Supporting Information

Radical ring-opening polymerization of sustainably-derived thionoisochromanone

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## Materials, Methods, and General Considerations

All polymerizations were either purged with N_2 or Ar for 30 minutes or prepared through freeze-pump-thaw techniques followed by back-filling with nitrogen. All reagents were purchased from commercial sources and were used as received, unless otherwise noted. Comonomers were passed through a basic alumina plug and bubbled with either Ar or N_2 gas for 10 min before use. Nuclear magnetic resonance (NMR) spectroscopy experiments were performed with either a Bruker Avance AV-500, a Bruker Avance HD-500, or a Bruker Avance AX-400 spectrometer. Diffusion-ordered spectroscopy (DOSY) were obtained on a Bruker Avance AV-500 spectrometer using ledbpgp2s pulse sequence, CD_2Cl_2 solvent, and gradient range of 2-98%. Chemical shifts for ^1H and ^{13}C NMR spectra were referenced to residual protium in the deuterated solvent (for ^1H NMR) and the deuterated solvent itself (for ^{13}C NMR). Molecular weights (M_n and M_w) and dispersities (M_w/M_n) of polymer samples were determined in DMF at 25 °C with a flow rate of 1 mL/min on an Agilent 1260 Infinity II HPLC with Polargel-m columns connected to a Wyatt DAWN Heleos II light scattering detector and a Wyatt OPTILAB T-rEX refractive index detector. Differential scanning calorimetry experiments were conducted via a TA Instruments Discovery DSC, using samples hermetically sealed in aluminum pans, at a heating rate of 10 °C/min. Reported T_g values are from the second heating ramp. GC-MS spectra were obtained on an Agilent 6953 gas chromatograph with an Agilent HP-5 column (0.25 µm film thickness, 15 mlength× 0.32 mm ID) connected to an Agilent 5975 MSD at 70 eV in electron ionization mode. Elemental Analysis was performed by Atlantic Microlab, Inc. in Norcross, Georgia. Energy Dispersive X-Ray Analysis (EDX) was performed on a JEOL 6500F SEM with an Oxford Instruments XMax 80mm2 EDS detector using the Oxford Instruments Aztec software at a 10mm working distance, 10kV accelerating voltage, and a probe current of ~5nA.

Synthesis and Characterization

Synthesis of TIC. An oven-dried round bottom flask was sequentially charged with a stir bar and a solution of 3-isochromanone (3.0 g, 20.2 mmol) in toluene (0.3 M, 65 mL). After addition of Lawesson's reagent (1 equiv., 20.2 mmol), the reaction mixture was stirred at reflux for 1 h. Following the reflux, the reaction mixture was cooled to room temperature before being placed in a –20 °C freezer overnight to induce precipitation. Subsequently, the reaction was filtered via gravity filtration and the filtrate concentrated *in vacuo*. The monomer (**TIC**) was purified from the

filtrate via column chromatography by hand (4:1 hexanes:EtOAc, Rf = 0.3) as an orange-brown solid followed by further purification on an Interchim PuriFlash automated column system using Teledyne Isco normal phase pre-column cartridges and RediSep Rf gold performance columns (1.3 g, 39.4%). ^{1}H NMR (500 MHz, CD$_2$Cl$_2$) δ 7.36 (m, 3H, ArH), 7.26 (d, J = 7.2 Hz, 1H, ArH), 5.42 (s, 2H, CH_2C=SC-OCH$_2$), 4.16 (s, 2H, CH$_2$C=SC-OCH_2). ^{13}C{^{1}H} NMR (125 MHz, CD$_2$Cl$_2$) δ 218.34, 131.78, 131.40, 129.76, 128.04, 126.77, 125.26, 74.46, 49.08.

NMR and IR Spectra for TIC
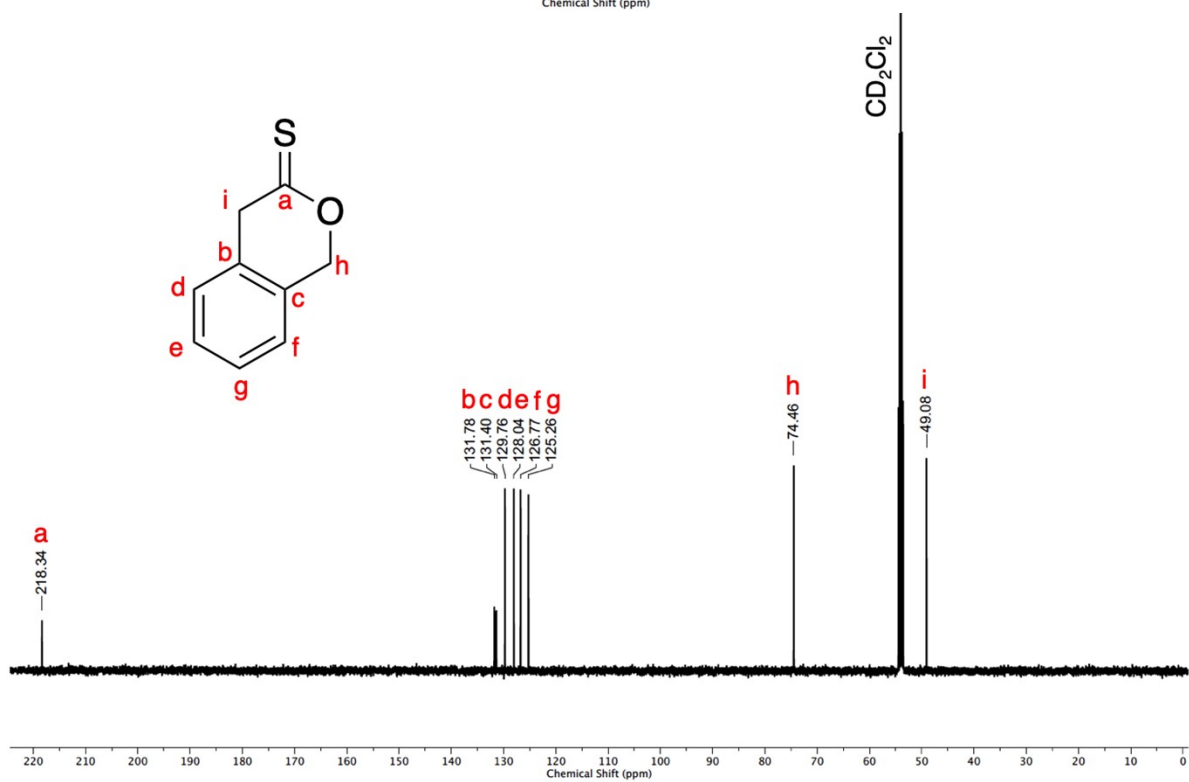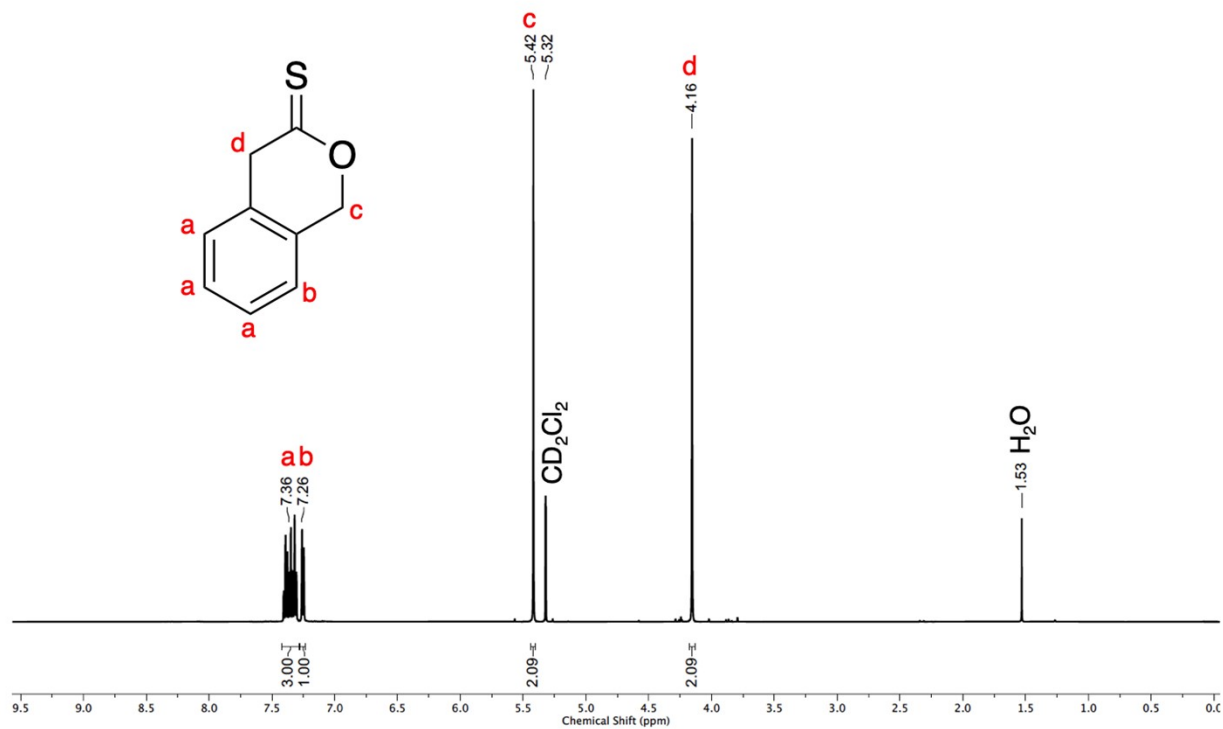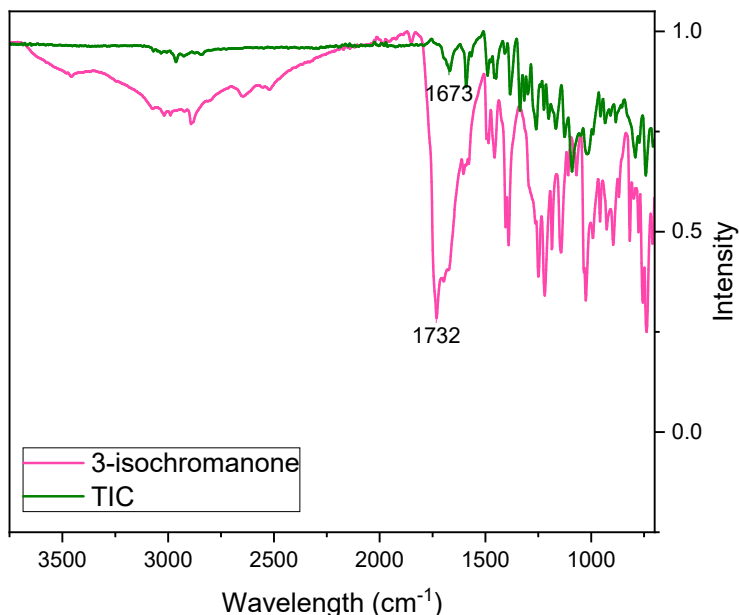
Figure S2. IR Spectrum of 3-isochromanone (pink trace) and TIC (green trace), highlighting the shift in carbonyl stretch from 1732 cm^{-1} of ester (OC=O) in 3-isochromanone to 1673 cm^{-1} of thioester (SC=O) in TIC.

Polymerization Experiments and Analysis

Homopolymerizations were performed in DMF (3.05 M) at 70 °C. An example free radical homopolymerization of **TIC** was completed as follows. A stock solution of initiator AIBN (0.609 M, DMF) was prepared. An oven-dried bomb flask was sequentially charged with a stir bar, TIC (20 equiv., 0.61 mmol), AIBN stock (1 equiv., 50 µL), and DMF (0.2 mL, 3.05 M). Freeze, pump, thaw was performed three times on the bomb flask and upon warming back to room temperature, the flask was backfilled with nitrogen, submerged in an oil bath, and stirred at 70 °C. After a specified amount of time, the polymerization was quenched by rapid cooling and exposure to air. An aliquot of the polymerization was removed and subjected to ^{1}H NMR analysis. The rest of the reaction mixture was precipitated into cold MeOH. Once precipitated, the mixture was centrifuged to collect a solid. This process was repeated before drying the polymer under vacuum for ~18 h before being submitted for analysis via NMR, SEC (M_n, Đ), and DSC (T_g).

Copolymerizations were performed in bulk (minimal DMF was used in the case of **TIC** homopolymerization studies) at 70 °C. An example free radical copolymerization of **TIC** and styrene was completed as follows. A stock solution of initiator AIBN (0.609 M, DMF) was prepared. An oven-dried bomb flask was sequentially charged with a stir bar, TIC (20 equiv., 0.61 mmol), AIBN stock solution (1 equiv., 50 µL), and styrene (380 equiv., 11.59 mmol). Freeze, pump, thaw was performed three times on the bomb flask and upon warming back to room temperature, the flask was back-filled with N_2, submerged in an oil bath, and stirred at 70 °C. After a specified amount of time, the polymerization was quenched by rapid cooling and exposure to air. An aliquot of the polymerization was removed and subjected to ^{1}H NMR analysis. The rest of the reaction mixture was precipitated into cold MeOH. Once precipitated, the mixture was centrifuged to collect a solid. This process was repeated before drying the polymer under vacuum for ~18 h before being submitted for analysis via NMR, SEC (M_n, Đ), TGA and DSC (T_g).

Block copolymerizations were performed as follows. A stock solution of initiator AIBN (0.609 M, DMF) was prepared. An oven-dried Schlenk flask was sequentially charged with a stir bar, TIC (20 equiv., 0.61 mmol), and AIBN stock solution (1 equiv., 50 µL). Freeze, pump, thaw was performed three times on the Schlenk flask and upon warming back to room temperature the flask was back-filled with N_2, submerged in an oil bath, and stirred at 70 °C for 4 days. An aliquot was removed using air-free techniques and submitted for NMR and crude SEC (M_n, Đ) analysis. Styrene monomer (380 equiv., 11.59 mmol) was sparged with N_2 for 20 minutes, taken up in an air-free syringe (pumped with N_2 3 times), and added to the Schlenk flask. The flask was left stirring at 70 °C for 3 days before quenching by rapid cooling and exposure to air. An aliquot of the polymerization was removed and subjected to ^{1}H NMR analysis. The rest of the reaction mixture was precipitated into cold MeOH and centrifuged to collect a solid. This process was repeated before drying the polymer under vacuum and submitting for analysis via NMR, SEC (M_n, Đ), and DSC (T_g).

