	-4.047561	0.141447	0.124562
C	-2.713660	-0.071631	-0.131824
N	-1.933045	0.757367	-0.767576
C	-2.490221	2.033634	-1.189591
C	-3.953753	1.901419	-1.606146
C	-4.744462	1.291972	-0.455064
C	-4.108354	-1.834552	1.632056
C	-2.973513	-2.362309	0.763525
N	-2.162210	-1.232451	0.351076
C	-4.905259	-0.804483	0.840634
H	-1.888020	2.411882	-2.020466
H	-2.403813	2.780002	-0.384818
H	-4.019494	1.252725	-2.485839
H	-4.384792	2.869803	-1.876768
H	-4.925216	2.041615	0.327344
H	-5.726994	0.953243	-0.802580
H	-5.557985	-0.233806	1.510955
H	-5.561823	-1.312700	0.119135
H	-3.684393	-1.377002	2.530461
H	-4.772846	-2.642946	1.947998
H	-3.380038	-2.919328	-0.094968
H	-2.340011	-3.052104	1.325420
H	-0.501333	0.195478	-1.516977

62 atoms
7-isomer, structure TSr in toluene

O	0.268893	-0.150447	-2.234457
O	1.122523	-1.047754	-0.362305
C	1.437429	-0.311947	-1.552914
C	2.449812	-1.046939	-2.446293
H	3.459742	-0.765874	-2.136859
H	2.307354	-0.634628	-3.448441
C	2.309395	-2.575863	-2.463018
H	1.249354	-2.848954	-2.491644
H	2.745903	-2.953834	-3.393854
C	3.021568	-3.274258	-1.291523
H	4.076213	-2.969394	-1.300035
H	3.022836	-4.356071	-1.466567
C	2.441154	-3.014396	0.106273
H	1.474226	-3.522484	0.210339
H	3.107696	-3.452419	0.856456
C	2.217738	-1.536804	0.430911
H	3.111789	-0.947210	0.214039
C	1.829147	-1.277913	1.899956
H	1.591367	-0.214749	1.998019
C	2.870969	-1.639492	2.856283
H	0.908011	-1.825916	2.130811
C	3.737773	-1.928939	3.638345
H	4.503302	-2.181735	4.333450
O	2.058830	0.912245	-1.122390
C	1.513278	2.183691	-1.481501
C	1.331849	3.051356	-0.256882
H	0.565047	2.043788	-2.001445
H	2.206379	2.667103	-2.179321
C	2.118405	4.188149	-0.062849
C	0.372305	2.722773	0.709584
C	1.952841	4.989036	1.068198
H	2.871133	4.450069	-0.801449
C	0.206873	3.517755	1.840162
H	-0.249477	1.844654	0.562990
H	2.573921	5.869174	1.203371
C	0.997102	4.654407	2.023479
H	-0.542654	3.253759	2.580216
H	0.866997	5.273135	2.905921
H	-0.798271	-1.449431	0.151187
N	-3.903088	-0.563421	0.192330
C	-2.561848	-0.513535	-0.099543
N	-1.991816	0.392353	-0.847247
C	-2.821914	1.470232	-1.365440
C	-4.231236	0.987275	-1.701703
C	-4.845672	0.346135	-0.463659

C	-3.499522	-2.333067	1.892372
C	-2.295788	-2.697139	1.032441
N	-1.760908	-1.471318	0.469259
C	-4.518357	-1.589413	1.036951
H	-2.336557	1.878712	-2.256460
H	-2.879126	2.297113	-0.641010
H	-4.175690	0.252227	-2.511347
H	-4.866628	1.809011	-2.044608
H	-5.166580	1.116494	0.250550
H	-5.738740	-0.228692	-0.733160
H	-5.265257	-1.103099	1.674400
H	-5.063234	-2.300691	0.399266
H	-3.166553	-1.700766	2.720422
H	-3.965572	-3.225568	2.317790
H	-2.589579	-3.419059	0.254814
H	-1.513795	-3.167933	1.632290
H	-0.516706	0.054625	-1.631369

62 atoms
7-isomer, structure I3r in toluene

O	0.184796	-0.052244	-2.170046
O	0.924957	-0.951434	-0.246614
C	1.305516	-0.162579	-1.392659
C	2.434587	-0.795239	-2.215793
H	3.396234	-0.461258	-1.817079
H	2.343972	-0.361120	-3.213659
C	2.394517	-2.327833	-2.286664
H	1.360581	-2.663657	-2.418359
H	2.933107	-2.644037	-3.186258
C	3.043910	-3.023779	-1.078732
H	4.071350	-2.650641	-0.976994
H	3.135523	-4.095259	-1.289425
C	2.319846	-2.858792	0.264689
H	1.382219	-3.428754	0.256933
H	2.939895	-3.286829	1.059092
C	1.973643	-1.412649	0.621726
H	2.844404	-0.760987	0.509194
C	1.440964	-1.247799	2.059536
H	1.131798	-0.206187	2.187951
C	2.412821	-1.597651	3.090865
H	0.536695	-1.855640	2.178971
C	3.221938	-1.876133	3.936007
H	3.936230	-2.120124	4.686625
O	1.814759	1.083240	-0.938500
C	0.852276	1.997928	-0.418740
C	1.555759	3.144861	0.266480

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H      0.181639     1.491576     0.281714
H      0.233495     2.375450    -1.241687
C      2.841341     3.544698    -0.108577
C      0.895705     3.859209     1.271510
C      3.451515     4.635683     0.507942
H      3.363424     2.989552    -0.878667
C      1.501481     4.954208     1.884187
H     -0.100743     3.554487     1.580469
H      4.452509     4.931017     0.208576
C      2.783975     5.346407     1.504012
H      0.975144     5.495215     2.664510
H      3.260767     6.195299     1.983789
H     -1.002059    -1.585896     0.005665
N     -4.158288    -0.931157    -0.184316
C     -2.803646    -0.764653    -0.348527
N     -2.242632     0.229515    -0.978561
C     -3.103926     1.281399    -1.497227
C     -4.437496     0.726886    -1.994599
C     -5.106955    -0.046402    -0.865046
C     -3.770628    -2.801600     1.408049
C     -2.468406    -3.006048     0.644094
N     -1.983806    -1.702266     0.230078
C     -4.763401    -2.065753     0.516045
H     -2.574487     1.788143    -2.309069
H     -3.289677     2.045746    -0.726197
H     -4.253663     0.059710    -2.843037
H     -5.102195     1.524301    -2.339502
H     -5.550083     0.644422    -0.134929
H     -5.924780    -0.662390    -1.255444
H     -5.602464    -1.690387     1.112556
H     -5.188586    -2.760228    -0.223458
H     -3.565799    -2.216792     2.309411
H     -4.200982    -3.757332     1.718235
H     -2.632208    -3.680688    -0.210564
H     -1.709690    -3.467714     1.279908
H     -0.662106     0.065095    -1.636305


62 atoms
7-isomer, structure TS34 in toluene
O     -0.137153    -0.579776     2.123342
O      0.110786     1.107713     0.287044
C      0.798609     0.198611     1.867884
C      1.113796     1.377122     2.778914
H      2.068702     1.819121     2.486148
H      1.278532     0.920922     3.762157
C      0.023512     2.456983     2.882919
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H	-0.950993	2.005787	2.676388
H	-0.015127	2.808474	3.920335
C	0.260104	3.690119	1.991361
H	1.285085	4.044278	2.165671
H	-0.391950	4.501280	2.338888
C	0.044068	3.518735	0.480390
H	-1.031165	3.432089	0.272603
H	0.386130	4.431252	-0.022893
C	0.726689	2.281054	-0.128327
H	1.789064	2.281714	0.173699
C	0.729678	2.333101	-1.686901
H	1.124422	1.374354	-2.037497
C	1.504820	3.425023	-2.267647
H	-0.306945	2.389518	-2.042676
C	2.159306	4.327701	-2.722812
H	2.737846	5.123502	-3.128632
O	1.980415	-0.275023	1.327041
C	1.861168	-1.464876	0.552615
C	3.191194	-1.801261	-0.076148
H	1.103296	-1.295866	-0.220341
H	1.514540	-2.289379	1.182954
C	4.091547	-0.803174	-0.461347
C	3.523393	-3.136460	-0.324980
C	5.292511	-1.134827	-1.085434
H	3.850146	0.233301	-0.257727
C	4.720298	-3.470228	-0.956099
H	2.841268	-3.924972	-0.017700
H	5.982363	-0.347896	-1.374591
C	5.610639	-2.468502	-1.338438
H	4.961932	-4.512884	-1.138586
H	6.546871	-2.725228	-1.824064
H	-1.464469	0.751659	-0.031440
N	-3.999132	-1.229718	-0.707168
C	-2.830368	-0.793522	-0.177362
N	-2.031399	-1.637755	0.486802
C	-2.349337	-3.047545	0.664636
C	-3.860245	-3.219761	0.762945
C	-4.516571	-2.580315	-0.453809
C	-4.056529	0.817716	-2.103486
C	-3.303076	1.467996	-0.949092
N	-2.450744	0.479555	-0.305110
C	-4.826650	-0.388079	-1.580922
H	-1.850115	-3.384439	1.573738
H	-1.950902	-3.641446	-0.167648
H	-4.221668	-2.743006	1.678719
H	-4.130793	-4.277178	0.808228
H	-4.357158	-3.197956	-1.346700

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H     -5.597728    -2.499083    -0.307097
H     -5.174869    -1.010206    -2.411103
H     -5.715215    -0.065621    -1.024072
H     -3.342760     0.505391    -2.871272
H     -4.753333     1.522157    -2.563579
H     -4.008242     1.900799    -0.227964
H     -2.664212     2.278921    -1.300399
H     -1.257344    -1.230900     1.042214


62 atoms
7-isomer, structure I4 in toluene
O      0.419861    -1.224387     2.142431
O      0.465489     1.195523    -0.065214
C      1.332925    -0.433684     2.248994
C      1.247124     0.951214     2.846591
H      1.819273     1.608484     2.191785
H      1.811415     0.921449     3.786147
C     -0.184287     1.469672     3.079898
H     -0.902377     0.772631     2.643921
H     -0.387977     1.467327     4.155229
C     -0.453396     2.885077     2.537079
H      0.396159     3.538922     2.774423
H     -1.303926     3.301914     3.088619
C     -0.786823     3.008695     1.040036
H     -1.683146     2.418855     0.811731
H     -1.050303     4.055028     0.849041
C      0.311541     2.600986     0.045265
H      1.277814     2.978198     0.397713
C      0.072683     3.212407    -1.362424
H      0.801922     2.761497    -2.042981
C      0.193443     4.665972    -1.410874
H     -0.918325     2.911943    -1.721375
C      0.310755     5.863582    -1.427233
H      0.411433     6.922971    -1.450604
O      2.597038    -0.701127     1.870942
C      2.869491    -1.959923     1.206647
C      3.676386    -1.712401    -0.041675
H      1.916384    -2.441057     0.985880
H      3.418093    -2.586458     1.912894
C      3.262395    -0.756744    -0.978101
C      4.828127    -2.460190    -0.294646
C      3.993911    -0.563300    -2.146807
H      2.376491    -0.158127    -0.786160
C      5.554924    -2.270812    -1.469980
H      5.163088    -3.195735     0.431610
H      3.668066     0.181936    -2.865864
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C      5.139133    -1.320338    -2.398727
H      6.448552    -2.859099    -1.653197
H      5.705442    -1.165940    -3.311797
H     -0.377833     0.770612    -0.380078
N     -3.788958    -1.419869    -0.901515
C     -2.623379    -0.883186    -0.401888
N     -2.296626    -1.205523     0.897504
C     -2.899870    -2.336696     1.582630
C     -4.401510    -2.289298     1.342516
C     -4.662587    -2.329460    -0.157419
C     -2.957629    -0.795507    -3.134255
C     -2.213496     0.316791    -2.400058
N     -1.836304    -0.070670    -1.048394
C     -4.161641    -1.214250    -2.302014
H     -2.663199    -2.251431     2.644768
H     -2.491756    -3.298306     1.233978
H     -4.803979    -1.367581     1.773004
H     -4.905127    -3.132146     1.822953
H     -4.525778    -3.353779    -0.534669
H     -5.701223    -2.052265    -0.370293
H     -4.581685    -2.152550    -2.680682
H     -4.957870    -0.459834    -2.367380
H     -2.286959    -1.650421    -3.270182
H     -3.285538    -0.471219    -4.126228
H     -2.842199     1.221689    -2.384069
H     -1.303905     0.587033    -2.945084
H     -1.336218    -1.003817     1.147176


62 atoms
7-isomer, structure I5 in toluene
O     -3.991748    -1.705050    -1.647178
O      3.139900     0.794162    -1.702039
C     -4.078430    -0.795880    -0.856257
C     -2.943688     0.098866    -0.404626
H     -2.827631    -0.038692     0.677067
H     -3.266104     1.138367    -0.527883
C     -1.627695    -0.164342    -1.134426
H     -1.348219    -1.215571    -1.009707
H     -1.776195    -0.021659    -2.210254
C     -0.492755     0.740449    -0.642503
H     -0.336910     0.579909     0.431873
H     -0.792539     1.787980    -0.745605
C      0.815589     0.486605    -1.396812
H      1.057927    -0.581442    -1.352096
H      0.685750     0.720636    -2.460770
C      2.053370     1.237943    -0.902066
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H	2.238573	0.987949	0.152871
C	1.950257	2.785705	-1.015608
H	2.972110	3.179327	-1.001970
C	1.192334	3.450337	0.041384
H	1.540102	3.043741	-1.998864
C	0.604170	4.007141	0.931424
H	0.072427	4.495385	1.713591
O	-5.232880	-0.450080	-0.247074
C	-6.400620	-1.247938	-0.591204
C	-7.572500	-0.709574	0.178808
H	-6.192205	-2.290004	-0.342568
H	-6.556273	-1.184353	-1.669463
C	-7.867995	-1.196338	1.455615
C	-8.372554	0.301933	-0.360705
C	-8.942346	-0.684353	2.179321
H	-7.252950	-1.982091	1.884601
C	-9.447863	0.816656	0.359685
H	-8.151958	0.687614	-1.351765
H	-9.163064	-1.073452	3.168055
C	-9.734654	0.323714	1.631811
H	-10.063079	1.599399	-0.072169
H	-10.574080	0.721407	2.193019
H	3.992913	0.991088	-1.225096
N	6.697813	-0.928624	0.832671
C	5.691810	-0.466502	0.016970
N	4.931099	-1.411525	-0.632288
C	4.902515	-2.806122	-0.233239
C	6.335879	-3.250652	0.027643
C	6.955986	-2.346972	1.086360
C	6.805912	1.359782	1.755465
C	6.305661	1.788407	0.377009
N	5.430940	0.789354	-0.215093
C	7.490379	0.003257	1.637976
H	4.454563	-3.383784	-1.044460
H	4.286365	-2.971052	0.664759
H	6.904129	-3.185022	-0.904654
H	6.369979	-4.288194	0.369951
H	6.570108	-2.614936	2.081256
H	8.041176	-2.494000	1.120382
H	7.631360	-0.440541	2.629907
H	8.489154	0.112919	1.193832
H	5.953714	1.286436	2.439231
H	7.503983	2.089839	2.175550
H	7.167498	1.985595	-0.279992
H	5.755352	2.731121	0.448299
H	4.136316	-1.023337	-1.125779

Table S9: Cartesian coordinates (in Angstroms) of all intermediates and transition states of the second step of the TBD catalyzed ROP of 3-/7-isomer (i.e. addition of another 3-/7-isomer unit to the 3-/7-isomer chain end) optimized in toluene using the PCM B3LYP/6-311G(d) method

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85 atoms
addition of another 3-isomer unit to the 3-isomer chain end,
structure I1, in toluene
N      3.185703     3.642610     1.346295
C      3.391873     2.285440     1.434800
N      4.183643     1.837480     2.458271
C      4.819982     2.700720     3.438217
C      5.143462     4.046765     2.800779
C      3.871441     4.619581     2.190469
C      1.259882     3.108356    -0.110700
C      2.126261     1.916893    -0.517637
N      2.887167     1.404591     0.612630
C      2.158665     4.198113     0.461866
H      5.723518     2.200359     3.791057
H      4.171704     2.849503     4.313411
H      5.902849     3.910300     2.024655
H      5.542016     4.745340     3.541388
H      3.193971     4.965756     2.985426
H      4.104696     5.494169     1.572741
H      1.567750     4.924665     1.033095
H      2.648461     4.755161    -0.348344
H      0.537655     2.782690     0.645084
H      0.693140     3.508249    -0.956845
H      2.796121     2.216194    -1.339344
H      1.508460     1.103708    -0.908261
H      4.521194     0.888701     2.363748
O      5.601023    -0.816548     2.189476
C      5.199909    -1.854809     1.707210
O      4.796449    -2.820803     2.550697
C      4.159552    -4.040605     2.096785
H      3.337981    -3.783078     1.425074
H      3.732423    -4.450257     3.011667
C      5.139164    -5.029885     1.479321
H      6.014941    -5.098193     2.134985
H      4.666665    -6.018786     1.493403
C      5.562427    -4.694907     0.046256
H      4.691439    -4.788486    -0.614404
H      6.285033    -5.443167    -0.296326
C      6.166360    -3.298811    -0.140680
H      7.092263    -3.200989     0.439233
H      6.451348    -3.189210    -1.190210
C      5.205362    -2.134706     0.208750
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H	4.185373	-2.411286	-0.073681
C	5.556097	-0.830633	-0.543950
H	4.877343	-0.037702	-0.215736
C	5.460142	-0.966337	-1.995250
H	6.565312	-0.508323	-0.268073
C	5.374096	-1.075421	-3.190588
H	5.294433	-1.163921	-4.248267
O	-0.889195	-3.118906	7.292194
C	-1.343148	-2.123496	6.776472
O	2.247106	-1.248849	1.106927
C	1.112336	-1.267738	1.955758
H	0.655936	-2.259100	1.853437
H	0.362754	-0.536611	1.615396
C	1.450232	-1.004421	3.425665
H	2.194025	-1.740560	3.750799
H	1.935867	-0.024816	3.505137
C	0.221698	-1.053044	4.339739
H	-0.274577	-2.025461	4.227151
H	-0.510875	-0.303552	4.013842
C	0.569473	-0.813357	5.812965
H	1.256923	-1.591303	6.163837
H	1.100580	0.138696	5.909521
C	-0.648988	-0.770630	6.757705
H	-1.362293	-0.027585	6.393509
C	-0.243276	-0.411247	8.210968
H	-1.117569	-0.497190	8.865822
C	0.309227	0.933713	8.341659
H	0.478998	-1.150690	8.570313
C	0.750542	2.047477	8.447416
H	1.145589	3.030540	8.550228
O	-2.528126	-2.088521	6.138892
C	-3.260945	-3.348790	6.078267
C	-4.551192	-3.099346	5.352240
H	-3.424232	-3.697394	7.099177
H	-2.637321	-4.083227	5.566416
C	-4.638573	-3.291810	3.970565
C	-5.679186	-2.649787	6.045617
C	-5.830109	-3.041775	3.293438
H	-3.768581	-3.640405	3.421833
C	-6.871671	-2.397682	5.372110
H	-5.622382	-2.497265	7.119470
H	-5.885700	-3.198240	2.221073
C	-6.948961	-2.593875	3.993745
H	-7.740913	-2.051986	5.922129
H	-7.878631	-2.401181	3.468134
H	2.529911	-0.305769	0.975742

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

N	4.276591	-3.224355	-1.206307
C	3.658272	-2.132347	-0.686239
N	3.470986	-2.031714	0.635474
C	4.034264	-2.983213	1.580897
C	3.993011	-4.377096	0.970494
C	4.705712	-4.356246	-0.375515
C	4.561910	-1.987095	-3.333104
C	3.299386	-1.236187	-2.931989
N	3.219476	-1.155555	-1.481631
C	4.577398	-3.342410	-2.638321
H	3.440609	-2.930699	2.494478
H	5.064232	-2.708591	1.844599
H	2.951607	-4.685012	0.839110
H	4.475548	-5.105031	1.626721
H	5.793030	-4.305606	-0.234949
H	4.495704	-5.274104	-0.932788
H	5.563055	-3.807854	-2.731470
H	3.853534	-4.023420	-3.103730
H	5.441107	-1.406085	-3.039355
H	4.603752	-2.130980	-4.415245
H	2.412530	-1.736914	-3.343161
H	3.300586	-0.215694	-3.317706
H	3.070244	-1.156801	1.026306
O	2.395703	0.238584	1.812002
C	2.695134	1.221235	1.104556
O	3.995944	1.181917	0.602165
C	4.463470	2.223733	-0.266071
H	3.635033	2.609346	-0.863187
H	5.163649	1.735152	-0.949253
C	5.179048	3.316786	0.520317
H	5.921112	2.831734	1.165742
H	5.740363	3.946729	-0.181306
C	4.246662	4.195064	1.361485
H	3.665495	4.845607	0.694988
H	4.854303	4.864848	1.980861
C	3.266453	3.431863	2.263979
H	3.809383	2.764053	2.943128
H	2.758081	4.166071	2.896681
C	2.185852	2.628573	1.500415
H	1.921243	3.173915	0.593575
C	0.907846	2.477442	2.359033
H	0.220104	1.779967	1.878325
C	0.214013	3.742543	2.592640

H	1.173821	2.014923	3.314338
C	-0.362130	4.784288	2.771780
H	-0.878817	5.700729	2.932686
O	-5.308439	1.997566	0.514672
C	-4.932882	1.149800	-0.261682
O	1.860771	0.965538	-0.573318
C	0.550828	0.477610	-0.540872
H	0.298096	0.119906	0.472356
H	0.466015	-0.415788	-1.189978
C	-0.487071	1.503295	-1.016472
H	-0.435157	2.394592	-0.380379
H	-0.204805	1.832458	-2.024300
C	-1.918244	0.956605	-1.027293
H	-2.191166	0.636527	-0.014337
H	-1.960698	0.051385	-1.647157
C	-2.940406	1.971266	-1.551082
H	-2.941384	2.863967	-0.915214
H	-2.639740	2.301226	-2.550625
C	-4.385400	1.435674	-1.650824
H	-4.381985	0.499791	-2.214898
C	-5.330318	2.446097	-2.350653
H	-6.361035	2.078077	-2.299804
C	-4.986225	2.686707	-3.748954
H	-5.318240	3.387751	-1.793459
C	-4.706735	2.871863	-4.904034
H	-4.463318	3.044511	-5.925798
O	-4.939704	-0.168220	0.014838
C	-5.407944	-0.538483	1.345806
C	-5.357206	-2.035148	1.455243
H	-6.420748	-0.151956	1.470006
H	-4.767843	-0.051264	2.082658
C	-4.235198	-2.671541	1.993381
C	-6.425508	-2.815447	1.001985
C	-4.181280	-4.061132	2.079458
H	-3.399643	-2.075530	2.348168
C	-6.374524	-4.204505	1.084798
H	-7.302553	-2.330896	0.582828
H	-3.305834	-4.542440	2.503236
C	-5.251222	-4.830005	1.624821
H	-7.211612	-4.798542	0.732488
H	-5.211997	-5.912372	1.694047
H	2.747113	-0.300547	-1.063044