Characterization of Polymers

NMR Spectra

Poly(TIC)
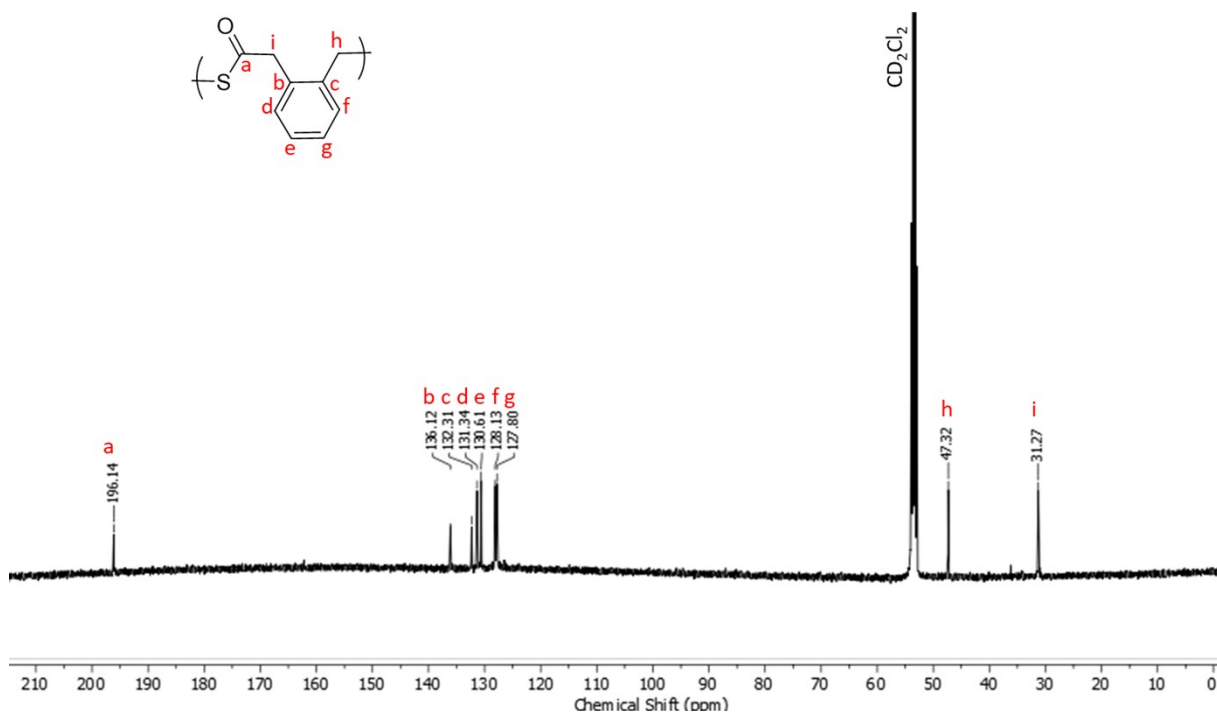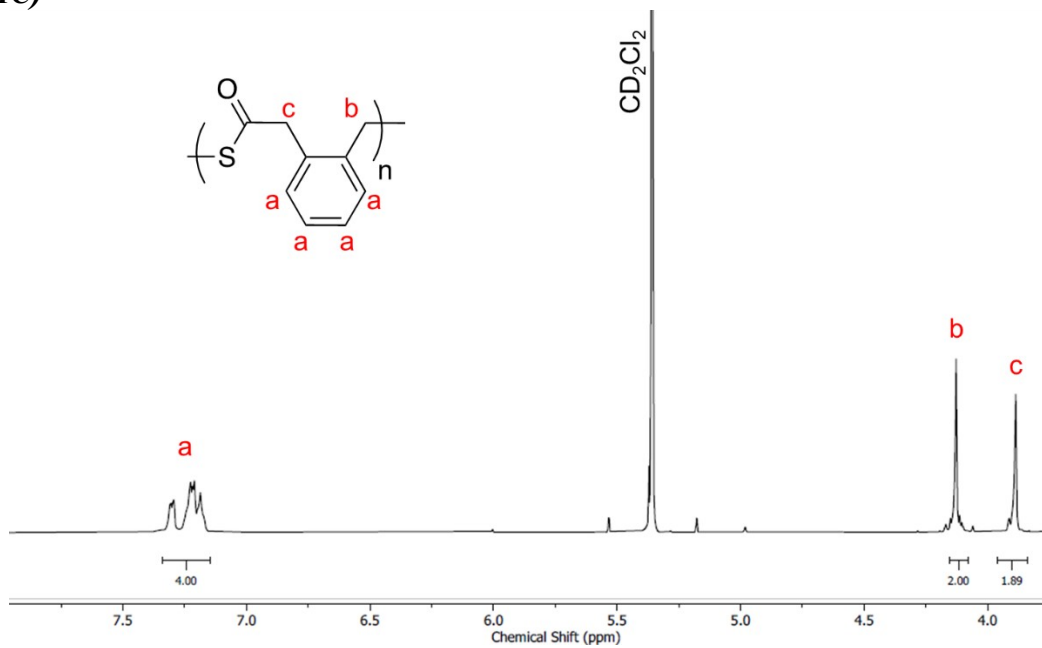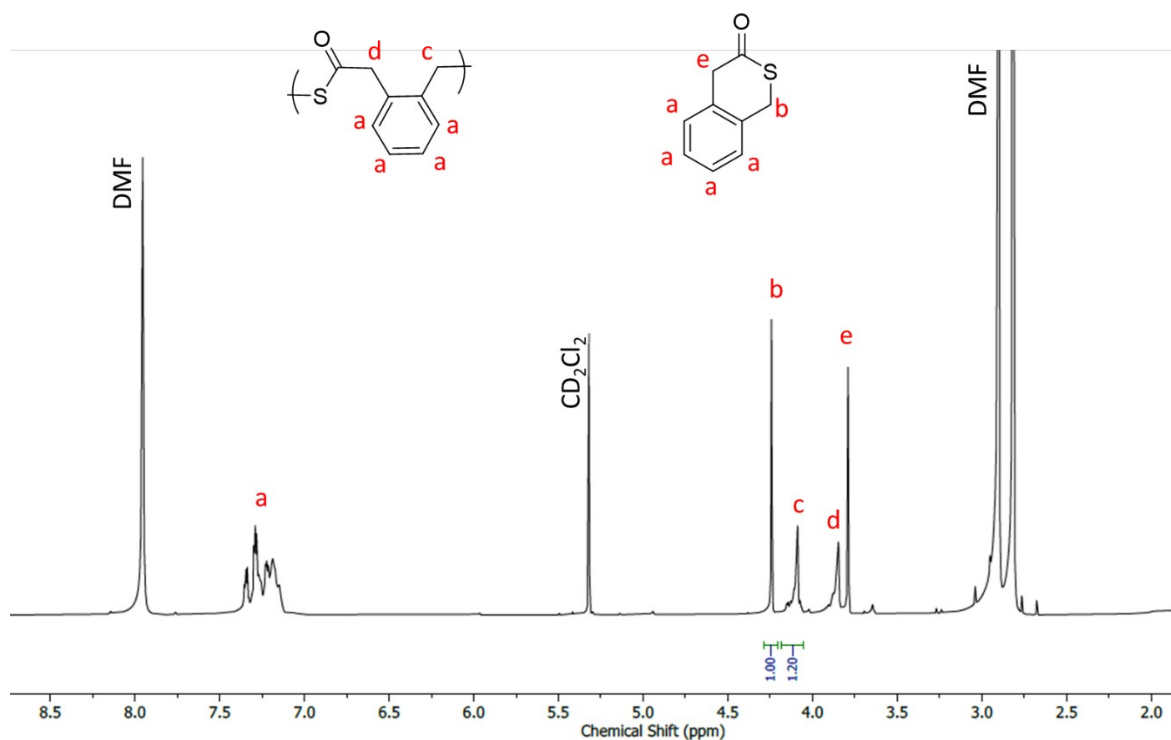
Figure S3. ^{1}H (top), ^{13}C (middle) NMR spectra of **p(TIC)** in CD$_2$Cl$_2$. ^{1}H (bottom) NMR crude spectrum of auto-initiated p(TIC).
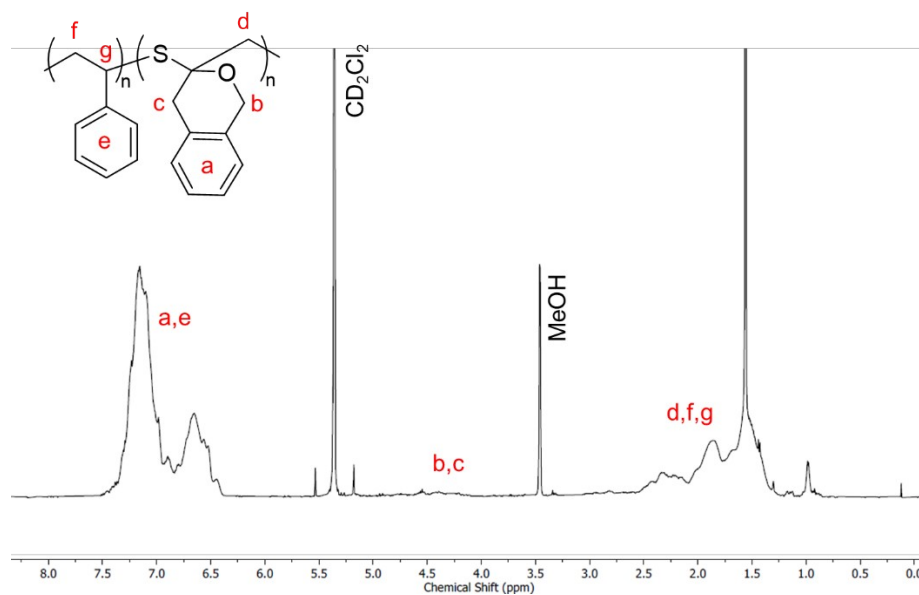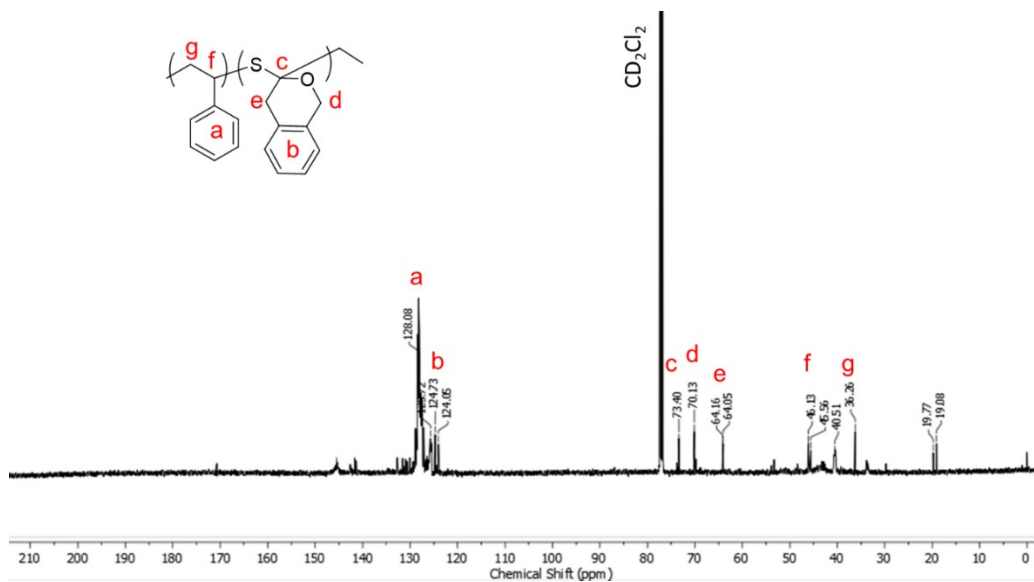
Figure S4. ^{1}H (top) and ^{13}C (bottom) NMR spectrum of poly(TIC-*co*-styrene) in CD$_2$Cl$_2$. Due to signal-to-noise, ^{13}C NMR is shown of crude material.
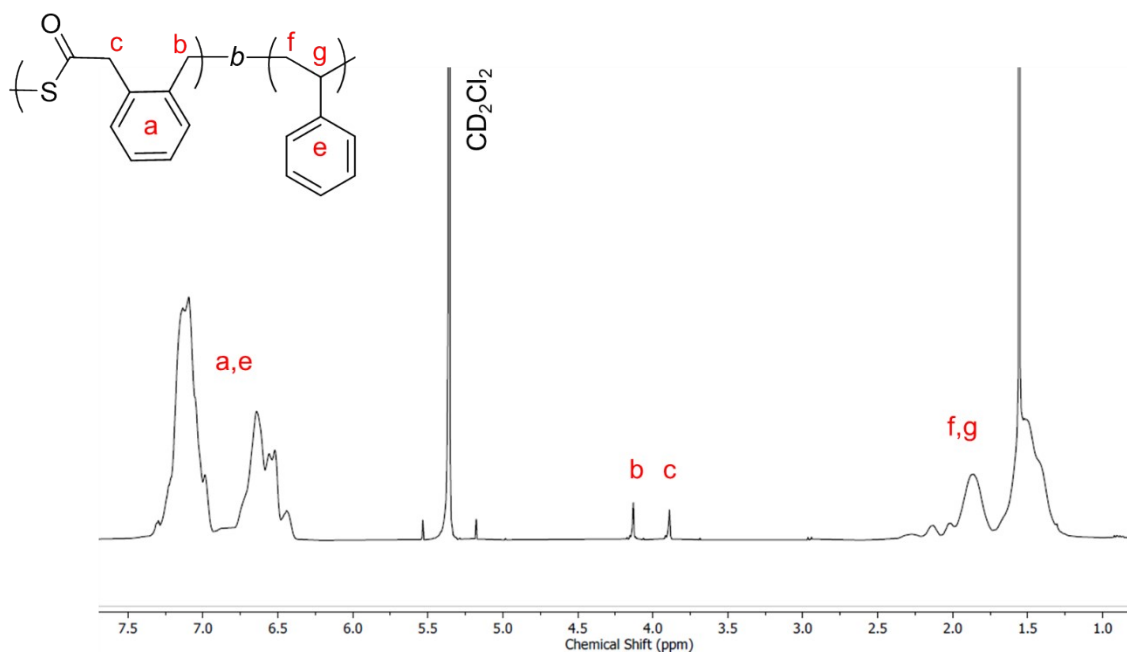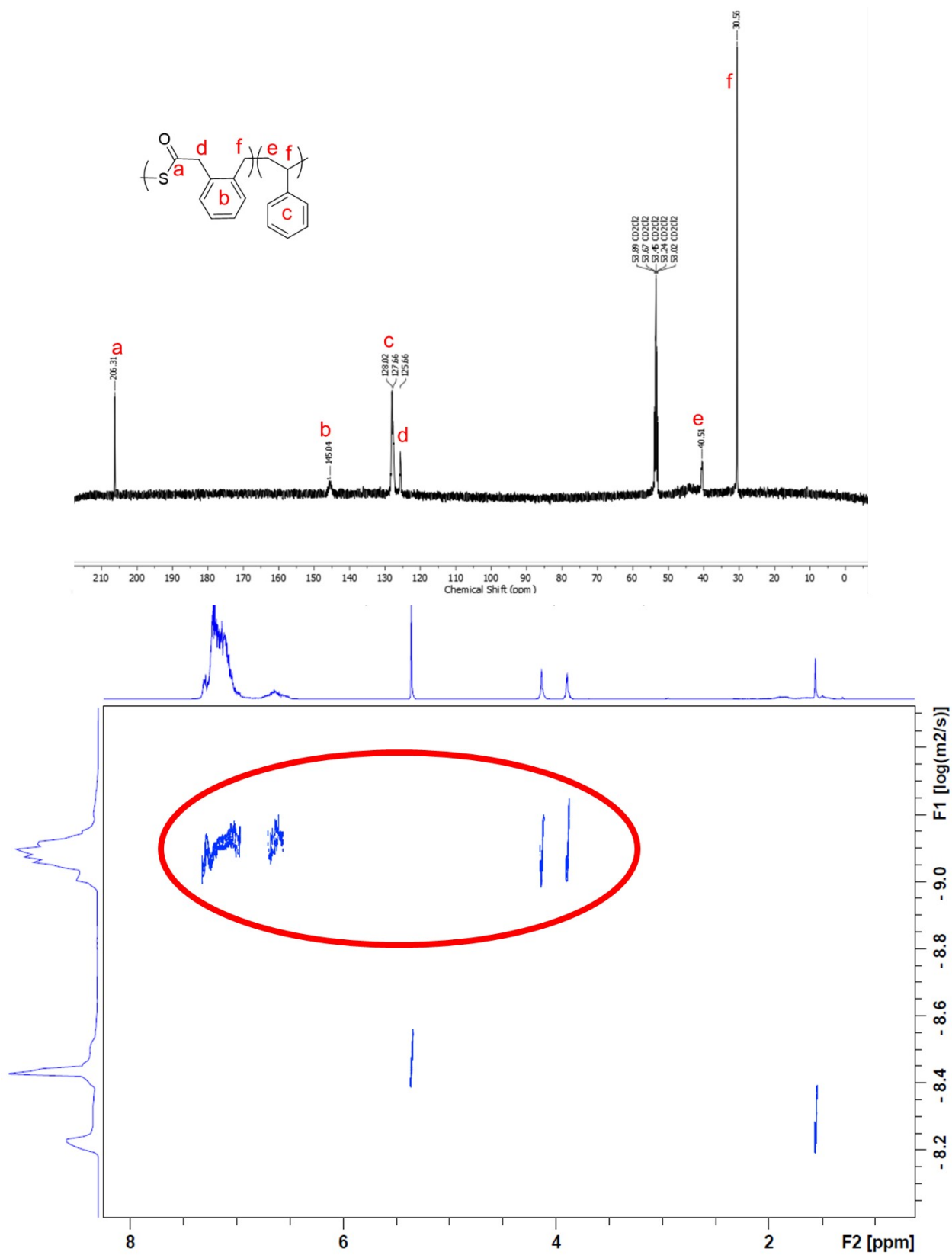
Figure S5. ^{1}H (top), ^{13}C (middle) and DOSY (bottom) NMR spectrum of purified poly(TIC-*b*-styrene) in CD_2Cl_2.
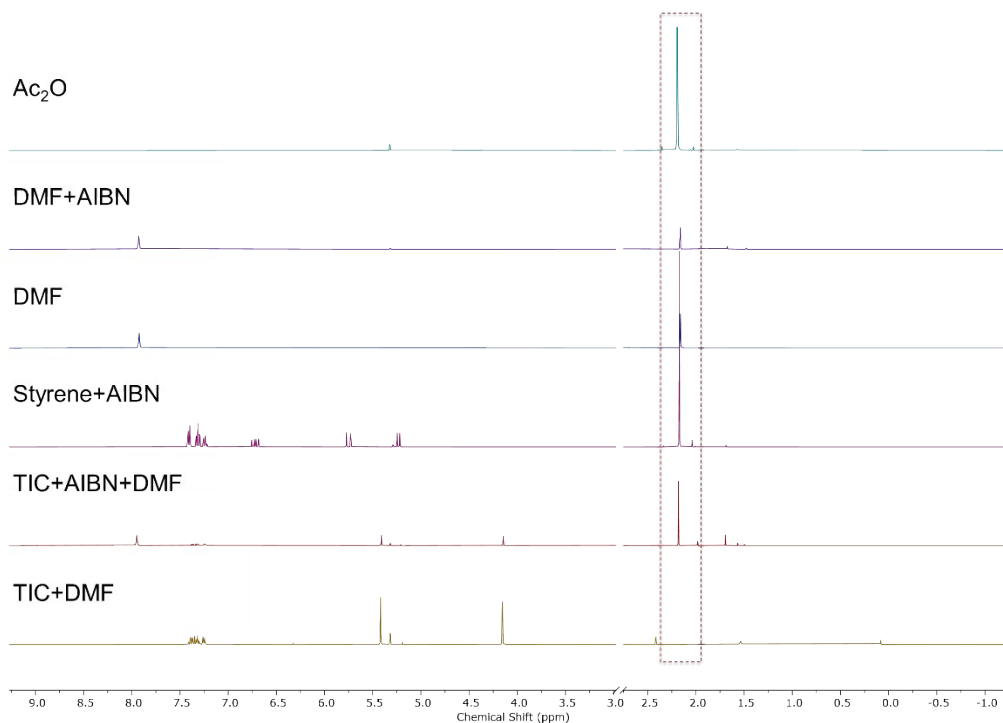
Figure S6. ^{1}H NMR spectra of acetic anhydride nucleophile-trapping experiments. All experiments were sparged with N_2 and heated at 70 °C for 5 hours before the addition of acetic anhydride, with the exception of the styrene+AIBN sample, which was sparged and heated at 70 °C for 30 minutes before adding acetic anhydride.
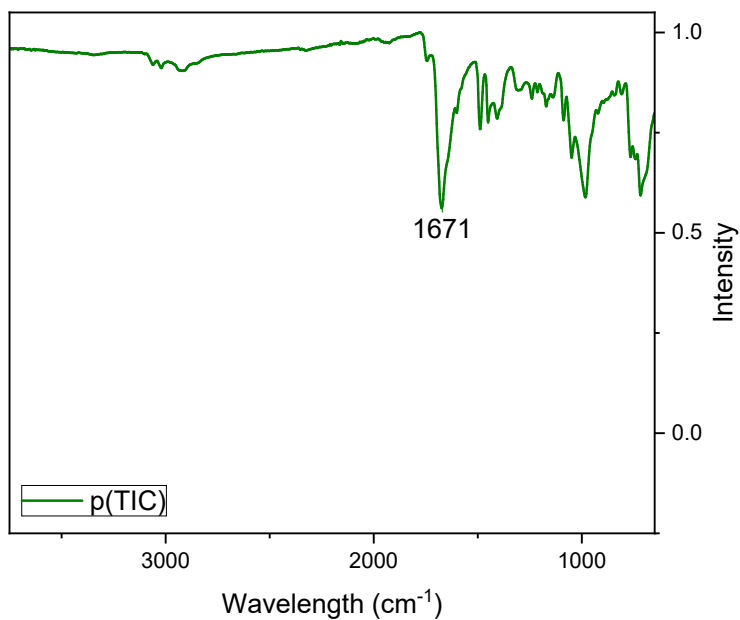
Figure S7. IR Spectrum of p(TIC), highlighting the thioester (SC=O) stretch at 1671 cm^{-1}.
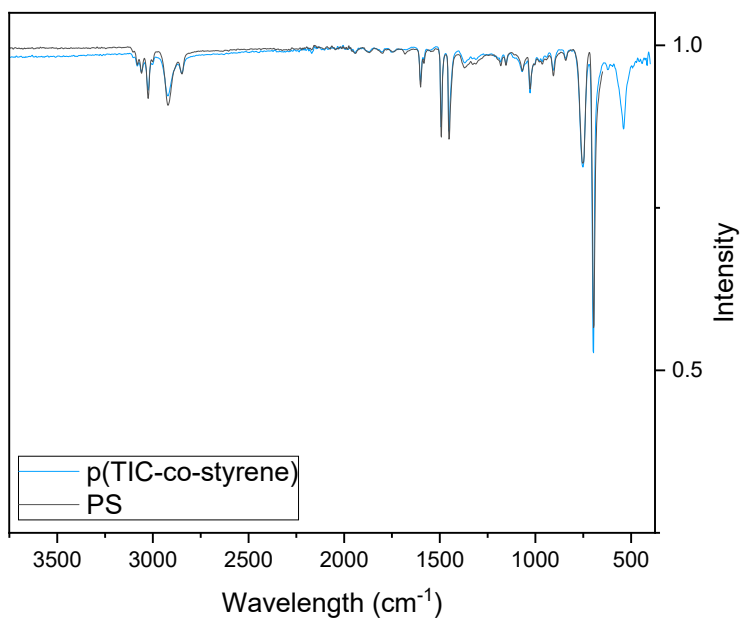
Figure S8. IR spectrum of polystyrene (black trace) and p(TIC-*co*-styrene), showing nearly complete overlap and no notable thioester stretch around 1670 cm^{-1}.
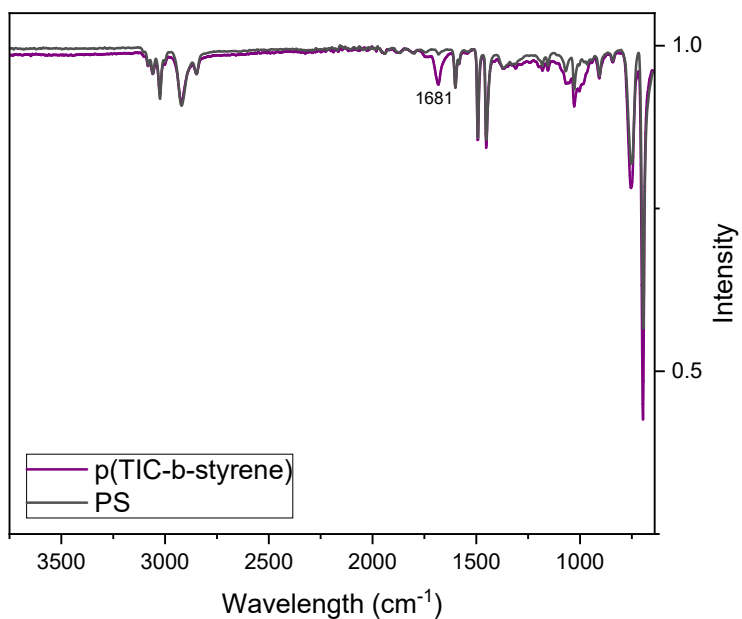
Figure S9. IR spectrum of polystyrene (black trace) and p(TIC-*b*-styrene) (purple trace), showing thioester (SC=O) stretch at 1681 cm^{-1}.

Elemental Analysis

Analysis provided by Atlantic Microlab, Inc. (6180 Atlantic Blvd. Suite M, Norcross, GA 30071)

Anal. Calcd. (S) for **p(TIC-*co*-styrene)** based on feed ratio of 1:19 of **TIC**:styrene: S, 1.50. Found: S, 1.34.

Energy-dispersive X-Ray Spectroscopy (EDX)

Table S1. EDX data for p(TIC-*co*-styrene).

Entry	Styrene: TIC	Concentration	Carbon content (%)	Oxygen content (%)	Sulfur content (%)
1	1:0	Bulk	98.7	1.5	0
2	19:1	Bulk	98.0	1.4	0.6
3	50:1	Bulk	98.2	1.5	0.3
4	38:1	3.05 M	98.4	1.5	0.1

Polymerization Results

Table S2. Polymerization data for **p(TIC)** kinetics.

Entry	Time	Temp. (°C)	TIC Conv.^{a}	M_n (kDa)^b	Đ ^{b}
1	6 h	70	6%	e	e
2	1 d	70	19%	1.66	1.28
3	2 d	70	26%	1.45	1.16
4	4 d	70	57%	1.75	1.07
5	8 d	70	74%	1.83	1.04

^{a}Determined by ^{1}H NMR spectroscopy. ^{b}Determined by SEC using light scattering (MALLS) detection with DMF eluent. ^{c}Determined by DSC measurement. ^{e}No M_n measured. ^{f}Significant isomerization to thiolactone analog.

Table S3. Additional Polymerization data for **p(TIC-*co*-styrene)**.

Entry	Styrene: TIC	Concentration (DMF)	Time	Temp. (°C)	Styrene Conv.[a]	TIC Conv.[a]	M_n (kDa)[b]	Đ [b]
1	19:1	N/A	6 h	70	9%	26%	4.77*	1.14
2	19:1	N/A	1 d	70	14%	42%	4.29*	1.15
3	19:1	N/A	2 d	70	17%	53%	4.97*	1.15
4	19:1	N/A	4 d	70	19%	79%	5.24*	1.16
5	19:1	N/A	8 d	70	22%	90%	4.95*	1.28
6	38:1	0.48 M	4 d	70	14%	8%	X	X
7	38:1	3.05 M	4 d	70	7%	18%	3.03*	1.15
8	50:1	3.05 M	4 d	70	12%	22%	5.26*	1.25
9	5:1	3.05 M	4 d	70	12%	8%	3.16	1.05
10[c]	19:1	N/A	4 d	70	6%	39%	X	X

[a]Determined by ^{1}H NMR spectroscopy. [b]Determined by SEC using light scattering (MALLS) detection with THF eluent. *All samples were bimodal with a first peak of large size but small concentration, as time increased relative concentration of second peak increased, M_n value shown for second peak. [c]Blank sample run without AIBN present.

∂n/∂c Measurements Data in Offline Batch Mode

A stock solution of p(TIC) was made in DMF (LiBr 0.05 M). Five solutions were made from stock and DMF (LiBr 0.05 M) to achieve a concentration range of 0.21-2.1 mg/mL. Samples were injected at a flow rate of 0.1 mL/min into a Wyatt Optilab T-rEX refractive index detector (25 °C, λ_0= 660 nm). Refractive indices were measured at each concentration and the ∂n/∂c is determined from the slope. ∂n/∂c= 0.1517
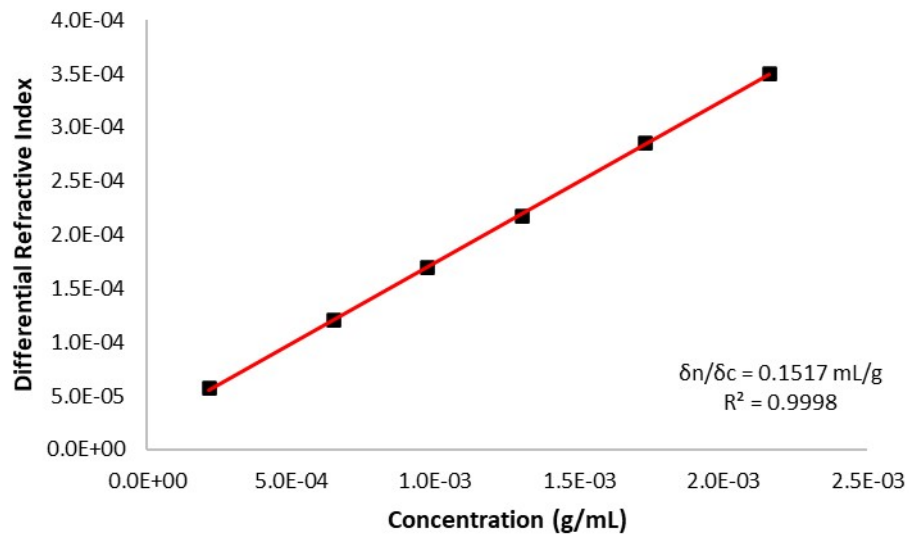
Figure S10. $\partial n/\partial c$ batch measurement for purified p(TIC)