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

N	1.406565	-4.588084	1.198072
C	1.828962	-3.277450	1.226791
N	2.318495	-2.678808	2.276522
C	2.499145	-3.462919	3.488313
C	1.386409	-4.493520	3.665230
C	1.331908	-5.379710	2.427338
C	1.260275	-4.521690	-1.279124
C	0.996706	-3.032525	-1.098539
N	1.747988	-2.573186	0.053274
C	0.882675	-5.251350	0.003703
H	2.523316	-2.776549	4.339887
H	3.474578	-3.974463	3.478786
H	0.431437	-3.972506	3.791360
H	1.545911	-5.111049	4.554095
H	2.151696	-6.111074	2.441914
H	0.397227	-5.951993	2.406913
H	1.272424	-6.275429	-0.014619
H	-0.211933	-5.332409	0.081128
H	2.320692	-4.672664	-1.501173
H	0.680595	-4.926594	-2.112848
H	-0.084663	-2.853751	-0.988261
H	1.329648	-2.465388	-1.970305
H	2.910602	-1.087413	2.343005
O	3.186216	-0.120355	2.475820
C	3.289955	0.499269	1.269135
O	4.159346	-0.268547	0.469960
C	4.526655	0.228009	-0.825293
H	3.763655	0.913946	-1.203597
H	4.539423	-0.643685	-1.484905
C	5.905160	0.873875	-0.772106
H	6.598704	0.140866	-0.344376
H	6.247714	1.068764	-1.796062
C	5.949341	2.170098	0.043667
H	5.445686	2.970142	-0.514683
H	6.993605	2.486831	0.142739
C	5.323250	2.087488	1.445329
H	5.758595	1.258852	2.013226
H	5.591547	3.004327	1.978920
C	3.783366	1.965598	1.463132
H	3.382027	2.545949	0.627492
C	3.218493	2.572916	2.774536
H	2.161169	2.329520	2.892372
C	3.368130	4.025514	2.841336
H	3.722516	2.106391	3.625396
C	3.477718	5.223187	2.883336
H	3.572938	6.282362	2.928741
O	-2.734845	5.142031	3.495243

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C     -3.133796     4.106704     3.014603
O      2.033930     0.449711     0.525221
C      0.798398     0.722258     1.197040
H      0.949200     0.686533     2.278015
H      0.124463    -0.105385     0.948647
C      0.173074     2.040295     0.746683
H      0.847739     2.872336     0.974835
H      0.066248     2.020344    -0.344016
C     -1.190633     2.284599     1.402446
H     -1.069488     2.307146     2.491902
H     -1.856535     1.437907     1.193250
C     -1.854764     3.578397     0.919380
H     -1.210668     4.436423     1.142763
H     -1.962487     3.543291    -0.169266
C     -3.251720     3.840491     1.521710
H     -3.874907     2.954051     1.381277
C     -3.946623     5.058443     0.860757
H     -4.882348     5.274243     1.388099
C     -4.240386     4.857719    -0.555118
H     -3.315048     5.942181     0.992627
C     -4.492083     4.681674    -1.717920
H     -4.715952     4.536622    -2.748471
O     -3.513142     3.042317     3.746080
C     -3.400862     3.188765     5.194127
C     -3.863988     1.908654     5.827287
H     -4.010807     4.041427     5.496694
H     -2.361493     3.414110     5.436648
C     -2.945866     0.913499     6.173694
C     -5.224315     1.686768     6.064038
C     -3.376908    -0.280704     6.747693
H     -1.886853     1.075414     5.995824
C     -5.659023     0.493911     6.635686
H     -5.946148     2.454091     5.799872
H     -2.653108    -1.043315     7.016141
C     -4.734814    -0.492327     6.979293
H     -6.717028     0.335195     6.817500
H     -5.071991    -1.420521     7.429300
H      1.996611    -1.592389     0.119040


85 atoms
addition of another 3-isomer unit to the 3-isomer chain end,
structure TS23, in toluene
N      1.200672    -4.349107     1.166634
C      1.753315    -3.088055     1.185308
N      2.250276    -2.511157     2.243695
C      2.291716    -3.275615     3.480606
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C	1.067558	-4.176773	3.626910
C	0.976101	-5.088961	2.410114
C	1.191956	-4.344515	-1.315611
C	1.075340	-2.830736	-1.191160
N	1.799201	-2.413634	-0.006574
C	0.670344	-4.989027	-0.037647
H	2.350655	-2.571989	4.316143
H	3.206028	-3.887865	3.529510
H	0.169628	-3.553435	3.692652
H	1.117626	-4.781275	4.537358
H	1.707479	-5.905247	2.486059
H	-0.014424	-5.555179	2.354646
H	0.946519	-6.049058	-0.008250
H	-0.429115	-4.949278	-0.019207
H	2.241327	-4.611224	-1.471698
H	0.619575	-4.714804	-2.170179
H	0.014506	-2.537616	-1.153213
H	1.517130	-2.329511	-2.054759
H	2.937537	-0.961593	2.313489
O	3.272739	-0.012958	2.445698
C	3.410225	0.605200	1.241470
O	4.179367	-0.246795	0.415645
C	4.652793	0.246782	-0.845353
H	3.997527	1.038034	-1.220806
H	4.578442	-0.595107	-1.538864
C	6.102541	0.702292	-0.725614
H	6.672957	-0.129887	-0.297603
H	6.505908	0.873466	-1.731509
C	6.296336	1.960654	0.127876
H	5.937493	2.836358	-0.428600
H	7.370020	2.120772	0.276990
C	5.601194	1.942043	1.499072
H	5.903827	1.061625	2.075093
H	5.952785	2.814400	2.057966
C	4.060126	2.004838	1.429701
H	3.773616	2.600437	0.558218
C	3.478011	2.711378	2.680470
H	2.388184	2.637422	2.686538
C	3.840284	4.125321	2.760974
H	3.819052	2.187175	3.577347
C	4.128493	5.292331	2.816030
H	4.380817	6.324899	2.871458
O	-2.960768	4.988998	3.424984
C	-3.303997	3.914720	2.988725
O	2.148515	0.722135	0.525339
C	0.921280	0.874450	1.248137
H	1.119323	0.935134	2.319425

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H      0.327819    -0.034216     1.090510
C      0.151740     2.090732     0.743829
H      0.749815     2.994712     0.906541
H      0.022867     1.998639    -0.340801
C     -1.214792     2.237573     1.421909
H     -1.073252     2.330231     2.505403
H     -1.798922     1.320629     1.273737
C     -2.011898     3.433874     0.891157
H     -1.453892     4.361421     1.062217
H     -2.131394     3.336037    -0.192403
C     -3.418072     3.584717     1.508353
H     -3.957536     2.639717     1.410040
C     -4.235050     4.707607     0.818539
H     -5.179574     4.852543     1.354476
C     -4.528719     4.429487    -0.584214
H     -3.688160     5.651112     0.908618
C     -4.779385     4.188802    -1.735593
H     -5.003001     3.986487    -2.756509
O     -3.618580     2.860601     3.764261
C     -3.507693     3.070416     5.204667
C     -3.908674     1.796811     5.891005
H     -4.155001     3.905598     5.476512
H     -2.478710     3.352815     5.431612
C     -2.945537     0.852976     6.258344
C     -5.255261     1.528446     6.156291
C     -3.319052    -0.336484     6.880384
H     -1.896688     1.051567     6.058674
C     -5.632510     0.340122     6.776266
H     -6.011744     2.255819     5.876413
H     -2.560857    -1.058919     7.164594
C     -4.663818    -0.594812     7.139976
H     -6.680470     0.145186     6.979754
H     -4.956224    -1.519293     7.627392
H      2.181084    -1.477715     0.038618


85 atoms
addition of another 3-isomer unit to the 3-isomer chain end,
structure I3, in toluene
N      3.010361    -3.614225    -2.361896
C      3.183865    -2.346353    -2.866059
N      3.964737    -1.439111    -2.350569
C      4.776454    -1.809583    -1.202039
C      4.038159    -2.775448    -0.277520
C      3.602205    -3.996791    -1.078076
C      1.780730    -4.294556    -4.408905
C      1.403075    -2.823144    -4.523498
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N	2.508304	-2.031678	-4.017904
C	2.120829	-4.611838	-2.957877
H	5.048322	-0.895813	-0.665823
H	5.724076	-2.266380	-1.528176
H	3.159385	-2.273867	0.140701
H	4.667865	-3.091064	0.559746
H	4.455353	-4.665991	-1.254730
H	2.856624	-4.573011	-0.518621
H	2.612164	-5.588839	-2.889892
H	1.198533	-4.680491	-2.362040
H	2.644276	-4.491946	-5.050669
H	0.961523	-4.938226	-4.739845
H	0.467146	-2.631040	-3.975342
H	1.230983	-2.544147	-5.565430
H	4.209802	0.132153	-2.974292
O	4.513652	1.055899	-3.246647
C	3.544378	1.805946	-3.851450
O	2.760883	0.895065	-4.640882
C	1.836787	1.443243	-5.591001
H	1.500974	2.430735	-5.262245
H	0.963446	0.784667	-5.576509
C	2.455014	1.470051	-6.985502
H	2.816949	0.458811	-7.205377
H	1.665246	1.683082	-7.716700
C	3.597212	2.479367	-7.157575
H	3.180599	3.494102	-7.196038
H	4.065313	2.311294	-8.133901
C	4.682988	2.445963	-6.068853
H	5.107953	1.441380	-5.973526
H	5.498739	3.098314	-6.394428
C	4.196114	2.930815	-4.691164
H	3.428763	3.696291	-4.836694
C	5.327702	3.583952	-3.860060
H	4.955809	3.779872	-2.850691
C	5.819280	4.831478	-4.440164
H	6.150648	2.872630	-3.751599
C	6.213382	5.861694	-4.921744
H	6.566904	6.774517	-5.339528
O	0.039732	2.461571	3.705681
C	-0.428176	1.615774	2.979468
O	2.688220	2.480181	-2.940221
C	2.127971	1.687141	-1.891649
H	2.919749	1.371491	-1.203931
H	1.670438	0.783996	-2.310023
C	1.087642	2.531396	-1.171221
H	1.565803	3.448320	-0.808869
H	0.325078	2.843925	-1.893733

C	0.427782	1.788261	-0.005117
H	1.197575	1.486885	0.715553
H	-0.024555	0.857544	-0.370115
C	-0.645560	2.631071	0.692258
H	-0.198547	3.546906	1.094891
H	-1.392409	2.944882	-0.043690
C	-1.384367	1.901768	1.831952
H	-1.769338	0.948472	1.462402
C	-2.566035	2.741096	2.385932
H	-2.992386	2.237557	3.260723
C	-3.626954	2.961072	1.407594
H	-2.181523	3.700547	2.745371
C	-4.504356	3.129090	0.602446
H	-5.283927	3.286460	-0.105195
O	-0.156322	0.301780	3.094260
C	0.750753	-0.069566	4.173291
C	0.872132	-1.566658	4.191309
H	0.340302	0.320235	5.106783
H	1.712775	0.415088	4.002020
C	2.058421	-2.190754	3.799601
C	-0.204532	-2.358467	4.606604
C	2.172293	-3.580583	3.826478
H	2.900822	-1.586927	3.475521
C	-0.096759	-3.745489	4.627608
H	-1.131653	-1.883758	4.913694
H	3.102783	-4.051815	3.526932
C	1.094404	-4.360041	4.239069
H	-0.938468	-4.348192	4.953040
H	1.181103	-5.441543	4.262182
H	2.592482	-1.059094	-4.294065

85 atoms
addition of another 3-isomer unit to the 3-isomer chain end, structure TSr, in toluene

N	3.706604	-3.892185	-2.838823
C	3.583587	-2.559412	-3.156897
N	4.458470	-1.638782	-2.868797
C	5.695709	-2.049665	-2.223470
C	5.466636	-3.202696	-1.247979
C	4.804381	-4.358329	-1.988932
C	1.748201	-4.445962	-4.264345
C	1.289962	-3.022890	-3.970000
N	2.468873	-2.184764	-3.864271
C	2.700036	-4.903196	-3.165343
H	6.113442	-1.183501	-1.702687
H	6.444278	-2.347514	-2.974439

H	4.815383	-2.860497	-0.436765
H	6.403987	-3.542657	-0.797909
H	5.540934	-4.893086	-2.604007
H	4.397915	-5.086166	-1.277432
H	3.221489	-5.816563	-3.472934
H	2.130987	-5.155571	-2.258149
H	2.254867	-4.463012	-5.233638
H	0.898172	-5.131253	-4.317025
H	0.680537	-3.004591	-3.052749
H	0.666899	-2.637412	-4.780073
H	4.206269	0.043684	-2.964954
O	4.243981	1.046015	-2.855780
C	3.326402	1.742661	-3.600356
O	2.586239	0.768799	-4.347345
C	1.752523	1.221939	-5.423803
H	1.404714	2.239977	-5.227624
H	0.871712	0.573629	-5.411796
C	2.481533	1.097123	-6.757932
H	2.854881	0.069216	-6.831685
H	1.754111	1.223502	-7.569434
C	3.637200	2.087383	-6.947157
H	3.228688	3.089017	-7.132952
H	4.185018	1.814242	-7.855885
C	4.626211	2.181242	-5.773644
H	5.045548	1.196663	-5.539116
H	5.464962	2.805732	-6.095164
C	4.021482	2.797293	-4.499106
H	3.260596	3.530375	-4.782485
C	5.076620	3.549690	-3.651834
H	4.621781	3.843953	-2.702038
C	5.607999	4.736943	-4.316705
H	5.890784	2.863746	-3.403296
C	6.036496	5.717395	-4.867850
H	6.418539	6.587231	-5.347623
O	-0.123948	2.710651	3.926544
C	-0.664250	1.937050	3.170406
O	2.440369	2.485182	-2.782911
C	1.822396	1.762906	-1.714755
H	2.592449	1.382083	-1.037369
H	1.274149	0.902294	-2.116747
C	0.876097	2.711088	-0.994427
H	1.446408	3.577163	-0.640383
H	0.142534	3.094813	-1.712720
C	0.156224	2.041728	0.180856
H	0.899742	1.654622	0.887713
H	-0.401719	1.167651	-0.177857
C	-0.805807	2.994742	0.898096

H	-0.253166	3.853035	1.296682
H	-1.524644	3.393991	0.175731
C	-1.604833	2.347036	2.047901
H	-2.105606	1.449431	1.677451
C	-2.667351	3.314955	2.630347
H	-3.134963	2.857089	3.509072
C	-3.711629	3.669272	1.673692
H	-2.165208	4.218054	2.990667
C	-4.576518	3.947392	0.885670
H	-5.343909	4.202470	0.193385
O	-0.490809	0.602894	3.219551
C	0.416038	0.114720	4.253143
C	0.454938	-1.383876	4.167995
H	0.045861	0.462013	5.219133
H	1.398089	0.560044	4.088309
C	1.495587	-2.032786	3.498480
C	-0.559940	-2.152134	4.748109
C	1.525309	-3.423490	3.411911
H	2.289101	-1.446487	3.044686
C	-0.535435	-3.541187	4.660594
H	-1.372739	-1.657904	5.272170
H	2.342529	-3.915159	2.894148
C	0.509244	-4.179859	3.992443
H	-1.327146	-4.126031	5.117497
H	0.532259	-5.262997	3.928753
H	2.390558	-1.182805	-3.997932

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

N	4.725764	-3.899243	-3.957607
C	4.265640	-2.607555	-3.860057
N	4.992156	-1.579812	-3.516233
C	6.411675	-1.795300	-3.280484
C	6.677648	-3.155232	-2.638024
C	6.079651	-4.245823	-3.518345
C	2.597586	-4.612583	-5.027154
C	1.975191	-3.456658	-4.254322
N	2.951106	-2.385027	-4.185917
C	3.887597	-5.038518	-4.336402
H	6.777949	-0.990107	-2.637213
H	6.977075	-1.718189	-4.222304
H	6.212261	-3.181092	-1.647226
H	7.748343	-3.335528	-2.504743
H	6.714432	-4.422425	-4.397271
H	6.026109	-5.193310	-2.970446

H	4.473715	-5.688586	-4.995641
H	3.654218	-5.628989	-3.438131
H	2.806318	-4.285617	-6.049903
H	1.915683	-5.465311	-5.079742
H	1.658892	-3.795703	-3.255564
H	1.086736	-3.077422	-4.763447
H	4.254050	-0.171010	-2.888494
O	3.850042	0.605809	-2.388644
C	3.093182	1.419148	-3.197678
O	2.251780	0.531457	-3.957651
C	1.494501	1.070955	-5.050594
H	1.261288	2.123160	-4.862550
H	0.546295	0.526344	-5.050427
C	2.221627	0.863532	-6.376390
H	2.480409	-0.199043	-6.447405
H	1.521904	1.069537	-7.195977
C	3.482157	1.718478	-6.553053
H	3.190145	2.761195	-6.733068
H	4.000931	1.391493	-7.461192
C	4.469145	1.690161	-5.374610
H	4.774589	0.662308	-5.151428
H	5.373670	2.220744	-5.687328
C	3.930949	2.367281	-4.100257
H	3.267044	3.186496	-4.392033
C	5.059538	2.993297	-3.244124
H	4.637780	3.324076	-2.291284
C	5.715423	4.124101	-3.896689
H	5.800673	2.226435	-3.000902
C	6.248689	5.058058	-4.436989
H	6.721341	5.887488	-4.907544
O	-0.512915	3.119800	4.075484
C	-1.096763	2.321847	3.379226
O	2.305728	2.270141	-2.405672
C	1.572415	1.649566	-1.341704
H	2.269850	1.275673	-0.587342
H	1.009054	0.795634	-1.732446
C	0.637788	2.694846	-0.752742
H	1.231662	3.560305	-0.437725
H	-0.039972	3.051703	-1.536663
C	-0.168792	2.156018	0.433206
H	0.522199	1.788907	1.201562
H	-0.756329	1.285463	0.115763
C	-1.107307	3.209224	1.031799
H	-0.526068	4.069379	1.382824
H	-1.778344	3.582286	0.251793
C	-1.977571	2.695900	2.196946
H	-2.518251	1.801828	1.877792

C	-2.999450	3.762596	2.669700
H	-3.523069	3.396126	3.559664
C	-3.987642	4.107558	1.652027
H	-2.455983	4.658657	2.984939
C	-4.806578	4.379232	0.814242
H	-5.533304	4.628223	0.077311
O	-1.032851	0.989357	3.557205
C	-0.185454	0.530056	4.653356
C	-0.261827	-0.968538	4.701289
H	-0.543243	0.989422	5.575927
H	0.830286	0.884204	4.471348
C	0.648088	-1.750050	3.983359
C	-1.257498	-1.604143	5.449309
C	0.566317	-3.140329	4.012688
H	1.426111	-1.266919	3.399683
C	-1.342762	-2.993866	5.480585
H	-1.968957	-1.006391	6.011600
H	1.281265	-3.735615	3.454060
C	-0.429940	-3.764566	4.761758
H	-2.118009	-3.475141	6.067928
H	-0.492761	-4.847659	4.788307
H	2.633877	-1.436799	-4.012095

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

N	3.713404	3.574203	0.883876
C	3.413255	2.282384	0.594936
N	3.545848	1.828302	-0.661825
C	4.036175	2.655073	-1.754551
C	3.594789	4.097037	-1.535420
C	4.048298	4.555104	-0.155020
C	3.776894	2.944874	3.281045
C	2.749444	1.885197	2.898151
N	2.987750	1.442257	1.533155
C	3.732488	4.077622	2.262816
H	3.629934	2.249152	-2.681607
H	5.130019	2.597741	-1.824341
H	2.505319	4.159283	-1.612308
H	4.021259	4.755869	-2.295438
H	5.131333	4.732850	-0.145742
H	3.565350	5.500097	0.111993
H	4.609260	4.723840	2.370390
H	2.847318	4.705690	2.424281
H	4.773189	2.493261	3.297236
H	3.577422	3.345232	4.277948

H	1.732426	2.285354	3.004907
H	2.820132	1.011118	3.546893
H	3.148112	0.906298	-0.888745
O	2.327695	-0.516693	-1.476847
C	2.364127	-1.633749	-0.944569
O	2.793764	-1.094585	0.978262
C	3.394184	-1.974168	1.870993
H	3.012082	-3.003182	1.729989
H	3.131395	-1.713283	2.915809
C	4.927719	-1.984075	1.758674
H	5.269952	-0.943764	1.841196
H	5.358415	-2.520793	2.616415
C	5.486051	-2.602078	0.469385
H	5.354268	-3.691652	0.504886
H	6.571207	-2.439781	0.452160
C	4.902371	-2.091072	-0.860760
H	4.883764	-0.998138	-0.879056
H	5.589300	-2.402032	-1.654958
C	3.497291	-2.628453	-1.198047
H	3.291138	-3.523087	-0.607138
C	3.375973	-3.029528	-2.698683
H	2.336026	-3.294400	-2.915276
C	4.236528	-4.146168	-3.078283
H	3.607510	-2.154997	-3.316135
C	4.944273	-5.071118	-3.381699
H	5.564825	-5.892242	-3.652604
O	-5.905708	-1.830793	-1.218381
C	-5.420280	-1.228535	-0.288852
O	1.215240	-2.321572	-0.672144
C	0.045543	-1.520423	-0.462649
H	-0.192872	-0.972177	-1.379360
H	0.270620	-0.794459	0.322606
C	-1.088993	-2.446756	-0.057267
H	-1.237273	-3.197404	-0.842278
H	-0.792644	-2.993073	0.844809
C	-2.396442	-1.688918	0.195589
H	-2.679121	-1.140972	-0.711648
H	-2.235563	-0.928101	0.969514
C	-3.538490	-2.615207	0.626871
H	-3.736960	-3.353725	-0.158090
H	-3.232520	-3.176796	1.514987
C	-4.855641	-1.885807	0.960821
H	-4.658374	-1.103987	1.697961
C	-5.927463	-2.853972	1.526559
H	-6.874669	-2.317056	1.649757
C	-5.553225	-3.445890	2.807427
H	-6.118186	-3.640707	0.790214

C	-5.245709	-3.920854	3.868628
H	-4.977473	-4.348977	4.805630
O	-5.310218	0.112617	-0.245735
C	-5.806846	0.832655	-1.413471
C	-5.627253	2.302127	-1.162930
H	-6.855033	0.565700	-1.556780
H	-5.249677	0.494293	-2.288254
C	-4.491635	2.970505	-1.628442
C	-6.587578	3.019836	-0.442827
C	-4.318601	4.330987	-1.382140
H	-3.739331	2.423057	-2.188574
C	-6.417030	4.378865	-0.192790
H	-7.474255	2.510103	-0.077282
H	-3.434486	4.839167	-1.753343
C	-5.281279	5.037314	-0.663345
H	-7.171098	4.925157	0.364496
H	-5.149562	6.097657	-0.473295
H	2.903186	0.381830	1.294320