SEC Traces
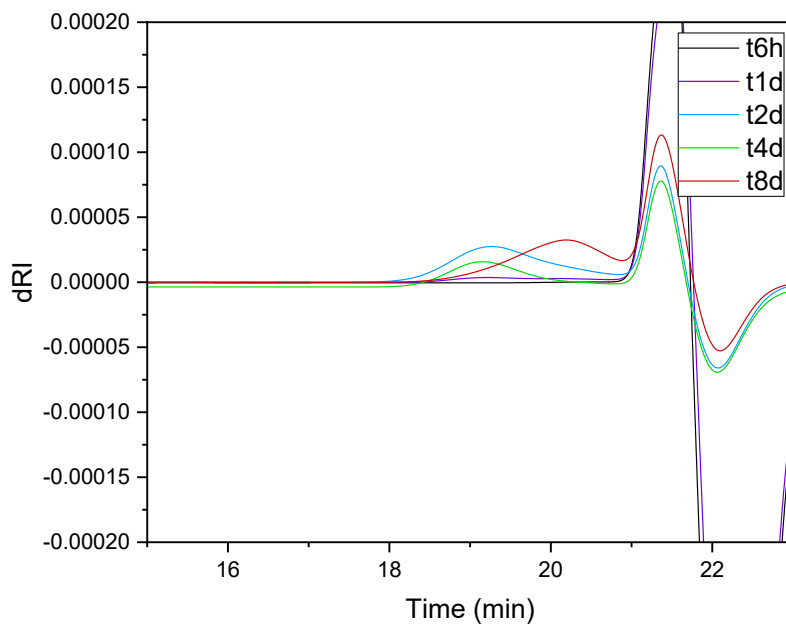
Figure S11. DMF SEC traces of p(TIC) kinetics, at time intervals of 6 hours, 1 day, 2 days, 4 days, and 8 days.
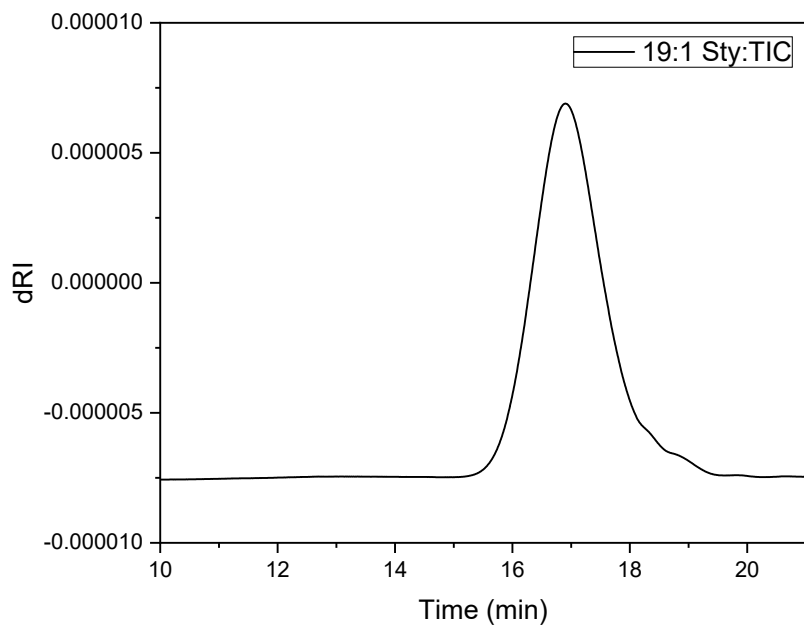
Figure S12. DMF SEC trace of 19:1 styrene:TIC copolymer
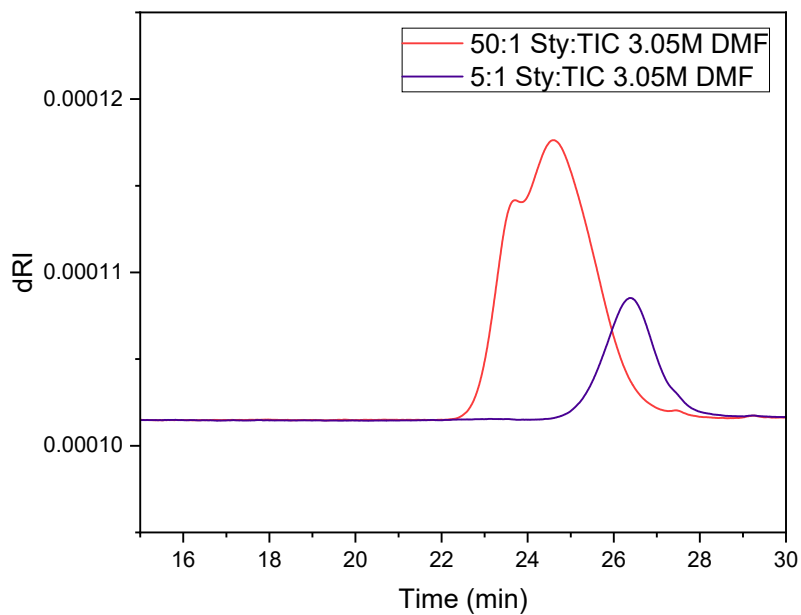
Figure S13. THF SEC trace of 50:1 and 5:1
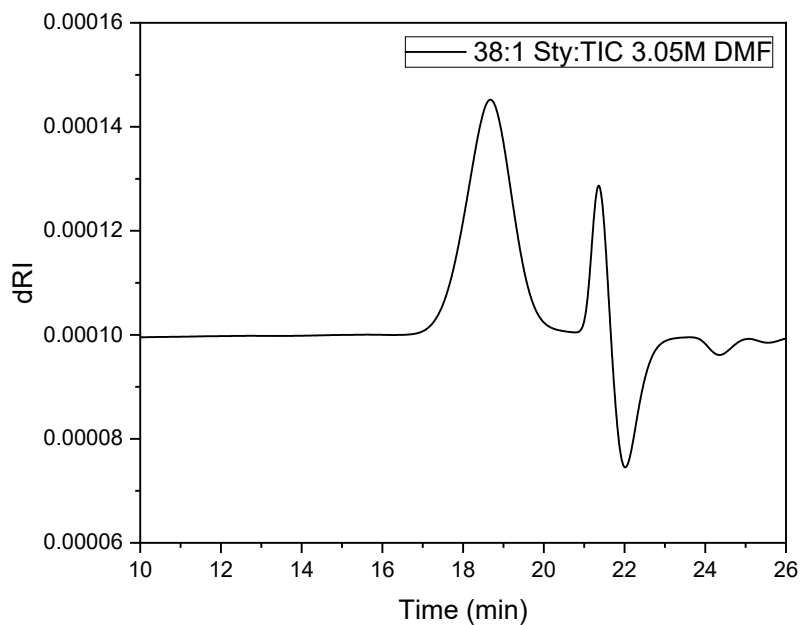
Figure S14. DMF SEC trace of 38:1 styrene:TIC ratio run in 3.05M DMF
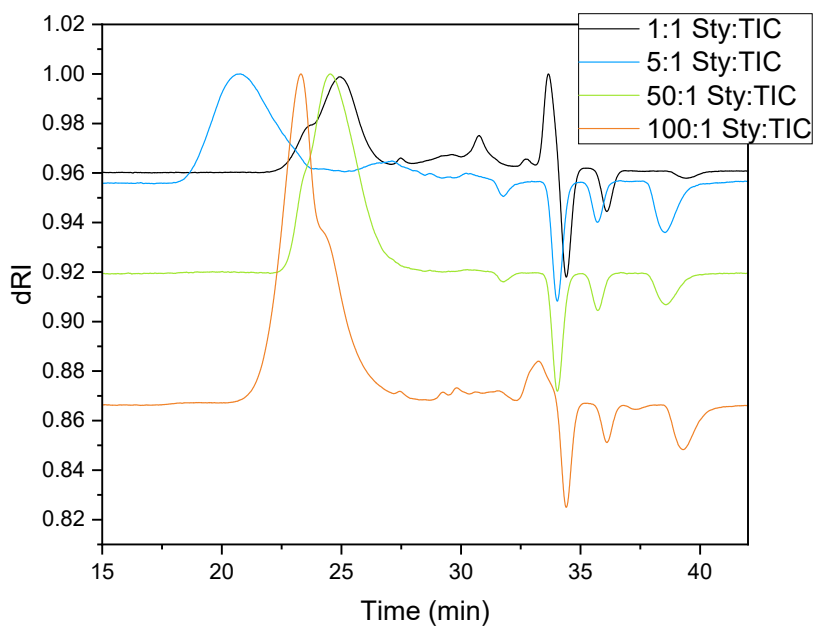
Figure S15. THF SEC traces of various ratios of styrene:TIC copolymerizations, run in bulk
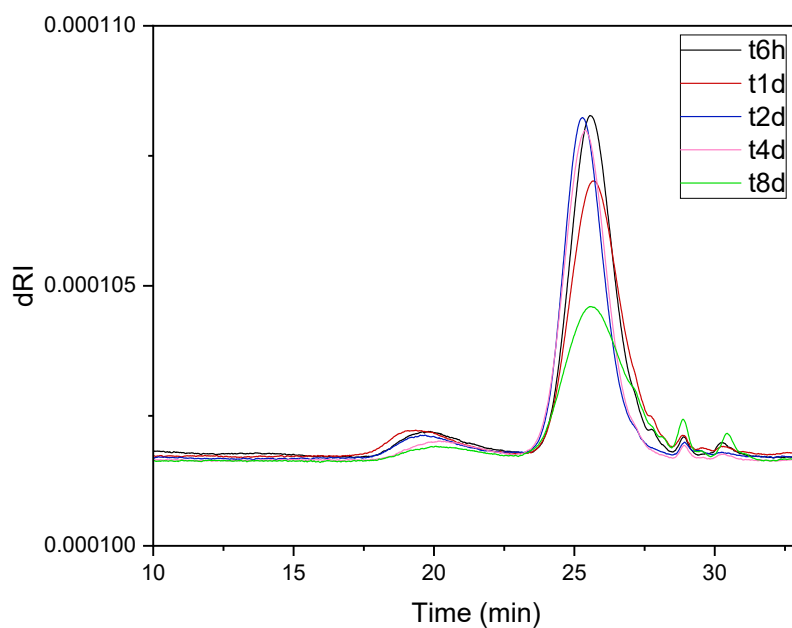
Figure S16. THF SEC traces of 19:1 styrene:TIC copolymer kinetics, at time intervals of 6 hours, 1 day, 2 days, 4 days, and 8 days.
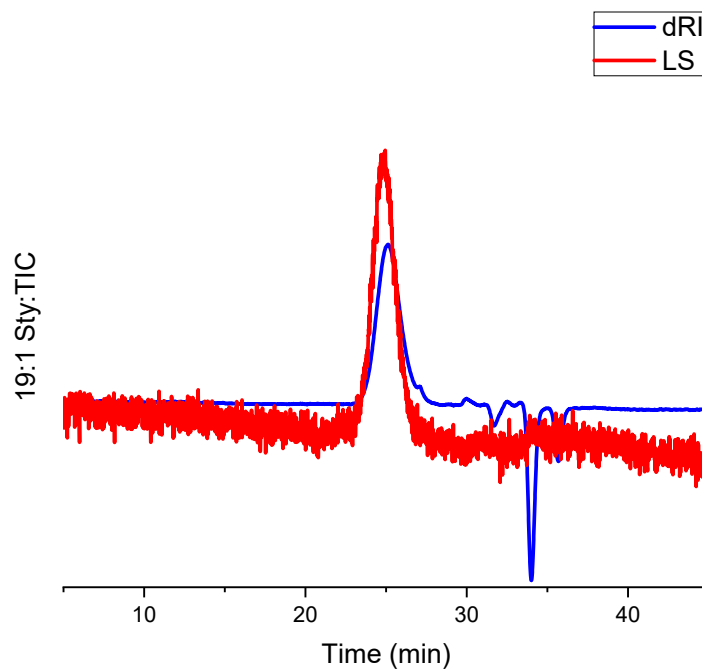
Figure S17. DMF SEC trace of 19:1 styrene:TIC copolymer, dRI (blue) and LS (red).
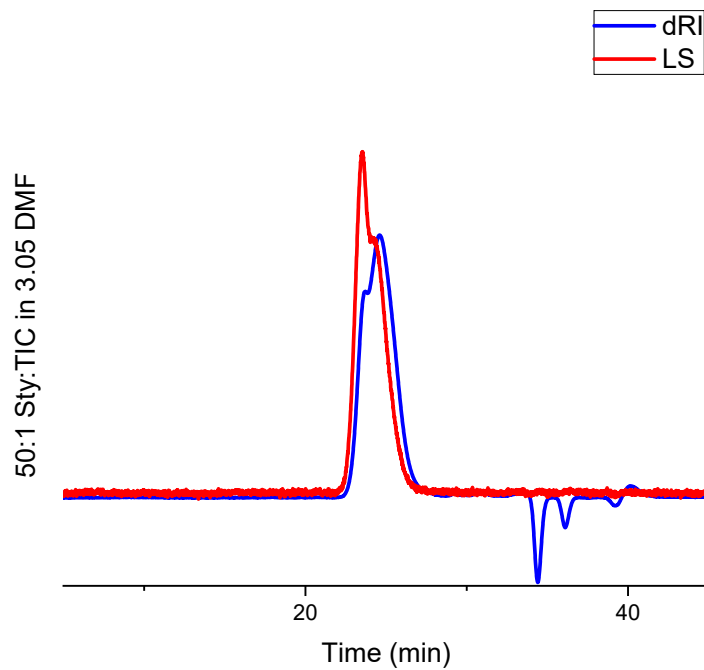
Figure S18. DMF SEC trace of 50:1 styrene:TIC copolymer run in 3.05M DMF, dRI (blue) and LS (red).
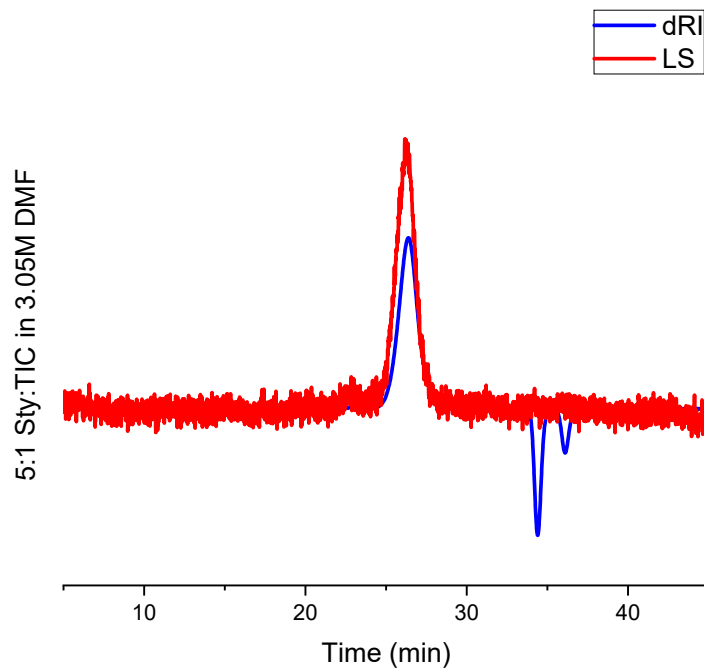
Figure S19. THF SEC trace of 5:1 styrene:TIC copolymer run in 3.05M DMF, dRI (blue) and LS (red).
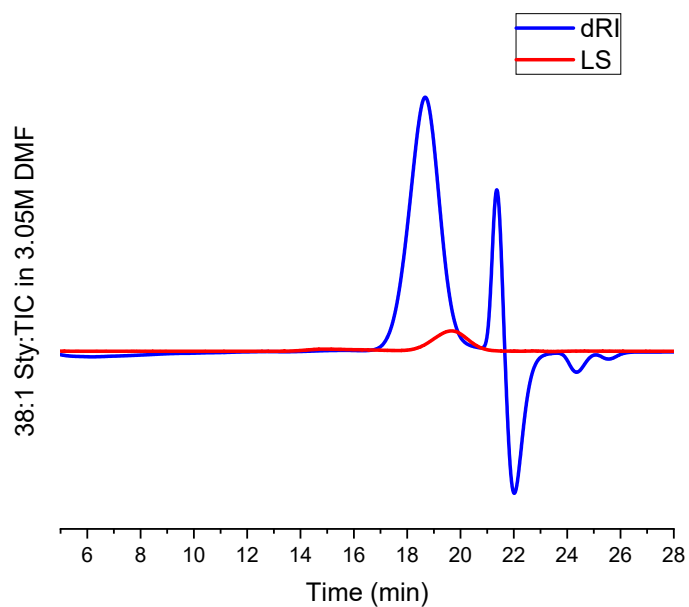
Figure S20. DMF SEC trace of 38:1 styrene:TIC copolymer run in 3.05M DMF, dRI (blue) and LS (red).
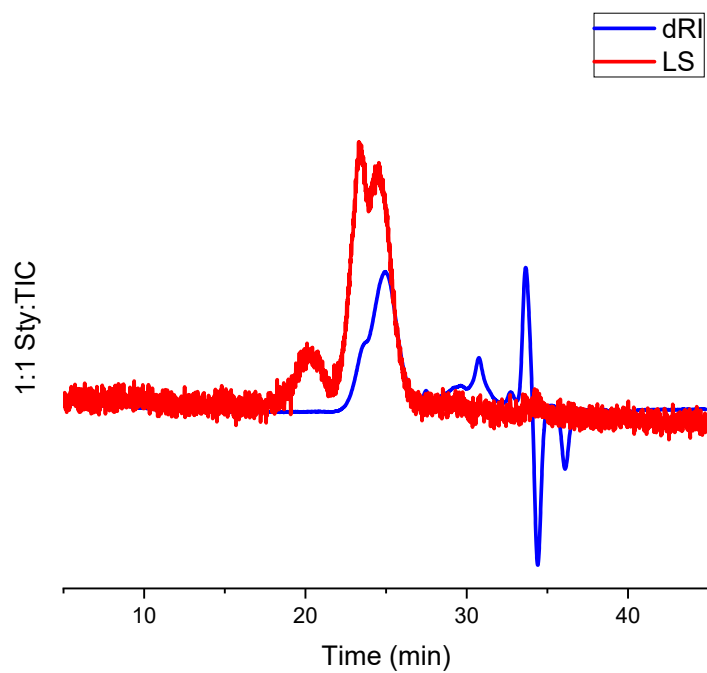
Figure S21. THF SEC trace of 1:1 styrene:TIC copolymer, dRI (blue) and LS (red).
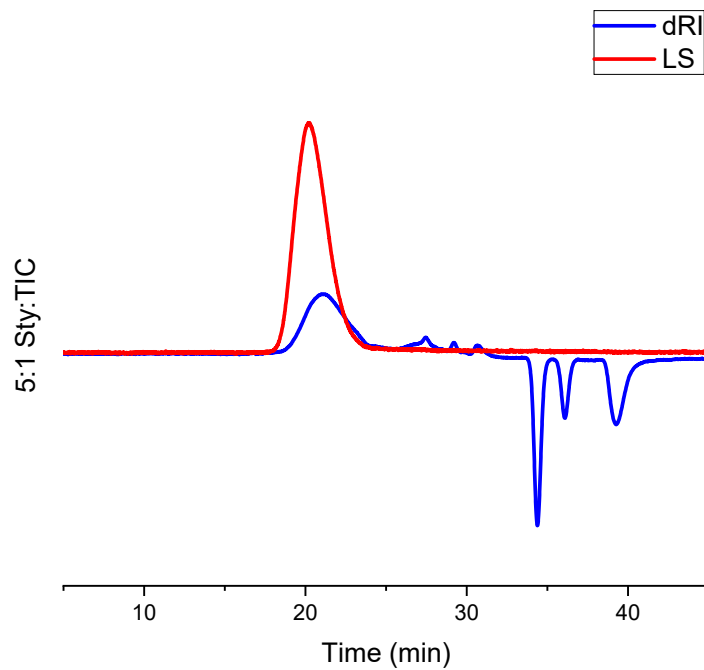
Figure S22. THF SEC trace of 5:1 styrene:TIC copolymer, dRI (blue) and LS (red).
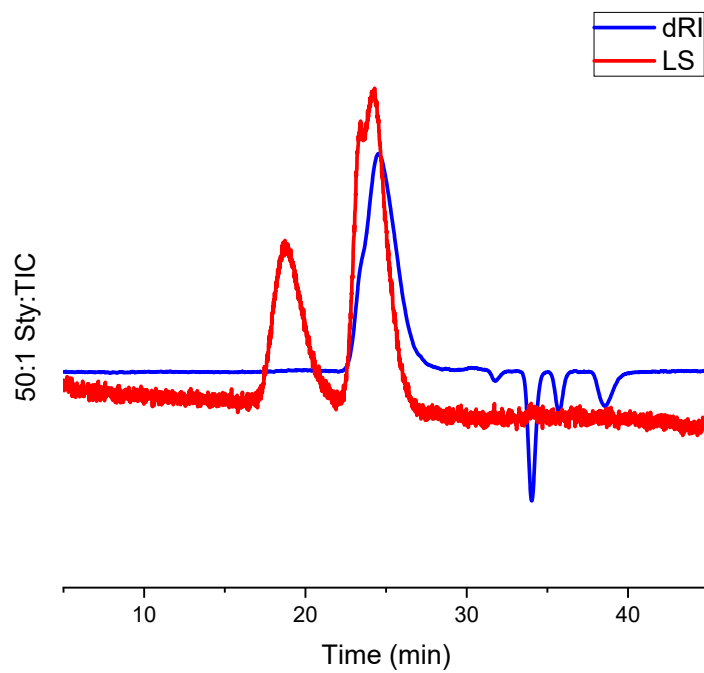
Figure S23. THF SEC trace of 50:1 styrene:TIC copolymer, dRI (blue) and LS (red).
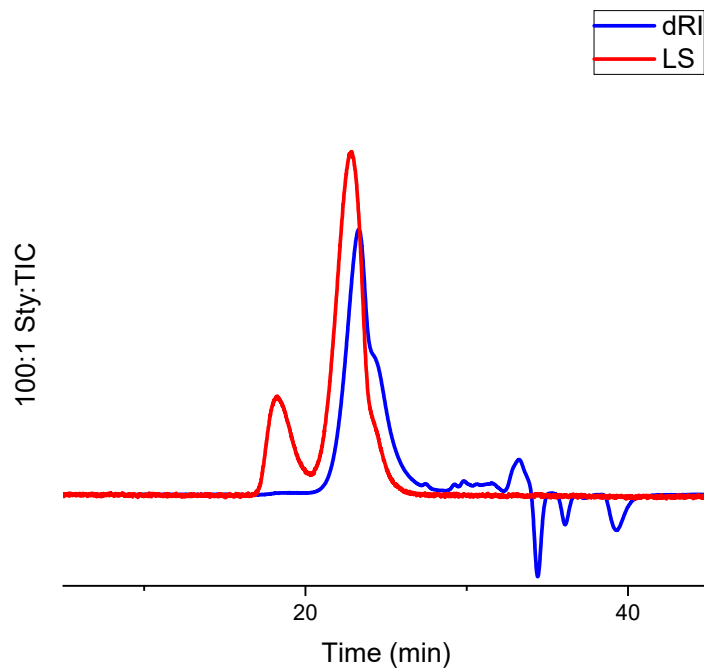
Figure S24. THF SEC trace of 100:1 styrene:TIC copolymer, dRI (blue) and LS (red).
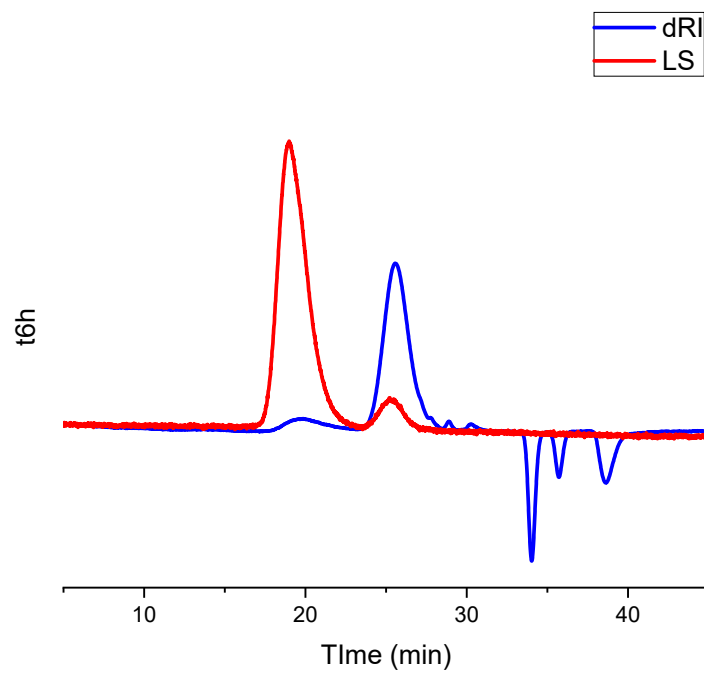
Figure S25. THF SEC trace of 19:1 styrene:TIC copolymer kinetics at 6 hour timepoint, dRI (blue) and LS (red).
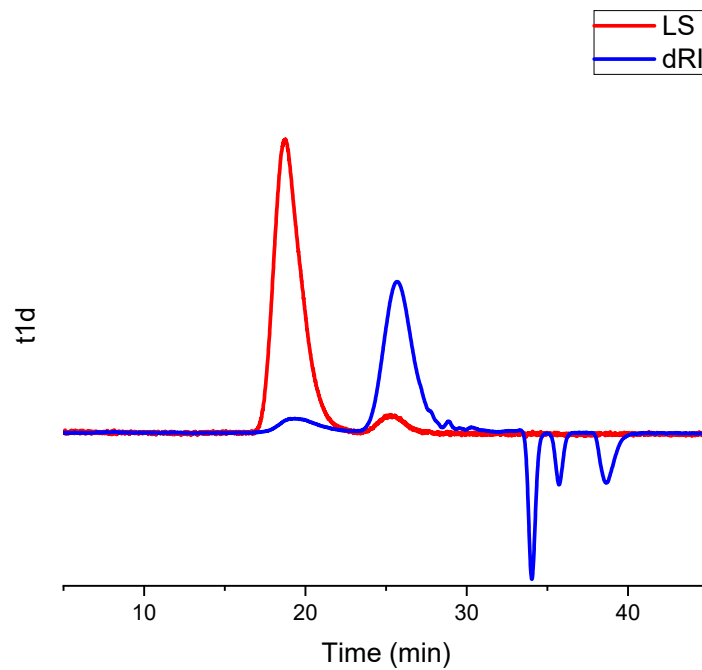
Figure S26. THF SEC trace of 19:1 styrene:TIC copolymer kinetics at 1 day timepoint, dRI (blue) and LS (red).
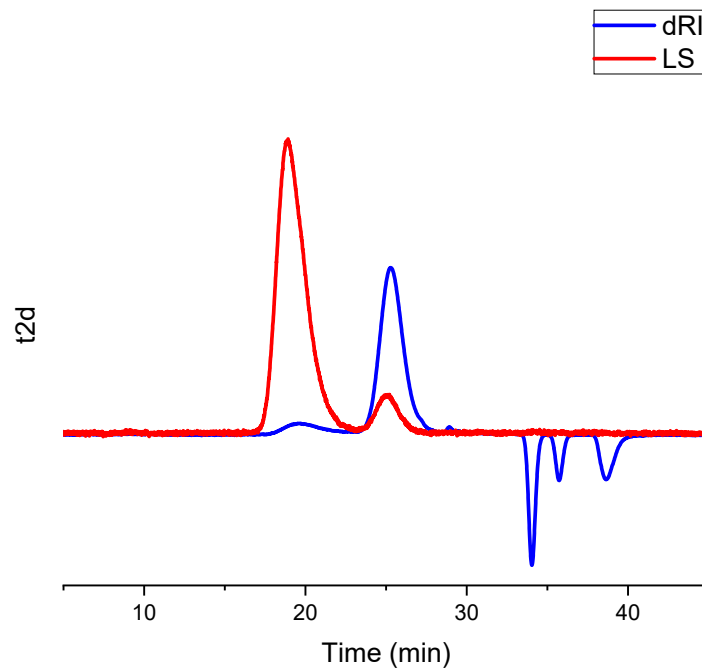
Figure S27. THF SEC trace of 19:1 styrene:TIC copolymer kinetics at 2 day timepoint, dRI (blue) and LS (red).
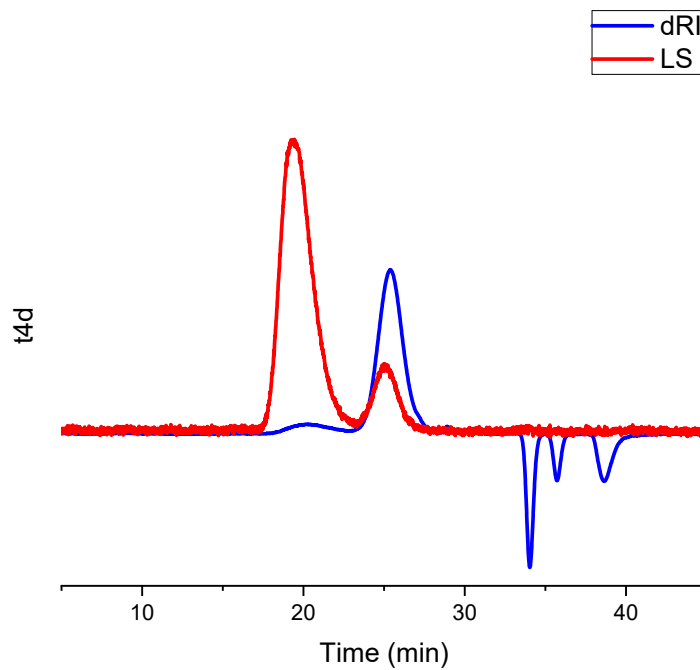
Figure S28. THF SEC trace of 19:1 styrene:TIC copolymer kinetics at 4 day timepoint, dRI (blue) and LS (red).
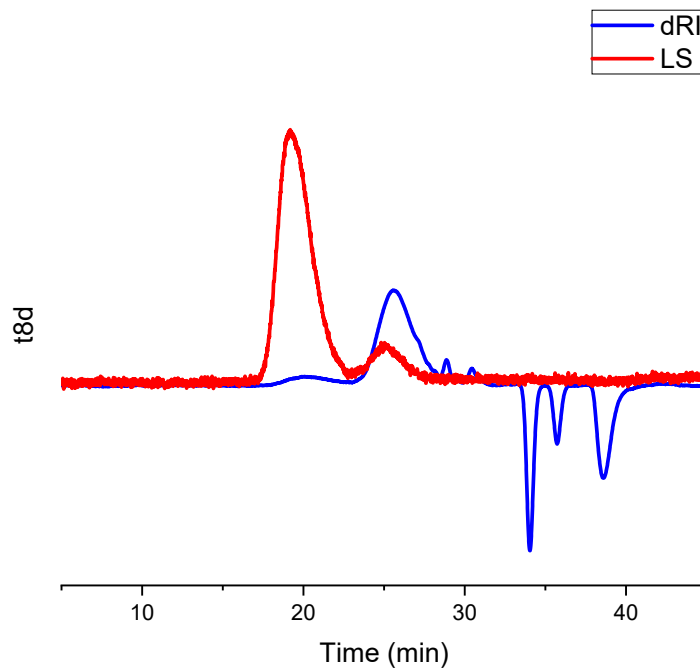
Figure S29. THF SEC trace of 19:1 styrene:TIC copolymer kinetics at 8 day timepoint, dRI (blue) and LS (red).

DSC Measurements

A few example DSC thermograms from various polymerizations with a heating ramp of 10 °C/min are shown. Corresponding T_g values were determined from the second heating ramp.
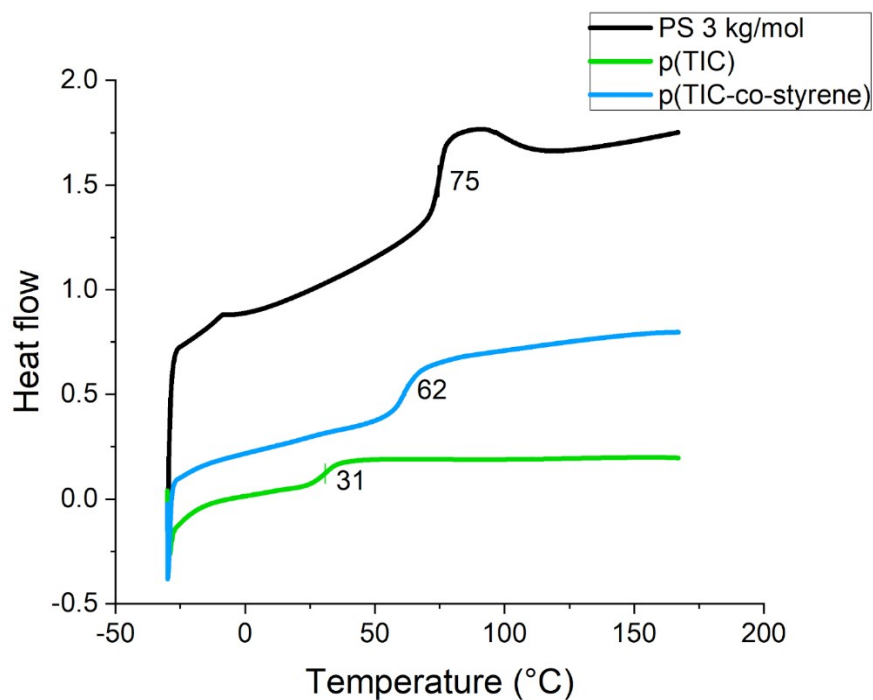
Figure S30. DSC thermogram of p(TIC) (green trace), p(TIC-*co*-styrene) (blue trace), and polystyrene with M_n of 3 kDa (black trace).
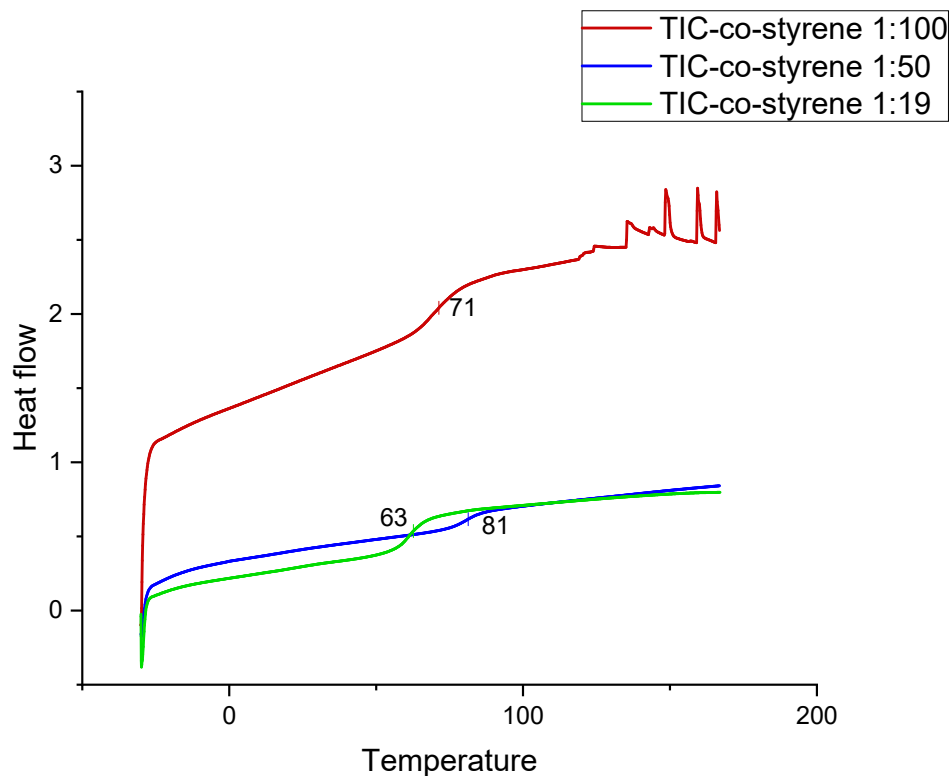
Feed ratio TIC:Styrene	Incorporation percentage of TIC (FTIC in polymer)	M_n (kDa)
1:100	2.6%	8.9
1:50	8.7%	3.3
1:19	17.9%	2.9

Figure S31. DSC thermogram of p(TIC-*co*-styrene) at different feed ratios of TIC and styrene. The feed ratios as well as resulting incorporation ratios and M_n are shown.

Polymer Degradation Studies

An example polymer degradation experiment was completed as follows.

To a Teflon-capped vial with a stir bar, p(TIC) (6.2 mg, 1 equiv., 0.037 mmol) and NaSCH$_3$ (20.7 mg, 8 equiv., 0.296 mmol) were suspended in DCM (0.4 mL). The vial was sealed, sparged with N$_2$ for 20 minutes, and stirred at room temperature overnight. The solution was quenched

with 1 N HCl, extracted with DCM, washed with water, sodium bicarbonate, and brine before being concentrated. Residue was submitted for ^{1}H NMR, SEC, and GC-MS analysis.
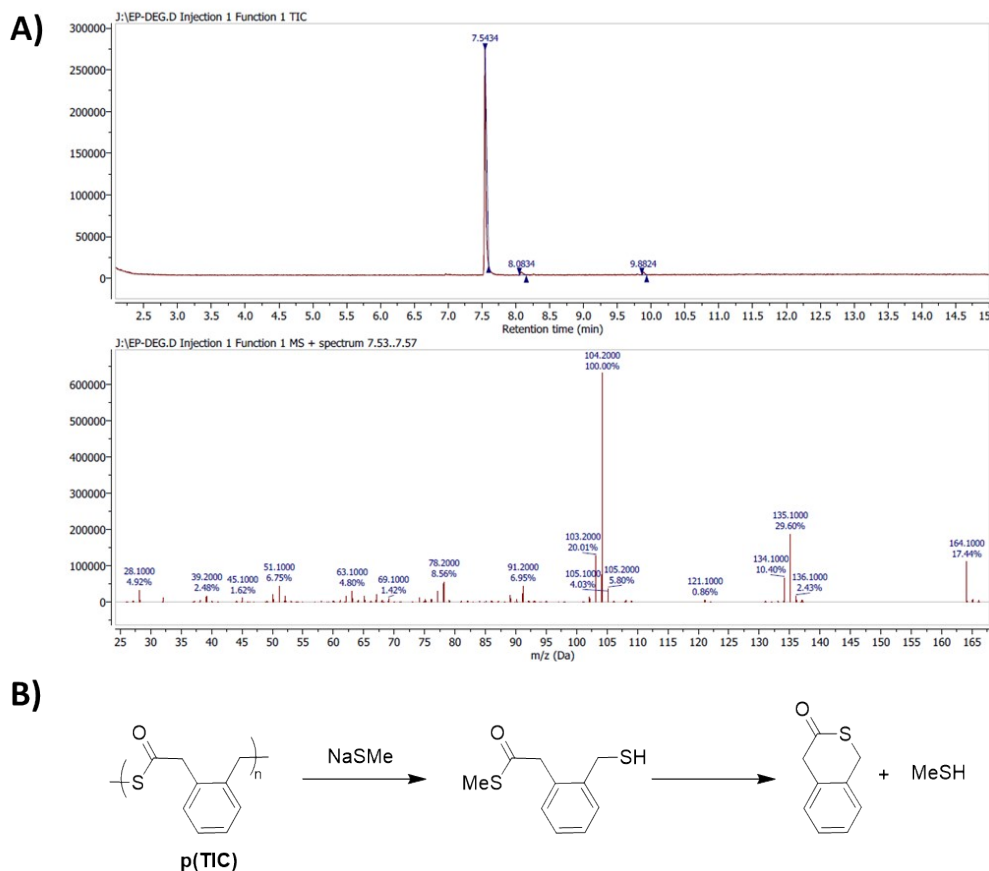
Figure S32. A) GC-MS chromatogram of degraded p(TIC) and B) Proposed degradation mechanism to yield thioester analog of TIC.

Theory

Computational Details and Cartesian Coordinates

Detailed conformational analysis of reactants and products of isodesmic reaction was done using regimes in the MacroModel package from Schrödinger[1] and the Merck Molecular Force Field (MMFFs). Monte-Carlo Molecular Mechanics (MCMM) was utilized with an extended torsional sampling.[2] Conformers within a range of 5 kcal mol−1 of the global minimum were considered for further analysis using Density Functional Theory (DFT). DFT optimizations were carried out at the M06-L/6-31G(d,p) level, chosen to take advantage of the speed of the local functional.[3] Following single point calculations at the SMD(DMF)/M06-2X/6-311++G(d,p) level of theory,[4]

all conformers having Gibbs free energies within a range of 5 kcal mol−1 of the global minimum were carried out further for use in Boltzmann-weighted free energies computed as described in the text. All DFT optimizations were carried out using the Gaussian16 electronic structure suite.[5] All reactants, products, intermediates, and transition-state structures (TSs) were optimized at the (U)M06-2X/6-31+G(d,p) level of theory. To verify the nature of stationary points, as well as to compute vibrational partitions functions for use in free energy calculations, vibrational frequency computations were carried out at the same level of theory. TS structures were confirmed with one and only one imaginary frequency along the reaction coordinate. Intrinsic Reaction Coordinate (IRC) calculations were carried out for the TS structures to confirm that they are connected to their respective reactants and products. Further solvent single point calculations were carried out using the SMD solvation model[6] at the (U)M06-2X, (U)ωB97XD[7], (U)PBE0-D3[8] and (U)MN15[9] level of theory along with 6-311++G(d,p) basis set for all atoms. Experimental studies were performed under dimethylformamide (DMF) solvent; SMD model is defined for n,n-DiMethylFormamide (DMF, $\square$ = 37.22) for calculations. Gibbs free energies for all stationary points were computed by adding the zero-point vibrational energy (ZPVE) and thermal energy corrections from standard statistical mechanics approximations at 343.15 K and 1 atm pressure, except that vibrational modes below 50 cm-1 were replaced with a value of exactly 50 cm-1 in vibrational partition function calculations.

Density functional theory (DFT) calculations were used first to compare the ring strains present in TIC and DOT by computing isodesmic reaction free energies for opening with *S-methyl* ethanethionate (Figure S13). Both TIC and DOT have essentially identical reaction energies of about ~4 kcal/mol, consistent with both monomers showing similar ring-opening reactivity.
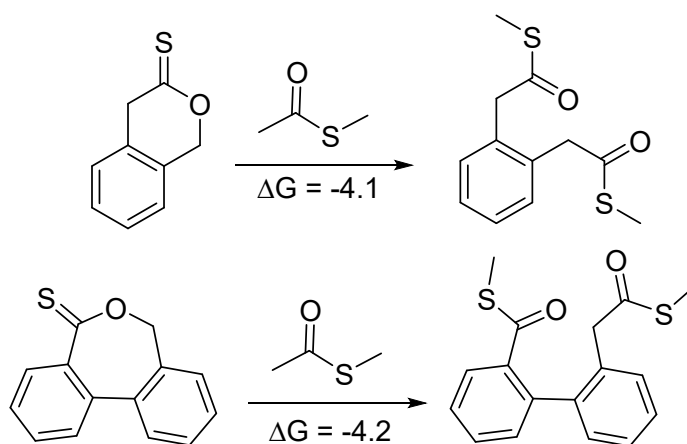
Figure S33. Isodesmic reactions of TIC or DOT with S-methyl ethanethionate to compare ring-strain Gibbs free energy values (kcal/mol; 298.15K; SMD(DMF)/M06-2X/6-311++G(d,p)//M06-L/6-31G(d,p) level of theory)

DFT was also used to develop insight at the atomic level for the mechanistic details of homopolymerization of DOT; Figure S14 shows reaction coordinates with Gibbs free-energy profiles for DOT analogous to TIC discussed in the manuscript. The homopolymerization follows the same pathway as that of p(TIC), the respective energies for p(DOT) intermediates shown below.
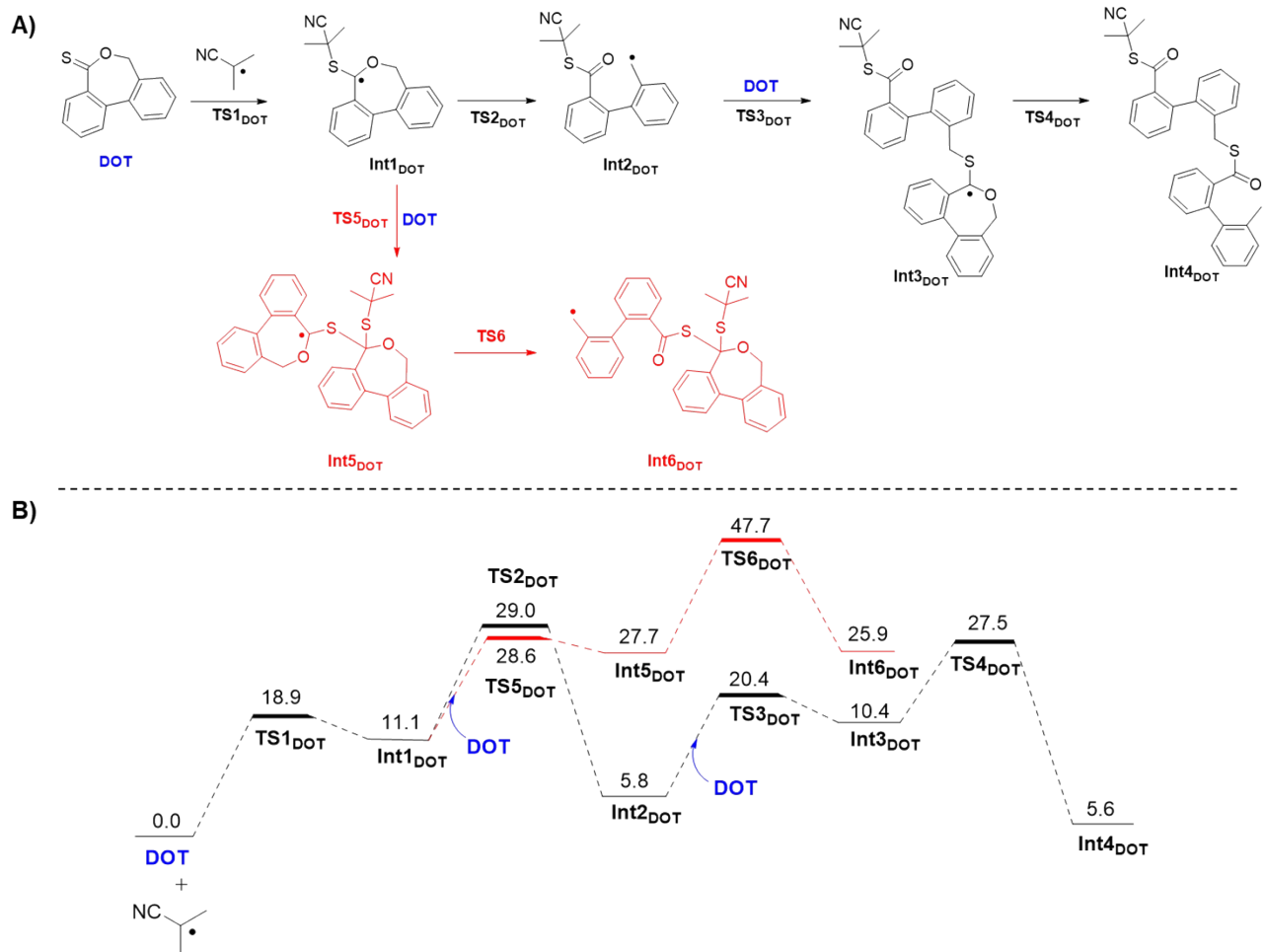
Figure S34. A) key mechanistic steps for the homopolymerization of DOT and B) Gibbs free energy (kcal/mol; 343.15K; SMD$_{(DMF)}$/PBE0-D3/6-311++G(d,p)//M06-2X/6-31+G(d,p) level of theory) profile on the potential energy surface for homopolymerization of DOT.
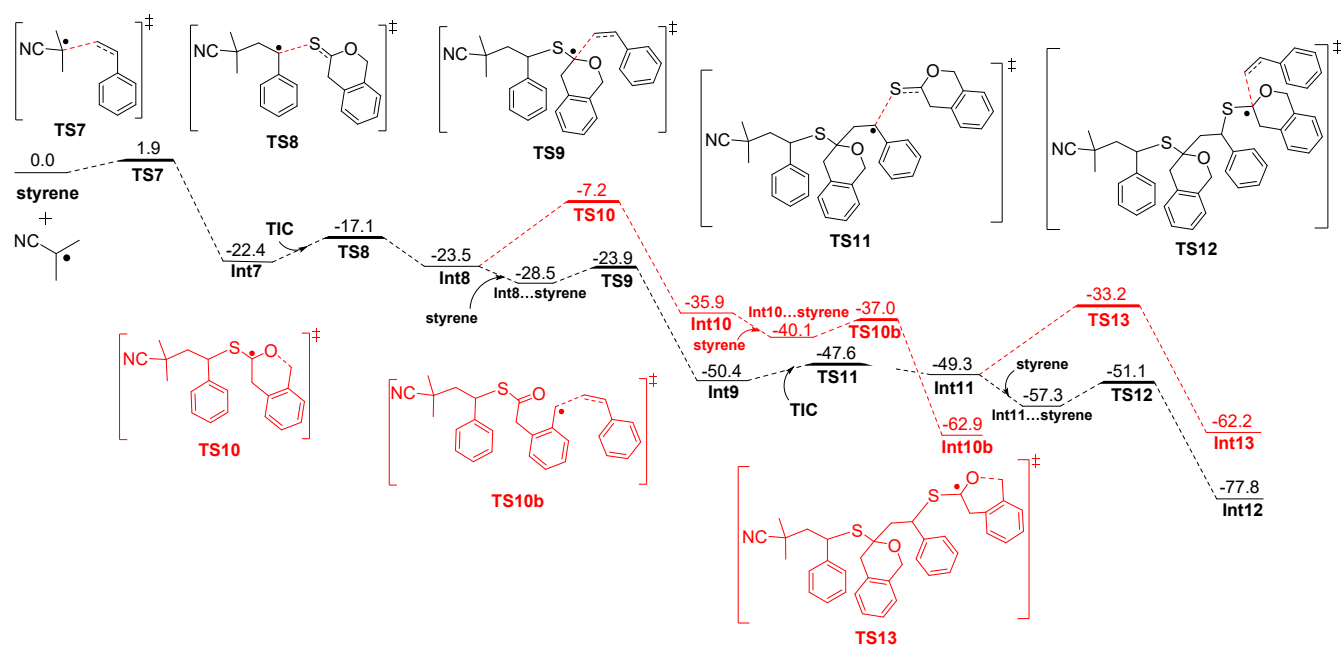
Figure S35. The enthalpy profile (in kcal/mol; 343.15 K; SMD(DMF)/PBE0-D3/6-311++G(d,p)//M06-2X/6-31+G(d,p) level of theory) for copolymerization of styrene and TIC.

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Cartesian Coordinates for Stationary Points
TIC
19

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O,0,0.0511419464,0.6513270462,-0.2600356019
S,0,0.1677191881,2.948411889,-1.4195489206
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AIBN radical

11

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Styrene

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TS2a-TIC

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C,0,3.6695013922,1.7759786962,-0.9927003406
C,0,3.9023794876,1.2324372884,1.7255326434
C,0,5.0446658791,1.3455098113,0.9428921875
C,0,4.9299914138,1.6254310348,-0.4200559066

H,0,3.5774107479,1.9518819983,-2.0613931338

H,0,5.8184214932,1.7058669377,-1.0379260597

H,0,6.0235260653,1.2060053113,1.3903951737

H,0,3.9859170786,1.0010194561,2.7839248105

TS2b-TIC

30

C,0,-2.5316268086,0.0844901217,-0.8493708495

C,0,-2.0896518282,-1.3688444575,-0.624563191

H,0,-2.1524711288,-1.634829651,0.4324122273

H,0,-1.0644645914,-1.4980295165,-0.9738866205

H,0,-2.7461319519,-2.0319003091,-1.1953786115

C,0,-2.4494724686,0.4892855049,-2.3289741336

H,0,-1.4153669575,0.4022929442,-2.6652856048

H,0,-2.7940429105,1.5158503877,-2.4682197017

H,0,-3.0809096098,-0.1792563701,-2.9221639621

C,0,-3.9250520827,0.2349264787,-0.3916094369

N,0,-5.0266340566,0.3390965708,-0.0553512617

C,0,0.0915620491,0.8175704986,-0.1022558622

C,0,1.5381602901,1.6237345908,-2.0569510746

C,0,2.4914961518,1.5086208977,0.2346372962

C,0,2.6908586358,1.5696541064,-1.1618370414

H,0,1.6788175478,1.2776699383,-3.0768339945

H,0,0.8150505216,2.4285257874,-1.9485696807

O,0,0.4630404622,0.3308766475,-1.2031532784

C,0,1.0972112496,1.4929991892,0.8112484473

H,0,1.0939394581,1.0095104588,1.7949062517

H,0,0.7519661509,2.5241324981,0.9803470905

S,0,-1.5954258911,1.2694291907,0.2322609878

C,0,3.5989758188,1.4122429116,1.0772791664

C,0,3.9969328834,1.4922244216,-1.6691565569
C,0,5.0911576919,1.4156923384,-0.8166499548
C,0,4.8933323782,1.384609451,0.5643586253
H,0,3.4431578074,1.3491632756,2.1514658935
H,0,5.7417061768,1.3201390583,1.2378542534
H,0,6.0952580696,1.3729361377,-1.2261562643
H,0,4.1452616124,1.5083411883,-2.7455179584

TS2c-TIC
30

C,0,-2.4964728988,-0.2887151176,0.4095010185
C,0,-1.9598439297,-1.6686957559,0.0024188065
H,0,-1.9657585596,-1.7830992676,-1.0832949782
H,0,-0.9429982418,-1.7915873323,0.3774961647
H,0,-2.5969187564,-2.4412869746,0.4424892814
C,0,-2.4934626814,-0.096520147,1.9335566
H,0,-1.4689119276,-0.1738503365,2.3002992792
H,0,-2.9045948955,0.8789752357,2.2006123845
H,0,-3.1044333274,-0.8769425128,2.3974398362
C,0,-3.8783082181,-0.1500831122,-0.0855350123
N,0,-4.9706761629,-0.0587914188,-0.4540590594
C,0,0.1041723436,0.682315738,-0.1105683758
C,0,1.4421886708,1.2852813789,1.9902897283
C,0,2.4727289234,1.5301391317,-0.2567687514
C,0,2.6243305154,1.4098597649,1.1418460194
H,0,1.5680849584,0.8107088126,2.9591083663
H,0,0.6809451946,2.0611886559,1.9627719709
O,0,0.4654661656,0.069788916,0.9292556858
C,0,1.1002541759,1.5263993971,-0.8833301078
H,0,1.1536344623,1.1847626967,-1.9233980772

H,0,0.7053554768,2.5528914107,-0.9224870616
S,0,-1.5934529338,1.0880996115,-0.450735663
C,0,3.6097086833,1.6022940363,-1.0616999942
C,0,3.9160150369,1.3273423768,1.6839659917
C,0,5.0390651394,1.4200619674,0.8714363714
C,0,4.8868534691,1.5671765275,-0.5078954625
H,0,3.4912262335,1.6783279128,-2.1397950878
H,0,5.7583708284,1.6349903382,-1.1508077609
H,0,6.0305851928,1.3704368852,1.3098039466
H,0,4.0293940229,1.2041852914,2.7576574204

TS2d-TIC
30

C,0,-2.1050563286,1.5735711839,1.8034489943
C,0,-1.6476739798,0.2970974306,2.5197338987
H,0,-0.569560659,0.1469947104,2.4333177077
H,0,-2.1525935336,-0.5604470902,2.0687560461
H,0,-1.9101134834,0.354599996,3.5803612942
C,0,-3.6301028104,1.7410544387,1.9142893481
H,0,-4.1207476912,0.8733775889,1.4662888689
H,0,-3.9658160152,2.64579264,1.4029211122
H,0,-3.9133010399,1.806702192,2.968123524
C,0,-1.4643503533,2.7533304061,2.410000459
N,0,-0.9690093475,3.673278176,2.9071492827
C,0,0.0058203082,1.1033331331,-0.0866369336
C,0,1.5467038538,1.6193291622,-2.1061369609
C,0,2.4230440297,1.7386132297,0.2002287332
C,0,2.6702232984,1.5859344091,-1.1817590865
H,0,1.6645225309,1.1413130257,-3.0734328147
H,0,0.8690256948,2.4687567671,-2.0953414842