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

N	0.524053	3.667490	1.361100
C	1.219361	2.564246	0.920711
N	1.498015	2.500301	-0.418094
C	1.327892	3.614156	-1.329994
C	0.028947	4.329499	-0.979471
C	0.072081	4.748545	0.484681
C	1.212036	3.015127	3.644111
C	1.188155	1.597699	3.074944
N	1.598784	1.571013	1.678715
C	0.316242	3.905237	2.791411
H	1.299319	3.218105	-2.347068
H	2.171450	4.319779	-1.280457
H	-0.812831	3.652436	-1.152590
H	-0.115330	5.213445	-1.606493
H	0.734245	5.618731	0.606745
H	-0.923425	5.062048	0.818639
H	0.521419	4.962890	2.994632
H	-0.740799	3.734518	3.037103
H	2.239776	3.392611	3.624142
H	0.872240	3.040292	4.683759
H	0.177299	1.175716	3.193226
H	1.860206	0.943929	3.637693
H	2.005633	1.680390	-0.726877
O	2.943079	0.118325	-1.562472

C	3.223383	-0.968127	-1.096442
O	3.859288	-0.036565	1.492955
C	4.953087	0.849864	1.655426
H	5.686052	0.356499	2.307167
H	4.624202	1.760536	2.175374
C	5.643730	1.254105	0.349009
H	4.908780	1.709857	-0.322811
H	6.355617	2.049241	0.607708
C	6.418667	0.135601	-0.381077
H	6.792940	-0.587421	0.355524
H	7.314168	0.582847	-0.827456
C	5.715736	-0.626522	-1.518786
H	5.315507	0.085591	-2.246949
H	6.491570	-1.195593	-2.040134
C	4.603128	-1.613123	-1.127999
H	4.774708	-2.005872	-0.123532
C	4.538928	-2.827549	-2.104819
H	3.663554	-3.436161	-1.864308
C	5.729760	-3.670762	-2.056089
H	4.395393	-2.462012	-3.128881
C	6.708491	-4.368065	-2.005155
H	7.571745	-4.989212	-1.960419
O	-4.702596	-3.378711	-1.030242
C	-4.379145	-2.517500	-0.245423
O	2.318593	-1.794413	-0.558432
C	0.950124	-1.321828	-0.470968
H	0.615372	-1.032704	-1.470711
H	0.934167	-0.438741	0.170711
C	0.111760	-2.449085	0.103841
H	0.193518	-3.329085	-0.544095
H	0.524329	-2.734884	1.077140
C	-1.358576	-2.043437	0.255787
H	-1.755903	-1.744436	-0.721506
H	-1.429354	-1.155085	0.894690
C	-2.215804	-3.165197	0.851404
H	-2.183117	-4.047187	0.201653
H	-1.794038	-3.469798	1.814135
C	-3.691460	-2.779828	1.085433
H	-3.733114	-1.862665	1.677638
C	-4.469440	-3.897240	1.827200
H	-5.530210	-3.628555	1.880557
C	-3.977206	-4.142484	3.179490
H	-4.419750	-4.816759	1.236095
C	-3.574491	-4.330504	4.296951
H	-3.220740	-4.506178	5.285525
O	-4.574492	-1.202721	-0.459417
C	-5.206657	-0.847942	-1.725371

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C     -5.316601     0.648334    -1.787699
H     -6.183304    -1.333947    -1.762374
H     -4.600461    -1.247746    -2.539095
C     -4.411946     1.398356    -2.543233
C     -6.322667     1.314057    -1.079393
C     -4.510560     2.788012    -2.594416
H     -3.627540     0.892324    -3.098285
C     -6.421498     2.701690    -1.124451
H     -7.032045     0.740502    -0.490125
H     -3.805948     3.357981    -3.191286
C     -5.515199     3.441794    -1.884007
H     -7.208062     3.206031    -0.572604
H     -5.595577     4.523270    -1.924882
H      3.029861     0.502741     1.458261
```

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

```
N     -6.029017    -3.964079    -4.371826
C     -5.477716    -2.898538    -3.697232
N     -5.979186    -2.627738    -2.445094
C     -6.766604    -3.583486    -1.689997
C     -7.787646    -4.205068    -2.634210
C     -7.058502    -4.840555    -3.811781
C     -4.102668    -3.803601    -5.909281
C     -4.110019    -2.322013    -5.535657
N     -4.551088    -2.111133    -4.166803
C     -5.489764    -4.385983    -5.666148
H     -7.260492    -3.049924    -0.875170
H     -6.144749    -4.370811    -1.235225
H     -8.466943    -3.424068    -2.987928
H     -8.385204    -4.964799    -2.123559
H     -6.598491    -5.790270    -3.499886
H     -7.769125    -5.083391    -4.609754
H     -5.451553    -5.481204    -5.677783
H     -6.179539    -4.083911    -6.466197
H     -3.367889    -4.326476    -5.287941
H     -3.817710    -3.954741    -6.954747
H     -4.754431    -1.771410    -6.239434
H     -3.108039    -1.896827    -5.645387
H     -5.471564    -1.903974    -1.949390
O      0.785725    -2.795254     2.692877
C      1.232020    -2.467667     1.617576
O     -4.036772    -0.365465    -2.090880
C     -2.706621    -0.396847    -1.597112
H     -2.674948     0.289904    -0.744546
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H	-2.007793	-0.002999	-2.350718
C	-2.252324	-1.790685	-1.157495
H	-2.952304	-2.162694	-0.399276
H	-2.328822	-2.471926	-2.012871
C	-0.824556	-1.807411	-0.602337
H	-0.757374	-1.109016	0.241042
H	-0.130139	-1.428238	-1.362813
C	-0.376419	-3.205419	-0.162577
H	-1.038131	-3.577472	0.627971
H	-0.474676	-3.897812	-1.004549
C	1.079738	-3.280030	0.341142
H	1.744560	-2.855832	-0.415027
C	1.516092	-4.738698	0.635759
H	2.514957	-4.736325	1.085987
C	1.538923	-5.587049	-0.552178
H	0.845447	-5.163930	1.388726
C	1.569564	-6.277950	-1.536144
H	1.597918	-6.896810	-2.401806
O	6.177370	3.216519	4.880530
C	5.000057	3.470272	4.990879
O	1.915687	-1.328042	1.410214
C	2.091364	-0.457961	2.557527
H	2.611674	-1.015160	3.340304
H	1.105940	-0.184146	2.941984
C	2.881201	0.753821	2.098524
H	3.837511	0.418882	1.682334
H	2.338584	1.244192	1.283182
C	3.124602	1.749117	3.238521
H	3.651667	1.242522	4.055889
H	2.163933	2.076338	3.654254
C	3.922415	2.974132	2.778642
H	4.901679	2.660443	2.400060
H	3.401591	3.453123	1.943879
C	4.135647	4.037076	3.874456
H	3.169316	4.317305	4.299832
C	4.829451	5.308345	3.318739
H	5.048184	5.993547	4.145141
C	4.029155	6.013823	2.322281
H	5.797589	5.026809	2.893174
C	3.359220	6.596417	1.511089
H	2.773640	7.117287	0.790577
O	4.296095	3.273448	6.120041
C	5.035277	2.714039	7.248419
C	4.085362	2.578726	8.402838
H	5.866170	3.383913	7.474891
H	5.450008	1.752457	6.942976
C	3.398710	1.381186	8.621947

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C      3.858331     3.656813     9.263989
C      2.502441     1.261132     9.681736
H      3.568183     0.536912     7.960070
C      2.962497     3.540932    10.323710
H      4.387430     4.591642     9.103386
H      1.977968     0.324952     9.842837
C      2.282810     2.341684    10.534290
H      2.797149     4.383835    10.986821
H      1.586947     2.249039    11.361824
H     -4.083177    -0.859147    -2.950210
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85 atoms
addition of another 3-isomer unit to the 7-isomer chain end, structure I1, in toluene

```
N      4.928319    -3.712914     3.963660
C      3.579344    -3.862412     4.201004
N      2.735116    -3.631335     3.141031
C      3.206790    -3.625626     1.766967
C      4.471006    -2.781378     1.705830
C      5.502534    -3.366027     2.661913
C      5.300159    -4.900368     6.092290
C      3.951344    -4.309493     6.494336
N      3.055508    -4.163287     5.357048
C      5.910350    -4.031655     5.000802
H      2.416361    -3.205072     1.143125
H      3.409190    -4.642302     1.395210
H      4.227966    -1.753833     1.991585
H      4.883675    -2.759625     0.693794
H      5.959460    -4.263061     2.218043
H      6.315307    -2.649981     2.829146
H      6.750161    -4.549515     4.523912
H      6.312029    -3.102156     5.427768
H      5.150779    -5.917803     5.715510
H      5.983676    -4.960169     6.944466
H      4.116444    -3.338026     6.988112
H      3.462063    -4.948128     7.236218
H      1.785441    -3.953305     3.275314
O     -0.161695    -4.582978     2.616197
C     -0.386159    -5.532447     3.336611
O      0.626463    -6.381449     3.582943
C      0.558680    -7.421804     4.591400
H      0.219063    -6.978362     5.529132
H      1.602288    -7.708170     4.715840
C     -0.276235    -8.617946     4.155482
H      0.022310    -8.892342     3.136983
H     -0.002184    -9.464911     4.795004
```

C	-1.790083	-8.400227	4.232134
H	-2.081633	-8.281181	5.283137
H	-2.298551	-9.302701	3.876792
C	-2.311993	-7.194869	3.442419
H	-2.108826	-7.320798	2.372016
H	-3.400097	-7.166674	3.544746
C	-1.761348	-5.828643	3.919887
H	-1.644235	-5.851977	5.007643
C	-2.715228	-4.662820	3.574264
H	-2.226489	-3.716270	3.816378
C	-3.991574	-4.744229	4.280033
H	-2.889099	-4.639569	2.493548
C	-5.037423	-4.812357	4.870632
H	-5.964012	-4.862506	5.392212
O	-0.190449	2.986615	4.346633
O	0.367001	-4.449635	6.029155
C	-0.846286	2.926117	5.359367
C	-1.037744	1.696727	6.221555
H	-2.114874	1.543640	6.351119
H	-0.660144	1.934670	7.222906
C	-0.363715	0.444340	5.663804
H	-0.759063	0.234090	4.664413
H	0.704796	0.639463	5.525395
C	-0.557765	-0.777027	6.569079
H	-1.630628	-0.966926	6.701914
H	-0.169384	-0.553998	7.567715
C	0.116997	-2.031442	6.003695
H	-0.234370	-2.198534	4.979321
H	1.199003	-1.869839	5.925141
C	-0.124979	-3.341239	6.769338
H	-1.203301	-3.507440	6.867810
C	0.488645	-3.373005	8.199226
H	0.567011	-4.429234	8.475845
C	-0.270238	-2.678446	9.235571
H	1.513951	-2.985820	8.163851
C	-0.910901	-2.142722	10.102074
H	-1.477053	-1.657973	10.861926
O	-1.512959	3.981695	5.875156
C	-1.400302	5.230688	5.136910
C	-2.199622	6.272941	5.865644
H	-1.770397	5.067127	4.123291
H	-0.344502	5.498872	5.069981
C	-3.555668	6.456630	5.579496
C	-1.605302	7.059982	6.856388
C	-4.303577	7.408992	6.267733
H	-4.027567	5.850069	4.812009
C	-2.349636	8.013608	7.546931

H	-0.552533	6.925189	7.087067
H	-5.354615	7.543888	6.033577
C	-3.701026	8.189731	7.253208
H	-1.875279	8.620501	8.311377
H	-4.281644	8.934464	7.788018
H	1.317559	-4.302952	5.766746

85 atoms
addition of another 3-isomer unit to the 7-isomer chain end, structure TS12, in toluene

N	3.820732	3.873844	-0.145371
C	3.458680	2.568421	-0.224973
N	3.145977	2.020533	-1.400102
C	3.268325	2.739704	-2.658999
C	2.935481	4.208379	-2.435155
C	3.813457	4.757772	-1.318128
C	4.708346	3.445412	2.123711
C	3.665114	2.339859	2.210081
N	3.403503	1.812645	0.879002
C	4.248714	4.490268	1.115727
H	2.580244	2.279449	-3.369401
H	4.280946	2.632984	-3.069593
H	1.880178	4.305253	-2.163968
H	3.099391	4.788199	-3.346319
H	4.843672	4.897765	-1.669298
H	3.447728	5.735707	-0.991999
H	5.064274	5.181432	0.884593
H	3.424598	5.087897	1.525739
H	5.666179	3.020094	1.810130
H	4.855378	3.916677	3.098141
H	2.742831	2.723262	2.666503
H	4.014603	1.512571	2.829566
H	2.934310	0.994082	-1.444064
O	2.515367	-0.604087	-1.597071
C	3.117445	-1.327958	-0.761391
O	4.465894	-0.958869	-0.606319
C	5.306288	-1.661159	0.315805
H	4.710197	-2.037728	1.149476
H	5.994160	-0.909814	0.715147
C	6.088634	-2.768410	-0.380615
H	6.583285	-2.332047	-1.256574
H	6.886604	-3.114264	0.288871
C	5.224665	-3.958865	-0.806460
H	4.913187	-4.518263	0.085551
H	5.838781	-4.650477	-1.394794
C	3.970892	-3.598871	-1.616342

H	4.241910	-3.006165	-2.497690
H	3.542519	-4.533037	-1.993455
C	2.864355	-2.861098	-0.826321
H	2.835393	-3.269858	0.186743
C	1.488875	-3.115985	-1.493852
H	0.739680	-2.433298	-1.090149
C	1.018959	-4.491352	-1.339013
H	1.561785	-2.864018	-2.556032
C	0.632437	-5.622941	-1.199700
H	0.284181	-6.621056	-1.076603
O	-4.306471	2.090262	-0.499519
O	2.624741	-0.862439	0.886212
C	-4.584960	0.997356	-0.065242
C	-3.613005	0.010119	0.544233
H	-3.815712	-0.976044	0.114247
H	-3.868358	-0.081802	1.607241
C	-2.146978	0.404153	0.370220
H	-1.915820	0.475741	-0.698298
H	-1.994116	1.409619	0.776071
C	-1.186765	-0.581866	1.044698
H	-1.358439	-1.589469	0.643556
H	-1.420305	-0.643575	2.111829
C	0.282117	-0.195629	0.835885
H	0.480497	-0.093544	-0.234494
H	0.469159	0.794393	1.274108
C	1.343792	-1.175823	1.377640
H	1.061461	-2.199086	1.087412
C	1.463485	-1.177589	2.931009
H	2.411390	-1.672110	3.164915
C	0.396964	-1.847111	3.670994
H	1.562950	-0.142320	3.279821
C	-0.453165	-2.427909	4.294844
H	-1.214758	-2.939449	4.834342
O	-5.842106	0.503259	-0.055061
C	-6.875952	1.375449	-0.591031
C	-8.191341	0.659084	-0.477519
H	-6.627858	1.610083	-1.627535
H	-6.868461	2.308182	-0.024053
C	-8.673375	-0.115034	-1.536730
C	-8.943671	0.738968	0.698355
C	-9.884321	-0.794936	-1.425683
H	-8.096497	-0.185331	-2.454278
C	-10.154109	0.060103	0.813841
H	-8.578176	1.337284	1.527896
H	-10.248519	-1.390108	-2.256831
C	-10.627011	-0.708214	-0.249366
H	-10.729702	0.132659	1.731001

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H    -11.571693    -1.235208    -0.162051
H      3.108569     0.816308     0.805588