O,0,0.373064727,0.4846270769,-1.1132080677

C,0,1.0140404274,1.9381289025,0.6908406414

H,0,0.9531178954,1.7577805641,1.7691742718

H,0,0.7101545356,2.9870569891,0.5542640354

S,0,-1.7509117398,1.498778745,-0.0072505296

C,0,3.4871904763,1.653643594,1.0979101215

C,0,3.975065754,1.3099354743,-1.6179666474

C,0,5.0279756266,1.247145344,-0.714092163

C,0,4.7860770699,1.4287183036,0.6489438505

H,0,3.2935290783,1.7618954757,2.1621347144

H,0,5.6038573365,1.378633268,1.3605252927

H,0,6.0349629051,1.0510686729,-1.0681911908

H,0,4.1562734337,1.1605811906,-2.6789153183

Int2-TIC

30

C,0,-2.7587033747,-1.0651025559,0.1603472989

C,0,-2.6530280396,-2.2919968844,-0.7577177945

H,0,-2.9899752003,-2.0497876186,-1.7674139877

H,0,-1.619827995,-2.6382650649,-0.7866722567

H,0,-3.2860820075,-3.0894768885,-0.357767776

C,0,-2.3166744521,-1.3687907685,1.6001453469

H,0,-1.2747632103,-1.6901931946,1.6030442788

H,0,-2.4308756255,-0.4867671086,2.2334381119

H,0,-2.9402900372,-2.1731672251,2.0012057183

C,0,-4.1598580041,-0.6059061651,0.179900498

N,0,-5.2653409192,-0.2674516624,0.2047625364

C,0,-0.1473405176,-0.1702199819,-0.5358047386

C,0,1.2050785552,1.6099244867,1.7456357093

C,0,2.1576966774,0.8319115852,-0.4166611744

C,0,2.2987176074,1.19211007,0.9584450003

H,0,1.3539329074,1.8657534948,2.7876873021

H,0,0.1995326592,1.6991769274,1.3531276939

O,0,0.2034221249,-1.2656212546,-0.1815884394

C,0,0.8054600306,0.8939717188,-1.076110489

H,0,0.9000505376,0.6986522488,-2.1505749268

H,0,0.3463064033,1.8835694633,-0.9696029715

S,0,-1.8481610511,0.3980135379,-0.5305404304

C,0,3.2677209424,0.415774668,-1.1368743337

C,0,3.595528429,1.1133052789,1.533233274

C,0,4.6902592522,0.6994151426,0.7952304669

C,0,4.5336100518,0.3463495047,-0.5482363389

H,0,3.1466339181,0.1361605541,-2.1800786178

H,0,5.3861590907,0.0178396162,-1.1329779839

H,0,5.6690626161,0.6483023926,1.2613039153

H,0,3.7143138354,1.3864416824,2.5781053771

TS3-TIC

49

C,0,-2.4340087825,-0.7606075816,-0.9982366788

C,0,-1.7532524445,-1.7007255438,-2.00451541

H,0,-1.5246685608,-1.1732351293,-2.9325863742

H,0,-0.8355686404,-2.097338798,-1.5700997059

H,0,-2.4298247108,-2.5305151665,-2.2292854629

C,0,-2.7964773741,-1.4717695852,0.3146418816

H,0,-1.8898987679,-1.854527667,0.7841667386

H,0,-3.3033858745,-0.7868310839,0.9972838639

H,0,-3.4660512667,-2.3083682566,0.093966992

C,0,-3.6684113402,-0.2318063905,-1.6075771553

N,0,-4.6458713508,0.156536666,-2.0883550779

C,0,0.0734986951,0.1044815964,0.0362786428

C,0,0.034772938,1.2850506156,3.0600950226

C,0,1.9582465908,0.8864013479,1.5170666001

C,0,1.414643055,0.9435143287,2.8253306462

H,0,-0.3416923667,1.1927663435,4.0732990986

H,0,-0.7029299287,1.1580541574,2.2751762309

O,0,0.2661966487,-1.0667369093,0.241212218

C,0,1.0872789816,1.2037162833,0.3308179397

H,0,1.6987518238,1.3002801433,-0.5746371501

H,0,0.5719603975,2.1615825279,0.4758100242

S,0,-1.428717407,0.7683758822,-0.6863489625

C,0,3.2998650948,0.5678113321,1.3421127985

C,0,2.2806922083,0.7363243758,3.9157595142

C,0,3.6223717629,0.4272076701,3.7268878575

C,0,4.1355039842,0.3292388364,2.4352243958

H,0,3.7021800486,0.5101166782,0.3334211447

H,0,5.1817693363,0.0873546925,2.2779792726

H,0,4.268599213,0.2689966397,4.5846235827

H,0,1.8770244784,0.8122299611,4.9226640984

C,0,1.5562517876,4.1390066718,2.7991511074

C,0,3.5265286856,4.37752401,1.4502916753

C,0,3.7999287818,4.0365727943,3.8713784101

C,0,4.3623357848,3.8979506264,2.602376611

O,0,2.1435454727,4.0156282034,1.5937525495

S,0,-0.0258704487,3.6931196702,2.9518018315

C,0,2.4220560405,4.6476829809,3.926322549

C,0,4.5122869225,3.621955687,4.9942213666

C,0,5.6369603576,3.3584865916,2.4516121666

C,0,5.7945503774,3.0948448574,4.8464788965

C,0,6.3588110136,2.9659591942,3.5774532721

H,0,4.0664096016,3.7134270036,5.9811224761

H,0,6.3522729097,2.7783515849,5.7224345207

H,0,7.3542550839,2.5484078046,3.464491807

H,0,6.0615943247,3.2372349241,1.4580727026

H,0,2.5104900675,5.7417775187,3.8197050379

H,0,1.9202120535,4.4556583488,4.8748542026

H,0,3.8410792109,3.930148284,0.5056451602

H,0,3.5790855312,5.4712552776,1.3548110712

TS3a-TIC

49

C,0,-2.6615264723,0.0699494098,0.9405027612

C,0,-3.1006302042,-0.8694055238,-0.1919078966

H,0,-3.5083500588,-0.3016449695,-1.0304291197

H,0,-2.2452240749,-1.4567790946,-0.5268926157

H,0,-3.8731216494,-1.5464214118,0.1844443704

C,0,-2.1084187082,-0.6942138237,2.1533603845

H,0,-1.2395749014,-1.279223616,1.8502700772

H,0,-1.8253439456,-0.0030170513,2.9500232658

H,0,-2.8808432788,-1.3700129438,2.5321125424

C,0,-3.8153877711,0.8804009385,1.3732602471

N,0,-4.7172834901,1.5171402389,1.718522321

C,0,-0.0435579518,0.3906337144,-0.1637633559

C,0,2.0701677289,1.4469822997,2.0240602207

C,0,2.4394127523,0.7859240743,-0.3575522313

C,0,2.8979049573,0.8978117139,0.9795767883

H,0,2.4541962357,1.4202452418,3.0384925487

H,0,0.9889651462,1.4099009306,1.9415298189

O,0,0.0080896388,-0.8087389531,-0.0881743429

C,0,1.0619629253,1.2747831807,-0.7230267934

H,0,0.9319654516,1.2584504229,-1.8118492026

H,0,0.9120475641,2.3102140044,-0.3906748602

S,0,-1.4710691562,1.363565767,0.3478123143

C,0,3.2789192457,0.2560893629,-1.3307182206

C,0,4.2194483779,0.5029404118,1.267918544

C,0,5.0480733185,-0.0193458628,0.2840850467

C,0,4.5775452039,-0.1518558039,-1.0222249151

H,0,2.9152490796,0.1661136744,-2.3509620495

H,0,5.216126137,-0.5620337188,-1.7975998124

H,0,6.0591975979,-0.3245915422,0.5342105697

H,0,4.5828095547,0.6039987009,2.287155147

C,0,0.6289187015,4.4170203777,1.7629425226

C,0,-1.4879818265,4.8469194757,0.7292993519

C,0,-0.8291015013,6.1992627328,2.663407749

C,0,-1.568800501,6.1437544353,1.4802943759

O,0,-0.1284942544,4.3725103534,0.6493152646

S,0,2.1703828495,3.8261371584,1.7037921496

C,0,-0.0428324106,4.9568280778,3.0020836847

C,0,-0.8353937287,7.3596095439,3.4319331099

C,0,-2.3215431715,7.2382334596,1.0659081225

C,0,-1.5997874848,8.4535663087,3.0252856361

C,0,-2.3427416767,8.3935491643,1.8470155013

H,0,-0.2466664488,7.4094152913,4.3437579226

H,0,-1.6091579523,9.357538038,3.6258320015

H,0,-2.9299179486,9.2495984311,1.5310020708

H,0,-2.8873052401,7.1909635113,0.1393055834

H,0,-0.7319675936,4.1818984173,3.3808926011

H,0,0.7083716049,5.1340098425,3.771352718

H,0,-1.8203393003,4.9384012471,-0.3052298114

H,0,-2.0891713697,4.0702233622,1.2221688937

TS3b-TIC

C,0,-2.5882773946,-0.5021185155,0.9665053731
C,0,-2.6417875844,-1.9026874733,0.3359775846
H,0,-3.0411139632,-1.854855409,-0.6790070697
H,0,-1.6413780106,-2.3341309484,0.318184749
H,0,-3.2949952273,-2.5380083692,0.9414157626
C,0,-2.0437539562,-0.520751033,2.4031314815
H,0,-1.0277710165,-0.9184303838,2.3980548596
H,0,-2.0461093349,0.4848663088,2.8313985014
H,0,-2.6765565479,-1.1681244602,3.0179249754
C,0,-3.9542524729,0.0536690258,0.9757855106
N,0,-5.0328245428,0.4717082949,0.9893357035
C,0,-0.0023784208,-0.0111814213,-0.134991206
C,0,1.9038453275,1.6768387279,1.6988942812
C,0,2.3891203551,0.708568407,-0.5560011068
C,0,2.8182152946,1.1438309102,0.7243999152
H,0,2.2918650539,1.9133385935,2.6834616074
H,0,0.850701338,1.4203499166,1.6665873648
O,0,0.2969126332,-1.0426295561,0.4060255733
C,0,0.9447810408,0.8509456603,-0.9568464336
H,0,0.8062717893,0.5481361231,-2.0017086996
H,0,0.6256062617,1.8984805684,-0.8762952666
S,0,-1.6528091237,0.7079425281,-0.0852252461
C,0,3.3172467086,0.199164955,-1.4574962126
C,0,4.1964330234,1.0881409622,1.0188982339
C,0,5.111443593,0.5838890825,0.1057181502
C,0,4.6739156615,0.1274284109,-1.1380675171
H,0,2.9765780094,-0.1401863757,-2.4323691423
H,0,5.3807802818,-0.2728923055,-1.8572520284
H,0,6.1653940549,0.5439105636,0.3621529903

H,0,4.534371768,1.4418687276,1.9891270171
C,0,0.2369246955,4.4298494329,1.9830693055
C,0,-0.5866592586,5.0832783806,4.1307209368
C,0,-2.1183826716,3.9245597377,2.6054195029
C,0,-1.7888994804,4.2066915352,3.9331524685
O,0,0.4989586922,4.6817051738,3.2786995516
S,0,1.4861148331,3.9637962528,1.0120732943
C,0,-1.2106637879,4.5202138525,1.5562285063
C,0,-3.2333032441,3.1394702242,2.3207276346
C,0,-2.5599581917,3.7008389129,4.9759926394
C,0,-4.0199078871,2.6468953198,3.3635790572
C,0,-3.6825577315,2.9242446708,4.6881794281
H,0,-3.4956966012,2.9163758799,1.2898425364
H,0,-4.888345232,2.0383821112,3.1324525806
H,0,-4.2908023922,2.5316310378,5.4966978533
H,0,-2.2881831329,3.9134140833,6.0067405259
H,0,-1.460896341,5.5858693532,1.4247796662
H,0,-1.3295847465,4.036828867,0.5858097675
H,0,-0.1918525272,5.0265304796,5.1455788411
H,0,-0.8243775939,6.1324461796,3.905377198

TS3c-TIC
49

C,0,-2.5839481784,-1.0387051147,-0.3536043224
C,0,-2.1439370749,-1.9824487868,-1.4829737692
H,0,-2.3008628399,-1.5178083346,-2.4582938412
H,0,-1.0905845828,-2.2342554388,-1.3593246859
H,0,-2.7388033907,-2.8990228387,-1.4307418113
C,0,-2.4031716452,-1.6646707605,1.0378067757
H,0,-1.350611305,-1.8997351055,1.1983728733

H,0,-2.7509906367,-0.9827993099,1.8163318922

H,0,-2.9880530139,-2.5876098613,1.0915853498

C,0,-4.0078548185,-0.7057307861,-0.5437161873

N,0,-5.1304973327,-0.4709091216,-0.691324112

C,0,-0.0194080843,0.1908704662,-0.245828553

C,0,0.774028644,1.5358634041,2.5882943764

C,0,2.1231592883,1.2870312713,0.4977604974

C,0,2.0259855353,1.3151543037,1.9125208323

H,0,0.7504502824,1.4192366611,3.6657370542

H,0,-0.1693207533,1.3667110869,2.0791493774

O,0,0.387902326,-0.9283921562,-0.0688043822

C,0,0.8795811661,1.4201464231,-0.3404152444

H,0,1.1421109986,1.5229119739,-1.3999950944

H,0,0.3120875418,2.3157928652,-0.056884145

S,0,-1.7472006404,0.6149958071,-0.465568994

C,0,3.3694923938,1.1635025106,-0.1064894078

C,0,3.2169751847,1.2493782487,2.6627696412

C,0,4.4568609763,1.1319637412,2.0447663494

C,0,4.5398993675,1.0897142775,0.6527123799

H,0,3.430618095,1.1330723646,-1.1913038729

H,0,5.5023652046,0.9954850305,0.1608682836

H,0,5.3586609458,1.0693337199,2.6469796146

H,0,3.1498499656,1.2932363048,3.7471489926

C,0,2.1861958353,4.370618859,2.5662395278

C,0,4.2408620229,4.6260344601,3.7515427084

C,0,3.9688282922,5.8177814758,1.6278741507

C,0,4.5993796775,5.7896466562,2.8735569436

O,0,2.8220105887,4.3852568213,3.7488108778

S,0,0.5905735996,3.9371367452,2.5295911098

C,0,3.0204334349,4.6794570898,1.3472435527

C,0,4.2277724274,6.8623561246,0.744893231

C,0,5.4904341785,6.7942099911,3.2384464536
C,0,5.1319268564,7.863014088,1.1022374456
C,0,5.7640561713,7.8293055574,2.3445042946
H,0,3.7254014489,6.894978958,-0.217963278
H,0,5.3367013006,8.6757399739,0.4126474481
H,0,6.4596699685,8.6146273988,2.6217895343
H,0,5.9661168104,6.7724401664,4.2154449585
H,0,3.6023057048,3.7716191307,1.1033240764
H,0,2.3621257204,4.8800898552,0.5013346845
H,0,4.5012772613,4.7969331992,4.796500397
H,0,4.732341081,3.7056556038,3.4037190166

Int3-TIC
49

C,0,-3.8074535111,-2.2763919021,-2.5470801185
C,0,-3.2722190114,-3.409786707,-3.4352771823
H,0,-3.0015837364,-3.0315853968,-4.4229602651
H,0,-2.4010814245,-3.8639488673,-2.962758799
H,0,-4.0516878715,-4.1686145361,-3.5511250323
C,0,-4.2255077962,-2.7727761132,-1.1543604038
H,0,-3.3632773335,-3.2111041817,-0.650810302
H,0,-4.6251201941,-1.9513906179,-0.5560436452
H,0,-5.0008358222,-3.536663072,-1.2651749094
C,0,-4.9809376212,-1.6746887055,-3.2071559079
N,0,-5.9140421319,-1.2282486328,-3.7242039915
C,0,-1.1811892633,-1.6189529473,-1.6720693268
C,0,-0.948137974,-0.3605446015,1.2559356518
C,0,0.8969827111,-0.9324584137,-0.4089807722
C,0,0.4505198545,-0.7892127407,0.9178594172
H,0,-1.1403803988,-0.5227069293,2.318092123

H,0,-1.7049277799,-0.9125904654,0.6896209859

O,0,-1.1381690565,-2.7661814497,-1.3038322949

C,0,-0.0192946155,-0.6409814621,-1.5695582867

H,0,0.529124905,-0.7281041612,-2.5154194473

H,0,-0.4031383309,0.3840387136,-1.5118791013

S,0,-2.6144300898,-0.8586320718,-2.4336034956

C,0,2.2147876823,-1.318182021,-0.6476507315

C,0,1.3493426341,-1.0241546464,1.9604280057

C,0,2.6665089647,-1.405623911,1.7142294018

C,0,3.1012808939,-1.5549597559,0.4026479782

H,0,2.5526640711,-1.4348030194,-1.6742896563

H,0,4.1252932354,-1.8486085748,0.1933454042

H,0,3.3471133736,-1.5711021279,2.5431985861

H,0,1.0101165104,-0.8973905517,2.9860287699

C,0,0.2241137576,2.2156958822,0.9711516112

C,0,2.3054059224,2.6412770803,-0.1058033091

C,0,2.3052649138,2.2023190579,2.3201188279

C,0,3.0238105359,2.1554558928,1.1228009702

O,0,0.9657911359,2.1420784274,-0.1697335897

S,0,-1.3209715884,1.4444805404,0.8819628624

C,0,0.8846931668,2.7117858793,2.2290304484

C,0,2.9072066759,1.7810977832,3.5035372652

C,0,4.3344712987,1.6867791172,1.1073899003

C,0,4.2270963336,1.3297346397,3.4922634795

C,0,4.9413191398,1.2819829382,2.2957638391

H,0,2.3451590042,1.8065008755,4.4338163513

H,0,4.6958123365,1.0080502872,4.4172789837

H,0,5.9646058629,0.9200712228,2.2865464079

H,0,4.878944173,1.6316645949,0.1679326701

H,0,0.9025710536,3.8154741599,2.2366133346

H,0,0.2923982444,2.4039888576,3.0937333582

H,0,2.790399681,2.2976989555,-1.0212962637

H,0,2.2640156392,3.7404686475,-0.1214650615

TS4-TIC

49

C,0,-0.1799020416,0.8822860258,0.6272217846

C,0,0.8011903706,0.3336044725,-1.644924227

C,0,1.903889211,2.0233928632,-0.2074550669

C,0,1.9782248673,1.123459025,-1.2932139479

H,0,0.957365378,-0.5896466504,-2.1970264986

H,0,-0.1243314476,0.8497864414,-1.883836262

O,0,0.2455983686,-0.1630610674,0.056238468

C,0,0.6259920668,2.1642813367,0.5801668

H,0,0.8404982183,2.5091414457,1.5985435369

H,0,-0.0109853998,2.9337630661,0.1193548535

S,0,-1.9005036369,1.090201033,1.0013224419

C,0,3.0410544034,2.7459507142,0.1543750779

C,0,3.2036021796,0.9465338704,-1.9536224418

C,0,4.3229803225,1.6857553537,-1.591948099

C,0,4.239900739,2.5981523893,-0.5388283507

H,0,2.9862637362,3.4295400271,0.9981602822

H,0,5.109706873,3.1780886351,-0.2472811932

H,0,5.2593203443,1.5479091745,-2.1233930698

H,0,3.2644264778,0.2281237817,-2.7671010128

C,0,-2.5525342619,1.8783967283,-3.5673533699

C,0,-1.4408447204,1.7876457344,-4.6286498491

H,0,-0.5089680766,1.4057942095,-4.2038990976

H,0,-1.7641810661,1.1271919906,-5.4376529805

H,0,-1.2554728562,2.7840630297,-5.037955381

C,0,-3.8437648445,2.4297845367,-4.1833825816

H,0,-4.1592645298,1.7671009684,-4.993273443

H,0,-4.6361808165,2.5066782768,-3.4402669575

H,0,-3.6465715346,3.423915553,-4.5959476813

C,0,-2.0775954484,2.7469042976,-2.4767581117

N,0,-1.6408767896,3.4493961673,-1.6683972436

C,0,-4.0014994661,0.3728795078,-1.6383209879

C,0,-2.3735554837,-0.6730328916,1.1575363772

C,0,-4.810164124,-0.8595867673,0.4284660838

C,0,-3.8490309598,-0.7537312999,1.4479666124

O,0,-4.4786910958,1.435758942,-1.3512663961

S,0,-2.7607833529,0.1605383939,-2.9259280627

C,0,-4.4108565944,-0.9619651026,-1.0233724049

C,0,-6.1650512006,-0.8807470627,0.7662664103

C,0,-4.2759534293,-0.6748966438,2.7766543019

C,0,-6.5791388349,-0.7997858306,2.0925016662

C,0,-5.6278566621,-0.6989487675,3.1044001904

H,0,-6.9054607131,-0.960804577,-0.0251909338

H,0,-7.6373205955,-0.8172226495,2.3323351145

H,0,-5.935545238,-0.6375223391,4.1432679567

H,0,-3.5287829122,-0.5865632486,3.56137289

H,0,-5.2664890562,-1.303130474,-1.6187105533

H,0,-3.6118669921,-1.6939049686,-1.1783419464

H,0,-1.7919788619,-1.110130263,1.9728904314

H,0,-2.0863245133,-1.176097388,0.2324738719

TS4a-TIC

49

C,0,-0.424210815,1.1838919932,0.6658224516

C,0,0.6699336241,-0.1468716325,-1.2776017345

C,0,1.5818906518,2.0393761272,-0.5799164293

C,0,1.7922914413,0.7828766703,-1.1877480921

H,0,0.9035612259,-1.2027292261,-1.3810009995

H,0,-0.2358577838,0.1805932151,-1.7823464248

O,0,0.0261240525,0.01964238,0.468549969

C,0,0.2169114978,2.3637480694,-0.0361999721

H,0,0.2346185099,3.2436304172,0.6146992084

H,0,-0.4524354216,2.6024161922,-0.8802101994

S,0,-2.0932998324,1.4886710495,1.2469420966

C,0,2.6473773501,2.928643535,-0.452595847

C,0,3.0823587807,0.4390943258,-1.6153488309

C,0,4.1338864506,1.3405776258,-1.4965374593

C,0,3.9160332101,2.5931801455,-0.920825184

H,0,2.4836497644,3.8903312427,0.0272134183

H,0,4.7344815429,3.2988371666,-0.8213883158

H,0,5.1238172701,1.066601202,-1.8472376762

H,0,3.2494525657,-0.5386722591,-2.059023982

C,0,-4.556400107,2.8265642312,-2.4986570348

C,0,-5.942034111,3.4803145779,-2.6435520864

H,0,-6.6414197362,2.8183368532,-3.1585001992

H,0,-6.3377325508,3.721099065,-1.6532020467

H,0,-5.8437740194,4.4046453818,-3.218665967

C,0,-3.5860924668,3.7735942886,-1.7826885756

H,0,-3.9878548916,4.0127032747,-0.7947002052

H,0,-2.6033249197,3.316760028,-1.6714121971

H,0,-3.4862310296,4.6955951464,-2.3635541903

C,0,-4.0661663693,2.4843697195,-3.844313065

N,0,-3.7346057116,2.2621031028,-4.9296726916

C,0,-3.2227022162,0.5321774262,-1.5780279954

C,0,-2.4793191478,-0.1497125457,1.9683767758

C,0,-4.11827345,-1.0474297033,0.229688312

C,0,-3.8308837445,-0.6774511138,1.5574214645

O,0,-2.2968004414,1.0253836248,-2.17449341
S,0,-4.8469895343,1.2885963725,-1.5218660661
C,0,-3.1254255273,-0.8253192166,-0.8852779949
C,0,-5.3650875699,-1.600804068,-0.0696039577
C,0,-4.8156895088,-0.8453778445,2.5332850312
C,0,-6.3389765432,-1.7664408345,0.9127206941
C,0,-6.0639319111,-1.3801474697,2.2202546128
H,0,-5.5768434615,-1.8982039519,-1.0939240721
H,0,-7.3021453574,-2.1949366388,0.6556185686
H,0,-6.8117607478,-1.5004327828,2.9975159768
H,0,-4.5958295144,-0.5572030017,3.557793163
H,0,-3.2843919392,-1.5655302668,-1.6796306187
H,0,-2.0861254485,-0.9219475543,-0.554797384
H,0,-2.4288000001,-0.0622888264,3.0550662998
H,0,-1.6729811085,-0.8128005134,1.6412468626

TS4b-TIC

49

C,0,0.2743521768,0.9106131956,0.9153208743
C,0,1.1139609275,-0.3796455961,-1.1767928415
C,0,2.3802012913,1.5485337358,-0.2957377122
C,0,2.3747085623,0.3417049754,-1.0278012971
H,0,1.1695934728,-1.4437624481,-1.3881290602
H,0,0.2692083478,0.139723328,-1.6227068182
O,0,0.5243091377,-0.2858038232,0.5934988081
C,0,1.0930180984,2.0345146397,0.3133477342
H,0,1.2620580543,2.8305969102,1.0453386684
H,0,0.4630969986,2.4614496448,-0.4856006916
S,0,-1.3141252421,1.4231504742,1.5716843935
C,0,3.5787357692,2.2357730072,-0.112250207

C,0,3.5858352187,-0.162407258,-1.5221380277

C,0,4.7724127524,0.540048726,-1.3457050317

C,0,4.7696993785,1.7473594941,-0.6455592466

H,0,3.5806910952,3.158378779,0.4627655745

H,0,5.6940294927,2.2972913984,-0.5010049278

H,0,5.6998295611,0.145671061,-1.7486870021

H,0,3.5848942209,-1.1049607537,-2.0628555712

C,0,-3.5693190761,3.5135815928,-1.9524993383

C,0,-4.834491408,4.3884512665,-2.0022425274

H,0,-5.6324123833,3.9009025423,-2.5662568745

H,0,-5.1823377971,4.5859420253,-0.9847168629

H,0,-4.5935747246,5.3397141369,-2.4837249657

C,0,-2.4580514754,4.2186583266,-1.1658320234

H,0,-2.8115027577,4.4145336132,-0.1502467974

H,0,-1.5586879813,3.6055283587,-1.1223262655

H,0,-2.2175367993,5.1686319887,-1.6528173501

C,0,-3.1458581405,3.2380598593,-3.3355774964

N,0,-2.8588275882,3.0788647922,-4.4444544778

C,0,-2.6146672968,0.9531732651,-1.2966125445

C,0,-1.9553414104,-0.1946709058,2.1418149966

C,0,-3.7380547086,-0.6364405724,0.3692242117

C,0,-3.3793922337,-0.4534843108,1.7184017683

O,0,-1.6248771597,1.3504400938,-1.8611845726

S,0,-4.0957517841,1.9491087014,-1.1286544659

C,0,-2.7347578946,-0.4661166147,-0.7455627136

C,0,-5.0616951379,-0.9484531212,0.0515210578

C,0,-4.3674901558,-0.5583907191,2.6997481668

C,0,-6.0385879973,-1.0534411758,1.0392191469

C,0,-5.6896647855,-0.8506728145,2.3702427066

H,0,-5.3304754598,-1.102945817,-0.990783412

H,0,-7.0615932835,-1.292790881,0.7679387955

H,0,-6.4383167158,-0.9270164842,3.1522574822

H,0,-4.092223694,-0.4143840124,3.7411407679

H,0,-3.0232034524,-1.084839844,-1.6047330642

H,0,-1.7221761433,-0.7647813079,-0.4556195037

H,0,-1.87940655,-0.2251678472,3.2301164305

H,0,-1.2720413195,-0.943660625,1.7307091071

TS4c-TIC

49

C,0,0.5722703542,1.1138920951,0.671086828

C,0,1.234435761,1.9512574791,-1.6495265613

C,0,2.7892832204,2.2393335679,0.2631560062

C,0,2.5803187933,2.1864962121,-1.1321366049

H,0,1.1486911931,1.5285875436,-2.6461715153

H,0,0.437245876,2.6409012389,-1.3827352704

O,0,0.7000690433,0.6017358848,-0.4737267076

C,0,1.6337235985,2.0510747083,1.2139134164

H,0,1.990962908,1.6929182623,2.1862409225

H,0,1.1481064728,3.0197260187,1.4064779951

S,0,-1.0212368175,1.2400984434,1.4501612953

C,0,4.0833992017,2.4160111461,0.7529600854

C,0,3.6864409673,2.2725634346,-1.9911515684

C,0,4.9674622032,2.4661977208,-1.489375159

C,0,5.1677377419,2.5480985716,-0.1105912911

H,0,4.2438874803,2.4394563642,1.828135637

H,0,6.1656083802,2.6938496045,0.2902150323

H,0,5.8095079346,2.5451532965,-2.1695799185

H,0,3.5269633556,2.1989379572,-3.0635655583

C,0,-2.7784859349,-5.7916013573,2.6679258349

C,0,-3.3975869215,-6.9238056774,3.5055858084

H,0,-2.9629506597,-6.9615676516,4.5066859125

H,0,-4.4770077248,-6.7702420388,3.5867671715

H,0,-3.2140577922,-7.8787104025,3.0064765579

C,0,-3.3920115624,-5.7555038663,1.2632927856

H,0,-4.4714907508,-5.608858306,1.3511456215

H,0,-2.9607641348,-4.9548252737,0.6634432476

H,0,-3.2024406922,-6.7115963161,0.7660654432

C,0,-1.3231336816,-6.0061689969,2.5993963225

N,0,-0.1919991217,-6.2434951634,2.5649528856

C,0,-2.2597966674,-3.0094914874,2.6302353989

C,0,-1.8668984294,-0.1416876196,0.5891043962

C,0,-3.5627715288,-0.9180911237,2.3234582598

C,0,-3.273441809,-0.2599311787,1.1158038743

O,0,-1.6080213087,-3.2825085202,1.6555615646

S,0,-3.1225077433,-4.2406307963,3.6072739985

C,0,-2.4757062803,-1.5921672035,3.140104721

C,0,-4.8845094388,-0.9832718856,2.7706189366

C,0,-4.3194769271,0.3318505684,0.4022820747

C,0,-5.9193701006,-0.3993627464,2.0450427171

C,0,-5.6343060442,0.2640637811,0.8545835077

H,0,-5.1027846899,-1.4992182153,3.7025230322

H,0,-6.9392650446,-0.4590518007,2.4109707234

H,0,-6.4299848335,0.7282004558,0.2808329735

H,0,-4.0916549124,0.8531967271,-0.5237703713

H,0,-2.7641893486,-1.6147872948,4.1946240328

H,0,-1.5219530111,-1.0634547881,3.0548853324

H,0,-1.2847981523,-1.0525133061,0.7443000222

H,0,-1.8701234214,0.0842269346,-0.4778028493

TS4d-TIC

49

C,0,-1.2569935496,1.2312411082,0.691005786

C,0,1.0168563837,0.2967690265,-0.1033978851

C,0,0.8779116981,1.646984458,1.9739475708

C,0,1.5676855723,0.6998764811,1.1859191679

H,0,1.3196392796,-0.6666869852,-0.5021033762

H,0,0.8110757309,1.0545706166,-0.8543540569

O,0,-0.7908348564,0.0953887994,0.403637348

C,0,-0.4435236054,2.20626946,1.5135506538

H,0,-1.0388495547,2.5440242099,2.3697341596

H,0,-0.2784982491,3.0988325868,0.8895522841

S,0,-2.6050186412,1.9386177578,-0.2200524594

C,0,1.4049185388,2.0199229802,3.2106705504

C,0,2.7339421121,0.1086842726,1.6965756784

C,0,3.2539160312,0.4987312374,2.9247714057

C,0,2.5962277367,1.4717887184,3.6796716594

H,0,0.8659900026,2.7431263258,3.81875118

H,0,2.99555793,1.7823989431,4.640181844

H,0,4.1671803496,0.0439871466,3.2950551955

H,0,3.2409928999,-0.6507132641,1.1076798356

C,0,-0.8197368181,-1.5882828195,5.0207688011

C,0,0.3283691555,-0.6878774886,5.5083537161

H,0,1.2012516586,-0.7702572846,4.8564748726

H,0,-0.0038456964,0.3543477541,5.5184212901

H,0,0.609452388,-0.981785733,6.5232961509

C,0,-2.0432030426,-1.4538548129,5.9347893155

H,0,-2.3713746264,-0.4112004723,5.9358659432

H,0,-2.8591867405,-2.0938282058,5.6003058207

H,0,-1.7649281535,-1.7405665795,6.9536231711

C,0,-0.331669687,-2.9779112304,4.9984662755

N,0,0.1112928856,-4.0456931486,5.0311770488

C,0,-2.4178408925,-2.2115285662,2.7910446119
C,0,-3.6062873244,0.4237485495,-0.4823229865
C,0,-4.2283170306,-0.9709321623,1.5881012194
C,0,-4.4837092098,0.0863069246,0.6990900574
O,0,-2.7449391244,-3.1462589837,3.4789970795
S,0,-1.1719779917,-1.0246576521,3.3000135547
C,0,-3.0380183664,-1.9100180884,1.4383729619
C,0,-5.1295586272,-1.2061953397,2.6370592305
C,0,-5.6210607112,0.8814439597,0.9002732885
C,0,-6.2513720735,-0.4092209847,2.8234486963
C,0,-6.499286788,0.6482401483,1.9487251829
H,0,-4.9450596931,-2.0375399523,3.3118395132
H,0,-6.9309101325,-0.6152348429,3.6442301636
H,0,-7.3721298688,1.2797710752,2.0791425237
H,0,-5.8091070531,1.7038866903,0.2138114539
H,0,-2.2723686912,-1.4912175994,0.7849146589
H,0,-3.3684324828,-2.873463551,1.0355289038
H,0,-2.9182411784,-0.3736217298,-0.7637274552
H,0,-4.224595893,0.6509612468,-1.3540506059