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure I2, in toluene
N     -2.176464    -0.903848    -4.831223
C     -1.724476    -0.405857    -3.629909
N     -1.471746     0.850217    -3.394556
C     -1.745119     1.813545    -4.449791
C     -1.451898     1.234868    -5.831985
C     -2.258169    -0.044835    -6.014668
C     -2.655391    -3.101581    -3.781093
C     -1.539713    -2.739684    -2.809521
N     -1.564558    -1.304312    -2.603947
C     -2.462047    -2.318210    -5.073232
H     -1.132902     2.701900    -4.269680
H     -2.793430     2.148551    -4.406236
H     -0.382180     1.014556    -5.909244
H     -1.700979     1.944008    -6.626866
H     -3.310931     0.189856    -6.223756
H     -1.883491    -0.613538    -6.873378
H     -3.363813    -2.381659    -5.692606
H     -1.644209    -2.760666    -5.661502
H     -3.618919    -2.851002    -3.327899
H     -2.654698    -4.172490    -4.000635
H     -0.572043    -3.088811    -3.204065
H     -1.688880    -3.224909    -1.842453
H     -0.956596     1.495493    -1.913605
O     -0.564408     1.952888    -1.097393
C     -0.705233     1.166531     0.005410
O     -2.058091     0.784532     0.070723
C     -2.502414    -0.017733     1.173231
H     -1.667585    -0.589830     1.587365
H     -3.213941    -0.732371     0.751467
C     -3.175618     0.849150     2.228031
H     -3.974697     1.417054     1.737941
H     -3.660682     0.198613     2.966467
C     -2.213579     1.808305     2.934396
H     -1.545715     1.238161     3.593705
H     -2.793119     2.464908     3.592768
C     -1.357554     2.681524     2.003390
H     -1.989952     3.194903     1.271580
H     -0.897406     3.462392     2.616605
C     -0.214601     1.950711     1.264536
H      0.223454     1.225198     1.957128
```

C	0.886826	2.980691	0.885943
H	1.579026	2.566453	0.151156
C	1.645884	3.449379	2.043693
H	0.413817	3.828529	0.382848
C	2.274443	3.820250	3.000536
H	2.834103	4.153201	3.842484
O	5.304511	1.007498	-5.512781
O	-0.027922	-0.120840	-0.146113
C	5.983563	0.977861	-4.513851
C	5.495306	0.646243	-3.119496
H	5.875080	1.413340	-2.436573
H	5.990791	-0.282942	-2.812810
C	3.976607	0.513538	-3.019752
H	3.509364	1.455257	-3.326827
H	3.632029	-0.237443	-3.737940
C	3.510643	0.137650	-1.608914
H	3.866308	0.891156	-0.894182
H	3.981024	-0.803227	-1.308732
C	1.983622	0.029268	-1.521796
H	1.534514	0.955854	-1.885468
H	1.626306	-0.761150	-2.193206
C	1.406393	-0.232554	-0.123439
H	1.823236	0.477407	0.596012
C	1.663975	-1.657897	0.423100
H	0.948788	-1.824432	1.234438
C	3.009268	-1.903041	0.935103
H	1.420547	-2.390230	-0.355377
C	4.098084	-2.117526	1.398857
H	5.067774	-2.298112	1.799169
O	7.308917	1.234631	-4.509875
C	7.902634	1.551374	-5.800779
C	9.365681	1.813909	-5.584982
H	7.387678	2.421000	-6.212553
H	7.733319	0.709989	-6.474986
C	9.817065	3.099327	-5.270900
C	10.295376	0.773652	-5.672323
C	11.170594	3.341796	-5.049583
H	9.103269	3.914857	-5.200039
C	11.650071	1.012037	-5.452131
H	9.955794	-0.229038	-5.915240
H	11.508260	4.344841	-4.809672
C	12.089950	2.297545	-5.140173
H	12.361900	0.196260	-5.526442
H	13.145345	2.485575	-4.971254
H	-1.136264	-0.924987	-1.767842

85 atoms
addition of another 3-isomer unit to the 7-isomer chain end, structure TS23, in toluene

N	-2.018469	-0.841772	-4.870048
C	-1.775237	-0.335435	-3.613787
N	-1.429041	0.894086	-3.360260
C	-1.360559	1.829600	-4.472284
C	-0.858079	1.155768	-5.747207
C	-1.752275	-0.036541	-6.064518
C	-2.915273	-2.942570	-3.890733
C	-2.000091	-2.631838	-2.713323
N	-1.950793	-1.190987	-2.553225
C	-2.389117	-2.233093	-5.132444
H	-0.698024	2.651955	-4.187479
H	-2.347707	2.280793	-4.658940
H	0.171644	0.817525	-5.592897
H	-0.853755	1.848300	-6.593983
H	-2.704367	0.300213	-6.496951
H	-1.276235	-0.683010	-6.810380
H	-3.148344	-2.240172	-5.922607
H	-1.516231	-2.772181	-5.529954
H	-3.925780	-2.595581	-3.656453
H	-2.964053	-4.018158	-4.079902
H	-1.003220	-3.068263	-2.884285
H	-2.388819	-3.064871	-1.789287
H	-0.954097	1.483890	-1.838057
O	-0.575355	1.920734	-1.005624
C	-0.702620	1.105279	0.079157
O	-2.041415	0.648476	0.093177
C	-2.482942	-0.175632	1.182620
H	-1.634916	-0.707688	1.622209
H	-3.146383	-0.922358	0.737941
C	-3.234181	0.653512	2.214060
H	-4.040085	1.185871	1.696163
H	-3.715440	-0.023872	2.930460
C	-2.345776	1.652092	2.960651
H	-1.676382	1.109876	3.641547
H	-2.980103	2.276003	3.599999
C	-1.499590	2.570514	2.065470
H	-2.129494	3.058790	1.314483
H	-1.099045	3.368040	2.698759
C	-0.298591	1.900230	1.362342
H	0.151239	1.189350	2.062586
C	0.763199	2.987417	1.031363
H	1.499151	2.617051	0.316088
C	1.459372	3.478342	2.218994
H	0.265597	3.816961	0.521725

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C      2.037598     3.866892     3.200236
H      2.552569     4.215935     4.063904
O      5.225008     1.009069    -5.534263
O      0.032440    -0.138648    -0.059473
C      5.934224     0.996740    -4.556048
C      5.485558     0.704309    -3.139756
H      5.870187     1.499436    -2.492288
H      6.002545    -0.206520    -2.814550
C      3.971920     0.553774    -2.998993
H      3.483888     1.480456    -3.319300
H      3.621698    -0.220572    -3.689190
C      3.542799     0.207059    -1.569055
H      3.898212     0.985344    -0.881284
H      4.037312    -0.716947    -1.255341
C      2.020353     0.071866    -1.450113
H      1.546745     0.984284    -1.818529
H      1.664665    -0.735870    -2.101476
C      1.468646    -0.182299    -0.040627
H      1.859207     0.560972     0.660099
C      1.794439    -1.582996     0.532724
H      1.088149    -1.768024     1.347805
C      3.150038    -1.752031     1.048248
H      1.585319    -2.340297    -0.231535
C      4.248504    -1.901427     1.514924
H      5.226096    -2.025113     1.917592
O      7.261297     1.240159    -4.599022
C      7.817692     1.519847    -5.914889
C      9.290052     1.767483    -5.751350
H      7.300972     2.386821    -6.330101
H      7.616427     0.665889    -6.564007
C      9.766827     3.052223    -5.474142
C     10.203805     0.714337    -5.851165
C     11.129671     3.281366    -5.301229
H      9.065514     3.877680    -5.394022
C     11.567775     0.939380    -5.679390
H      9.844457    -0.287953    -6.065617
H     11.487037     4.283949    -5.089607
C     12.032997     2.224282    -5.403941
H     12.266946     0.113613    -5.762919
H     13.095543     2.401871    -5.272793
H     -1.663745    -0.809507    -1.661877


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure I3, in toluene
N     -2.497578    -1.007262    -4.807319
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C	-2.182842	-0.404301	-3.611119
N	-1.223367	0.461451	-3.443283
C	-0.466839	0.881769	-4.612520
C	-0.285428	-0.259641	-5.610535
C	-1.654160	-0.811544	-5.988446
C	-4.587545	-1.928798	-3.832450
C	-3.842754	-1.870131	-2.505248
N	-2.968935	-0.712231	-2.528620
C	-3.575628	-1.983295	-4.970170
H	0.505553	1.253658	-4.277810
H	-0.964234	1.728643	-5.110828
H	0.317562	-1.048524	-5.148871
H	0.240402	0.073045	-6.510071
H	-2.160535	-0.136763	-6.692226
H	-1.550366	-1.777863	-6.494841
H	-4.071503	-1.786064	-5.927229
H	-3.144741	-2.993206	-5.041038
H	-5.215457	-1.038195	-3.927707
H	-5.238091	-2.805976	-3.881409
H	-3.288872	-2.808210	-2.341374
H	-4.539064	-1.755109	-1.671511
H	-0.814033	1.155316	-1.951690
O	-0.511355	1.662663	-1.127261
C	-0.540131	0.885463	-0.008918
O	-1.853261	0.336727	0.078074
C	-2.180661	-0.478716	1.214989
H	-1.270588	-0.904454	1.643555
H	-2.777535	-1.310869	0.831097
C	-2.974512	0.327934	2.232265
H	-3.845401	0.754368	1.721193
H	-3.363881	-0.352636	2.999568
C	-2.161265	1.444539	2.893791
H	-1.431451	1.004418	3.585979
H	-2.834250	2.047307	3.513527
C	-1.417661	2.378635	1.925525
H	-2.102646	2.768857	1.165846
H	-1.072664	3.241215	2.503760
C	-0.180244	1.768916	1.230363
H	0.330525	1.125778	1.953985
C	0.797208	2.910558	0.832878
H	1.557416	2.554232	0.135783
C	1.459993	3.515046	1.986922
H	0.240087	3.672645	0.281298
C	2.013184	3.997452	2.940572
H	2.504902	4.429871	3.779721
O	5.438316	1.355931	-5.506015
O	0.276353	-0.295122	-0.108644

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C      6.146486     1.284184    -4.529691
C      5.699509     0.893564    -3.136912
H      6.062994     1.656517    -2.440190
H      6.236686    -0.022890    -2.865001
C      4.189272     0.700510    -3.011377
H      3.681199     1.631864    -3.283608
H      3.858696    -0.043804    -3.743164
C      3.767151     0.268108    -1.602897
H      4.110282     1.013309    -0.873660
H      4.279693    -0.662400    -1.341037
C      2.248267     0.097170    -1.487473
H      1.755922     1.017464    -1.809865
H      1.901968    -0.684732    -2.174194
C      1.710690    -0.238308    -0.089619
H      2.051717     0.505019     0.637849
C      2.128034    -1.634599     0.433934
H      1.415576    -1.907844     1.218084
C      3.477465    -1.720415     0.984831
H      1.998744    -2.371769    -0.366573
C      4.570479    -1.804083     1.479946
H      5.543184    -1.869142     1.907383
O      7.471099     1.543552    -4.553392
C      8.026371     1.918046    -5.845883
C      9.495402     2.171226    -5.661923
H      7.500595     2.804839    -6.203626
H      7.836181     1.107030    -6.551163
C      9.961650     3.451217    -5.348331
C     10.416562     1.126020    -5.778715
C     11.321599     3.684015    -5.156589
H      9.254713     4.270412    -5.254541
C     11.777118     1.354490    -5.587398
H     10.065255     0.127393    -6.021671
H     11.670775     4.683159    -4.916877
C     12.232018     2.635081    -5.275909
H     12.482062     0.535084    -5.684088
H     13.292146     2.815386    -5.129732
H     -2.619868    -0.348721    -1.647655


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure TSr, in toluene
N     -1.986549    -0.598945    -4.948917
C     -1.820077    -0.129652    -3.666565
N     -0.967951     0.792953    -3.316234
C     -0.191595     1.435687    -4.365290
C      0.187963     0.452611    -5.470223
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C	-1.080179	-0.185461	-6.023038
C	-4.038887	-1.821451	-4.271158
C	-3.405190	-1.865594	-2.886760
N	-2.644561	-0.644781	-2.698674
C	-2.943807	-1.643197	-5.315284
H	0.706067	1.868309	-3.914298
H	-0.751756	2.278699	-4.799648
H	0.842321	-0.319695	-5.053661
H	0.736345	0.945728	-6.277815
H	-1.602628	0.512088	-6.691966
H	-0.833554	-1.071463	-6.619056
H	-3.383270	-1.377032	-6.283085
H	-2.408220	-2.592870	-5.463184
H	-4.741920	-0.984536	-4.314613
H	-4.595015	-2.739205	-4.479724
H	-2.779575	-2.766643	-2.786434
H	-4.170531	-1.914109	-2.108865
H	-0.723868	1.311176	-1.719811
O	-0.517263	1.744196	-0.826166
C	-0.606248	0.868755	0.212805
O	-1.855976	0.195054	0.090689
C	-2.189011	-0.813790	1.061050
H	-1.276918	-1.214284	1.507349
H	-2.661191	-1.626831	0.502366
C	-3.141859	-0.254774	2.106051
H	-4.017930	0.152995	1.588427
H	-3.503613	-1.080061	2.731894
C	-2.508728	0.826399	2.985320
H	-1.765992	0.369100	3.652273
H	-3.282546	1.241224	3.640643
C	-1.843702	1.982706	2.221902
H	-2.527614	2.382999	1.466008
H	-1.669851	2.790692	2.939003
C	-0.484166	1.667143	1.560065
H	0.093041	1.046686	2.252683
C	0.289027	3.001775	1.356490
H	1.136548	2.868361	0.683179
C	0.765153	3.578965	2.612054
H	-0.367573	3.712589	0.847045
C	1.166295	4.043571	3.647169
H	1.524616	4.459292	4.559132
O	5.219622	0.813020	-5.603208
O	0.339321	-0.212263	0.130791
C	5.963608	0.958206	-4.662122
C	5.574623	0.866999	-3.201791
H	5.797759	1.836162	-2.740391
H	6.253102	0.156179	-2.717531

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C      4.113764     0.478608    -2.981789
H      3.467400     1.197796    -3.495019
H      3.921292    -0.488381    -3.459100
C      3.740392     0.407649    -1.497062
H      3.930318     1.381312    -1.027184
H      4.399457    -0.302470    -0.989199
C      2.271747     0.018360    -1.294324
H      1.635999     0.696462    -1.867598
H      2.087721    -0.984267    -1.699743
C      1.751356     0.047292     0.148084
H      1.956413     1.021602     0.597031
C      2.346444    -1.043431     1.072182
H      1.684224    -1.129873     1.939082
C      3.703019    -0.794849     1.552175
H      2.300052    -2.009514     0.556400
C      4.803444    -0.591117     1.993082
H      5.781097    -0.404941     2.370713
O      7.278802     1.233405    -4.792041
C      7.774370     1.358720    -6.155055
C      9.246235     1.650216    -6.087649
H      7.221640     2.158743    -6.650718
H      7.566116     0.427755    -6.685002
C      9.706776     2.968147    -6.013919
C     10.177026     0.607231    -6.075759
C     11.070398     3.239807    -5.931491
H      8.992398     3.786216    -6.022086
C     11.541548     0.874646    -5.993526
H      9.830243    -0.420512    -6.132275
H     11.414942     4.267479    -5.878172
C     11.990570     2.192501    -5.921382
H     12.253876     0.055949    -5.988636
H     13.053525     2.402633    -5.860521
H     -2.408997    -0.353379    -1.755563


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure I3r, in toluene
N     -2.873971     4.237417     0.078538
C     -3.120808     2.888208    -0.008745
N     -3.129935     2.063138     1.001180
C     -2.936241     2.610084     2.336668
C     -1.966669     3.789333     2.330001
C     -2.465753     4.842196     1.348450
C     -3.576130     4.552239    -2.283247
C     -3.130960     3.108365    -2.474549
N     -3.417458     2.382775    -1.250957
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C	-2.859426	5.139912	-1.073752
H	-2.558759	1.813546	2.982413
H	-3.899548	2.928736	2.764753
H	-0.975936	3.436671	2.025286
H	-1.867396	4.231270	3.325761
H	-3.309995	5.399705	1.776549
H	-1.677299	5.573150	1.136783
H	-3.333517	6.081027	-0.773922
H	-1.817989	5.380527	-1.334166
H	-4.658622	4.573080	-2.127700
H	-3.351808	5.154408	-3.167498
H	-2.062121	3.075450	-2.739700
H	-3.681777	2.634012	-3.289920
H	-3.651368	0.448505	0.903887
O	-4.033916	-0.484362	0.997115
C	-3.569844	-1.374653	0.067414
O	-3.290334	-0.613607	-1.114325
C	-3.042221	-1.320610	-2.338681
H	-2.621826	-2.306689	-2.123850
H	-2.272203	-0.747763	-2.862595
C	-4.310929	-1.399005	-3.182356
H	-4.696426	-0.379035	-3.298921
H	-4.041919	-1.744560	-4.188184
C	-5.406247	-2.304733	-2.605814
H	-5.113846	-3.354312	-2.737728
H	-6.316797	-2.171212	-3.200386
C	-5.739378	-2.080966	-1.121320
H	-6.010598	-1.036442	-0.935037
H	-6.626643	-2.676804	-0.887956
C	-4.610150	-2.498754	-0.161399
H	-4.068224	-3.342198	-0.598362
C	-5.149799	-2.974876	1.209564
H	-4.306493	-3.134445	1.887131
C	-5.928686	-4.207954	1.123190
H	-5.756052	-2.180913	1.653829
C	-6.562454	-5.228186	1.046675
H	-7.123267	-6.130832	0.987216
O	4.851717	-1.962654	-1.711726
O	-2.385163	-2.055643	0.469901
C	4.898448	-1.173504	-0.798160
C	3.730740	-0.747046	0.066132
H	3.614827	0.337172	-0.048652
H	4.017114	-0.895019	1.113078
C	2.428182	-1.475561	-0.260235
H	2.187031	-1.330027	-1.318344
H	2.575530	-2.553565	-0.134211
C	1.259572	-1.004832	0.612535

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H      1.106473     0.072179     0.468185
H      1.518947    -1.130172     1.667624
C     -0.037172    -1.755392     0.290580
H     -0.228038    -1.693207    -0.786297
H      0.083030    -2.822436     0.514874
C     -1.305813    -1.257889     0.989290
H     -1.475958    -0.205585     0.748019
C     -1.325255    -1.431972     2.527957
H     -2.366612    -1.319657     2.840105
C     -0.510874    -0.490579     3.291941
H     -1.033312    -2.460463     2.770830
C      0.125511     0.291956     3.948531
H      0.700977     0.978178     4.523627
O      6.031001    -0.544263    -0.418279
C      7.227391    -0.865418    -1.183229
C      8.366300    -0.064973    -0.619273
H      7.040446    -0.627505    -2.231785
H      7.406254    -1.939429    -1.109057
C      8.643620     1.215969    -1.105925
C      9.152875    -0.579794     0.415389
C      9.686775     1.968073    -0.570955
H      8.039106     1.625676    -1.909936
C     10.197062     0.169047     0.953119
H      8.946469    -1.573913     0.801020
H      9.893913     2.959633    -0.960334
C     10.465829     1.445114     0.460229
H     10.802292    -0.243783     1.753688
H     11.281202     2.028379     0.875797
H     -3.437910     1.369065    -1.278275


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure TSr2, in toluene
N     -3.581015     4.362132     0.089651
C     -3.595488     2.993228    -0.033475
N     -3.992916     2.163940     0.888127
C     -4.518661     2.714857     2.128230
C     -3.798385     4.002087     2.523507
C     -3.889095     4.997598     1.373222
C     -3.056019     4.606804    -2.327459
C     -2.416158     3.230657    -2.195148
N     -3.195746     2.466063    -1.238828
C     -3.106868     5.269957    -0.956150
H     -4.408539     1.958944     2.910539
H     -5.598605     2.909588     2.036701
H     -2.748743     3.773635     2.735214
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H	-4.229357	4.442835	3.427169
H	-4.891233	5.445176	1.328575
H	-3.180495	5.819924	1.522469
H	-3.773345	6.139337	-0.980971
H	-2.109274	5.645641	-0.684291
H	-4.066792	4.491087	-2.729184
H	-2.491024	5.240108	-3.016354
H	-1.362267	3.331505	-1.891123
H	-2.429116	2.700284	-3.149861
H	-3.795648	0.486726	0.904099
O	-3.726415	-0.486039	1.174918
C	-3.343552	-1.345003	0.176437
O	-3.114115	-0.539903	-0.984135
C	-2.982678	-1.192661	-2.257171
H	-2.580318	-2.200408	-2.123690
H	-2.233140	-0.617732	-2.807893
C	-4.311405	-1.186216	-3.006491
H	-4.674478	-0.152040	-3.024733
H	-4.126863	-1.469698	-4.050014
C	-5.383728	-2.104637	-2.408112
H	-5.129706	-3.149165	-2.629256
H	-6.333037	-1.912410	-2.920142
C	-5.595649	-1.971662	-0.891331
H	-5.836445	-0.937600	-0.621122
H	-6.470977	-2.571186	-0.624894
C	-4.400257	-2.456955	-0.050928
H	-3.900146	-3.274051	-0.578797
C	-4.840717	-3.014056	1.324856
H	-3.950811	-3.217648	1.926676
C	-5.635105	-4.235829	1.222860
H	-5.405084	-2.244861	1.858922
C	-6.283038	-5.246059	1.133147
H	-6.855007	-6.140781	1.061510
O	5.026365	-2.124145	-1.846831
O	-2.150530	-2.038050	0.513564
C	5.114965	-1.330384	-0.940311
C	3.975291	-0.852695	-0.065399
H	3.883203	0.230606	-0.208204
H	4.277834	-0.979055	0.979657
C	2.649900	-1.557529	-0.348781
H	2.392977	-1.434048	-1.405906
H	2.774286	-2.635145	-0.196926
C	1.508370	-1.037388	0.531673
H	1.376110	0.038653	0.361703
H	1.784653	-1.140020	1.585224
C	0.190532	-1.768421	0.254388
H	-0.024800	-1.726936	-0.819037

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H      0.296352    -2.832293     0.499956
C     -1.049839    -1.233856     0.975026
H     -1.226100    -0.191808     0.698127
C     -1.009902    -1.336706     2.519451
H     -2.042908    -1.248675     2.862445
C     -0.213482    -0.314742     3.193872
H     -0.660563    -2.335847     2.805620
C      0.406966     0.542357     3.767085
H      0.965950     1.294943     4.271010
O      6.275269    -0.741658    -0.580177
C      7.448988    -1.116310    -1.355610
C      8.629440    -0.373530    -0.798106
H      7.266588    -0.866597    -2.402174
H      7.576077    -2.197989    -1.285516
C      9.011055     0.860225    -1.332685
C      9.352429    -0.896540     0.278468
C     10.094989     1.558167    -0.804454
H      8.456766     1.275980    -2.169122
C     10.435766    -0.201576     0.810123
H      9.064707    -1.854638     0.701428
H     10.383323     2.513266    -1.231487
C     10.809302     1.027913     0.268588
H     10.990520    -0.620113     1.643632
H     11.655755     1.568755     0.679361
H     -3.098358     1.457315    -1.215842


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure I3r2, in toluene
N     -4.961848     4.250334    -0.029228
C     -4.447199     2.977119    -0.066910
N     -4.823630     1.996020     0.706869
C     -5.913655     2.240336     1.639611
C     -5.876615     3.664484     2.190009
C     -5.897716     4.647403     1.025896
C     -3.759003     4.835017    -2.125401
C     -2.759356     3.769725    -1.693303
N     -3.492351     2.714784    -1.017660
C     -4.513994     5.338378    -0.900984
H     -5.836977     1.513599     2.453360
H     -6.885815     2.059185     1.155209
H     -4.960176     3.799699     2.773602
H     -6.723354     3.861872     2.853830
H     -6.909488     4.725282     0.605440
H     -5.617803     5.650314     1.367000
H     -5.394902     5.912863    -1.208479
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H	-3.876520	6.023590	-0.323263
H	-4.455846	4.397902	-2.846387
H	-3.255705	5.674730	-2.611606
H	-1.984785	4.215328	-1.050176
H	-2.252380	3.334196	-2.556867
H	-3.793237	0.684094	0.993861
O	-3.148618	-0.037223	1.289894
C	-2.876971	-0.948751	0.297029
O	-2.589844	-0.166353	-0.873461
C	-2.487976	-0.833686	-2.141523
H	-2.144480	-1.862270	-1.998285
H	-1.703305	-0.304835	-2.689059
C	-3.806112	-0.762716	-2.906599
H	-4.114746	0.288359	-2.937146
H	-3.623855	-1.064464	-3.945469
C	-4.932012	-1.618958	-2.315112
H	-4.725411	-2.678066	-2.516223
H	-5.861940	-1.388670	-2.846868
C	-5.164066	-1.449778	-0.804848
H	-5.360312	-0.400517	-0.559587
H	-6.071810	-2.002881	-0.545351
C	-4.010441	-1.986186	0.064226
H	-3.553250	-2.839425	-0.445410
C	-4.502155	-2.499792	1.439830
H	-3.633966	-2.733297	2.061805
C	-5.350757	-3.684986	1.340727
H	-5.042182	-1.700220	1.955168
C	-6.044197	-4.664761	1.253809
H	-6.655123	-5.533502	1.183886
O	5.349284	-2.644970	-1.726649
O	-1.749395	-1.712973	0.655696
C	5.522982	-1.777433	-0.903951
C	4.447938	-1.135325	-0.052743
H	4.452409	-0.060820	-0.270287
H	4.756939	-1.216578	0.995143
C	3.059437	-1.734374	-0.269358
H	2.795183	-1.660383	-1.329398
H	3.089364	-2.806007	-0.044858
C	1.985011	-1.054155	0.586043
H	1.947716	0.015607	0.344424
H	2.268119	-1.111091	1.641177
C	0.602241	-1.678705	0.371295
H	0.374994	-1.685833	-0.700363
H	0.616000	-2.730218	0.684013
C	-0.572662	-0.987769	1.068114
H	-0.659196	0.046889	0.731603
C	-0.525609	-1.010759	2.615087

H	-1.540390	-0.804284	2.961101
C	0.374699	-0.036227	3.226022
H	-0.269973	-2.022096	2.953020
C	1.082593	0.785229	3.747536
H	1.716499	1.507915	4.204355
O	6.733769	-1.246928	-0.629485
C	7.853125	-1.782945	-1.390677
C	9.099792	-1.076568	-0.940331
H	7.655655	-1.626323	-2.452526
H	7.906130	-2.858586	-1.213852
C	9.528301	0.088659	-1.582734
C	9.838755	-1.562141	0.142689
C	10.673330	0.755874	-1.153436
H	8.961983	0.474792	-2.425278
C	10.983815	-0.897776	0.575372
H	9.514886	-2.466705	0.649113
H	10.997203	1.657490	-1.663244
C	11.403302	0.263180	-0.072843
H	11.550184	-1.287032	1.415236
H	12.297299	0.779984	0.260965
H	-3.075038	1.793115	-0.942736

85 atoms
addition of another 3-isomer unit to the 7-isomer chain end, structure TS34, in toluene

N	-3.626908	4.207842	-0.076607
C	-3.497974	2.857053	-0.077652
N	-4.191777	2.117482	0.804260
C	-5.111192	2.695761	1.773403
C	-4.603278	4.068633	2.196697
C	-4.382615	4.925751	0.956631
C	-2.594411	4.231160	-2.330623
C	-1.860554	2.977709	-1.865955
N	-2.699023	2.234778	-0.937943
C	-3.014737	5.047005	-1.114007
H	-5.167679	2.012350	2.621255
H	-6.120425	2.776092	1.349836
H	-3.664326	3.954793	2.746211
H	-5.319098	4.562756	2.857723
H	-5.343291	5.251832	0.537753
H	-3.819938	5.828903	1.211952
H	-3.744196	5.811689	-1.398762
H	-2.151212	5.569778	-0.683824
H	-3.475356	3.939732	-2.910131
H	-1.959896	4.843225	-2.976157
H	-0.905615	3.248192	-1.395948

H	-1.630119	2.319076	-2.704372
H	-3.932058	1.130166	0.910260
O	-3.416328	-0.488748	1.408297
C	-3.159952	-1.425135	0.644895
O	-2.778481	-0.352705	-1.097384
C	-3.000491	-0.864930	-2.370121
H	-2.672484	-1.920250	-2.437134
H	-2.385877	-0.328438	-3.120907
C	-4.469748	-0.768782	-2.813829
H	-4.791072	0.271332	-2.668964
H	-4.541108	-0.968036	-3.892943
C	-5.439787	-1.708279	-2.085168
H	-5.250770	-2.741489	-2.405529
H	-6.458443	-1.479656	-2.423132
C	-5.427522	-1.670027	-0.546597
H	-5.477662	-0.638892	-0.186787
H	-6.345169	-2.159499	-0.204142
C	-4.226674	-2.378434	0.112509
H	-3.745883	-3.047107	-0.603694
C	-4.667877	-3.246539	1.329922
H	-3.778536	-3.635933	1.835553
C	-5.530152	-4.366679	0.965066
H	-5.181559	-2.604137	2.053541
C	-6.235208	-5.291381	0.655322
H	-6.855214	-6.112917	0.384294
O	5.179282	-2.297865	-1.759736
O	-1.955835	-2.072768	0.695463
C	5.277971	-1.462988	-0.892413
C	4.156287	-0.967683	-0.004527
H	4.070041	0.114937	-0.154024
H	4.477216	-1.088004	1.036192
C	2.820644	-1.665489	-0.255243
H	2.533419	-1.535661	-1.303699
H	2.944088	-2.744248	-0.111925
C	1.707824	-1.143156	0.659995
H	1.581881	-0.064317	0.503612
H	2.011995	-1.259669	1.704650
C	0.374944	-1.855841	0.409242
H	0.116998	-1.780517	-0.651634
H	0.478172	-2.926353	0.626158
C	-0.828064	-1.316792	1.182566
H	-0.999997	-0.267367	0.941425
C	-0.764105	-1.486439	2.719837
H	-1.786068	-1.387399	3.093087
C	0.068827	-0.510501	3.417783
H	-0.431379	-2.503306	2.959421
C	0.721887	0.305725	4.013687

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H      1.310236     1.023362     4.534845
O      6.437959    -0.839609    -0.591329
C      7.596669    -1.232379    -1.379504
C      8.780045    -0.450761    -0.884530
H      7.384878    -1.030399    -2.430899
H      7.741336    -2.308210    -1.266701
C      9.117410     0.774486    -1.466570
C      9.549916    -0.927697     0.180757
C     10.203425     1.509130    -0.995709
H      8.526421     1.154470    -2.294844
C     10.635893    -0.196056     0.654997
H      9.296914    -1.878754     0.640197
H     10.457012     2.457098    -1.459167
C     10.964805     1.024531     0.066632
H     11.227284    -0.579246     1.480289
H     11.813116     1.593918     0.432610
H     -2.734920     1.140837    -1.000307


85 atoms
addition of another 3-isomer unit to the 7-isomer chain end,
structure I4, in toluene
N     -1.358200     4.087571     0.027770
C     -1.929688     2.836803    -0.035700
N     -2.929193     2.564658     0.856936
C     -3.506607     3.538805     1.762136
C     -2.406707     4.479939     2.237802
C     -1.722659     5.094771     1.023742
C     -0.443847     3.625342    -2.221727
C     -0.438402     2.175848    -1.738756
N     -1.570486     1.896889    -0.868343
C     -0.433044     4.548786    -1.009620
H     -3.954415     2.999938     2.599384
H     -4.310702     4.115244     1.280328
H     -1.682205     3.915890     2.832728
H     -2.815057     5.274138     2.868420
H     -2.378881     5.848726     0.563632
H     -0.808135     5.617194     1.326561
H     -0.722394     5.566125    -1.299288
H      0.578903     4.615498    -0.587120
H     -1.346252     3.800507    -2.816700
H      0.418381     3.844976    -2.858422
H      0.513758     1.969308    -1.223229
H     -0.482169     1.485799    -2.585995
H     -3.287170     1.618688     0.849721
O     -4.046722    -0.214142     1.068697
C     -3.862039    -1.279262     0.516363
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O	-3.029582	-0.226601	-1.890369
C	-3.931246	0.343350	-2.822762
H	-4.016727	-0.353061	-3.666708
H	-3.514664	1.279172	-3.221322
C	-5.330608	0.632805	-2.268372
H	-5.241710	1.264013	-1.376654
H	-5.841873	1.245308	-3.023222
C	-6.225317	-0.588701	-1.974918
H	-6.049436	-1.357490	-2.739113
H	-7.266575	-0.275840	-2.114702
C	-6.163907	-1.239845	-0.581301
H	-6.294407	-0.474631	0.189415
H	-7.033413	-1.900005	-0.507838
C	-4.915286	-2.074124	-0.244745
H	-4.428011	-2.424212	-1.156679
C	-5.268974	-3.331089	0.608795
H	-4.345716	-3.828719	0.916836
C	-6.109118	-4.290148	-0.102277
H	-5.777759	-3.014467	1.527324
C	-6.793827	-5.081344	-0.695409
H	-7.397093	-5.785313	-1.218467
O	4.553295	-2.773695	-1.289718
O	-2.707397	-1.960306	0.583155
C	4.628106	-1.831781	-0.537323
C	3.485080	-1.241421	0.261184
H	3.459419	-0.163988	0.064895
H	3.743833	-1.333909	1.322601
C	2.134008	-1.890998	-0.032490
H	1.901453	-1.780939	-1.096817
H	2.204615	-2.968648	0.147515
C	1.003488	-1.293554	0.812053
H	0.934102	-0.215176	0.624294
H	1.245319	-1.401497	1.873417
C	-0.347557	-1.946946	0.501604
H	-0.545571	-1.871015	-0.571962
H	-0.310882	-3.018064	0.734814
C	-1.551694	-1.326912	1.207073
H	-1.604751	-0.257341	1.003490
C	-1.651059	-1.578908	2.727889
H	-2.681122	-1.374225	3.033068
C	-0.767675	-0.753667	3.547398
H	-1.466354	-2.640308	2.929132
C	-0.072222	-0.065838	4.246994
H	0.553364	0.540315	4.858781
O	5.776481	-1.163683	-0.295693
C	6.957577	-1.649561	-0.994590
C	8.125421	-0.805146	-0.571269