Int4-TIC
49

C,0,1.5751397411,0.1684302792,1.5582082195
C,0,2.4481220818,-0.1421945571,-1.4700361737
C,0,3.6077984626,1.0636863135,0.3642271585
C,0,3.6320090245,0.3148844063,-0.8517023243
H,0,2.5014017241,-0.7466800989,-2.368815938
H,0,1.4630158679,0.0540033434,-1.0643952549
O,0,2.130319221,-0.8089330185,1.9936230329
C,0,2.2922009734,1.3997442995,1.0140648169

H,0,2.4555403256,2.0580042906,1.8756032958

H,0,1.6231028658,1.9355160436,0.32995287

S,0,-0.2082022597,0.3249659911,1.5323713727

C,0,4.8023594346,1.4720305216,0.9395800339

C,0,4.8956971968,0.0222183813,-1.4288665515

C,0,6.0745992019,0.4447282437,-0.8398190713

C,0,6.0352293511,1.1742109033,0.3517545557

H,0,4.774513772,2.0343062619,1.8691768359

H,0,6.9545651159,1.5062202199,0.8225786007

H,0,7.0273396001,0.2068297735,-1.3022781893

H,0,4.9223859389,-0.5490547664,-2.3529705961

C,0,-1.1212444116,1.1228293472,-2.9874809944

C,0,-0.0771721202,1.1985117435,-4.1153782129

H,0,0.9182854487,0.9303891481,-3.7531704643

H,0,-0.3644523284,0.5211727589,-4.9242090263

H,0,-0.0459028791,2.2193773149,-4.5050442921

C,0,-2.5048121316,1.5445930842,-3.4947198774

H,0,-2.794994462,0.8836724645,-4.3154870942

H,0,-3.2489671912,1.4934255707,-2.7011880516

H,0,-2.4518572786,2.5716000961,-3.8689304983

C,0,-0.6704791313,1.9918775239,-1.8868858269

N,0,-0.2614774867,2.6912783668,-1.0613416552

C,0,-2.1572530589,-0.5543118296,-0.9499738453

C,0,-0.6253174545,-1.2730903301,2.3192353019

C,0,-2.8417492926,-1.7651360935,1.1575228107

C,0,-2.1199192578,-1.4681054588,2.3264959267

O,0,-2.7921110383,0.4210937669,-0.6582669095

S,0,-1.0865841171,-0.6275020395,-2.4010265909

C,0,-2.166498207,-1.875901095,-0.1857170412

C,0,-4.2254491704,-1.933121407,1.2320151662

C,0,-2.8114944034,-1.3428039561,3.5348092146

C,0,-4.9038379635,-1.8083193255,2.4406237857

C,0,-4.1914713092,-1.5111937687,3.5992359536

H,0,-4.7784141672,-2.1604961385,0.3240114998

H,0,-5.9802102707,-1.9414419596,2.4756159146

H,0,-4.7057667109,-1.4106334752,4.5495436635

H,0,-2.2533512867,-1.1096377189,4.4375365746

H,0,-2.6965673793,-2.5975513077,-0.8201117297

H,0,-1.1328030155,-2.227661929,-0.1085151055

H,0,-0.2318479014,-1.2667526665,3.3372339001

H,0,-0.0959937772,-2.057237201,1.7713016491

TS5-TIC

49

C,0,0.6579299969,-0.2480897979,-4.6237474376

C,0,2.163361102,-0.4591801115,-4.4393286279

H,0,2.5565629363,0.1426389029,-3.6176926583

H,0,2.3523701833,-1.5111208608,-4.2123906412

H,0,2.686198692,-0.1830362653,-5.3607082859

C,0,0.1279403435,-1.0554538138,-5.8183463648

H,0,0.3474520535,-2.1142047561,-5.6598365447

H,0,-0.9513142409,-0.9291189267,-5.9337899205

H,0,0.6192425544,-0.7211591223,-6.736452106

C,0,0.3824356528,1.1795349837,-4.8566042452

N,0,0.1821172754,2.3036643052,-5.0479706572

C,0,-1.9728769929,0.3270258187,0.3527297205

C,0,-3.8223202452,1.7962823488,-0.0366845763

C,0,-1.9932623225,2.6120004461,1.3885253926

C,0,-3.0447471643,2.9465667924,0.5339454076

O,0,-2.9617965425,0.7317350253,-0.466331911

S,0,-1.0980805603,-1.0041538435,-0.07800652

C,0,-1.7287205391,1.1425766022,1.6042215379

C,0,-1.2527406597,3.6217970777,1.9993791733

C,0,-3.3439640456,4.2812830443,0.2695775005

C,0,-1.5619609582,4.9583150376,1.7518666698

C,0,-2.6023563972,5.2894546746,0.8833861464

H,0,-0.4275975149,3.3602962737,2.6559732215

H,0,-0.9837194,5.7434951284,2.2292543282

H,0,-2.8318724121,6.3305541431,0.6807869348

H,0,-4.1518402196,4.5320777696,-0.4127570867

H,0,-2.4028010284,0.7632352949,2.38983426

H,0,-0.7063910964,0.9623442587,1.9454207927

H,0,-4.3907600756,2.08082851,-0.9227694619

H,0,-4.5184787604,1.3884904137,0.7098931312

C,0,0.5171615571,-0.2083524847,-1.7524206759

C,0,2.1878208552,-0.7139186905,-0.1409447208

C,0,1.3657626098,1.6626191458,-0.3168157999

C,0,2.1634354985,0.7169234553,0.3295254992

O,0,1.6554957403,-0.8992327814,-1.4525877909

S,0,-0.3382281319,-0.8424983487,-3.1616364227

C,0,0.5437126756,1.2751183103,-1.5213968966

C,0,1.3633723529,2.9833530077,0.1422594482

C,0,2.9326423321,1.0930591581,1.4344620893

C,0,2.1340988522,3.35741981,1.2372273456

C,0,2.9195022199,2.4063879851,1.8918121093

H,0,0.7389008509,3.7174913105,-0.3620664774

H,0,2.1202095781,4.3871108306,1.5823242892

H,0,3.5253074848,2.6903470248,2.7465047277

H,0,3.5507475678,0.3501256651,1.9336990686

H,0,0.9542376907,1.7789834231,-2.4102429795

H,0,-0.4870334771,1.6386456425,-1.4235216363

H,0,3.214043885,-1.0854881419,-0.1947048828

H,0,1.6166408538,-1.3465954355,0.5498779939

TS5a-TIC
49

C,0,0.6677616719,-0.4127775368,-4.7023292659
C,0,2.1482317195,-0.7867289478,-4.5821608308
H,0,2.6587148194,-0.1661118432,-3.8427094396
H,0,2.2322017392,-1.8311379514,-4.2726789265
H,0,2.6404583225,-0.6488759872,-5.5502187925
C,0,-0.0150182947,-1.2199852159,-5.816598495
H,0,0.0905995006,-2.2863106238,-5.6013174476
H,0,-1.0775643976,-0.9751785408,-5.8871503037
H,0,0.4594066513,-1.0000943927,-6.7771619496
C,0,0.5464456414,1.0226061595,-5.0065277788
N,0,0.4685158556,2.1525564413,-5.2465364728
C,0,-1.8015021705,0.5279764125,0.3202951675
C,0,-3.6844588256,1.9272697559,-0.1651763793
C,0,-2.0633969068,2.7369427986,1.4994972108
C,0,-3.0426945917,3.0723437977,0.563849539
O,0,-2.7263976415,0.9426446677,-0.5713483214
S,0,-0.8521207474,-0.7611620626,-0.0748656449
C,0,-1.7103645933,1.2770330977,1.6331807916
C,0,-1.4664373097,3.7403701716,2.2609435699
C,0,-3.4039138327,4.4037739117,0.3654225527
C,0,-1.8370185001,5.0711151956,2.0766264943
C,0,-2.8002444948,5.4051476266,1.1236220261
H,0,-0.7062038913,3.4761563432,2.9910675263
H,0,-1.3692005144,5.8502505127,2.6705168591
H,0,-3.0776864947,6.4430089394,0.9706801284
H,0,-4.1540702782,4.6571131332,-0.3791944636

H,0,-2.4098461305,0.7993457838,2.3385263533

H,0,-0.7056800349,1.1400048754,2.0407171136

H,0,-4.1748299455,2.2487351758,-1.084950592

H,0,-4.4307129611,1.4327814632,0.4730535251

C,0,0.6703413743,-0.1217999553,-1.8449509209

C,0,2.8515115562,-0.2855501114,-0.8357997691

C,0,1.4747157513,1.7409521591,-0.4216992841

C,0,2.4709233082,0.8775260599,0.0389060375

O,0,1.7607744735,-0.8834519827,-1.5456165837

S,0,-0.3041938472,-0.7985991631,-3.1592026752

C,0,0.7903965089,1.373754797,-1.7110081736

C,0,1.1560491045,2.8812321841,0.3116136515

C,0,3.1305833489,1.142551059,1.2367009238

C,0,1.8361431265,3.1623206823,1.4965603677

C,0,2.8182137195,2.2904614434,1.9643498252

H,0,0.3736315766,3.5485928092,-0.042489771

H,0,1.5938135784,4.0611121304,2.0557771635

H,0,3.3388291814,2.5018681978,2.8929355002

H,0,3.8919400099,0.4563973896,1.5991612332

H,0,1.3614517595,1.7796066282,-2.5636373229

H,0,-0.2114687712,1.8107616895,-1.7733030414

H,0,3.3021016727,-1.0916719216,-0.2530073732

H,0,3.5861597237,0.0457112638,-1.5855719107

Int5-TIC

49

C,0,0.9040434459,-1.6091955666,-3.7442511328

C,0,2.389378611,-1.8992673938,-3.4996091121

H,0,2.7996964337,-1.27868819,-2.7025306509

H,0,2.50532763,-2.9456530025,-3.2082701143

H,0,2.9463913742,-1.7097991182,-4.4227723668

C,0,0.3871952529,-2.4331305995,-4.9378772405

H,0,0.5438747596,-3.4952138735,-4.7342937101

H,0,-0.6767371456,-2.2555098009,-5.1122646063

H,0,0.940405946,-2.155144323,-5.8391300194

C,0,0.720880945,-0.1810844772,-4.0603854149

N,0,0.5946998837,0.9380873276,-4.327364996

C,0,-1.5113112127,-0.6091017479,1.0042177934

C,0,-3.417943457,0.7755792119,0.6994905408

C,0,-1.7198602449,1.4745034121,2.3493866051

C,0,-2.7512440479,1.8647403826,1.4924778273

O,0,-2.4685415755,-0.1473567168,0.1579826077

S,0,-0.6888076928,-2.0435386878,0.5060083944

C,0,-1.3416701533,0.0118242029,2.3644387031

C,0,-1.088108733,2.4298883751,3.1437333197

C,0,-3.1367891803,3.2020849392,1.4159129772

C,0,-1.4830338724,3.7648663922,3.0808348803

C,0,-2.5046394258,4.1536600173,2.213851132

H,0,-0.2762460595,2.1275377892,3.7999935538

H,0,-0.9869908117,4.5049513048,3.7012473744

H,0,-2.8029059025,5.1954672712,2.1554130971

H,0,-3.9283449033,3.4987790533,0.7325677567

H,0,-1.9659880334,-0.5125829558,3.1095050156

H,0,-0.3011917165,-0.1150397772,2.6828325285

H,0,-3.9660424155,1.1706844485,-0.1570106435

H,0,-4.1172031509,0.2105013647,1.3329833018

C,0,0.544586218,-1.4496951269,-0.8186009047

C,0,2.3967597159,-1.8474240128,0.6439729665

C,0,1.4884567626,0.5002991881,0.4222419464

C,0,2.3041425318,-0.410875744,1.0983142378

O,0,1.7638918817,-2.1065820406,-0.6065447251

S,0,-0.2105742479,-2.0999135606,-2.3472154494
C,0,0.7378003996,0.0586208958,-0.8096391044
C,0,1.3948587204,1.8144249572,0.888496232
C,0,3.011425723,-0.0015394808,2.2314586963
C,0,2.1102679883,2.2224345699,2.0094493417
C,0,2.9214619235,1.3104171349,2.6865320907
H,0,0.7424154296,2.5156773091,0.373064014
H,0,2.0254105826,3.2464126198,2.3605285716
H,0,3.4813082909,1.6207344681,3.5632131687
H,0,3.6387074463,-0.7174516092,2.758377254
H,0,1.321964902,0.3245336239,-1.6986113025
H,0,-0.2253769586,0.5679437067,-0.8985610657
H,0,3.4405409822,-2.138596683,0.4966259332
H,0,1.9590751454,-2.5029165657,1.4081798876

TS6-TIC

49

C,0,1.5378627096,-1.7271900022,-3.7070550916
C,0,2.9889086428,-2.0403706978,-3.3238650686
H,0,3.3603826055,-1.3662646661,-2.5520953872
H,0,3.0444352882,-3.061201802,-2.938983466
H,0,3.6191923939,-1.9477469621,-4.2140329587
C,0,1.0861311284,-2.6282028628,-4.8714798526
H,0,1.1886821157,-3.6751040686,-4.5753996969
H,0,0.0464917269,-2.433139404,-5.1450466166
H,0,1.7184574788,-2.4389131822,-5.7430387515
C,0,1.4295008566,-0.3237780526,-4.1440021833
N,0,1.3657150337,0.7739527666,-4.505006987
C,0,-1.0448413714,-0.1768530137,0.8962033671
C,0,-3.3853912357,0.9477916503,0.9183471247