```
H      6.774758    -1.585351    -2.068605
H      7.100232    -2.701199    -0.740150
C      8.484713     0.330891    -1.301960
C      8.857824    -1.131773     0.574172
C      9.555792     1.125165    -0.898273
H      7.922915     0.593877    -2.193529
C      9.928519    -0.339998     0.981626
H      8.587622    -2.012806     1.149006
H      9.826974     2.002286    -1.476931
C     10.279646     0.790680     0.245020
H     10.491004    -0.606668     1.870562
H     11.116309     1.406408     0.559064
H     -2.545094     0.512028    -1.438796
```

85 atoms
addition of another 3-isomer unit to the 7-isomer chain end, structure I5, in toluene

```
N      5.578138    -3.159363     1.296918
C      4.213195    -2.984995     1.267264
N      3.442870    -4.119967     1.162578
C      3.957816    -5.447513     1.438499
C      5.321113    -5.573446     0.770746
C      6.234546    -4.467392     1.284898
C      5.717966    -0.815063     2.061956
C      4.419368    -0.631121     1.277825
N      3.602744    -1.833483     1.292688
C      6.470663    -2.017523     1.505235
H      3.253915    -6.177221     1.032810
H      4.046719    -5.645044     2.518526
H      5.196185    -5.486608    -0.312465
H      5.774146    -6.546029     0.980217
H      6.582403    -4.709875     2.300295
H      7.129028    -4.393203     0.656304
H      7.261978    -2.326445     2.197648
H      6.961625    -1.758751     0.557047
H      5.478951    -0.984648     3.117194
H      6.352319     0.074640     2.006404
H      4.656566    -0.336769     0.243014
H      3.832989     0.190298     1.700029
H      2.447911    -3.947704     1.249886
O     -1.671450    -4.001125     7.620256
C     -1.472684    -2.809229     7.645105
O      0.922763    -2.494347     1.304917
C      0.209941    -2.071778     2.456855
H     -0.808813    -2.459784     2.352206
H      0.133289    -0.973956     2.479820
```

C	0.822873	-2.569112	3.768138
H	0.881846	-3.663751	3.732606
H	1.854128	-2.203345	3.835336
C	0.031925	-2.131216	5.004832
H	-0.999044	-2.498373	4.921195
H	-0.035760	-1.035859	5.028134
C	0.655298	-2.626192	6.314238
H	0.701679	-3.720512	6.313322
H	1.686788	-2.266798	6.382943
C	-0.093762	-2.169477	7.577717
H	-0.221016	-1.084670	7.562142
C	0.666834	-2.557353	8.877085
H	0.045482	-2.321302	9.748338
C	1.949421	-1.875100	9.019116
H	0.815670	-3.641891	8.890299
C	2.998995	-1.300025	9.136590
H	3.929930	-0.795697	9.247336
O	-6.739724	2.262908	3.899242
O	-2.448858	-1.884483	7.761354
C	-6.099478	1.485990	3.231019
C	-5.255059	0.347532	3.764648
H	-4.210820	0.570698	3.514762
H	-5.501209	-0.553981	3.194190
C	-5.419990	0.121440	5.266503
H	-5.200869	1.052921	5.797730
H	-6.468932	-0.106874	5.484742
C	-4.523122	-1.002415	5.793872
H	-3.474465	-0.762458	5.587853
H	-4.738996	-1.931213	5.250391
C	-4.707022	-1.242795	7.295272
H	-4.504650	-0.319899	7.851720
H	-5.748851	-1.508562	7.500871
C	-3.827283	-2.351443	7.855857
H	-3.912200	-3.262757	7.261803
C	-4.112058	-2.683891	9.334096
H	-3.358325	-3.397087	9.680182
C	-5.439069	-3.253504	9.545704
H	-3.993181	-1.773997	9.932959
C	-6.530481	-3.730336	9.709574
H	-7.495454	-4.153887	9.860685
O	-6.041657	1.535434	1.884425
C	-6.795558	2.608115	1.250206
C	-6.615973	2.483785	-0.235601
H	-6.422389	3.561185	1.629354
H	-7.842075	2.515002	1.544702
C	-5.529487	3.090944	-0.872579
C	-7.518945	1.740103	-1.000625

```
C     -5.348379     2.958465    -2.247022
H     -4.821345     3.670481    -0.287523
C     -7.341839     1.605889    -2.375856
H     -8.366171     1.263726    -0.515910
H     -4.501955     3.436216    -2.729639
C     -6.255332     2.215205    -3.001385
H     -8.051790     1.028163    -2.958823
H     -6.116881     2.113255    -4.072895
H      1.808780    -2.048455     1.281303
```

85 atoms
addition of another 7-isomer unit to the 3-isomer chain end, structure I1, in toluene

```
O     -2.670355    -0.259157    -2.587403
O     -4.162065    -1.065930    -1.199731
C     -3.078937    -1.229047    -1.983897
C     -2.469443    -2.605746    -2.127916
H     -1.990894    -2.863025    -1.177713
H     -1.674902    -2.499143    -2.866786
C     -3.454660    -3.712376    -2.553702
H     -4.081332    -3.351324    -3.377683
H     -2.865951    -4.538486    -2.964175
C     -4.332027    -4.256588    -1.421257
H     -3.684058    -4.691502    -0.649914
H     -4.938344    -5.082455    -1.808266
C     -5.260050    -3.228399    -0.766111
H     -6.000140    -2.860703    -1.487216
H     -5.821134    -3.719831     0.034676
C     -4.541327    -2.022165    -0.168373
H     -3.634901    -2.312343     0.366740
C     -5.420260    -1.182757     0.774465
H     -4.856268    -0.280755     1.032430
C     -5.808058    -1.895398     1.987153
H     -6.313549    -0.854950     0.230370
C     -6.120826    -2.483488     2.988573
H     -6.395415    -2.999092     3.878458
N     -3.376845     3.847641     0.708839
C     -3.170492     2.552339     0.284386
N     -3.322329     2.310235    -1.052795
C     -3.414218     3.357852    -2.050204
C     -4.315496     4.459042    -1.507346
C     -3.751807     4.948405    -0.179518
C     -2.253347     3.192648     2.810692
C     -2.839061     1.816217     2.504112
N     -2.875168     1.553303     1.072715
C     -3.077388     4.248587     2.085051
```

H	-3.826429	2.918971	-2.960686
H	-2.426597	3.771534	-2.307663
H	-5.323864	4.059117	-1.365775
H	-4.381213	5.297253	-2.206148
H	-2.873892	5.587280	-0.358057
H	-4.489844	5.569209	0.341484
H	-2.536709	5.202064	2.052588
H	-4.017716	4.436376	2.621475
H	-1.215100	3.226303	2.463972
H	-2.249717	3.402425	3.884491
H	-3.848159	1.746246	2.941229
H	-2.247451	1.028547	2.978962
H	-3.132421	1.367550	-1.370334
O	5.334440	-1.274413	2.405010
C	5.130468	-1.289002	1.212931
O	-1.570051	-0.842404	0.611696
C	-0.217500	-0.525046	0.326194
H	0.091223	0.372770	0.881729
H	-0.088267	-0.297713	-0.743863
C	0.675587	-1.696318	0.715177
H	0.536052	-1.898838	1.783435
H	0.331678	-2.592328	0.184092
C	2.156866	-1.453119	0.411071
H	2.485824	-0.540898	0.924405
H	2.285346	-1.258163	-0.660967
C	3.045451	-2.631894	0.822705
H	2.967648	-2.796483	1.903392
H	2.683152	-3.545246	0.340450
C	4.534062	-2.465699	0.456277
H	4.622263	-2.262050	-0.613366
C	5.360346	-3.733247	0.798238
H	6.422892	-3.535054	0.618411
C	4.965102	-4.907162	0.025584
H	5.266600	-3.939226	1.869011
C	4.644720	-5.867962	-0.622937
H	4.365358	-6.723854	-1.190902
O	5.400837	-0.252856	0.397609
C	5.950972	0.937907	1.036912
C	6.196058	1.965417	-0.029863
H	6.869314	0.655234	1.553466
H	5.235614	1.284052	1.784567
C	5.184241	2.854177	-0.405433
C	7.432607	2.034832	-0.678112
C	5.403140	3.794635	-1.409010
H	4.219648	2.808815	0.091540
C	7.655533	2.974470	-1.681934
H	8.225606	1.349160	-0.394214

```
H      4.610303     4.480265    -1.689907
C      6.640264     3.856357    -2.048997
H      8.620992     3.020172    -2.175278
H      6.813219     4.590661    -2.829121
H     -2.083611     0.004441     0.688432
```

85 atoms
addition of another 7-isomer unit to the 3-isomer chain end, structure TS12, in toluene

```
O     -2.444093     0.071911    -2.303849
O     -4.005234    -0.850152    -1.027727
C     -2.744682    -0.920525    -1.617278
C     -2.284325    -2.310940    -2.057845
H     -2.002349    -2.918949    -1.198195
H     -1.382218    -2.148328    -2.649669
C     -3.345127    -3.055642    -2.892066
H     -3.847995    -2.355352    -3.568768
H     -2.835983    -3.784317    -3.532185
C     -4.372281    -3.808467    -2.034030
H     -3.833737    -4.529828    -1.405519
H     -5.021540    -4.404116    -2.686070
C     -5.257424    -2.932955    -1.137112
H     -5.949368    -2.344169    -1.751934
H     -5.872737    -3.583619    -0.506521
C     -4.497974    -1.948319    -0.244075
H     -3.660298    -2.426423     0.268037
C     -5.405735    -1.293353     0.815394
H     -4.827262    -0.503538     1.302384
C     -5.912515    -2.223547     1.819573
H     -6.242123    -0.799626     0.306749
C     -6.317069    -2.991881     2.652232
H     -6.676122    -3.672730     3.387479
N     -3.360970     3.724305     0.924392
C     -3.030867     2.541281     0.342820
N     -3.048732     2.421410    -0.989838
C     -3.367972     3.527220    -1.879785
C     -4.392225     4.434832    -1.211769
C     -3.864156     4.865102     0.150388
C     -2.291246     2.927653     3.010881
C     -2.689666     1.534994     2.540221
N     -2.686019     1.488299     1.085585
C     -3.216891     3.951796     2.367411
H     -3.756373     3.100229    -2.805353
H     -2.463784     4.094844    -2.136130
H     -5.335847     3.893998    -1.094459
H     -4.588026     5.318697    -1.823196
```

H	-3.061881	5.605517	0.035931
H	-4.657774	5.338760	0.736153
H	-2.823901	4.963637	2.505879
H	-4.208349	3.923486	2.837161
H	-1.254115	3.126754	2.724977
H	-2.358152	3.007837	4.098384
H	-3.679838	1.273051	2.936837
H	-1.991408	0.775604	2.894803
H	-2.844813	1.500762	-1.425788
O	4.858133	-1.092526	2.506041
C	4.844806	-1.220758	1.303296
O	-1.758257	-0.750949	0.036454
C	-0.388251	-0.542755	-0.147911
H	-0.067759	0.384505	0.367887
H	-0.163295	-0.371733	-1.214843
C	0.469343	-1.699637	0.383195
H	0.228800	-1.850243	1.443231
H	0.177222	-2.623393	-0.130132
C	1.974971	-1.471324	0.216052
H	2.251494	-0.525182	0.699787
H	2.210932	-1.344771	-0.848349
C	2.819857	-2.613257	0.791550
H	2.629755	-2.709355	1.866626
H	2.513392	-3.559102	0.333883
C	4.337559	-2.455067	0.574609
H	4.541493	-2.328388	-0.491052
C	5.131268	-3.683211	1.095017
H	6.205890	-3.483525	1.015922
C	4.829492	-4.915211	0.372296
H	4.922643	-3.813384	2.161595
C	4.587406	-5.924652	-0.234932
H	4.374214	-6.821855	-0.766654
O	5.282158	-0.276438	0.449193
C	5.765343	0.959274	1.053491
C	6.257912	1.853526	-0.047756
H	6.555121	0.711816	1.763762
H	4.940268	1.408373	1.609830
C	5.353944	2.590878	-0.819727
C	7.623009	1.949239	-0.329401
C	5.806002	3.407460	-1.852413
H	4.290403	2.521502	-0.611353
C	8.079606	2.768496	-1.360366
H	8.333719	1.379599	0.262192
H	5.094709	3.974341	-2.444300
C	7.171239	3.498618	-2.123898
H	9.142863	2.836075	-1.566592
H	7.524681	4.137378	-2.926881

H -2.362272 0.579100 0.614208

85 atoms
addition of another 7-isomer unit to the 3-isomer chain end, structure I2, in toluene
O -2.275743 0.716318 -2.034053
O -3.736313 -0.796988 -1.256966
C -2.421112 -0.607991 -1.733102
C -2.086603 -1.440019 -2.982674
H -1.747167 -2.435097 -2.678551
H -1.237555 -0.949945 -3.462890
C -3.248662 -1.571214 -3.979772
H -3.769066 -0.611870 -4.062462
H -2.829780 -1.779633 -4.970032
C -4.236838 -2.696947 -3.635546
H -3.676101 -3.637586 -3.553356
H -4.928314 -2.834327 -4.474447
C -5.062553 -2.492220 -2.359175
H -5.785840 -1.681688 -2.508114
H -5.641110 -3.399911 -2.157591
C -4.237563 -2.135064 -1.121939
H -3.405124 -2.832412 -0.987613
C -5.073406 -2.128247 0.173228
H -4.441602 -1.740625 0.977528
C -5.595669 -3.438685 0.548059
H -5.896971 -1.414962 0.054301
C -6.010712 -4.523740 0.860166
H -6.383370 -5.482064 1.135688
N -3.462667 2.930912 2.268642
C -2.988259 2.087011 1.289737
N -2.929380 2.375887 0.022298
C -3.343843 3.704586 -0.400116
C -4.499653 4.233958 0.445975
C -4.094022 4.203530 1.914141
C -2.614135 1.413456 4.043210
C -2.806925 0.313185 3.008272
N -2.504484 0.865933 1.700520
C -3.515158 2.590468 3.691071
H -3.633869 3.652793 -1.453596
H -2.498179 4.408514 -0.348064
H -5.377723 3.598517 0.290667
H -4.774639 5.253488 0.159963
H -3.406344 5.029916 2.140891
H -4.972013 4.336763 2.556324
H -3.221595 3.477040 4.264567
H -4.554538 2.363880 3.971782

```
H     -1.565711     1.725395     4.041277
H     -2.856942     1.057181     5.047715
H     -3.833310    -0.082388     3.067916
H     -2.127256    -0.522033     3.190071
H     -2.542959     1.284421    -1.243913
O      4.683941     1.167898     2.138637
C      4.730411     0.220893     1.387713
O     -1.590696    -0.989716    -0.605143
C     -0.179231    -0.822517    -0.778032
H      0.026689     0.193946    -1.128306
H      0.191735    -1.523796    -1.536023
C      0.507061    -1.087167     0.554472
H      0.129808    -0.373278     1.294570
H      0.225632    -2.086864     0.905151
C      2.032411    -0.976941     0.457502
H      2.298498     0.016386     0.077239
H      2.409196    -1.694169    -0.282078
C      2.723168    -1.227320     1.802350
H      2.380026    -0.492768     2.539823
H      2.431567    -2.211858     2.181333
C      4.264001    -1.182367     1.744622
H      4.615631    -1.866403     0.968769
C      4.905452    -1.580813     3.099001
H      5.990542    -1.440156     3.043062
C      4.630131    -2.961354     3.485693
H      4.550874    -0.895131     3.874684
C      4.410919    -4.103156     3.793273
H      4.220234    -5.112229     4.073744
O      5.191690     0.290646     0.125971
C      5.632878     1.607703    -0.323948
C      6.111536     1.476568    -1.740713
H      6.422459     1.948661     0.347420
H      4.792720     2.298026    -0.236350
C      5.240852     1.707582    -2.809487
C      7.431184     1.101465    -2.011237
C      5.679423     1.567835    -4.124385
H      4.214067     2.000496    -2.611090
C      7.872843     0.959726    -3.324208
H      8.116271     0.920543    -1.188037
H      4.994415     1.753522    -4.945218
C      6.996728     1.193224    -4.383630
H      8.900226     0.671098    -3.521169
H      7.340599     1.086663    -5.407384
H     -2.294534     0.222295     0.944600

85 atoms
```

addition of another 7-isomer unit to the 3-isomer chain end, structure TS23, in toluene

O	-2.104692	-0.996515	-1.947481
O	-3.789536	-1.206418	-0.464499
C	-2.468089	-1.630628	-0.792284
C	-2.344886	-3.146308	-1.021382
H	-2.233181	-3.651621	-0.057195
H	-1.407902	-3.294194	-1.562149
C	-3.507520	-3.766658	-1.811919
H	-3.801924	-3.087085	-2.617810
H	-3.148445	-4.680494	-2.297313
C	-4.719612	-4.135237	-0.943188
H	-4.386189	-4.825891	-0.157218
H	-5.438096	-4.697758	-1.549952
C	-5.454338	-2.956825	-0.292002
H	-5.976920	-2.369952	-1.056572
H	-6.219806	-3.346395	0.387076
C	-4.546811	-1.991088	0.472516
H	-3.866325	-2.532120	1.136391
C	-5.332923	-0.978315	1.327774
H	-4.612423	-0.283467	1.769428
C	-6.123134	-1.589003	2.392315
H	-5.981647	-0.388904	0.669570
C	-6.761449	-2.093495	3.278113
H	-7.329078	-2.538965	4.060773
N	-2.730622	3.908427	-1.255217
C	-2.685940	2.541630	-1.105951
N	-2.106205	1.719508	-1.931173
C	-1.398518	2.276581	-3.073505
C	-2.084682	3.531659	-3.608478
C	-2.225720	4.540933	-2.475854
C	-3.644403	4.167180	1.038736
C	-4.210343	2.768776	0.831594
N	-3.264962	2.016180	0.026599
C	-3.398840	4.813155	-0.318760
H	-1.344630	1.508669	-3.850673
H	-0.357480	2.515140	-2.804325
H	-3.074871	3.263885	-3.991741
H	-1.521048	3.978376	-4.432820
H	-1.260891	5.023019	-2.267031
H	-2.923676	5.337095	-2.757928
H	-2.775715	5.707329	-0.205540
H	-4.352759	5.146512	-0.753895
H	-2.707140	4.092369	1.597512
H	-4.332668	4.787801	1.618286
H	-5.204844	2.828942	0.361976
H	-4.332952	2.254331	1.786860

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H     -2.175386     0.004521    -1.859858
O      4.614010     2.044448     1.293371
C      4.609283     0.845663     1.454236
O     -1.701325    -1.200128     0.339134
C     -0.281420    -1.298677     0.233063
H      0.045906    -0.871552    -0.719954
H      0.032643    -2.351476     0.258209
C      0.326384    -0.538862     1.402951
H     -0.028845     0.496416     1.362587
H     -0.056492    -0.964659     2.337625
C      1.857786    -0.573513     1.400977
H      2.227107    -0.163321     0.453424
H      2.205039    -1.613697     1.435001
C      2.460971     0.199119     2.579011
H      2.151917     1.249587     2.532755
H      2.063741    -0.202739     3.516356
C      4.000503     0.142303     2.657463
H      4.323831    -0.901133     2.642332
C      4.539762     0.820447     3.943627
H      5.634535     0.847182     3.909557
C      4.124172     0.146838     5.170330
H      4.211533     1.864329     3.958253
C      3.788589    -0.418959     6.177116
H      3.493690    -0.912951     7.072793
O      5.135672    -0.026684     0.575368
C      5.717526     0.552689    -0.631455
C      6.258952    -0.568936    -1.469555
H      6.496896     1.254121    -0.329833
H      4.939451     1.114461    -1.150334
C      5.467226    -1.167072    -2.454075
C      7.557309    -1.045154    -1.263139
C      5.962611    -2.220523    -3.219300
H      4.457454    -0.804909    -2.623417
C      8.055667    -2.098587    -2.025465
H      8.181148    -0.587028    -0.501193
H      5.338838    -2.674195    -3.982571
C      7.258267    -2.688107    -3.005713
H      9.066043    -2.457153    -1.857618
H      7.646504    -3.506909    -3.602796
H     -3.343694     1.006966     0.010678


85 atoms
addition of another 7-isomer unit to the 3-isomer chain end,
structure I3, in toluene
O      0.615994    -0.016552     0.229987
O     -0.121155     2.076064    -0.147288
```

C	-0.483281	0.787794	0.348123
C	-1.642545	0.156762	-0.447951
H	-2.595196	0.462836	-0.004552
H	-1.562968	-0.922948	-0.305754
C	-1.641868	0.491262	-1.948369
H	-0.617708	0.450667	-2.332290
H	-2.197355	-0.292321	-2.474857
C	-2.297574	1.841046	-2.287733
H	-3.316049	1.842070	-1.877417
H	-2.414336	1.917284	-3.374621
C	-1.560014	3.093498	-1.793381
H	-0.637944	3.236996	-2.369866
H	-2.185870	3.973623	-1.975162
C	-1.170293	3.044650	-0.316459
H	-2.023220	2.763577	0.306174
C	-0.615747	4.378074	0.220949
H	-0.229796	4.193964	1.227601
C	-1.603875	5.451800	0.255538
H	0.239837	4.684728	-0.392299
C	-2.427602	6.327622	0.290587
H	-3.153121	7.105863	0.323975
N	4.851065	2.178403	1.208620
C	3.525258	1.909536	0.956244
N	2.863201	0.898668	1.443128
C	3.547875	0.023934	2.381627
C	5.021330	-0.150461	2.017686
C	5.680511	1.221556	1.944410
C	4.642476	4.404526	0.122367
C	3.531666	3.754757	-0.693477
N	2.850502	2.798198	0.157362
C	5.575143	3.320097	0.648136
H	3.037455	-0.943567	2.383423
H	3.467519	0.416071	3.407670
H	5.092991	-0.649276	1.045529
H	5.547105	-0.772621	2.748008
H	5.875536	1.608860	2.953761
H	6.650487	1.153053	1.438649
H	6.227453	3.727560	1.428901
H	6.233607	2.968832	-0.160223
H	4.195731	4.955871	0.954694
H	5.214365	5.113250	-0.482377
H	3.950490	3.284765	-1.597047
H	2.803876	4.498644	-1.024845
H	1.408879	0.378448	0.715491
O	0.195656	-2.688181	7.714457
C	-0.940487	-2.695267	7.299766
O	-0.838829	1.035348	1.709348

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C     -1.171831    -0.104837     2.499670
H     -0.449791    -0.906479     2.312921
H     -2.169385    -0.479234     2.230178
C     -1.143320     0.313317     3.962628
H     -0.141219     0.689993     4.194036
H     -1.832455     1.153940     4.103017
C     -1.512948    -0.830909     4.911714
H     -0.840613    -1.679127     4.734089
H     -2.522435    -1.192590     4.679830
C     -1.449919    -0.413899     6.385063
H     -0.430606    -0.102111     6.639583
H     -2.092506     0.457778     6.543371
C     -1.891325    -1.510566     7.375597
H     -2.891186    -1.858614     7.106038
C     -1.912700    -0.995731     8.838357
H     -2.134063    -1.829146     9.514346
C     -2.890251     0.064615     9.064723
H     -0.910563    -0.646484     9.105416
C     -3.705890     0.928808     9.249672
H     -4.423143     1.696783     9.419919
O     -1.510086    -3.758522     6.703115
C     -0.665640    -4.939874     6.556539
C     -1.479681    -6.011560     5.891192
H     -0.324491    -5.239079     7.548767
H      0.209833    -4.663503     5.967161
C     -1.463342    -6.157563     4.501148
C     -2.282614    -6.866694     6.652291
C     -2.233422    -7.139680     3.882086
H     -0.842826    -5.499382     3.900101
C     -3.054499    -7.848919     6.036999
H     -2.302024    -6.762466     7.733230
H     -2.209305    -7.244725     2.802319
C     -3.030720    -7.987036     4.649654
H     -3.671250    -8.508266     6.639056
H     -3.629178    -8.754232     4.169105
H      1.894511     2.535731    -0.053535


85 atoms
addition of another 7-isomer unit to the 3-isomer chain end,
structure TSr, in toluene
O     -0.421074     0.150743    -0.087140
O     -0.293477     2.398532    -0.034671
C     -1.151412     1.268442     0.189144
C     -2.392317     1.292094    -0.718885
H     -3.181785     1.860975    -0.220724
H     -2.740417     0.257299    -0.767776
```

C	-2.152224	1.848989	-2.130041
H	-1.190817	1.488030	-2.509614
H	-2.917348	1.441458	-2.799688
C	-2.227444	3.383787	-2.208050
H	-3.203225	3.700175	-1.816607
H	-2.214726	3.690412	-3.260080
C	-1.122507	4.152963	-1.469458
H	-0.168089	4.035831	-1.997415
H	-1.361013	5.221849	-1.482693
C	-0.899632	3.701665	-0.025440
H	-1.844188	3.657701	0.522357
C	0.055185	4.618932	0.763728
H	0.270907	4.130479	1.718380
C	-0.479838	5.956206	1.000310
H	1.008134	4.694587	0.226770
C	-0.933820	7.051965	1.200009
H	-1.332457	8.022505	1.379726
N	4.337012	0.417931	0.988231
C	3.009613	0.722652	0.799829
N	2.014408	-0.073426	1.078005
C	2.318436	-1.356876	1.690902
C	3.626063	-1.941245	1.160361
C	4.745684	-0.932031	1.382808
C	4.977116	2.773751	0.521450
C	3.713884	2.807714	-0.329408
N	2.717514	1.970819	0.312222
C	5.438329	1.329335	0.672299
H	1.485777	-2.037257	1.489728
H	2.380392	-1.259502	2.786637
H	3.518461	-2.147142	0.090396
H	3.877109	-2.884220	1.654977
H	5.055526	-0.926572	2.436708
H	5.628920	-1.204683	0.794213
H	6.185338	1.251417	1.470286
H	5.929484	0.994116	-0.253026
H	4.756798	3.205496	1.501943
H	5.776157	3.364420	0.065976
H	3.938199	2.476010	-1.355098
H	3.316833	3.822792	-0.397825
H	0.474874	0.149017	0.378604
O	-0.604106	-1.259482	8.098573
C	-1.376542	-1.898133	7.421739
O	-1.586052	1.366035	1.551702
C	-1.456515	0.221058	2.393483
H	-0.399317	-0.020522	2.548628
H	-1.933026	-0.650733	1.929911
C	-2.124299	0.552461	3.720493

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H     -1.634375     1.433318     4.150616
H     -3.165172     0.837053     3.530074
C     -2.073812    -0.614316     4.712217
H     -1.030181    -0.917726     4.860953
H     -2.583990    -1.485146     4.282163
C     -2.712813    -0.265887     6.060845
H     -2.163654     0.558215     6.530028
H     -3.734230     0.091448     5.897197
C     -2.780351    -1.442394     7.055337
H     -3.298788    -2.281879     6.586445
C     -3.523970    -1.055879     8.360581
H     -3.461726    -1.885010     9.074179
C     -4.929608    -0.723752     8.148203
H     -3.005248    -0.213056     8.827831
C     -6.089897    -0.463333     7.968757
H     -7.117099    -0.228424     7.817450
O     -1.086099    -3.101885     6.894015
C      0.255553    -3.609804     7.157488
C      0.387389    -4.945591     6.484375
H      0.391692    -3.680680     8.237388
H      0.973825    -2.882808     6.774149
C      0.633035    -5.024507     5.109406
C      0.250601    -6.128028     7.215788
C      0.738819    -6.260712     4.478468
H      0.739670    -4.111496     4.530997
C      0.359742    -7.367717     6.588150
H      0.058533    -6.078799     8.283602
H      0.929364    -6.308756     3.411232
C      0.603203    -7.435730     5.218029
H      0.254668    -8.278548     7.168575
H      0.688775    -8.399966     4.727540
H      1.735952     2.122079     0.106673


85 atoms
addition of another 7-isomer unit to the 3-isomer chain end,
structure I3r, in toluene
O     -0.966169     0.401078    -0.577299
O     -0.293367     2.234834     0.538449
C     -1.449852     1.529239     0.030595
C     -2.253928     2.347056    -0.988244
H     -3.005404     2.935737    -0.455289
H     -2.800498     1.611796    -1.582462
C     -1.411848     3.255631    -1.893937
H     -0.504636     2.727048    -2.204941
H     -1.979805     3.449353    -2.810104
C     -1.060474     4.612290    -1.260855
```

H	-1.993438	5.100070	-0.949557
H	-0.624983	5.263501	-2.027176
C	-0.098839	4.568245	-0.065564
H	0.908998	4.299690	-0.406351
H	-0.025604	5.569719	0.371226
C	-0.492128	3.570835	1.025269
H	-1.540139	3.696592	1.311471
C	0.367156	3.695699	2.300118
H	0.099911	2.872843	2.969870
C	0.202892	4.966716	2.998765
H	1.421537	3.549286	2.038354
C	0.053208	6.010866	3.576664
H	-0.077166	6.933955	4.090625
N	3.483315	-1.190161	0.492839
C	2.329077	-0.440578	0.504442
N	1.122261	-0.927855	0.545932
C	0.970395	-2.371918	0.634428
C	2.053572	-3.101497	-0.157789
C	3.422661	-2.646436	0.333809
C	4.860221	0.860073	0.780938
C	3.699321	1.579200	0.105649
N	2.469316	0.927334	0.518502
C	4.826225	-0.614093	0.396193
H	-0.022299	-2.632324	0.256299
H	0.997388	-2.700959	1.684746
H	1.942361	-2.861316	-1.220227
H	1.967836	-4.187057	-0.053858
H	3.667016	-3.128250	1.290104
H	4.201432	-2.942411	-0.377947
H	5.493036	-1.191579	1.046251
H	5.200614	-0.740647	-0.630525
H	4.765533	0.971468	1.864993
H	5.819275	1.290807	0.481789
H	3.831377	1.568116	-0.987509
H	3.653967	2.625642	0.415318
H	-0.207546	-0.024461	-0.071679
O	-1.928142	-0.570121	8.110198
C	-2.008280	-1.431075	7.264639
O	-2.339486	1.271132	1.101530
C	-1.933518	0.273722	2.042218
H	-0.911934	0.471031	2.383872
H	-1.935931	-0.709400	1.559679
C	-2.912281	0.300689	3.206262
H	-2.913879	1.303631	3.648320
H	-3.923289	0.130734	2.819018
C	-2.574396	-0.742555	4.276141
H	-1.563676	-0.556104	4.656906

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H     -2.542815    -1.740165     3.821119
C     -3.580835    -0.749855     5.431485
H     -3.625148     0.240971     5.898337
H     -4.581011    -0.953013     5.036313
C     -3.286605    -1.797912     6.527258
H     -3.142183    -2.774227     6.058322
C     -4.439489    -1.895346     7.558434
H     -4.144582    -2.566862     8.372222
C     -5.690757    -2.376430     6.980328
H     -4.590254    -0.913529     8.017407
C     -6.714833    -2.784133     6.499261
H     -7.625984    -3.141535     6.080581
O     -0.959567    -2.166321     6.849394
C      0.326553    -1.846571     7.459891
C      1.379806    -2.679553     6.788342
H      0.257054    -2.055421     8.528764
H      0.508326    -0.778237     7.336016
C      2.033495    -2.207414     5.646189
C      1.710017    -3.944820     7.282466
C      2.999848    -2.983368     5.010470
H      1.785618    -1.226118     5.252769
C      2.675844    -4.723845     6.649406
H      1.208618    -4.321451     8.169194
H      3.501585    -2.601239     4.127377
C      3.323096    -4.243643     5.511907
H      2.925392    -5.702955     7.045140
H      4.078490    -4.848187     5.020264
H      1.591645     1.425419     0.415876


85 atoms
addition of another 7-isomer unit to the 3-isomer chain end,
structure TS34, in toluene
O     -2.235598    -0.609019    -2.014351
O     -2.631057    -1.342368     0.318410
C     -2.220523    -1.745717    -1.495459
C     -3.285654    -2.787621    -1.833547
H     -2.982082    -3.759856    -1.438668
H     -3.234164    -2.875655    -2.925340
C     -4.726295    -2.461375    -1.406611
H     -4.865515    -1.376578    -1.377155
H     -5.407137    -2.833081    -2.181319
C     -5.159759    -3.100565    -0.074846
H     -4.938919    -4.175194    -0.126494
H     -6.251742    -3.029406     0.007078
C     -4.542824    -2.529162     1.209542
H     -4.960139    -1.532672     1.408033
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H	-4.842143	-3.167760	2.049598
C	-3.012221	-2.377838	1.166717
H	-2.568785	-3.328667	0.825745
C	-2.422333	-2.119094	2.585384
H	-1.360417	-1.888320	2.453614
C	-2.570132	-3.226350	3.524969
H	-2.888553	-1.219188	3.005389
C	-2.692796	-4.156825	4.279474
H	-2.797636	-4.978242	4.948038
N	-4.508146	3.159024	-0.049873
C	-3.953072	1.944151	-0.283223
N	-3.932048	1.432637	-1.520769
C	-4.382083	2.177427	-2.687608
C	-5.549262	3.071525	-2.294329
C	-5.138969	3.946781	-1.116972
C	-3.380503	3.197747	2.145549
C	-3.428261	1.677200	2.095662
N	-3.422472	1.227019	0.710760
C	-4.502476	3.765189	1.286644
H	-4.674107	1.454452	-3.450776
H	-3.562877	2.777966	-3.104459
H	-6.407388	2.451980	-2.017627
H	-5.851778	3.703888	-3.131962
H	-4.448281	4.734992	-1.442372
H	-6.014374	4.441378	-0.687103
H	-4.376329	4.843561	1.158077
H	-5.477166	3.606685	1.765230
H	-2.413782	3.547618	1.771281
H	-3.487769	3.552610	3.172971
H	-4.319935	1.308478	2.619532
H	-2.558418	1.241325	2.589892
H	-3.342243	0.590257	-1.684412
O	5.236950	-1.204594	1.874029
C	5.201806	-0.839346	0.721698
O	-1.015087	-2.396991	-1.323447
C	0.127292	-1.550163	-1.180451
H	-0.041550	-0.869025	-0.340432
H	0.249941	-0.943885	-2.083171
C	1.338277	-2.438180	-0.941364
H	1.170670	-3.033536	-0.036738
H	1.423142	-3.150378	-1.770359
C	2.637282	-1.637042	-0.807102
H	2.530035	-0.909702	0.007259
H	2.802893	-1.048343	-1.718029
C	3.855123	-2.531657	-0.552402
H	3.717108	-3.091106	0.379700
H	3.934093	-3.272937	-1.353709

C	5.196085	-1.774317	-0.477539
H	5.322600	-1.171904	-1.380068
C	6.401487	-2.741814	-0.344145
H	7.318888	-2.162158	-0.192315
C	6.579289	-3.606473	-1.506819
H	6.271428	-3.347246	0.558225
C	6.727692	-4.306904	-2.473066
H	6.862234	-4.933247	-3.323234
O	5.156970	0.454443	0.351571
C	5.126106	1.428265	1.436866
C	5.111983	2.801171	0.829035
H	6.001474	1.268821	2.067654
H	4.236518	1.236199	2.039391
C	3.913411	3.366366	0.381664
C	6.297326	3.527045	0.684870
C	3.900063	4.631989	-0.198201
H	2.986681	2.810171	0.487853
C	6.287500	4.795123	0.107282
H	7.233877	3.097414	1.028171
H	2.963495	5.059972	-0.540847
C	5.088153	5.349482	-0.335603
H	7.214595	5.349635	0.004399
H	5.078372	6.337457	-0.784547
H	-3.108925	0.236745	0.520036

85 atoms
addition of another 7-isomer unit to the 3-isomer chain end, structure I4, in toluene

O	-1.427955	-0.537717	-0.602485
O	-4.131090	-1.664444	2.188359
C	-1.264702	-1.732943	-0.454064
C	-2.358950	-2.714623	-0.126594
H	-2.615683	-2.533304	0.922428
H	-1.976960	-3.733447	-0.217111
C	-3.616242	-2.508594	-0.986122
H	-3.868933	-1.445530	-1.011852
H	-3.379021	-2.788526	-2.019184
C	-4.843693	-3.314168	-0.523700
H	-4.535225	-4.325461	-0.227441
H	-5.494887	-3.453006	-1.394106
C	-5.713635	-2.699772	0.588869
H	-6.004060	-1.679164	0.310147
H	-6.641552	-3.280877	0.631209
C	-5.121736	-2.661213	2.006598
H	-4.619354	-3.614439	2.208053
C	-6.225245	-2.490540	3.087277

H	-5.717144	-2.320079	4.041484
C	-7.129594	-3.629327	3.209833
H	-6.801224	-1.582733	2.872813
C	-7.855303	-4.585088	3.301526
H	-8.501750	-5.426240	3.388307
N	-5.210289	3.031905	0.512048
C	-4.673339	1.773885	0.681980
N	-3.738621	1.371946	-0.245508
C	-3.069750	2.311166	-1.129633
C	-4.120936	3.245626	-1.709422
C	-4.837487	3.950541	-0.565396
C	-6.017768	2.851386	2.832183
C	-6.048952	1.350216	2.558726
N	-5.012893	0.938520	1.622154
C	-6.124280	3.593561	1.507564
H	-2.568076	1.735563	-1.908193
H	-2.295498	2.893061	-0.605280
H	-4.832670	2.661911	-2.300733
H	-3.667230	3.989905	-2.369137
H	-4.198644	4.747988	-0.157406
H	-5.750760	4.435479	-0.928832
H	-5.871478	4.651600	1.639303
H	-7.154493	3.558033	1.126780
H	-5.074999	3.108788	3.326334
H	-6.832756	3.155459	3.495559
H	-7.046588	1.072165	2.182089
H	-5.907931	0.793491	3.490025
H	-3.203876	0.551154	0.005854
O	6.787121	-0.887836	0.896062
C	6.441531	-0.580155	-0.221113
O	-0.056010	-2.315349	-0.534721
C	1.076516	-1.444237	-0.773439
H	1.107015	-0.686137	0.012883
H	0.929176	-0.930555	-1.726794
C	2.325246	-2.307043	-0.780629
H	2.398737	-2.833117	0.177237
H	2.222060	-3.076040	-1.553920
C	3.594408	-1.483547	-1.025944
H	3.676454	-0.706900	-0.256204
H	3.512079	-0.953995	-1.982985
C	4.857875	-2.350787	-1.033448
H	4.969208	-2.855354	-0.067205
H	4.753424	-3.136673	-1.787809
C	6.154984	-1.574662	-1.336232
H	6.034096	-1.017163	-2.267890
C	7.376882	-2.520776	-1.469991
H	8.288226	-1.923277	-1.583238

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C      7.274150    -3.440350    -2.599115
H      7.495188    -3.081410    -0.537639
C      7.189145    -4.186744    -3.538243
H      7.121625    -4.853230    -4.365614
O      6.256251     0.690802    -0.622151
C      6.492435     1.721802     0.384185
C      6.298238     3.059737    -0.268576
H      7.505426     1.594231     0.768678
H      5.795737     1.562264     1.208452
C      5.076268     3.730250    -0.169455
C      7.335044     3.646377    -1.001527
C      4.892157     4.964875    -0.788797
H      4.264563     3.284551     0.397908
C      7.154032     4.878566    -1.623640
H      8.289369     3.134397    -1.083896
H      3.939596     5.477118    -0.700695
C      5.931072     5.540642    -1.517525
H      7.967057     5.324607    -2.187178
H      5.790319     6.503197    -1.998475
H     -4.465490    -0.765775     1.928197


85 atoms
addition of another 7-isomer unit to the 3-isomer chain end,
structure I5, in toluene
O      0.251488    -0.997523    11.096978
O     -6.789285    -0.605121     9.368230
C     -0.055633    -0.290558    10.166829
C     -1.463289     0.124551     9.795936
H     -1.612571    -0.101029     8.734458
H     -1.513230     1.217717     9.867370
C     -2.542843    -0.530595    10.655577
H     -2.459049    -1.619237    10.569817
H     -2.356175    -0.298816    11.709386
C     -3.954879    -0.089300    10.259332
H     -4.124206    -0.310486     9.201657
H     -4.041713     1.000528    10.364150
C     -5.044304    -0.766379    11.094558
H     -4.963606    -1.855171    10.984006
H     -4.876874    -0.549353    12.157157
C     -6.470347    -0.335450    10.721644
H     -6.554442     0.751640    10.831465
C     -7.500166    -0.989472    11.676738
H     -7.450455    -2.078586    11.554828
C     -8.871465    -0.537253    11.461893
H     -7.213128    -0.782861    12.714652
C     -9.999143    -0.149752    11.304712
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H	-10.996075	0.189739	11.151461
N	-5.289415	-3.388836	5.912187
C	-5.609063	-2.555115	6.958524
N	-5.432374	-1.199885	6.753445
C	-5.350476	-0.633142	5.417856
C	-4.377111	-1.479360	4.608780
C	-4.865442	-2.922523	4.590532
C	-6.515089	-5.150789	7.131866
C	-6.118092	-4.372055	8.384612
N	-6.021359	-2.943498	8.130446
C	-5.530632	-4.830035	6.013995
H	-4.996805	0.396134	5.506222
H	-6.330943	-0.600633	4.917547
H	-3.386609	-1.420619	5.069250
H	-4.292838	-1.111326	3.582970
H	-5.703030	-3.025508	3.884763
H	-4.070633	-3.587053	4.233701
H	-5.920870	-5.176286	5.050711
H	-4.577727	-5.351645	6.177414
H	-7.525404	-4.855241	6.830140
H	-6.527399	-6.229171	7.315529
H	-5.161949	-4.761134	8.768875
H	-6.852829	-4.531431	9.179565
H	-5.846937	-0.632470	7.483961
O	7.251433	-1.294121	6.588491
C	7.293025	-0.635835	7.602243
O	0.843320	0.242620	9.312255
C	2.235623	-0.062565	9.562179
H	2.362522	-1.147991	9.570640
H	2.505330	0.310845	10.553571
C	3.054238	0.595523	8.466245
H	2.719916	0.213298	7.495483
H	2.849496	1.671649	8.466695
C	4.556943	0.347902	8.638359
H	4.745058	-0.732014	8.668875
H	4.886754	0.740150	9.607965
C	5.383852	0.992656	7.520736
H	5.092565	0.571129	6.552084
H	5.161852	2.063362	7.476636
C	6.908020	0.833556	7.688377
H	7.204664	1.206814	8.671226
C	7.692839	1.607150	6.596763
H	8.761913	1.388012	6.693648
C	7.501437	3.052882	6.662409
H	7.394118	1.232537	5.612822
C	7.349352	4.243960	6.729132
H	7.219293	5.299350	6.779469