C,0,-1.7546646068,1.4067044603,2.7231806795

C,0,-2.8934157587,1.8038822988,1.9887420003

O,0,-1.7020205311,0.5339308767,0.1019782347

S,0,-0.3862796132,-1.771788453,0.4124265126

C,0,-1.0433567666,0.125089584,2.3796551721

C,0,-1.2606158599,2.2440372212,3.7238570967

C,0,-3.472871346,3.0561503702,2.249713833

C,0,-1.873480992,3.4617527509,4.0072695379

C,0,-2.978431341,3.8728908091,3.2585947629

H,0,-0.3709352597,1.9424912209,4.271606385

H,0,-1.4796122203,4.0972780726,4.7940404223

H,0,-3.4479201091,4.8306979879,3.458997974

H,0,-4.3291565571,3.3738783814,1.6609915569

H,0,-1.5273782278,-0.728339811,2.8815022256

H,0,-0.007419873,0.1429528918,2.7427575911

H,0,-3.983444145,1.4012482668,0.1341500171

H,0,-3.6208060572,-0.0911670241,1.1279699477

C,0,0.9260745735,-1.2841587243,-0.8534960064

C,0,2.6794825761,-1.5130779594,0.7687868566

C,0,1.6612599268,0.7621267338,0.3386694991

C,0,2.4268930868,-0.0741083688,1.1554981899

O,0,2.1344959243,-1.8960234924,-0.4936265572

S,0,0.299199558,-2.077487476,-2.374751629

C,0,1.1325756734,0.2217848778,-0.9668307605

C,0,1.3640876427,2.0597341054,0.7656291354

C,0,2.902636149,0.4008543665,2.3803803605

C,0,1.839821846,2.5301121195,1.9852369464

C,0,2.6176272815,1.6990598749,2.7942410026

H,0,0.7335467466,2.6897532178,0.1435555503

H,0,1.5912008324,3.5350535912,2.3113099794

H,0,2.9917803862,2.0587612739,3.7477620963

H,0,3.4909587876,-0.2556082754,3.0181519108

H,0,1.8728100328,0.3810518493,-1.7596739069

H,0,0.2133609278,0.7251605145,-1.2708474559

H,0,3.7520412224,-1.7117437578,0.6849899088

H,0,2.2654447179,-2.171777078,1.5432494986

Int6-TIC

49

C,0,1.3099664423,-1.7827731664,-3.8294681089

C,0,2.6867047665,-2.3581035067,-3.4766288226

H,0,3.1719304881,-1.7942496941,-2.6798430819

H,0,2.5659227313,-3.3897249772,-3.1381055233

H,0,3.3214851462,-2.3357969177,-4.3680380127

C,0,0.6976984622,-2.5496919385,-5.0164496215

H,0,0.6154234591,-3.6079953081,-4.7566723071

H,0,-0.2923981041,-2.1641197474,-5.2706273937

H,0,1.3482659839,-2.4452636231,-5.8887762482

C,0,1.4427326326,-0.3673670349,-4.2167900858

N,0,1.5698763226,0.7362355837,-4.540820464

C,0,-1.195826741,0.0660912367,0.6676596841

C,0,-4.3470638031,0.4752882876,1.4622688282

C,0,-2.2973022203,1.4805368707,2.4473120827

C,0,-3.6807116318,1.5421866147,2.1002173379

O,0,-1.3520947189,0.9063415409,-0.1717755503

S,0,-0.5320640626,-1.5949392804,0.3245897781

C,0,-1.490512421,0.2492342073,2.1497843847

C,0,-1.6894419426,2.5709307683,3.054252399

C,0,-4.3883741868,2.7339108401,2.4122283192

C,0,-2.4062692694,3.7343208517,3.3472110418

C,0,-3.7643648818,3.8073698106,3.0227427396

H,0,-0.6323593987,2.5108936116,3.3026962616

H,0,-1.9099320536,4.5731405925,3.823759241

H,0,-4.3302232015,4.7061209463,3.2467535044

H,0,-5.4423435385,2.7911676405,2.1544719331

H,0,-1.9633954676,-0.6659110308,2.5293285934

H,0,-0.5039131521,0.3062542004,2.6300598595

H,0,-5.396773241,0.5624513481,1.209995096

H,0,-3.8467480635,-0.4438184829,1.1848971045

C,0,0.803045823,-1.3103054821,-0.9645847891

C,0,2.5074245444,-1.8409227845,0.6554579165

C,0,1.839048289,0.567039402,0.27027376

C,0,2.4404474002,-0.3935875022,1.087390855

O,0,1.8788349565,-2.1320750899,-0.5979196323

S,0,0.0468664258,-1.9703510004,-2.4883991854

C,0,1.2908868053,0.132162494,-1.0647953825

C,0,1.7141868025,1.8816487074,0.7255999602

C,0,2.9289493766,-0.0276819167,2.3431328739

C,0,2.210878154,2.2460190055,1.9742241109

C,0,2.8237851958,1.2887263409,2.7844052278

H,0,1.2079313787,2.611832605,0.0997440411

H,0,2.1127118237,3.2710890002,2.3178346172

H,0,3.2094466017,1.5650263334,3.7606486847

H,0,3.3851181938,-0.7799762647,2.9829195142

H,0,2.0936558774,0.1307392473,-1.8116022042

H,0,0.5075420284,0.7988166486,-1.4227263315

H,0,3.5463204814,-2.1603894231,0.5290222338

H,0,2.0465871291,-2.4683273088,1.4286823422

TS7

27

C,0,-0.6045300173,-0.488978676,1.504715399

C,0,-0.2826531817,-1.700700593,0.6765211907

H,0,-1.0928201212,-1.9502632101,-0.0129890651

H,0,0.6309035675,-1.5262710781,0.0994362477

H,0,-0.1106633295,-2.5699540767,1.325882974

C,0,0.480611396,0.0403347566,2.4004799065

H,0,1.4012031118,0.1701208033,1.8230946499

H,0,0.2048804302,0.9962271058,2.8522338704

H,0,0.6885438874,-0.6709210718,3.2107831882

C,0,-1.943739334,-0.3610491693,1.9690052194

N,0,-3.0492637239,-0.2055559378,2.2995819028

C,0,0.4700843082,1.2427497922,-0.6592012157

C,0,-0.7577304933,1.14473609,-0.0707221441

H,0,-1.0472550894,1.8632994211,0.6893312546

H,0,-1.5761912769,0.6132418123,-0.5478986409

H,0,1.204985604,1.9057175707,-0.2050889447

C,0,0.9421455298,0.4820618329,-1.8122421142

C,0,2.2954737694,0.5704406051,-2.1819176526

C,0,0.0996777562,-0.3434027612,-2.5805746541

C,0,2.7938091018,-0.1437016999,-3.2668381217

H,0,2.9588381166,1.2086473119,-1.6035893942

C,0,0.597525651,-1.0563265346,-3.6634395118

H,0,-0.9544590025,-0.4217215298,-2.3323595228

C,0,1.9472745659,-0.9631052954,-4.0117957418

H,0,3.8432536128,-0.0604197702,-3.5314489988

H,0,-0.0697426511,-1.6856516285,-4.2440900459

H,0,2.3319348123,-1.5210300694,-4.8593320349

TS7a

27

C,0,-0.8648080277,-0.2192782446,1.5801663387

C,0,-2.1571838813,-0.9093352321,1.2305274284

H,0,-3.0214934071,-0.2645500784,1.4075047312

H,0,-2.147315706,-1.2114500902,0.1789508751

H,0,-2.2827341684,-1.8163937012,1.8371282479

C,0,0.4178276145,-0.9133906715,1.2127775967

H,0,0.3941859359,-1.2063219165,0.1590521039

H,0,1.2845603618,-0.2682735128,1.3763373764

H,0,0.5447067773,-1.8216306433,1.8166182816

C,0,-0.8528954435,0.5097451932,2.8048342467

N,0,-0.8430624082,1.1653985139,3.7669216716

C,0,0.2336314455,1.6417875717,-0.4758692354

C,0,-0.9666522395,1.567810858,0.1756580525

H,0,-1.1862202509,2.2214458248,1.014303247

H,0,-1.8264313375,1.1673877509,-0.3519058213

H,0,0.3348524602,1.1391673946,-1.4364916159

C,0,1.4435852757,2.2697764299,0.0395672928

C,0,2.5776570975,2.3589267794,-0.7867820766

C,0,1.532487103,2.7722245555,1.3516826111

C,0,3.7536373689,2.9429627026,-0.3296400452

H,0,2.5249511133,1.9672939083,-1.7995798439

C,0,2.7110995894,3.3506014481,1.8077570402

H,0,0.684555619,2.6950253275,2.0262473472

C,0,3.8250036343,3.4424519847,0.9707822926

H,0,4.6160649896,3.0062865922,-0.9858141365

H,0,2.7623328321,3.7265149723,2.8246931649

H,0,4.7428876521,3.8949112832,1.3321848284

TS7b

27

C,0,-0.5959966652,-0.4696259337,1.5337624976

C,0,-2.0146333241,-0.4195686728,2.0322772453

H,0,-2.2518064096,0.5468331264,2.4837930461

H,0,-2.7109079751,-0.6073222625,1.2089770169

H,0,-2.1835886176,-1.1954283467,2.7912263756

C,0,-0.1772128241,-1.6508277125,0.7047536523

H,0,-0.9021087519,-1.8251734247,-0.0970047815

H,0,0.8062232962,-1.4965189836,0.254309124

H,0,-0.1344188623,-2.5586498975,1.3217113266

C,0,0.3980835495,0.0970297848,2.383498939

N,0,1.2154420311,0.6090550485,3.0341911653

C,0,0.5475319907,1.2372859744,-0.6367809163

C,0,-0.6667370252,1.1950028071,-0.0163918897

H,0,-0.8921880378,1.9141244817,0.7645746697

H,0,-1.5208503576,0.7056857026,-0.4780719848

H,0,1.3340057121,1.831560711,-0.175240976

C,0,0.9426736895,0.4671155054,-1.812195298

C,0,2.3002400499,0.4228881406,-2.1734551756

C,0,0.0234149157,-0.2420790118,-2.6075102503

C,0,2.7277539362,-0.3112996345,-3.2751964667

H,0,3.0227131126,0.9685116852,-1.5721577187

C,0,0.4504135635,-0.9749750539,-3.7073561259

H,0,-1.035940853,-0.2085851292,-2.3706478695

C,0,1.8050714695,-1.0165194087,-4.0461479531

H,0,3.7821990349,-0.333466478,-3.531888299

H,0,-0.2755699041,-1.5123753574,-4.309675687

H,0,2.1349622562,-1.5889116603,-4.9070576662

TS7c

27

C,0,-0.9239159801,-0.6292765906,1.3238854795

C,0,0.5512121665,-0.5683424651,1.610702751

H,0,1.1420125363,-0.8693089486,0.7420822746

H,0,0.8346150447,0.4506557825,1.8900549316

H,0,0.8031995162,-1.2338975124,2.4468868096

C,0,-1.8601899642,-0.0639194344,2.359505795

H,0,-1.5434988707,0.9454438903,2.6389494815

H,0,-2.8903082813,-0.0261528725,1.9968746322

H,0,-1.8442789095,-0.6819769178,3.267386885

C,0,-1.3788086741,-1.789646777,0.6324156567

N,0,-1.7593685152,-2.6966505866,0.0094340859

C,0,-0.0009480625,1.2608289058,-0.7898101812

C,0,-1.2378702687,0.8606743603,-0.3650024188

H,0,-1.8178918991,1.5280613326,0.2643389492

H,0,-1.80482161,0.1201717898,-0.9208295094

H,0,0.4373025027,2.1529662437,-0.3451659843

C,0,0.8439890528,0.5476075805,-1.7392024662

C,0,2.0507480827,1.1334409124,-2.1604974261

C,0,0.5111170819,-0.7267226825,-2.2365375342

C,0,2.8887889798,0.4820577663,-3.0585170154

H,0,2.3235948355,2.1136461602,-1.7775377985

C,0,1.3535603195,-1.3779530262,-3.1298037887

H,0,-0.400003076,-1.2207328391,-1.911187107

C,0,2.5428405593,-0.7774646683,-3.5479504723

H,0,3.8134286796,0.9545825681,-3.3749478228

H,0,1.0829558146,-2.3627778134,-3.4972061198

H,0,3.1969009394,-1.2905701581,-4.2456580872

Int7

27

C,0,-0.8891121926,-0.0934993178,1.9771164675

C,0,-0.6224080984,-1.5091939619,1.444067025

H,0,-1.3815600025,-1.805360308,0.7149603428

H,0,0.357628919,-1.5365966485,0.9588386787

H,0,-0.6307545365,-2.2337866795,2.2625467299

C,0,0.1378562442,0.2732532024,3.0596718986

H,0,1.146122177,0.2007037674,2.6423857195

H,0,-0.021570432,1.2920851058,3.4242143198

H,0,0.0641161851,-0.4130184326,3.9069760144

C,0,-2.2370952252,-0.0642535601,2.5802820621

N,0,-3.2964981781,-0.0345538086,3.0445183432

C,0,0.4438606332,1.1032737787,0.1511983288

C,0,-0.8826103827,0.9566639695,0.8209693146

H,0,-1.1783869252,1.9206941513,1.2519609065

H,0,-1.6623745641,0.6798595948,0.1039861423

H,0,1.1776190375,1.7417781145,0.6363658433

C,0,0.8326698803,0.498354483,-1.0744237212

C,0,2.1301399172,0.749939717,-1.5955318597

C,0,-0.0133022308,-0.3603335301,-1.8238841351

C,0,2.5528301463,0.1796156402,-2.7841291135

H,0,2.7958875724,1.4064152847,-1.0412871072

C,0,0.4183527682,-0.926043381,-3.0141801526

H,0,-1.0133017663,-0.5817718172,-1.4658158346

C,0,1.7007232924,-0.6641922186,-3.5046593335

H,0,3.5501945052,0.3905079994,-3.1573287274

H,0,-0.2492362955,-1.578769895,-3.5681624925

H,0,2.0317083406,-1.1108272511,-4.4362602513

TS8

46

C,0,2.2125444266,1.3556245984,1.3294947876

C,0,1.9481210145,4.3066330858,2.6475080277

C,0,-0.1665518124,4.9843874719,3.532120843

C,0,1.8649584841,5.7545882631,4.6723145726

C,0,0.5158242209,5.9968314609,4.4059166434

O,0,0.6606117017,4.6246113005,2.4114079082

S,0,2.8378414501,3.6479786324,1.4188801341

C,0,2.4481306966,4.5058875441,4.0602768901

C,0,2.586716791,6.6473998915,5.4599091493

C,0,-0.116107363,7.1212394317,4.9289292481

C,0,1.9520138618,7.7677794548,5.9961965748

C,0,0.6030495705,8.0038704603,5.7341862984

H,0,3.6406232952,6.4683109276,5.6545627364

H,0,2.5136135708,8.4620423442,6.6130457985

H,0,0.114698014,8.8806763101,6.1467655883

H,0,-1.1632064602,7.3094574507,4.7070202005

H,0,2.1363516212,3.6334837559,4.6609890301

H,0,3.5384780246,4.5149645845,4.05395319

H,0,-1.0897680454,5.3675980733,3.0969275609

H,0,-0.3989150003,4.0651060535,4.0899323126

C,0,0.8876710832,1.4198572171,2.0330568654

H,0,1.0301986267,1.9377948006,2.9900537198

H,0,0.1683801257,2.0201042855,1.4651465294

C,0,0.2437222181,0.0381632974,2.361329874

C,0,1.2100541096,-0.8547844923,3.1557513374

H,0,1.6001538084,-0.3314839738,4.033824954

H,0,0.7052734986,-1.7646225055,3.4902110415

H,0,2.048465691,-1.1411321589,2.514530462

C,0,-0.2460648561,-0.6961086395,1.1036212999

H,0,-0.9379887109,-0.0742486142,0.529095986

H,0,0.6066872283,-0.9431003506,0.4663780944

H,0,-0.758352437,-1.6216064216,1.3805049075

C,0,-0.9244630855,0.3384387742,3.2165975483

N,0,-1.8259885684,0.6090821454,3.8900824182

H,0,3.0387833498,0.9928592787,1.9387950662

C,0,2.3438498802,1.071799878,-0.0907874727

C,0,3.5181927405,0.4610203529,-0.5701660346

C,0,1.3555009752,1.4314991589,-1.0286072938

C,0,3.6854956411,0.1888837914,-1.9236132153

H,0,4.2992306205,0.1938226266,0.1375656036

C,0,1.5247850515,1.1584376504,-2.3792400377

H,0,0.4576619703,1.9427355519,-0.69420245

C,0,2.6870840339,0.5310789557,-2.8355177085

H,0,4.5965965076,-0.2905795899,-2.2679658234

H,0,0.7506697655,1.443570644,-3.0850183415

H,0,2.8150696702,0.3199562426,-3.8921968246

TS8a

46

C,0,2.2555215758,1.3650054889,1.9729247979

C,0,1.5381719989,4.4621844027,2.7938887943

C,0,-0.7068956325,5.2215154327,3.1182868475

C,0,1.0508860291,6.1496708436,4.5546818847

C,0,-0.2025917253,6.3488394678,3.9724874132

O,0,0.3227273042,4.712201352,2.2575078956

S,0,2.6791632335,3.7148216207,1.864232057

C,0,1.7197498334,4.8332942925,4.2482500619

C,0,1.609092941,7.1442854729,5.3531857008

C,0,-0.9030679524,7.5316610955,4.1899538894

C,0,0.902932605,8.3249582354,5.5838935291

C,0,-0.351222279,8.5186601027,5.006172916

H,0,2.5919550261,6.9979493504,5.7926881828

H,0,1.336663506,9.0992934453,6.2085447676

H,0,-0.8929876233,9.4425323656,5.1805482864

H,0,-1.8716726837,7.6851750122,3.7214464897

H,0,1.2593857554,4.0430496431,4.867230519

H,0,2.7844622516,4.8433050817,4.4824052445

H,0,-1.5115897745,5.5354246871,2.4525423322

H,0,-1.0721549059,4.390569366,3.7409547416

C,0,0.7593949083,1.3700682396,2.0903957749

H,0,0.4829461762,2.0046438602,2.9438036499

H,0,0.2961785282,1.8269996055,1.2086945004

C,0,0.0937048147,-0.0093388747,2.3618097779

C,0,-1.3883356527,0.2181239901,2.707906707

H,0,-1.8927471374,0.7782105331,1.915737344

H,0,-1.9076332926,-0.7337861781,2.8448351585

H,0,-1.4559647067,0.7896213833,3.6392632897

C,0,0.7966471042,-0.7577700341,3.5045681458

H,0,1.8229464352,-1.0186502224,3.235994779

H,0,0.8168345229,-0.1195848601,4.3947423806

H,0,0.2583241807,-1.6775608891,3.7476170508

C,0,0.1408097338,-0.8504662846,1.1478427054

N,0,0.1275882205,-1.5261308194,0.2088600191

H,0,2.7905252471,1.2169527276,2.9092171151

C,0,2.965941867,0.9051626489,0.7948045254

C,0,4.3155971471,0.5171185328,0.9153305866

C,0,2.3837374724,0.8895463199,-0.4875440564

C,0,5.0449416054,0.1055706549,-0.1925683285

H,0,4.784008539,0.5414473696,1.8964062868

C,0,3.1143564997,0.4746727278,-1.5925890216

H,0,1.350862037,1.1961984297,-0.6175149864

C,0,4.4460470416,0.0786756211,-1.4530875649

H,0,6.0811493227,-0.1960637077,-0.0750572958

H,0,2.6422599449,0.4563416727,-2.5696650089

H,0,5.0120309574,-0.2466912058,-2.3199918857

TS8b

46

C,0,1.2426009287,1.3215412619,1.728260018

C,0,1.1392091011,4.2043743053,0.3814727718

C,0,3.055652962,5.1846412119,-0.6433116569

C,0,0.8750316736,5.5056215594,-1.7138148698

C,0,2.1618954335,6.0128778999,-1.5205305287

O,0,2.3643408191,4.7383510196,0.5361923286

S,0,0.3942592737,3.5295630695,1.6976655067

C,0,0.5686221928,4.2048820621,-1.0151715535

C,0,-0.0320579136,6.2057137596,-2.5043561888

C,0,2.5477007513,7.2098480394,-2.1162283748

C,0,0.3566984263,7.3984891369,-3.1149115117

C,0,1.6436501365,7.8997230187,-2.9239193669

H,0,-1.0385356544,5.8206884023,-2.6433534926

H,0,-0.3494615486,7.9420995706,-3.734502982

H,0,1.9391205266,8.8323446033,-3.3935067856

H,0,3.5466694033,7.6043348679,-1.9492893691

H,0,1.0380444343,3.3728816427,-1.5711508696

H,0,-0.5003112166,3.9956460447,-0.9664780179

H,0,3.9163045106,5.7460730072,-0.2782109712

H,0,3.4091992514,4.2907308643,-1.1778441602

C,0,0.0996032745,0.654926135,2.4397100343

H,0,-0.1293556751,1.2322370354,3.3451413924

H,0,-0.8070324492,0.6720048819,1.8250000185

C,0,0.3564319149,-0.8016976557,2.920081071

C,0,-0.8355719219,-1.2577765317,3.7791892444

H,0,-1.77416255,-1.1688304817,3.2255374142

H,0,-0.7141286486,-2.2980203655,4.0916996698

H,0,-0.8956910593,-0.6287731877,4.6726562704

C,0,1.6603502638,-0.905384474,3.7261158304

H,0,2.5316577456,-0.685763172,3.1050587264

H,0,1.628873184,-0.1900496199,4.5547071486

H,0,1.7755989927,-1.9114181733,4.137702961

C,0,0.4461593415,-1.709511846,1.7575126944

N,0,0.4931173742,-2.4476724528,0.8678173496

H,0,2.0984294039,1.5640023233,2.3541493829

C,0,1.5603765563,1.0970393722,0.3300361373

C,0,2.8175680873,1.5102125574,-0.1550532571

C,0,0.6278791417,0.5965635661,-0.5999081465

C,0,3.1354552909,1.4143413843,-1.50571917

H,0,3.5434215804,1.9136667759,0.5476644921

C,0,0.9476076095,0.5014704414,-1.9484293798

H,0,-0.3510869116,0.2697516954,-0.2647465045

C,0,2.1993032719,0.9139885523,-2.4126193496

H,0,4.1167427046,1.7256074343,-1.8529667037

H,0,0.2171571206,0.1000697586,-2.6437847283

H,0,2.4453468653,0.8351566993,-3.4666065241

TS8c

46

C,0,1.959173877,1.3869896671,1.5651301068

C,0,3.5374438102,4.0966278167,1.0097753755

C,0,5.8890157449,4.1189532033,0.6173865293

C,0,4.4795429557,5.6354597073,-0.693281269

C,0,5.7473195615,5.3967534688,-0.1581770071

O,0,4.7755465637,3.91864439,1.5052408055

S,0,2.238087527,3.7033418693,1.9584398514

C,0,3.438497899,4.5804814813,-0.4157698695

C,0,4.2449691434,6.7979956676,-1.4222526718

C,0,6.7805371787,6.3085644254,-0.3520795223

C,0,5.2828862694,7.7067073078,-1.6310021742

C,0,6.5486773261,7.4631665114,-1.0995288094

H,0,3.2553582407,6.9927925962,-1.8263915686

H,0,5.1008960854,8.610946884,-2.2031139437

H,0,7.3508734848,8.1768323741,-1.2567832819

H,0,7.7604128954,6.1215661085,0.0795576821

H,0,3.6129555245,3.7132350665,-1.078444521

H,0,2.4239133503,4.9312387406,-0.6064215841

H,0,6.7721852573,4.1164127918,1.2571172424

H,0,5.9321442289,3.2532311778,-0.0596888536

C,0,0.4923895376,1.285711905,1.8739093294

H,0,0.3082903815,1.7650127425,2.8444231648

H,0,-0.1010284439,1.8396284875,1.1382272675

C,0,-0.0766649809,-0.1561599846,1.99920053

C,0,-1.5308093443,-0.0738594636,2.4947592025

H,0,-2.1362350478,0.549298211,1.8310544926

H,0,-1.9815163921,-1.0683148475,2.5440673173

H,0,-1.5443483303,0.3664821032,3.496500943

C,0,0.7631852901,-1.0095011854,2.9620978658

H,0,1.7725215607,-1.1694506705,2.5764151994

H,0,0.8320322105,-0.4989742198,3.9284801239

H,0,0.2944427273,-1.9850003228,3.1153183957

C,0,-0.0893037128,-0.811954488,0.6750130983

N,0,-0.136913357,-1.3400706829,-0.3533200021

H,0,2.6234934734,1.0792318953,2.3694587124

C,0,2.5124864145,1.2352063211,0.2320445298

C,0,3.8997794732,1.0294514806,0.0918310536

C,0,1.7502198543,1.4051550066,-0.9405539552

C,0,4.4974461875,0.9805055944,-1.1631219575

H,0,4.5051440152,0.9117825988,0.9880142691

C,0,2.3492549307,1.3558101743,-2.1929101065

H,0,0.679408279,1.5672344107,-0.8730349772

C,0,3.7258149181,1.1492592918,-2.3143666651

H,0,5.5665680729,0.8057188027,-1.245680842

H,0,1.7389299704,1.4764556493,-3.0823801254

H,0,4.1886903882,1.1087659351,-3.2950473811

TS8d

46

C,0,1.9170959438,1.3958828589,1.5013188966

C,0,3.5092291179,4.098002337,0.9702261346

C,0,5.8665493213,4.0950114392,0.6091632264

C,0,4.4953967397,5.660374963,-0.6846541037

C,0,5.7520683223,5.3924775729,-0.1375260511

O,0,4.7373076837,3.8872239095,1.4757557617

S,0,2.1916883982,3.7095243008,1.894635716

C,0,3.4369692838,4.6131817014,-0.4458256529

C,0,4.2852899103,6.8434759129,-1.3874367206

C,0,6.7991332212,6.2957217331,-0.2937137007

C,0,5.337201312,7.7438958218,-1.5584357387

C,0,6.5920599607,7.4712841799,-1.0152437575

H,0,3.3038304486,7.0612474202,-1.7995642307

H,0,5.1745165621,8.6647137358,-2.1094553116

H,0,7.4048550124,8.178848652,-1.1426106466

H,0,7.7700686605,6.0863004425,0.1476484402

H,0,3.6108347394,3.7574695841,-1.1237112575

H,0,2.4296972295,4.9807313242,-0.6433284826

H,0,6.7397933529,4.0659089832,1.2616578669

H,0,5.9093161401,3.2447529172,-0.0874165013

C,0,0.4514729755,1.2804627104,1.8141649745

H,0,0.2460458812,1.8203595015,2.7465854046

H,0,-0.1528026975,1.7639506107,1.0397255032

C,0,-0.0531535474,-0.1827151004,2.0052630843

C,0,0.6958322154,-0.8854483546,3.1492860628

H,0,0.6630657006,-0.2895028862,4.0657154678

H,0,0.2512046745,-1.8625367209,3.3544476014

H,0,1.7404959164,-1.0371814909,2.8641556312

C,0,0.0544603866,-1.0090614281,0.7137197833

H,0,-0.4894935343,-0.5322812796,-0.1062941398

H,0,1.1041117081,-1.1052949731,0.4237954865

H,0,-0.3602139416,-2.0088463851,0.8680982668

C,0,-1.4813374653,-0.090515056,2.3745648731

N,0,-2.600171533,-0.0122704246,2.6589164131

H,0,2.5890455763,1.0880199565,2.2993094588

C,0,2.4670264195,1.2609124052,0.1640139982

C,0,3.8496196546,1.0312827161,0.0139429572

C,0,1.706339594,1.4677444177,-1.0050204805

C,0,4.4422533495,0.9905273779,-1.2442575021

H,0,4.4560948822,0.888228022,0.9055332889

C,0,2.3007409317,1.4282633922,-2.2605104564

H,0,0.6431144923,1.6727620096,-0.9288265556

C,0,3.6722510565,1.1930192811,-2.3909520169

H,0,5.5078566752,0.7979977943,-1.3322647006

H,0,1.6928162684,1.5889959668,-3.1456401991

H,0,4.1320600001,1.162670148,-3.3733270913

TS8e

C,0,1.0192395679,1.3080092496,1.4801591059

C,0,0.4933116612,4.3496960422,0.7137762099

C,0,1.9494176919,5.520337317,-0.7681593689

C,0,-0.454726866,5.9748777561,-0.9019295864

C,0,0.8354711724,6.4663365876,-1.1120860969

O,0,1.713805176,4.8691589686,0.4926968307

S,0,0.245908242,3.4576907439,2.0867072188

C,0,-0.5433595511,4.5705312939,-0.359830256

C,0,-1.5553327324,6.7805082831,-1.1804252028

C,0,1.0311948623,7.7533258554,-1.603962628

C,0,-1.3624175394,8.0659263429,-1.6874270867

C,0,-0.0731433275,8.5518358756,-1.9011531907

H,0,-2.5594561852,6.4059002451,-1.0017002645

H,0,-2.2205481786,8.6929361307,-1.9076465041

H,0,0.0724715662,9.5556167304,-2.2868302192

H,0,2.038863591,8.1331785248,-1.7511601785

H,0,-0.3417439183,3.8513305459,-1.1746854226

H,0,-1.5301251346,4.3356206616,0.0399339817

H,0,2.9073814477,6.0289829257,-0.6553525338

H,0,2.04672675,4.7352457261,-1.5324562911

C,0,0.2199357078,0.4905389013,2.4558539095

H,0,0.2840084063,0.9598154493,3.4451815482

H,0,-0.8410688431,0.4866791427,2.1856264739

C,0,0.7048812045,-0.983632271,2.6096609501

C,0,2.1673033727,-1.0430804249,3.0802345199

H,0,2.3164418807,-0.438179566,3.9790793308

H,0,2.4558791115,-2.0733592845,3.3032452445

H,0,2.8220109705,-0.6671334012,2.2892314269

C,0,0.5307652553,-1.7917092937,1.313829905

H,0,-0.5085164121,-1.7738605276,0.9744222553

H,0,1.1596816127,-1.3672034792,0.5268598477

H,0,0.8239912464,-2.8326810793,1.4742388227

C,0,-0.1425242644,-1.5987813658,3.6527245299

N,0,-0.8118013229,-2.0762105124,4.4669069204

H,0,2.0504398087,1.4997573471,1.7681055064

C,0,0.783037072,1.3080925107,0.047261763

C,0,1.7833284709,1.8101660462,-0.8094645868

C,0,-0.4498412901,0.9401900124,-0.529503728

C,0,1.5706199434,1.9220967388,-2.179917245

H,0,2.734623018,2.1165226233,-0.3800915786

C,0,-0.660501195,1.0541745429,-1.8983783503

H,0,-1.2535220262,0.5729595273,0.1010718015

C,0,0.3449870709,1.5484713067,-2.7339517487

H,0,2.363633663,2.2995692034,-2.819453666

H,0,-1.6182133146,0.762433344,-2.3185316377

H,0,0.1762645574,1.6352957032,-3.8023087312

TS8f

46

C,0,1.3171203417,1.833014307,1.8146776401

C,0,0.5788814643,4.6745090276,0.5259584932

C,0,1.800129538,5.677705156,-1.2594036174

C,0,-0.6420825232,5.878368948,-1.2651732603

C,0,0.5719576724,6.4378594991,-1.6692234533

O,0,1.7207430267,5.2531698525,0.1125751799

S,0,0.5185680966,4.0419096394,2.057313385

C,0,-0.5459844265,4.5967692543,-0.4760465033

C,0,-1.8377185828,6.5140275757,-1.5882880363

C,0,0.5973611111,7.6231494016,-2.3978559703

C,0,-1.8159771709,7.6946074721,-2.3314232128
C,0,-0.6024952392,8.2480180444,-2.7377208676
H,0,-2.7824703552,6.0889895767,-1.2607014353
H,0,-2.74834212,8.1882462704,-2.5864865491
H,0,-0.5898179602,9.1712507718,-3.3078045769
H,0,1.5471482393,8.0593754397,-2.6961152445
H,0,-0.3285376899,3.7601576563,-1.1646051177
H,0,-1.4732605441,4.3534614616,0.0434497729
H,0,2.7046354146,6.2836233244,-1.3218606156
H,0,1.9271325549,4.7768797459,-1.8775292539
C,0,0.5459596291,1.0666553514,2.860153849
H,0,-0.457923127,1.4954957327,2.9822690567
H,0,0.3994097984,0.0336640714,2.5124436055
C,0,1.2300510978,1.0027320427,4.2475454469
C,0,1.4444581517,2.3997972812,4.8522559069
H,0,0.501650776,2.9506353483,4.9105653779
H,0,1.8625251411,2.3172658873,5.8588822828
H,0,2.1390944509,2.9731750451,4.2322567496
C,0,2.5603473747,0.232079324,4.1834929246
H,0,2.4144888355,-0.7644537848,3.7579588623
H,0,3.2787747406,0.7747496336,3.5637023408
H,0,2.9870062831,0.1238562495,5.1839090741
C,0,0.3168383374,0.251242134,5.1350795621
N,0,-0.3973370501,-0.3402741065,5.8267647726
H,0,2.3504470587,2.0799399379,2.0469341529
C,0,1.0558101915,1.5945764844,0.4046903346
C,0,1.9843037227,2.031076533,-0.5602531951
C,0,-0.1497652654,1.0241295491,-0.0477915876
C,0,1.7260893995,1.8898222567,-1.9194422208
H,0,2.9131925646,2.4881540074,-0.2265633781
C,0,-0.4065026303,0.8866180672,-1.4080044378

H,0,-0.8949669364,0.6977052307,0.6715778934

C,0,0.5258983985,1.3211149956,-2.3524177667

H,0,2.4637336572,2.2192180158,-2.645917975

H,0,-1.341682747,0.4424086612,-1.7349627313

H,0,0.3231492995,1.2110566266,-3.4127666571

TS8g

46

C,0,1.813663,1.443002,1.50084

C,0,1.1225,4.39393,0.446267

C,0,0.795804,4.844198,-1.870507

C,0,-0.66749,5.962697,-0.250845

C,0,-0.081178,6.01103,-1.517575

O,0,1.661156,4.490167,-0.778357

S,0,2.062352,3.825985,1.681226

C,0,-0.336235,4.753599,0.587184

C,0,-1.491338,7.002356,0.172216

C,0,-0.31982,7.088658,-2.365566

C,0,-1.743509,8.076098,-0.682081

C,0,-1.161721,8.11959,-1.948673

H,0,-1.932154,6.971707,1.16474

H,0,-2.388527,8.885314,-0.35462

H,0,-1.353366,8.961504,-2.606122

H,0,0.151248,7.126185,-3.344426

H,0,-0.929052,3.892747,0.229758

H,0,-0.575607,4.88894,1.642582

H,0,1.461965,5.05877,-2.706839

H,0,0.197733,3.955208,-2.116599

C,0,0.630836,0.986632,2.310884

H,0,-0.308653,1.218683,1.800208

H,0,0.682162,-0.114006,2.361727

C,0,0.501002,1.480354,3.77773

C,0,1.855672,1.609721,4.487123

H,0,2.474882,2.38874,4.038591

H,0,1.707284,1.85457,5.542096

H,0,2.386287,0.653597,4.425656

C,0,-0.392734,0.486207,4.547048

H,0,-1.346235,0.339714,4.031744

H,0,0.119775,-0.478059,4.617465

H,0,-0.597616,0.849239,5.557144

C,0,-0.214006,2.775568,3.806971

N,0,-0.860692,3.733127,3.871387

H,0,2.785055,1.279076,1.964492

C,0,1.810288,1.302821,0.054424

C,0,3.037088,1.316008,-0.642831

C,0,0.627336,1.245639,-0.707811

C,0,3.080113,1.270669,-2.027243

H,0,3.96015,1.387416,-0.073617

C,0,0.673729,1.193203,-2.099736

H,0,-0.341494,1.233119,-0.218568

C,0,1.895561,1.210351,-2.768798

H,0,4.03903,1.286388,-2.536028

H,0,-0.253635,1.137489,-2.663208

H,0,1.928136,1.170995,-3.852931

TS8h

46

C,0,2.078981428,2.4901658832,2.3361774859

C,0,3.6231910778,4.8390789472,0.8291100135

C,0,5.988054537,4.7619181221,0.5332782738

C,0,4.6201579175,5.6690193606,-1.2861136494

C,0,5.8680879183,5.6662014907,-0.659187835

O,0,4.842151067,4.8764450688,1.3945790807

S,0,2.2930941977,4.7950900913,1.8127863556

C,0,3.5761567796,4.7671947075,-0.6774122025

C,0,4.4056105147,6.4825004434,-2.3952685825

C,0,6.9019600722,6.4657003968,-1.1372494995

C,0,5.4447602572,7.2738441354,-2.885784063

C,0,6.6909683353,7.2651157154,-2.2606333245

H,0,3.4305552149,6.4982036388,-2.8744747926

H,0,5.2784878033,7.9053396176,-3.7527548684

H,0,7.4937528598,7.8890827072,-2.639818925

H,0,7.8656946382,6.4683383916,-0.6347250958

H,0,3.7830644469,3.7215037603,-0.9698115921

H,0,2.567280421,5.0026907382,-1.017197886

H,0,6.8453986558,5.0102130431,1.1596599009

H,0,6.0634851595,3.7098186963,0.2211491767

C,0,0.6113705037,2.459242413,2.654836552

H,0,0.3686587459,3.3210248276,3.2887819921

H,0,0.0041629708,2.5575429357,1.7479304363

C,0,0.1292545613,1.1825631098,3.4006037212

C,0,0.3269427059,-0.0868780208,2.5573922943

H,0,1.379332714,-0.2494560159,2.3157074428

H,0,-0.048226124,-0.9619450793,3.0947483702

H,0,-0.2316664721,0.0128111508,1.6209484155

C,0,-1.3538308406,1.3458863373,3.7713532627

H,0,-1.5094738488,2.2331177031,4.3904532177

H,0,-1.9426696947,1.4510787103,2.8547586155

H,0,-1.715786266,0.4716854637,4.3185369341

C,0,0.9111476921,1.0453288313,4.6474444939

N,0,1.5246458719,0.939129617,5.6225999353

H,0,2.731220747,2.5158480019,3.2072730127

C,0,2.660104848,1.8763973536,1.156757769

C,0,4.0496854613,1.6401117993,1.1272324045

C,0,1.9249418669,1.6077800685,-0.0161825096

C,0,4.6727237024,1.1429018774,-0.0128544392

H,0,4.6347947958,1.8543376571,2.0185397963

C,0,2.5497711613,1.1115991168,-1.1540895216

H,0,0.8569869249,1.801431337,-0.0412783742

C,0,3.9277889108,0.8788428704,-1.1638461313

H,0,5.7429868112,0.9564619361,-0.0038203996

H,0,1.9610127775,0.9111489681,-2.0441616323

H,0,4.4118281715,0.4910840742,-2.0542236292

TS8i

46

C,0,2.0044463791,1.8475784097,1.7852771626

C,0,3.7413828677,4.3878209327,0.8911626836

C,0,6.0795866275,4.2974512001,0.4337130549

C,0,4.6684847098,5.6993580921,-0.9973193802

C,0,5.9453077464,5.4863635845,-0.4731943189

O,0,4.9885761604,4.2253863524,1.3683489093

S,0,2.4618518664,4.1605623461,1.920679271

C,0,3.6113289272,4.709247341,-0.5769390798

C,0,4.4395286532,6.7828632021,-1.8409367928

C,0,6.9933935337,6.3446361571,-0.7914153819

C,0,5.4917477377,7.6366073658,-2.1733430663

C,0,6.766527769,7.4182884245,-1.6524903603

H,0,3.4431834288,6.9597816073,-2.2365988755

H,0,5.3138925654,8.479415081,-2.8337101301

H,0,7.5798715784,8.0902568411,-1.9063706574

H,0,7.980661035,6.1797614904,-0.3677467053

H,0,3.7464455554,3.7692929216,-1.1423983379

H,0,2.6001384569,5.0639108705,-0.7784607938

H,0,6.9811453799,4.3407087549,1.0456588859

H,0,6.0817891502,3.3620680253,-0.1448660094

C,0,0.511436407,1.7754611286,1.9870303594

H,0,0.0273673575,2.6661122194,1.5638914462

H,0,0.1149758452,0.914965902,1.4286253618

C,0,0.0676525994,1.6231353299,3.4624126604

C,0,0.5336400389,2.8023784082,4.3317879706

H,0,0.1883747153,3.7542808503,3.9190120348

H,0,0.1440479805,2.7014845533,5.3481150175

H,0,1.6259227009,2.8243434078,4.3778425467

C,0,0.5491430469,0.2890700409,4.059127954

H,0,0.215679564,-0.5547913957,3.4491223594

H,0,1.6409311845,0.273430403,4.1097256463

H,0,0.1592105963,0.1613728265,5.0721490761

C,0,-1.410920943,1.6078869417,3.4601738853

N,0,-2.567687078,1.5923668178,3.4559229281

H,0,2.6299947287,1.5778120064,2.6329466197

C,0,2.574608397,1.5252002205,0.4875563303

C,0,3.9520939114,1.2525214274,0.3790065632

C,0,1.8138153726,1.570222398,-0.6968785857

C,0,4.5416722682,1.0191356654,-0.8587776589

H,0,4.5561348856,1.2294903372,1.2832778376

C,0,2.4067836866,1.3391619441,-1.9338089948

H,0,0.7533965386,1.7993147627,-0.6479698446

C,0,3.7732693297,1.0662338762,-2.0244168659

H,0,5.6031031391,0.7948285553,-0.9171989404

H,0,1.8012003362,1.3768394605,-2.8341589058

H,0,4.2324242627,0.8848059122,-2.9907718786

TS8j

46

C,0,2.0900079925,2.5222332205,2.3700841436
C,0,3.6117976877,4.8629147011,0.8380082463
C,0,5.978475794,4.8398634128,0.5519708023
C,0,4.5937043791,5.6499110377,-1.3001146959
C,0,5.8388181064,5.7014485087,-0.6695738887
O,0,4.8276383985,4.9530615979,1.4069073411
S,0,2.2777067824,4.8151544275,1.8180513769
C,0,3.5716588922,4.740802106,-0.6653044345
C,0,4.3622537672,6.4206743218,-2.4360678582
C,0,6.8528436499,6.5123857765,-1.1701843238
C,0,5.3818051712,7.2233733239,-2.9488188905
C,0,6.6252356393,7.2688200676,-2.3197514015
H,0,3.3893632332,6.3938897115,-2.9191170799
H,0,5.2022732074,7.8211940886,-3.8367755263
H,0,7.412640236,7.9012498855,-2.7167744148
H,0,7.8142391574,6.5569993208,-0.6650868105
H,0,3.8053924795,3.6919033295,-0.9239731473
H,0,2.5581917101,4.9394038464,-1.0148966024
H,0,6.8277268284,5.1307626351,1.1711388502
H,0,6.0814083921,3.7806799429,0.2739531112
C,0,0.6126993208,2.4802521087,2.6397122465
H,0,0.3623724967,3.2975649574,3.3288084099
H,0,0.0426707922,2.6640622692,1.7224019313
C,0,0.0826563627,1.1821920868,3.3124200588
C,0,-1.3980216012,1.3826539895,3.6789359372
H,0,-1.9858380758,1.6566474315,2.7987301471
H,0,-1.8194377543,0.4697825959,4.1073989406