O	7.678312	-1.124365	8.794700
C	8.052715	-2.535623	8.819523
C	8.449300	-2.884982	10.224476
H	8.870719	-2.681177	8.112255
H	7.199949	-3.122365	8.475358
C	7.517574	-3.431104	11.111574
C	9.753236	-2.649703	10.671858
C	7.880334	-3.738048	12.421296
H	6.502261	-3.618792	10.774732
C	10.119032	-2.953720	11.980446
H	10.485476	-2.226520	9.990394
H	7.148236	-4.164533	13.099210
C	9.182207	-3.499169	12.857732
H	11.134667	-2.769091	12.315026
H	9.467037	-3.739716	13.876856
H	-6.591198	-1.550572	9.134138

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

N	4.094393	6.110485	3.691359
C	2.969883	5.446108	4.127911
N	2.382766	4.582555	3.250029
C	2.935316	4.225688	1.958294
C	3.601950	5.454030	1.352176
C	4.633328	5.989243	2.336606
C	4.546618	6.618611	6.068823
C	3.023087	6.613719	6.176182
N	2.430003	5.605563	5.309794
C	4.933407	6.874378	4.617684
H	2.115725	3.865260	1.334712
H	3.664353	3.405726	2.041790
H	2.842438	6.215432	1.150571
H	4.092418	5.209807	0.406145
H	5.516172	5.332793	2.349740
H	4.983011	6.979396	2.022607
H	5.979566	6.594660	4.443555
H	4.848032	7.943676	4.380852
H	4.930599	5.646677	6.394972
H	4.996828	7.382890	6.709232
H	2.638907	7.617691	5.933272
H	2.711036	6.411443	7.204867
H	1.509205	4.156599	3.527222
O	-0.158050	2.848696	3.245775
C	-0.980789	3.348742	3.982330
O	-0.999056	4.694201	4.076118

C	-1.703044	5.406750	5.133354
H	-1.475541	4.912112	6.079955
C	-3.205394	5.460385	4.868417
H	-3.355324	5.726299	3.815017
H	-3.623927	6.280311	5.460168
C	-3.956806	4.170535	5.212540
H	-3.880708	3.993349	6.292826
H	-5.022028	4.316400	5.004240
C	-3.472630	2.920039	4.471414
H	-3.627127	3.036297	3.392269
H	-4.095641	2.073037	4.774303
C	-2.004429	2.539106	4.746278
H	-1.780095	2.625590	5.814374
H	-1.823699	1.500871	4.468112
O	0.298629	-3.837278	7.046164
O	0.806029	3.703939	6.473211
C	1.390623	-3.651666	7.528624
C	2.041142	-2.304770	7.761973
H	3.029113	-2.324265	7.288749
H	2.240177	-2.216537	8.836428
C	1.209777	-1.126011	7.258997
H	1.024783	-1.244351	6.186039
H	0.224204	-1.150126	7.735760
C	1.884485	0.223950	7.525491
H	2.873162	0.238555	7.049277
H	2.069605	0.331891	8.598808
C	1.050745	1.399456	7.006522
H	0.826373	1.244665	5.945846
H	0.082486	1.423682	7.523711
C	1.682296	2.789987	7.114906
H	2.652095	2.787195	6.598653
C	1.917181	3.272150	8.576179
H	2.003022	4.362734	8.541544
C	3.101966	2.739216	9.243588
H	1.020196	3.058457	9.169527
C	4.099996	2.337213	9.783006
H	4.976273	1.967868	10.261140
O	2.199380	-4.651977	7.940121
C	1.679931	-6.001631	7.776822
C	2.716115	-6.961370	8.288090
H	1.460898	-6.162173	6.719866
H	0.742284	-6.079722	8.330036
C	3.683386	-7.488199	7.427414
C	2.742052	-7.325347	9.637755
C	4.656937	-8.363138	7.904172
H	3.673005	-7.211845	6.377092
C	3.713961	-8.199403	10.118552

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H      1.995427    -6.921581    10.315389
H      5.399995    -8.767782     7.224591
C      4.673529    -8.720412     9.251503
H      3.720928    -8.476436    11.167796
H      5.429364    -9.404374     9.623903
H      1.353290     4.421619     6.048630
C     -1.028941     6.789425     5.129627
H     -1.236036     7.283842     4.173511
C     -1.458201     7.640109     6.234643
H      0.053103     6.629411     5.177957
C     -1.808489     8.335110     7.151671
H     -2.113130     8.952573     7.963528
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85 atoms
addition of another 7-isomer unit to the 7-isomer chain end, structure TS12, in toluene

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N     -4.548705     3.379495     0.625397
C     -4.097034     2.215068     0.094479
N     -4.659345     1.712823    -1.007886
C     -5.731013     2.389684    -1.723698
C     -6.609423     3.138574    -0.729995
C     -5.738055     4.066491     0.106261
C     -2.460598     3.523945     1.955432
C     -2.481989     2.001579     1.915801
N     -3.081241     1.558563     0.665408
C     -3.875835     4.047009     1.747168
H     -6.296020     1.627646    -2.261710
H     -5.321648     3.081561    -2.470929
H     -7.120992     2.419728    -0.083376
H     -7.372949     3.724088    -1.247235
H     -5.420746     4.934611    -0.485292
H     -6.299402     4.449138     0.963958
H     -3.859859     5.120079     1.533450
H     -4.475354     3.907758     2.655458
H     -1.800467     3.898921     1.167804
H     -2.076173     3.885390     2.911940
H     -3.038304     1.607816     2.776772
H     -1.475657     1.584664     1.964642
H     -4.367012     0.772141    -1.351957
O     -3.918223    -0.682258    -2.083814
C     -3.465788    -1.497420    -1.249686
O     -4.233201    -1.583460    -0.086577
C     -3.900342    -2.537842     0.932357
H     -2.817172    -2.675621     0.954701
C     -4.635319    -3.855898     0.675999
H     -5.686061    -3.608635     0.480714
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H	-4.618064	-4.458141	1.590638
C	-4.068725	-4.692697	-0.478054
H	-3.093649	-5.098222	-0.177484
H	-4.720522	-5.560715	-0.630128
C	-3.893012	-3.953155	-1.812330
H	-4.854335	-3.566185	-2.168719
H	-3.560080	-4.678646	-2.562374
C	-2.861157	-2.810016	-1.749762
H	-2.014301	-3.119881	-1.134309
H	-2.474557	-2.599252	-2.747776
O	5.093860	0.332507	2.139461
O	-1.979004	-0.692089	-0.415226
C	5.307579	0.111895	0.970801
C	4.259339	-0.131631	-0.093787
H	4.472690	-1.103121	-0.554070
H	4.419332	0.603010	-0.891193
C	2.825114	-0.073211	0.429676
H	2.698645	-0.816741	1.223850
H	2.654162	0.899648	0.903503
C	1.785277	-0.303868	-0.672553
H	1.961666	-1.279855	-1.142790
H	1.924738	0.437104	-1.465546
C	0.349333	-0.248782	-0.138660
H	0.242901	-0.963817	0.685199
H	0.159505	0.743014	0.294666
C	-0.783918	-0.567116	-1.133384
H	-0.533800	-1.520295	-1.628631
C	-0.939999	0.504413	-2.263629
H	-1.942153	0.364664	-2.676804
C	0.027743	0.437385	-3.354251
H	-0.922678	1.504249	-1.811091
C	0.799546	0.361805	-4.276097
H	1.487295	0.293618	-5.085325
O	6.549965	0.053469	0.443568
C	7.648091	0.278302	1.371586
C	8.932027	0.212866	0.594944
H	7.603467	-0.483706	2.151673
H	7.506211	1.251759	1.844230
C	9.628532	-0.992598	0.471205
C	9.438568	1.353940	-0.034672
C	10.809282	-1.057900	-0.265335
H	9.243806	-1.885376	0.955551
C	10.618033	1.292777	-0.772573
H	8.905207	2.295870	0.054893
H	11.342020	-1.999484	-0.350751
C	11.306004	0.085524	-0.888859
H	11.002000	2.186421	-1.253940

H	12.227047	0.036997	-1.460778
H	-2.690982	0.694560	0.207539
C	-4.328926	-1.866856	2.251769
H	-5.413043	-1.705033	2.229900
C	-3.960729	-2.618527	3.447525
H	-3.865621	-0.876848	2.281840
C	-3.642401	-3.234604	4.430577
H	-3.362480	-3.781216	5.300030

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

N	-6.835602	3.679020	6.194909
C	-6.374494	2.518438	5.616481
N	-6.945262	1.906359	4.618885
C	-8.128092	2.513447	4.027268
C	-8.987279	3.217594	5.074887
C	-8.131822	4.241616	5.809781
C	-4.728416	3.918204	7.489268
C	-4.654990	2.400234	7.395907
N	-5.199178	2.000610	6.110574
C	-6.176869	4.356335	7.313023
H	-8.701727	1.727878	3.527105
H	-7.842699	3.232189	3.243223
H	-9.368645	2.475344	5.783788
H	-9.849495	3.714690	4.620801
H	-7.973729	5.131093	5.184610
H	-8.638152	4.580227	6.720752
H	-6.227190	5.436295	7.134085
H	-6.741568	4.163577	8.237273
H	-4.102389	4.354805	6.705625
H	-4.355634	4.272574	8.453779
H	-5.198280	1.945563	8.239308
H	-3.621596	2.051416	7.451248
H	-6.536935	0.355690	4.014291
O	-6.295696	-0.510043	3.551990
C	-5.568651	-1.306578	4.392776
O	-6.289804	-1.406539	5.600969
C	-5.890839	-2.390660	6.567243
H	-4.834280	-2.638940	6.428751
C	-6.773099	-3.630228	6.415897
H	-7.814984	-3.288925	6.433222
H	-6.637540	-4.278304	7.288071
C	-6.510117	-4.441489	5.141074
H	-5.546050	-4.958616	5.236363
H	-7.266466	-5.231343	5.073206

C	-6.504631	-3.640606	3.829424
H	-7.446240	-3.097663	3.703255
H	-6.446318	-4.351724	2.998736
C	-5.327086	-2.660068	3.702651
H	-4.419583	-3.123760	4.101531
H	-5.139741	-2.447751	2.648641
O	3.100251	-0.488044	6.166276
O	-4.325430	-0.669443	4.804387
C	3.100361	-0.652502	4.969195
C	1.882587	-0.610436	4.070251
H	1.942911	-1.451443	3.372408
H	1.971236	0.288729	3.448004
C	0.560141	-0.610249	4.835776
H	0.487377	-1.526110	5.432897
H	0.561119	0.215021	5.554636
C	-0.654937	-0.494663	3.909060
H	-0.643500	-1.317497	3.183296
H	-0.576393	0.423643	3.319870
C	-1.973834	-0.517199	4.688786
H	-2.010285	-1.419180	5.309339
H	-2.007070	0.330772	5.384341
C	-3.257542	-0.501054	3.852712
H	-3.247919	-1.346696	3.159487
C	-3.481713	0.800511	3.038039
H	-4.546093	0.856827	2.803739
C	-2.729238	0.876336	1.789136
H	-3.255796	1.666416	3.670519
C	-2.144604	0.932050	0.738825
H	-1.621500	0.983239	-0.186722
O	4.219283	-0.887997	4.252375
C	5.465774	-0.917055	5.004639
C	6.580693	-1.212144	4.042612
H	5.382675	-1.679811	5.780451
H	5.594213	0.049457	5.495363
C	6.976220	-2.530073	3.796254
C	7.225446	-0.174540	3.362654
C	7.997060	-2.807143	2.889840
H	6.482133	-3.343946	4.318886
C	8.246284	-0.447326	2.455323
H	6.925984	0.853215	3.546228
H	8.296989	-3.834542	2.710467
C	8.634082	-1.765276	2.217539
H	8.740931	0.367456	1.936558
H	9.431700	-1.979202	1.513436
H	-4.963342	1.080328	5.755506
C	-6.048715	-1.704995	7.938470
H	-7.101365	-1.431840	8.074165

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C     -5.592600    -2.517394     9.062055
H     -5.486139    -0.767416     7.911139
C     -5.199791    -3.184467     9.982703
H     -4.856979    -3.774680    10.799608


85 atoms
addition of another 7-isomer unit to the 7-isomer chain end,
structure TS23, in toluene
N     -7.352310     3.710761     5.743745
C     -6.716402     2.514022     5.515504
N     -6.708361     1.877214     4.379449
C     -7.376068     2.491971     3.241173
C     -8.615073     3.276118     3.667318
C     -8.215362     4.303334     4.719031
C     -6.222041     3.933820     7.942449
C     -6.178951     2.411889     7.932768
N     -5.998304     1.975766     6.559284
C     -7.346891     4.407561     7.031043
H     -7.646553     1.701424     2.535484
H     -6.685024     3.159947     2.704471
H     -9.352455     2.584013     4.087224
H     -9.082767     3.781238     2.817212
H     -7.699330     5.153077     4.251870
H     -9.103856     4.706085     5.217806
H     -7.249203     5.481192     6.835778
H     -8.318417     4.263691     7.526440
H     -5.261483     4.320223     7.589629
H     -6.386825     4.315210     8.953359
H     -7.097842     2.004999     8.383005
H     -5.336763     2.042484     8.521801
H     -6.108088     0.281841     4.104061
O     -5.752982    -0.605719     3.788831
C     -5.163893    -1.297997     4.810478
O     -6.058042    -1.288884     5.913202
C     -5.886964    -2.263031     6.957336
H     -4.838713    -2.571309     7.008480
C     -6.801613    -3.460034     6.691110
H     -7.800162    -3.060363     6.478458
H     -6.887111    -4.057151     7.604781
C     -6.341812    -4.368527     5.544149
H     -5.448892    -4.922087     5.863598
H     -7.115595    -5.124696     5.370626
C     -6.025836    -3.659364     4.218967
H     -6.899294    -3.109326     3.855396
H     -5.812057    -4.426027     3.466726
C     -4.821891    -2.707148     4.298386
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H	-4.038184	-3.142649	4.924567
H	-4.392342	-2.575977	3.303320
O	3.431639	-2.017656	5.766940
O	-3.999024	-0.626514	5.331618
C	3.371994	-1.507458	4.673406
C	2.129620	-0.926552	4.032066
H	2.032272	-1.362623	3.031995
H	2.315950	0.140542	3.862587
C	0.859980	-1.136131	4.855486
H	0.701636	-2.208908	5.010200
H	1.002205	-0.709330	5.853676
C	-0.375818	-0.516119	4.194187
H	-0.513168	-0.949044	3.195317
H	-0.204775	0.552418	4.033920
C	-1.643566	-0.732597	5.027191
H	-1.756407	-1.802018	5.237225
H	-1.535541	-0.244141	6.003614
C	-2.961129	-0.258826	4.404774
H	-3.126813	-0.758863	3.447202
C	-3.059643	1.269813	4.172397
H	-4.119797	1.515106	4.069493
C	-2.356272	1.767538	2.993099
H	-2.707490	1.792211	5.069777
C	-1.816710	2.186182	2.002226
H	-1.330392	2.551863	1.128961
O	4.438587	-1.378162	3.855862
C	5.702382	-1.886126	4.369613
C	6.754441	-1.652874	3.323316
H	5.581498	-2.946289	4.598227
H	5.929484	-1.364944	5.301315
C	7.038234	-2.634233	2.369299
C	7.450454	-0.441235	3.274433
C	7.999402	-2.411326	1.385842
H	6.503384	-3.579093	2.397744
C	8.411536	-0.214105	2.292471
H	7.237889	0.328177	4.010957
H	8.212617	-3.182938	0.653150
C	8.687916	-1.199953	1.345971
H	8.946815	0.729590	2.267454
H	9.439013	-1.025695	0.582268
H	-5.704981	1.021108	6.397140
C	-6.230818	-1.528167	8.267740
H	-7.264125	-1.167884	8.208103
C	-6.051978	-2.341582	9.466505
H	-5.591563	-0.643117	8.336209
C	-5.888656	-3.008601	10.453886
H	-5.747035	-3.599434	11.328029

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

N	6.701065	0.250454	7.428095
C	5.451185	-0.227385	7.114940
N	4.385439	0.509947	6.969538
C	4.528653	1.953855	7.093713
C	5.574160	2.329276	8.141031
C	6.894653	1.658456	7.784180
C	7.704043	-1.975921	6.969232
C	6.337524	-2.522484	7.361151
N	5.330452	-1.580188	6.907721
C	7.885154	-0.595614	7.587909
H	3.553127	2.372613	7.355188
H	4.803318	2.400741	6.125962
H	5.237679	1.986747	9.125154
H	5.714677	3.412568	8.198290
H	7.380449	2.183036	6.950330
H	7.587185	1.700124	8.632271
H	8.736239	-0.081873	7.126925
H	8.117417	-0.692089	8.658695
H	7.762201	-1.913335	5.878822
H	8.505512	-2.635768	7.311253
H	6.293071	-2.689275	8.448706
H	6.150083	-3.483572	6.877860
H	2.809201	-0.143867	7.087486
O	1.850362	-0.408406	7.256788
C	1.434466	-1.412957	6.430263
O	2.367092	-2.485432	6.545011
C	1.996371	-3.756491	5.979315
H	1.230801	-3.602662	5.215170
C	1.485141	-4.663717	7.098530
H	2.235720	-4.646010	7.897998
H	1.435808	-5.695289	6.734116
C	0.112654	-4.263018	7.657633
H	-0.659569	-4.513321	6.918417
H	-0.098565	-4.888002	8.532519
C	-0.051909	-2.783799	8.045477
H	0.696251	-2.491489	8.788848
H	-1.026759	-2.670439	8.531564
C	0.009016	-1.821678	6.848010
H	-0.504756	-2.265950	5.991512
H	-0.518197	-0.894483	7.083720
O	-4.393703	0.419724	0.478530
O	1.491297	-1.060594	5.039727

C	-3.967083	1.537099	0.649304
C	-2.807289	1.915530	1.545926
H	-3.211003	2.534806	2.356261
H	-2.143664	2.578475	0.981227
C	-2.049972	0.712748	2.106501
H	-2.751722	0.056192	2.630606
H	-1.649138	0.119242	1.277351
C	-0.912252	1.123096	3.047666
H	-1.321957	1.701477	3.885444
H	-0.231493	1.800468	2.523530
C	-0.144576	-0.089018	3.586593
H	-0.855760	-0.789958	4.036992
H	0.328337	-0.629886	2.757572
C	0.931470	0.201071	4.638674
H	0.493335	0.698203	5.507556
C	2.117697	1.060710	4.132858
H	2.950760	0.886220	4.819611
C	1.866635	2.497223	4.056671
H	2.439934	0.683380	3.154947
C	1.685380	3.686559	4.024014
H	1.515184	4.736604	3.988275
O	-4.489935	2.630112	0.053688
C	-5.632835	2.398200	-0.817702
C	-6.053953	3.721459	-1.390126
H	-6.427258	1.936173	-0.228779
H	-5.336829	1.692154	-1.595262
C	-6.965164	4.532936	-0.707527
C	-5.524260	4.171959	-2.602783
C	-7.341290	5.769565	-1.226239
H	-7.382844	4.192996	0.235701
C	-5.898200	5.407968	-3.125275
H	-4.815254	3.549914	-3.141311
H	-8.051991	6.388405	-0.688062
C	-6.807988	6.209211	-2.437151
H	-5.482058	5.744249	-4.069433
H	-7.102657	7.171069	-2.844286
H	4.373080	-1.900568	6.813318
C	3.255227	-4.301180	5.277568
H	4.032051	-4.486455	6.028799
C	3.015196	-5.520568	4.512165
H	3.634311	-3.516554	4.616124
C	2.805950	-6.518741	3.874737
H	2.624072	-7.401875	3.308860

85 atoms

addition of another 7-isomer unit to the 7-isomer chain end, structure TSr, in toluene

N	6.342617	0.489736	7.579323
C	5.192217	-0.136024	7.163091
N	4.167107	0.465295	6.623431
C	4.266478	1.899444	6.387224
C	5.060747	2.598338	7.488221
C	6.436146	1.951751	7.592896
C	7.449738	-1.709595	7.933285
C	6.037589	-2.226131	8.177567
N	5.138743	-1.500741	7.298889
C	7.480559	-0.206551	8.183283
H	3.254414	2.307317	6.324597
H	4.735564	2.099101	5.412301
H	4.527631	2.494003	8.439014
H	5.171116	3.667896	7.286990
H	7.081760	2.283710	6.768617
H	6.930903	2.250421	8.523926
H	8.401019	0.226916	7.776228
H	7.490145	-0.007328	9.264909
H	7.734259	-1.928274	6.900082
H	8.170434	-2.201569	8.591603
H	5.768951	-2.107396	9.238802
H	5.962901	-3.290012	7.942055
H	2.613248	-0.227711	6.724267
O	1.664394	-0.521502	6.916853
C	1.319495	-1.684327	6.294813
O	2.468792	-2.537112	6.328564
C	2.297620	-3.910176	5.935435
H	1.408365	-3.997199	5.306497
C	2.168185	-4.771601	7.192263
H	3.019987	-4.533110	7.841504
H	2.268673	-5.827067	6.918602
C	0.852678	-4.576282	7.960160
H	0.037501	-5.042223	7.391350
H	0.917904	-5.136121	8.899904
C	0.455030	-3.121876	8.267153
H	1.242281	-2.614644	8.834704
H	-0.423699	-3.145525	8.920549
C	0.109197	-2.301822	7.015574
H	-0.448625	-2.918413	6.306233
H	-0.539789	-1.460694	7.272451
O	-4.748800	0.729071	0.563458
O	0.974345	-1.536758	4.904071
C	-4.139378	1.767916	0.657457
C	-2.835084	1.967118	1.399916
H	-2.999946	2.743079	2.156389

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H     -2.114136     2.400368     0.697684
C     -2.290430     0.688092     2.033240
H     -3.042306     0.272006     2.711862
H     -2.143362    -0.066806     1.253453
C     -0.976107     0.919975     2.786849
H     -1.133112     1.669325     3.573240
H     -0.236787     1.351147     2.106604
C     -0.438622    -0.372630     3.411008
H     -1.228470    -0.830867     4.015947
H     -0.203598    -1.098567     2.622791
C      0.783243    -0.238751     4.327982
H      0.582278     0.483878     5.122032
C      2.101889     0.155688     3.613693
H      2.922432    -0.030358     4.313379
C      2.194274     1.542265     3.163574
H      2.254092    -0.522699     2.765866
C      2.303067     2.687558     2.810004
H      2.385946     3.700275     2.493206
O     -4.554336     2.924729     0.097656
C     -5.805309     2.862341    -0.644059
C     -6.097394     4.236655    -1.175152
H     -6.588589     2.509358     0.028891
H     -5.695052     2.129542    -1.445352
C     -6.843962     5.146208    -0.420438
C     -5.608417     4.634684    -2.422927
C     -7.098738     6.428042    -0.902425
H     -7.228776     4.847691     0.550374
C     -5.860706     5.915584    -2.908444
H     -5.027227     3.936078    -3.017715
H     -7.682651     7.123275    -0.307965
C     -6.607132     6.814878    -2.148305
H     -5.478032     6.210743    -3.880120
H     -6.807480     7.812099    -2.526695
H      4.235584    -1.902434     7.073531
C      3.523414    -4.260702     5.069089
H      4.433700    -4.152414     5.670035
C      3.469027    -5.599624     4.490345
H      3.590008    -3.515485     4.271191
C      3.410248    -6.699347     4.006835
H      3.362322    -7.672026     3.576934


85 atoms
addition of another 7-isomer unit to the 7-isomer chain end,
structure I3r, in toluene
N      5.091209     0.835480     3.107875
C      4.031950    -0.002437     2.856666
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N	2.828801	0.386195	2.539028
C	2.588703	1.813496	2.378008
C	3.425985	2.641503	3.350503
C	4.896258	2.285771	3.168836
C	6.657246	-1.096960	3.139204
C	5.441281	-1.898669	3.585952
N	4.276480	-1.353583	2.912999
C	6.433945	0.374699	3.466797
H	1.522983	2.000440	2.538463
H	2.803011	2.124044	1.345100
H	3.114841	2.417193	4.376184
H	3.284013	3.714199	3.189638
H	5.294673	2.747187	2.255072
H	5.490101	2.671791	4.004802
H	7.162026	0.995802	2.933065
H	6.598336	0.548737	4.540274
H	6.792649	-1.229080	2.062000
H	7.565541	-1.445681	3.637431
H	5.344772	-1.862540	4.682284
H	5.540376	-2.949246	3.304342
H	1.478655	-0.613885	2.751593
O	0.619316	-1.085436	3.003520
C	0.426873	-2.274461	2.363201
O	1.733759	-2.868808	2.197459
C	1.798042	-4.251508	1.807078
H	0.877465	-4.519772	1.281631
C	1.998449	-5.123207	3.049036
H	2.850737	-4.709959	3.603065
H	2.289613	-6.130838	2.734702
C	0.775038	-5.221190	3.969299
H	0.012405	-5.843464	3.483210
H	1.069259	-5.763028	4.875237
C	0.127929	-3.885071	4.366155
H	0.857737	-3.228956	4.852023
H	-0.641680	-4.091992	5.117299
C	-0.526853	-3.147138	3.191474
H	-1.026771	-3.857257	2.527611
H	-1.299673	-2.462637	3.548037
O	-5.483290	0.870768	-3.282345
O	-0.195338	-2.157566	1.081243
C	-4.689811	1.781409	-3.261328
C	-3.342672	1.768509	-2.570492
H	-3.342697	2.579211	-1.832463
H	-2.584971	2.053083	-3.308877
C	-3.004314	0.430230	-1.916337
H	-3.791863	0.166888	-1.202886
H	-3.017112	-0.356992	-2.677796

C	-1.644024	0.448478	-1.210410
H	-1.643087	1.232193	-0.441802
H	-0.864280	0.725292	-1.924402
C	-1.320781	-0.900961	-0.558531
H	-2.151063	-1.185203	0.095767
H	-1.258057	-1.683161	-1.325234
C	-0.058883	-0.953650	0.311893
H	-0.044046	-0.099968	0.994082
C	1.277648	-1.003399	-0.470187
H	2.072817	-1.210992	0.249441
C	1.639721	0.206797	-1.202972
H	1.239004	-1.854920	-1.159854
C	1.981324	1.194375	-1.799883
H	2.268757	2.070444	-2.331567
O	-4.907338	2.968884	-3.866765
C	-6.179483	3.107761	-4.560339
C	-6.233403	4.484947	-5.157486
H	-6.984115	2.942029	-3.841822
H	-6.244143	2.329400	-5.322517
C	-6.731836	5.560907	-4.416836
C	-5.766498	4.716012	-6.454679
C	-6.764863	6.842482	-4.961169
H	-7.097231	5.392569	-3.407988
C	-5.798065	5.996213	-7.002942
H	-5.377100	3.887370	-7.038998
H	-7.157542	7.668398	-4.376894
C	-6.297822	7.062159	-6.256383
H	-5.435907	6.161309	-8.012544
H	-6.326195	8.059547	-6.683217
H	3.443763	-1.924397	2.822698
C	2.966447	-4.363912	0.806166
H	3.899216	-4.084284	1.309308
C	3.103337	-5.690781	0.213122
H	2.810574	-3.625865	0.014891
C	3.201653	-6.782372	-0.282166
H	3.291812	-7.747313	-0.722626

85 atoms
addition of another 7-isomer unit to the 7-isomer chain end, structure TSr2, in toluene

N	4.553043	1.151993	2.951502
C	3.619728	0.161986	2.757022
N	2.398199	0.356779	2.344320
C	2.005358	1.712341	1.989208
C	2.668081	2.747423	2.895920
C	4.179678	2.563721	2.839569

C	6.340559	-0.548726	3.266746
C	5.211940	-1.449547	3.753349
N	4.022199	-1.128689	2.988483
C	5.918614	0.907919	3.419547
H	0.916295	1.783302	2.064014
H	2.256967	1.923588	0.938712
H	2.314799	2.603654	3.922292
H	2.410200	3.767893	2.597779
H	4.582711	2.974273	1.903814
H	4.662326	3.108326	3.658943
H	6.594775	1.558757	2.853829
H	5.997535	1.211957	4.473686
H	6.547759	-0.774641	2.216850
H	7.257850	-0.722018	3.835481
H	5.059701	-1.315348	4.835561
H	5.452425	-2.502210	3.589405
H	1.192163	-0.808469	2.585867
O	0.396004	-1.392218	2.806841
C	0.413044	-2.606556	2.183459
O	1.797044	-3.024400	2.144454
C	2.086062	-4.403441	1.859128
H	1.273917	-4.826209	1.260543
C	2.267466	-5.177757	3.167906
H	2.984937	-4.617121	3.780263
H	2.733492	-6.143593	2.946941
C	0.978751	-5.417204	3.963007
H	0.365888	-6.159237	3.434841
H	1.246532	-5.878043	4.920525
C	0.117452	-4.172518	4.222299
H	0.694031	-3.403738	4.747518
H	-0.695705	-4.457008	4.898382
C	-0.495989	-3.576502	2.949436
H	-0.818953	-4.372044	2.272729
H	-1.388991	-2.995094	3.188271
O	-5.587214	1.438926	-2.414171
O	-0.110002	-2.589189	0.854107
C	-4.625246	2.085593	-2.754275
C	-3.181611	1.767493	-2.427343
H	-2.760210	2.635357	-1.907166
H	-2.632062	1.705941	-3.373433
C	-3.007153	0.493029	-1.603411
H	-3.577188	0.582315	-0.672872
H	-3.450423	-0.349923	-2.144126
C	-1.537121	0.194163	-1.288964
H	-1.102208	1.037943	-0.738393
H	-0.972169	0.123875	-2.222917
C	-1.376813	-1.090312	-0.468942

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H     -2.012749    -1.029312     0.420598
H     -1.742542    -1.950005    -1.044280
C      0.032955    -1.415998     0.036759
H      0.408098    -0.590061     0.641612
C      1.073813    -1.737691    -1.062239
H      1.923941    -2.207004    -0.561892
C      1.573163    -0.594166    -1.821959
H      0.657157    -2.488233    -1.744017
C      2.026970     0.333022    -2.440132
H      2.414202     1.156965    -2.991485
O     -4.712497     3.212418    -3.493729
C     -6.055608     3.622476    -3.876454
C     -5.939823     4.867189    -4.709226
H     -6.637995     3.791035    -2.968998
H     -6.521818     2.803819    -4.427517
C     -6.024403     6.130258    -4.116869
C     -5.724255     4.780268    -6.088134
C     -5.898257     7.285115    -4.885986
H     -6.191431     6.209600    -3.046622
C     -5.596527     5.932087    -6.860291
H     -5.657081     3.803714    -6.558812
H     -5.969706     8.259711    -4.414003
C     -5.683911     7.187582    -6.259777
H     -5.432788     5.850843    -7.930013
H     -5.588375     8.086069    -6.860913
H      3.289263    -1.819732     2.880427
C      3.366377    -4.405847     0.997470
H      4.190619    -3.974550     1.576893
C      3.742650    -5.729802     0.511470
H      3.211043    -3.739052     0.145239
C      4.039541    -6.820729     0.101281
H      4.305229    -7.785120    -0.262908


85 atoms
addition of another 7-isomer unit to the 7-isomer chain end,
structure I3r2, in toluene
N     -0.118523     3.693673     4.398496
C      0.058725     2.709608     3.455338
N      0.718774     2.852248     2.339254
C      1.374683     4.127988     2.095873
C      0.560693     5.297090     2.646951
C      0.308227     5.069375     4.132169
C     -1.070111     2.039807     5.993744
C     -1.496688     1.280524     4.743617
N     -0.475210     1.475923     3.731939
C     -0.870113     3.509081     5.641519
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H	1.519107	4.238470	1.017402
H	2.380177	4.138346	2.545107
H	-0.393051	5.353407	2.112198
H	1.076813	6.250871	2.503210
H	1.212713	5.290275	4.715035
H	-0.475541	5.743859	4.494881
H	-0.330323	4.021286	6.445957
H	-1.846056	4.008059	5.549516
H	-0.137259	1.609894	6.369622
H	-1.821353	1.955196	6.783266
H	-2.486633	1.627394	4.408787
H	-1.580227	0.210178	4.944739
H	0.395223	1.814477	1.001435
O	0.118913	1.348104	0.152555
C	0.409179	0.008796	0.138993
O	0.213218	-0.449949	1.492582
C	0.190885	-1.866304	1.731715
H	0.754123	-2.373084	0.942662
C	-1.258164	-2.356352	1.770598
H	-1.798064	-1.722299	2.485127
H	-1.279421	-3.372815	2.177366
C	-1.977745	-2.344386	0.415580
H	-1.570022	-3.147227	-0.212394
H	-3.029131	-2.602909	0.584626
C	-1.902283	-1.027136	-0.372859
H	-2.284771	-0.193667	0.225809
H	-2.570108	-1.112070	-1.236566
C	-0.494660	-0.693298	-0.882518
H	0.005364	-1.598981	-1.235794
H	-0.545559	-0.014214	-1.736030
O	5.645515	5.622952	-3.033799
O	1.735383	-0.294099	-0.272091
C	6.111957	5.548063	-1.922038
C	5.787322	4.486091	-0.893052
H	5.541701	4.991699	0.047026
H	6.712936	3.934723	-0.688659
C	4.670013	3.536998	-1.323094
H	3.760622	4.113750	-1.523288
H	4.940442	3.069178	-2.275240
C	4.380945	2.457598	-0.274179
H	4.108073	2.933596	0.675764
H	5.297534	1.893872	-0.072647
C	3.258406	1.512441	-0.715439
H	2.370093	2.094314	-0.975269
H	3.555119	0.981182	-1.628540
C	2.811221	0.465483	0.311066
H	2.463964	0.952222	1.226123

C	3.901471	-0.571216	0.676876
H	3.393980	-1.466264	1.047607
C	4.862469	-0.132193	1.685134
H	4.428085	-0.880284	-0.233522
C	5.638603	0.199900	2.542163
H	6.327963	0.503742	3.294073
O	7.018170	6.424685	-1.437379
C	7.430114	7.484505	-2.346002
C	8.434169	8.343103	-1.631198
H	6.545399	8.050830	-2.641559
H	7.849878	7.024986	-3.242720
C	8.028273	9.488898	-0.941407
C	9.788945	7.996798	-1.628320
C	8.956824	10.275636	-0.263114
H	6.978518	9.767531	-0.936951
C	10.720009	8.779612	-0.950540
H	10.115406	7.108753	-2.161629
H	8.628836	11.165063	0.265161
C	10.304925	9.921728	-0.266515
H	11.768949	8.501489	-0.958840
H	11.030022	10.534955	0.258782
H	-0.391268	0.810373	2.972080
C	0.929364	-2.083143	3.068959
H	0.371820	-1.585281	3.870569
C	1.129652	-3.489458	3.404511
H	1.897302	-1.576555	3.014283
C	1.302353	-4.650618	3.666075
H	1.457640	-5.676994	3.902058

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

N	-0.639142	3.443679	4.533073
C	-0.357444	2.593998	3.515555
N	0.328874	3.020953	2.448751
C	0.832207	4.381715	2.328333
C	-0.129349	5.340000	3.020500
C	-0.346609	4.880607	4.456477
C	-1.150234	1.475004	5.949481
C	-1.572325	0.810971	4.644148
N	-0.757410	1.321232	3.551381
C	-1.241051	2.987152	5.792409
H	0.921581	4.605861	1.264961
H	1.834875	4.463310	2.766653
H	-1.081131	5.351858	2.481562
H	0.266325	6.358214	3.020666

H	0.537615	5.098095	5.068739
H	-1.189023	5.414887	4.905882
H	-0.720035	3.490607	6.612487
H	-2.287314	3.315606	5.824287
H	-0.124095	1.181675	6.189101
H	-1.789503	1.156571	6.776160
H	-2.637407	0.991513	4.450168
H	-1.432002	-0.269363	4.687458
H	0.368306	2.402470	1.620184
O	0.327420	1.525673	0.175017
C	0.566227	0.321861	-0.026027
O	0.320531	-0.407637	1.768617
C	0.210096	-1.784191	1.918493
H	0.759241	-2.299648	1.110732
C	-1.259267	-2.241554	1.882936
H	-1.806070	-1.636767	2.619121
H	-1.342859	-3.283987	2.214052
C	-1.941387	-2.113247	0.513073
H	-1.574526	-2.913343	-0.143830
H	-3.012049	-2.312846	0.646309
C	-1.781345	-0.774592	-0.230876
H	-2.033564	0.067539	0.419538
H	-2.515264	-0.764203	-1.044837
C	-0.385938	-0.549592	-0.835860
H	0.096527	-1.504277	-1.056597
H	-0.477454	-0.026056	-1.795032
O	5.887200	5.635360	-3.213378
O	1.859772	-0.117345	-0.255460
C	6.338152	5.598333	-2.093457
C	5.958139	4.605307	-1.015681
H	5.652794	5.174572	-0.130420
H	6.871168	4.078229	-0.715538
C	4.871172	3.620421	-1.442854
H	3.976685	4.174565	-1.746522
H	5.203344	3.081129	-2.336011
C	4.516681	2.622640	-0.334860
H	4.181716	3.169594	0.556214
H	5.418700	2.082836	-0.030298
C	3.426401	1.637656	-0.770033
H	2.551649	2.195309	-1.116317
H	3.776934	1.047224	-1.625885
C	2.925320	0.667726	0.305164
H	2.535576	1.215299	1.164424
C	3.965889	-0.364393	0.792941
H	3.406882	-1.192404	1.236993
C	4.920641	0.133883	1.779650
H	4.501090	-0.781406	-0.068144

C	5.693376	0.514868	2.619582
H	6.381933	0.857070	3.355493
O	7.271868	6.463281	-1.640880
C	7.732739	7.461169	-2.595081
C	8.764599	8.312993	-1.912555
H	6.873854	8.047309	-2.926085
H	8.140620	6.942520	-3.464590
C	8.401294	9.511960	-1.293099
C	10.102475	7.908311	-1.869727
C	9.355094	10.293783	-0.644692
H	7.365062	9.836265	-1.320476
C	11.058527	8.685988	-1.221541
H	10.395901	6.978572	-2.348351
H	9.060307	11.224816	-0.171376
C	10.685948	9.881501	-0.607785
H	12.094042	8.362191	-1.198435
H	11.430825	10.490617	-0.105912
H	-0.376869	0.643400	2.831413
C	0.904922	-2.212136	3.248260
H	0.342826	-1.795316	4.093565
C	1.059293	-3.652087	3.429258
H	1.887349	-1.730155	3.268672
C	1.186659	-4.843449	3.550285
H	1.301748	-5.895818	3.659709

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

N	-5.372451	3.415389	0.029273
C	-4.826770	2.158079	-0.102083
N	-4.348957	1.812460	-1.347951
C	-4.057212	2.815258	-2.359352
C	-5.233310	3.778242	-2.423475
C	-5.433967	4.403683	-1.049381
C	-5.175796	3.095132	2.463607
C	-5.325763	1.609953	2.145318
N	-4.766776	1.266181	0.845915
C	-5.805885	3.904963	1.338951
H	-3.912269	2.300789	-3.311183
H	-3.128890	3.366118	-2.141545
H	-6.129833	3.228369	-2.724688
H	-5.059037	4.566240	-3.160738
H	-4.672541	5.178308	-0.875140
H	-6.408059	4.903148	-0.997024
H	-5.517311	4.958946	1.417449
H	-6.902193	3.869432	1.404119

H	-4.111821	3.340651	2.545232
H	-5.648934	3.350669	3.416276
H	-6.392004	1.335872	2.194681
H	-4.819933	1.007654	2.905911
H	-3.737456	1.004848	-1.344433
O	-2.239033	-0.227254	-1.872627
C	-2.056290	-1.399259	-1.621957
O	-3.770047	-1.341178	0.646774
C	-4.767086	-2.331352	0.836060
H	-4.245487	-3.293052	0.778535
C	-5.865967	-2.281667	-0.236869
H	-6.193281	-1.239205	-0.334473
H	-6.732317	-2.842766	0.131174
C	-5.510904	-2.845552	-1.623383
H	-5.272255	-3.913165	-1.528745
H	-6.425032	-2.805047	-2.226873
C	-4.393548	-2.138909	-2.413377
H	-4.506756	-1.056930	-2.319930
H	-4.537596	-2.359394	-3.475463
C	-2.960184	-2.544209	-2.015919
H	-2.949960	-3.259195	-1.192728
H	-2.458039	-3.056439	-2.845570
O	6.590843	-2.142380	-1.245966
O	-0.956457	-1.860683	-0.996740
C	6.439340	-1.107433	-0.641383
C	5.110000	-0.474682	-0.287097
H	5.068081	0.501787	-0.784062
H	5.118472	-0.251078	0.785055
C	3.905626	-1.334380	-0.666538
H	3.943746	-1.558105	-1.737421
H	3.976922	-2.301342	-0.157123
C	2.573325	-0.661667	-0.319573
H	2.501613	0.301103	-0.840640
H	2.549321	-0.426022	0.748711
C	1.373617	-1.538028	-0.695075
H	1.442487	-1.810453	-1.754131
H	1.408296	-2.479623	-0.134155
C	0.004809	-0.895780	-0.482733
H	-0.094338	0.020415	-1.065108
C	-0.385258	-0.617446	0.987166
H	-1.477636	-0.589941	1.047761
C	0.153681	0.627800	1.526465
H	-0.068996	-1.462885	1.609308
C	0.571242	1.663467	1.973627
H	0.944403	2.578708	2.368558
O	7.464082	-0.352028	-0.193276
C	8.800573	-0.850790	-0.485054

C	9.792592	0.113485	0.099490
H	8.906304	-0.940036	-1.567621
H	8.897555	-1.848665	-0.054351
C	10.248020	1.203989	-0.647478
C	10.259242	-0.052649	1.406708
C	11.152875	2.110569	-0.100408
H	9.892196	1.342433	-1.664300
C	11.164331	0.851664	1.957486
H	9.912254	-0.896441	1.996003
H	11.501360	2.950890	-0.692107
C	11.612838	1.935456	1.204041
H	11.521557	0.709176	2.972249
H	12.320528	2.639020	1.630539
H	-4.168234	-0.428681	0.677096
C	-5.350054	-2.216240	2.270881
H	-5.942089	-1.296943	2.345662
C	-6.161587	-3.357912	2.680339
H	-4.505456	-2.100884	2.957609
C	-6.816887	-4.315508	2.999588
H	-7.399019	-5.157957	3.290094

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

N	-5.069683	-3.403889	9.706132
C	-5.898773	-2.311821	9.594652
N	-5.773642	-1.335511	10.555911
C	-4.644584	-1.251928	11.462146
C	-4.324981	-2.657783	11.953948
C	-4.060205	-3.558989	10.754282
C	-5.710852	-3.947736	7.383506
C	-7.017692	-3.236457	7.730935
N	-6.808005	-2.150701	8.674845
C	-5.052901	-4.436875	8.667982
H	-4.921272	-0.599140	12.292643
H	-3.756819	-0.810530	10.982081
H	-5.174549	-3.036198	12.529775
H	-3.449253	-2.655847	12.608141
H	-3.064450	-3.346970	10.337097
H	-4.052732	-4.609581	11.065123
H	-4.009253	-4.714069	8.481209
H	-5.559119	-5.337667	9.041101
H	-5.045561	-3.245463	6.870405
H	-5.878667	-4.793791	6.710621
H	-7.735738	-3.967792	8.134775
H	-7.478141	-2.825459	6.827482

H	-6.346210	-0.516265	10.394678
O	-2.024857	1.575083	5.274117
C	-1.976980	2.008738	6.399680
O	-7.911961	0.302634	9.226999
C	-8.109306	1.260843	8.199952
H	-8.157967	2.231775	8.705769
C	-6.963797	1.284783	7.181387
H	-6.885228	0.291514	6.721261
H	-7.222961	1.981808	6.376671
C	-5.613365	1.678205	7.785349
H	-5.374550	0.996473	8.607885
H	-5.694424	2.679111	8.229787
C	-4.474526	1.662377	6.761595
H	-4.380050	0.662108	6.327334
H	-4.712598	2.329737	5.926152
C	-3.135689	2.074908	7.371251
H	-2.881204	1.434216	8.224392
H	-3.178653	3.090861	7.778194
O	4.257867	-3.012034	5.785868
O	-0.850920	2.500988	6.968176
C	4.718906	-2.140598	5.087356
C	4.149405	-0.747777	4.917703
H	3.963264	-0.592329	3.849051
H	4.936855	-0.032018	5.179249
C	2.884944	-0.503487	5.738991
H	2.124627	-1.240534	5.460803
H	3.101517	-0.682794	6.797421
C	2.330693	0.913062	5.553556
H	2.109259	1.084615	4.493126
H	3.098703	1.644250	5.822911
C	1.062481	1.142732	6.383497
H	0.332776	0.366065	6.133447
H	1.286558	1.030831	7.451259
C	0.372615	2.491942	6.175376
H	0.092422	2.618745	5.128813
C	1.152771	3.726487	6.667813
H	0.427308	4.530737	6.824976
C	2.181528	4.201548	5.746656
H	1.593738	3.515342	7.648561
C	3.010891	4.627580	4.987720
H	3.747514	4.995565	4.312936
O	5.834261	-2.295261	4.344285
C	6.478183	-3.599233	4.418993
C	7.689488	-3.568177	3.531608
H	5.758695	-4.356481	4.102736
H	6.738875	-3.796365	5.460148
C	7.582469	-3.883988	2.173774

C	8.937186	-3.201547	4.044108
C	8.699800	-3.835382	1.343857
H	6.617753	-4.170343	1.765147
C	10.057415	-3.152395	3.217457
H	9.031957	-2.954167	5.097418
H	8.603926	-4.085941	0.292351
C	9.940134	-3.469307	1.865086
H	11.021075	-2.869703	3.628687
H	10.812370	-3.434351	1.220342
H	-7.671593	-0.587282	8.850099
C	-9.486891	1.011947	7.531119
H	-9.452053	0.059552	6.987816
C	-9.921526	2.077268	6.632953
H	-10.220014	0.883526	8.333493
C	-10.265417	2.972758	5.906329
H	-10.577116	3.758840	5.259883

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