H,0,-1.4795355873,2.1858436947,4.4177153768
C,0,0.8952904294,0.8281743008,4.567439331
H,0,1.9288636496,0.5795310131,4.316431253
H,0,0.8947029667,1.6847141195,5.2498173582
H,0,0.450190628,-0.0277644927,5.0812899478
C,0,0.1620786058,0.0520454481,2.3636427796
N,0,0.1869854967,-0.8446507961,1.6329170928
H,0,2.7197969761,2.5921960535,3.254045964
C,0,2.7177883135,1.8812158459,1.2294279556
C,0,4.1165162631,1.7076344099,1.2330088323
C,0,2.0139671203,1.5313654829,0.0601366042
C,0,4.7814629224,1.1942958074,0.1245152585
H,0,4.6767930081,1.9871635951,2.1226226037
C,0,2.6801942089,1.0188299197,-1.0458245977
H,0,0.9362383778,1.6511563636,0.0190794972
C,0,4.0672718794,0.8517427738,-1.025202391
H,0,5.8585656118,1.0557162261,0.1571713803
H,0,2.1144629305,0.7441782662,-1.9305522299
H,0,4.5827825438,0.448199247,-1.8906574153

Int8

46

C,0,-1.321109923,-0.4826506766,1.1213040216
C,0,0.0155957373,1.5061873196,-0.3040231567
C,0,2.3687233712,1.2845892869,-0.034707633
C,0,1.4895091299,2.1501929654,-2.1651331451
C,0,2.5563653332,2.1333154968,-1.2616024824
O,0,1.074021357,1.4681757433,0.5534712956
S,0,-1.5300019028,1.2476550717,0.4380502994
C,0,0.2795097625,1.3383407368,-1.773736307

C,0,1.5863091183,2.9033442172,-3.3320479489

C,0,3.713655729,2.8607990595,-1.5241257385

C,0,2.7512527763,3.6215708587,-3.603666258

C,0,3.8145699388,3.6003633377,-2.7025774698

H,0,0.752172459,2.9296362251,-4.0282460469

H,0,2.8251960312,4.205630927,-4.515637838

H,0,4.7160691728,4.167424415,-2.9111503164

H,0,4.5333944648,2.853316936,-0.8102231679

H,0,0.4645570468,0.2712510691,-2.0068425378

H,0,-0.6081239057,1.6335249548,-2.3381664047

H,0,3.0860390185,1.5321255685,0.7493009981

H,0,2.4747502875,0.219232304,-0.2898284511

C,0,-2.6787740658,-0.8889726512,1.6981545031

H,0,-3.0226809714,-0.073677445,2.3461341804

H,0,-3.4202403571,-0.9926696225,0.8960997934

C,0,-2.7105147261,-2.1991675687,2.5278885568

C,0,-2.6024070464,-3.4672035612,1.659884941

H,0,-1.6401153293,-3.540490693,1.1519978439

H,0,-2.7351447122,-4.3556278261,2.2832914571

H,0,-3.3934655408,-3.450567729,0.9031222413

C,0,-4.0263425078,-2.2410784231,3.3255850497

H,0,-4.110767979,-1.3806313318,3.9939726946

H,0,-4.8679082575,-2.2245894077,2.625771995

H,0,-4.0891768519,-3.1544176301,3.9223974826

C,0,-1.5837217171,-2.1924423913,3.4841184578

N,0,-0.6929928069,-2.1904121403,4.2226767539

H,0,-0.598375038,-0.3933713526,1.9377666716

C,0,-0.753001863,-1.3855080389,0.0597904103

C,0,0.5450009008,-1.8806620719,0.1992965065

C,0,-1.4750960244,-1.6974420742,-1.0988462865

C,0,1.1135381291,-2.6801227516,-0.7945948979

H,0,1.1086570596,-1.6396718174,1.0978630537

C,0,-0.9146761747,-2.499536596,-2.0871676634

H,0,-2.4744852642,-1.290593446,-1.2336456669

C,0,0.3850459566,-2.991641844,-1.9397529353

H,0,2.1234138571,-3.0592384781,-0.6705832089

H,0,-1.4857898627,-2.7348487353,-2.9800499806

H,0,0.8238281108,-3.6119191995,-2.7147697255

TS9

62

C,0,-1.0176652452,-0.7702109621,1.4335742217

C,0,-0.050938726,1.5562314384,0.1984232171

C,0,2.2511587398,0.9568880541,-0.0814306732

C,0,1.1204669686,2.2269129279,-1.8629192831

C,0,2.3250926408,1.9466212842,-1.2105377285

O,0,1.129373472,1.1950287224,0.7845598727

S,0,-1.4627552463,0.9989134816,1.1201664918

C,0,-0.1043728031,1.5464040938,-1.3112810804

C,0,1.1076407878,3.12225995,-2.9294892112

C,0,3.5075556474,2.5572653282,-1.619807692

C,0,2.294218151,3.7224422309,-3.3520557924

C,0,3.4932470538,3.4418532822,-2.6982910718

H,0,0.168501689,3.3516528098,-3.4270571963

H,0,2.2811570775,4.4174923796,-4.1857450054

H,0,4.4134201652,3.9182688773,-3.0208364714

H,0,4.4371343224,2.3452770546,-1.0976338124

H,0,-0.1509037519,0.5047636731,-1.6729491612

H,0,-1.0243422425,2.0459932068,-1.6292296264

H,0,3.131721357,1.0020780921,0.5616760047

H,0,2.1557495628,-0.0632186705,-0.4803586335

C,0,-2.1354666886,-1.3414997105,2.3166161581

H,0,-2.242112462,-0.678359154,3.1828568422

H,0,-3.0912168549,-1.3234864163,1.7774788866

C,0,-1.9328845684,-2.7889014801,2.8423403059

C,0,-2.2605726214,-3.8678295391,1.7915311265

H,0,-1.5841574033,-3.8367245019,0.9369470782

H,0,-2.1982320675,-4.8595844645,2.2477591902

H,0,-3.2832968713,-3.7138591879,1.4326416461

C,0,-2.8410046176,-2.9921516349,4.0691877674

H,0,-2.5927831321,-2.2866315328,4.8658755214

H,0,-3.8819762535,-2.8313918551,3.7711545491

H,0,-2.7444944238,-4.008494669,4.4591516636

C,0,-0.5283423367,-2.9611800124,3.2682545107

N,0,0.5756259665,-3.0933690857,3.5889217467

H,0,-0.0881779654,-0.7475769342,2.009775409

C,0,-0.7784758746,-1.5309868603,0.1534779581

C,0,0.441228345,-2.180536452,-0.0456026988

C,0,-1.7626574093,-1.6147892637,-0.8389742143

C,0,0.6765890422,-2.9078516754,-1.2144520648

H,0,1.201837077,-2.1305743553,0.7304753567

C,0,-1.5327644071,-2.3430245807,-2.0014278745

H,0,-2.7044115308,-1.0881637306,-0.7027662999

C,0,-0.309830435,-2.991635471,-2.1937334707

H,0,1.6285818914,-3.4106474522,-1.3542643185

H,0,-2.3035578955,-2.4008208789,-2.7638265413

H,0,-0.1299821934,-3.5560477832,-3.1031628719

C,0,-0.1387705195,3.7903598831,0.6438069925

C,0,-0.9761397507,4.4284883959,-0.2258293596

H,0,-0.4375921431,3.5555363549,1.6615059956

H,0,-0.5579911604,4.7836717152,-1.166891892

H,0,0.9315447783,3.8201851319,0.4634905483

C,0,-2.4145113403,4.6175848576,-0.0658184633

C,0,-3.1441527367,5.2402290829,-1.0942137831

C,0,-3.1185390093,4.2017591846,1.0797596902

C,0,-4.5163189681,5.4414069245,-0.987804603

H,0,-2.6168047492,5.5714023785,-1.9857521543

C,0,-4.489573611,4.4017827342,1.1850679933

H,0,-2.587991604,3.7159781135,1.8930368099

C,0,-5.1983329813,5.0219081362,0.1538888558

H,0,-5.0545337939,5.9268890045,-1.7963166387

H,0,-5.0111331565,4.0724272636,2.0787973516

H,0,-6.268963234,5.1769860162,0.2412854865

TS9a

62

C,0,-1.4943910158,-0.5716334678,1.009457236

C,0,-0.2260292081,1.6349831843,-0.1673030064

C,0,2.0994088963,1.2528763111,0.3867308012

C,0,1.4964940985,2.0559187401,-1.8964984876

C,0,2.4581807023,1.9637425439,-0.889975597

O,0,0.721835233,1.3665935488,0.7690797799

S,0,-1.8394874487,1.1352139048,0.3809345867

C,0,0.1506521783,1.4422286102,-1.6165135048

C,0,1.806428952,2.7119461649,-3.0889247891

C,0,3.732215945,2.4961321645,-1.089085357

C,0,3.0780991744,3.2443093194,-3.2877364667

C,0,4.0461911983,3.1291531588,-2.2883620786

H,0,1.0478012771,2.8032627767,-3.8622240233

H,0,3.3137222967,3.7520421733,-4.2177274491

H,0,5.0371671339,3.5455882298,-2.439216838

H,0,4.4700657736,2.4330275653,-0.2929995808

H,0,0.184183581,0.362908139,-1.8445901372

H,0,-0.6293986024,1.8772925765,-2.2487116755

H,0,2.6696633305,1.6593812114,1.2277919941

H,0,2.3213193105,0.1805148921,0.2914482394

C,0,-2.8174110204,-1.1032237459,1.5741861653

H,0,-3.2036482005,-0.3521096434,2.273027854

H,0,-3.5598510122,-1.2086823261,0.7729404673

C,0,-2.7520984159,-2.46293369,2.3213390228

C,0,-2.6763540377,-3.6753707107,1.3728229272

H,0,-1.7527937358,-3.6938214274,0.7935540018

H,0,-2.7422719805,-4.6012945479,1.9507197876

H,0,-3.5222510675,-3.6374471286,0.6788170326

C,0,-4.0067986204,-2.5936176082,3.2041567993

H,0,-4.0612713603,-1.78396118,3.9360055687

H,0,-4.8959679978,-2.5498989603,2.567125827

H,0,-4.0083134245,-3.5476226115,3.7372501638

C,0,-1.5613768155,-2.4808939535,3.1964546625

N,0,-0.6212043628,-2.495883355,3.870860116

H,0,-0.7853107964,-0.4427532094,1.832103624

C,0,-0.8586593117,-1.4402355516,-0.0456977159

C,0,0.4129205701,-1.9721031097,0.17523486

C,0,-1.5138796145,-1.7244177423,-1.2497728077

C,0,1.0230005638,-2.7791241835,-0.7874252623

H,0,0.9178458742,-1.7623713046,1.1154973349

C,0,-0.9114336756,-2.5330146348,-2.2077662904

H,0,-2.4932393858,-1.2914973144,-1.440527176

C,0,0.3623056995,-3.0616265654,-1.9801245237

H,0,2.0116755387,-3.1872893051,-0.6014984937

H,0,-1.4293867022,-2.747007601,-3.1376641474

H,0,0.8340255303,-3.6876611675,-2.7307793285

C,0,-0.5206941883,3.9027781223,-0.0237098743

C,0,-0.1869747145,4.1438109231,1.2771418064

H,0,0.1947549379,4.0619851115,-0.8267477101

H,0,-0.9617963413,4.0515552186,2.0356231518

H,0,-1.5663181476,3.868885729,-0.3173348906

C,0,1.1734091119,4.3189681274,1.7723271032

C,0,1.4498334756,4.0817468246,3.1319057257

C,0,2.2423296643,4.7009410276,0.9415383023

C,0,2.7403326357,4.195311098,3.6361778479

H,0,0.6358465365,3.7848908428,3.7881210096

C,0,3.532405217,4.8190627788,1.4476063433

H,0,2.062528713,4.9090895363,-0.1097488303

C,0,3.7925077561,4.5628234511,2.7948680624

H,0,2.9279916333,3.9960737101,4.6869222258

H,0,4.3399386199,5.1170425042,0.7844604354

H,0,4.8003186258,4.6579996254,3.1865964663

TS9b

62

C,0,-0.9607488833,-0.7296968535,1.2753805097

C,0,0.196485285,1.5363578059,0.1167908351

C,0,2.4833583571,0.8327521203,-0.0575622284

C,0,1.4797504621,2.1043029283,-1.9090227258

C,0,2.6443874091,1.8005849986,-1.1966889828

O,0,1.3364014749,1.1287816941,0.7549011307

S,0,-1.2688567725,1.0733812282,1.0044392521

C,0,0.2181927502,1.4596181098,-1.396849722

C,0,1.5376287432,2.9906352646,-2.9806142976

C,0,3.8598008342,2.3759472309,-1.5557834631

C,0,2.7581969208,3.5562920101,-3.3518815268

C,0,3.9178990769,3.2500238258,-2.6418486475

H,0,0.6296569491,3.2423535267,-3.5228315871

H,0,2.8014256582,4.2454789395,-4.1893173401

H,0,4.863984983,3.6995785451,-2.9256292024

H,0,4.7582358871,2.146337481,-0.9885647408

H,0,0.1891529955,0.4014215796,-1.7102094484

H,0,-0.6814016518,1.9344272892,-1.7973194934

H,0,3.3369439754,0.853350792,0.622091045

H,0,2.3666373541,-0.1894013231,-0.4462993559

C,0,-2.1181284402,-1.2320651089,2.1498839692

H,0,-2.1731790905,-0.5789266653,3.0282255193

H,0,-3.0705339528,-1.1303525646,1.6139856175

C,0,-2.0262383256,-2.700719164,2.6466373941

C,0,-2.4392150591,-3.7305321233,1.576820993

H,0,-1.7663568658,-3.7330177237,0.7188305315

H,0,-2.4498812055,-4.7333401248,2.0126673866

H,0,-3.4490924808,-3.4925215394,1.2275108861

C,0,-2.943546567,-2.8574234392,3.8734771602

H,0,-2.6393093747,-2.1885041807,4.682173437

H,0,-3.9697812488,-2.610554566,3.5833576675

H,0,-2.9247446419,-3.8856040665,4.243508517

C,0,-0.6379131906,-2.9896456153,3.0625792091

N,0,0.4535011509,-3.2139558145,3.3750027305

H,0,-0.0329149299,-0.7888424461,1.8523233517

C,0,-0.7773401795,-1.4850003564,-0.0170695601

C,0,0.3925163604,-2.2168052589,-0.2300997972

C,0,-1.7619134515,-1.4742523702,-1.0124765923

C,0,0.5796131753,-2.9285478383,-1.4172649283

H,0,1.1512249337,-2.242858112,0.5489993874

C,0,-1.5809462448,-2.1872233765,-2.1928563925

H,0,-2.663991483,-0.8853495589,-0.8634641784

C,0,-0.4062129123,-2.9154900343,-2.4006097522

H,0,1.4935422799,-3.4947379326,-1.5682254126

H,0,-2.351645501,-2.1712227046,-2.9574376487

H,0,-0.263604255,-3.4670290918,-3.3244348508

C,0,0.1691361578,3.7948162668,0.3968830604

C,0,-0.4720593546,4.1413191084,1.5528127141

H,0,1.2530874773,3.7461589658,0.3831099192

H,0,0.1015832784,4.1517945863,2.4772220591

H,0,-0.307205213,3.9455610121,-0.5692427592

C,0,-1.8957391706,4.4261548413,1.6897998969

C,0,-2.3987364492,4.8441234776,2.9343350346

C,0,-2.8066351176,4.2956183461,0.6247577331

C,0,-3.7478171369,5.1343827822,3.1076918172

H,0,-1.7120007665,4.9425466322,3.7712234058

C,0,-4.1544252017,4.5850035212,0.7976469219

H,0,-2.45796529,3.9491588624,-0.3440159135

C,0,-4.6347129,5.0083396254,2.0388154215

H,0,-4.1086657792,5.4588073458,4.0790870467

H,0,-4.8382734571,4.4743402977,-0.0386703531

H,0,-5.6883771854,5.2328694523,2.1705023102

TS9c

62

C,0,-1.3681266343,-0.625600866,1.1799238266

C,0,-0.4404188098,1.5742316533,-0.2971571262

C,0,1.9245900961,1.2767277486,-0.0451845474

C,0,1.0389415878,1.9688890632,-2.239773894

C,0,2.1161449205,2.0008668457,-1.3483671862

O,0,0.6362499535,1.5211814326,0.5415280709

S,0,-1.9321417167,0.9853190189,0.4726253522

C,0,-0.2065196061,1.2737566521,-1.7580414526

C,0,1.15497989,2.5794396056,-3.4853134385

C,0,3.2997548091,2.6462529144,-1.6963108436

C,0,2.347339443,3.209008296,-3.843296964

C,0,3.4176930121,3.2456489608,-2.951050016

H,0,0.3066695578,2.5831228664,-4.1661512846

H,0,2.4319270766,3.6868969678,-4.8145774996

H,0,4.3399451469,3.7471278758,-3.2269887678

H,0,4.1276366514,2.6799380776,-0.9925251522

H,0,-0.1035262527,0.1839961989,-1.899163822

H,0,-1.0873285444,1.5924814698,-2.3245891727

H,0,2.651622741,1.5876221727,0.7070943563

H,0,2.0202983044,0.1926739172,-0.2023489136

C,0,-2.5524420216,-1.1795367057,1.984575764

H,0,-2.871642492,-0.396185591,2.6815506045

H,0,-3.4006542928,-1.3837006001,1.3186169676

C,0,-2.290903314,-2.4733787311,2.8031614969

C,0,-2.3257945948,-3.7528577924,1.9445004732

H,0,-1.5249675862,-3.7807386425,1.205089818

H,0,-2.2355837546,-4.6326354682,2.5874990796

H,0,-3.2860018337,-3.80193581,1.420955848

C,0,-3.3641928618,-2.5781843795,3.9023957065

H,0,-3.3256853351,-1.7184556532,4.5757995904

H,0,-4.3522464687,-2.6101698364,3.4322306519

H,0,-3.2298127962,-3.4895557843,4.4903472251

C,0,-0.9666646021,-2.3806335878,3.4524278439

N,0,0.0759909211,-2.3068241189,3.9488740419

H,0,-0.5572200119,-0.3795296541,1.8720576346

C,0,-0.836779837,-1.561400807,0.1226397928

C,0,0.4589548427,-2.0682491115,0.2375088455

C,0,-1.6226705161,-1.9475692527,-0.9697160972

C,0,0.9646412865,-2.9497652397,-0.7205396584

H,0,1.0659028911,-1.7848376466,1.0945667957
C,0,-1.1236363126,-2.8298565215,-1.9219812331
H,0,-2.6231352662,-1.5356091572,-1.0795588131
C,0,0.1746453515,-3.3329048499,-1.8011656218
H,0,1.9733907013,-3.3374601401,-0.6172651097
H,0,-1.7422789268,-3.1213191214,-2.7652001465
H,0,0.5652094876,-4.0168522525,-2.5478890373
C,0,-0.944812669,3.7794817828,-0.291980318
C,0,-1.946124267,4.0257462631,-1.1879559499
H,0,-1.1674164871,3.6574010158,0.7629896677
H,0,-2.9741211902,3.8236008209,-0.8899619257
H,0,0.0884528507,4.018506602,-0.5362571559
C,0,-1.7461991248,4.4355445938,-2.578132346
C,0,-2.7009862881,4.098029936,-3.55466347
C,0,-0.6252235737,5.1806063437,-2.9841389751
C,0,-2.5276728962,4.460340545,-4.8866853526
H,0,-3.5806739878,3.5324203329,-3.2567571028
C,0,-0.4568871996,5.5516117769,-4.3134923767
H,0,0.115442177,5.4761189703,-2.2464338224
C,0,-1.4016298939,5.1885095668,-5.2745848446
H,0,-3.2738550519,4.1787663306,-5.6236049639
H,0,0.4165405077,6.1297427545,-4.6010747899
H,0,-1.2687971902,5.4802179486,-6.3115982622

TS9d
62

C,0,-1.2842124148,-0.4704900921,0.9582963408
C,0,0.4875712853,1.5748516476,0.1833500154
C,0,2.567333989,0.5676205514,0.8418050477
C,0,2.4652292454,1.7881291708,-1.2963640027

C,0,3.2520386179,1.389740301,-0.2126701658
O,0,1.2673360212,1.0725935246,1.1865480633
S,0,-1.2443229635,1.3210174586,0.5017474768
C,0,1.0056107118,1.4267746495,-1.2301539738
C,0,3.0421924775,2.5034553867,-2.3431109809
C,0,4.6024485342,1.7265316112,-0.1606580366
C,0,4.3979413341,2.8259051343,-2.3013841231
C,0,5.1776641068,2.4443028364,-1.2093119529
H,0,2.4247479632,2.8346348346,-3.1746601929
H,0,4.8418818921,3.390602315,-3.1156313993
H,0,6.2297923054,2.7083803489,-1.172246097
H,0,5.2039102436,1.4291715082,0.6947488804
H,0,0.8674551176,0.3810694016,-1.555351327
H,0,0.409444019,2.0539979156,-1.8990546609
H,0,3.1302184051,0.5495477744,1.7768062594
H,0,2.4409552553,-0.4652728024,0.486872226
C,0,-2.7282558215,-0.7723267913,1.3827857247
H,0,-3.0063306012,-0.0389654449,2.1483738224
H,0,-3.4107298331,-0.6285375457,0.5353249957
C,0,-3.0009374176,-2.1905300438,1.9545513947
C,0,-3.1349009271,-3.2701490422,0.8627894935
H,0,-2.2084354624,-3.4187637877,0.3075684452
H,0,-3.4240026088,-4.221803437,1.3170591915
H,0,-3.9182108018,-2.968229228,0.1600898029
C,0,-4.3038905473,-2.1419435886,2.7737807611
H,0,-4.2238350602,-1.4337338156,3.6020814615
H,0,-5.1228794089,-1.8248785091,2.120307029
H,0,-4.5445495074,-3.1281510656,3.1785051361
C,0,-1.8959108714,-2.5724288613,2.8583037361
N,0,-1.0214894951,-2.870024697,3.5553338801
H,0,-0.6321169205,-0.5663730205,1.8315097048

C,0,-0.7561355565,-1.3541282259,-0.1439848213

C,0,0.3071337708,-2.2209260296,0.1155903804

C,0,-1.3210765198,-1.3366538003,-1.4248750717

C,0,0.7992113147,-3.061429462,-0.8854077283

H,0,0.7366621128,-2.2499049638,1.1145389365

C,0,-0.8366324711,-2.1766471725,-2.4218891786

H,0,-2.1321303201,-0.6451598885,-1.6411515538

C,0,0.2281535345,-3.0417173738,-2.1551783719

H,0,1.6251255428,-3.7318640064,-0.6688087412

H,0,-1.2823287728,-2.1536582455,-3.4115949325

H,0,0.6091537414,-3.692791118,-2.9354750988

C,0,0.4998439184,3.8204819676,0.5707688502

C,0,1.3628247034,4.4639784582,-0.269881204

H,0,-0.573427983,3.8950939735,0.4155802177

H,0,2.4119768424,4.5375827112,0.0128061054

H,0,0.8133811145,3.5615951897,1.5765321549

C,0,1.0255709753,4.9968178485,-1.5856486687

C,0,1.9927085826,5.722274435,-2.3046067162

C,0,-0.2261133228,4.7895277858,-2.1955290178

C,0,1.7227639992,6.2264351049,-3.5720563254

H,0,2.9697705768,5.8795027687,-1.854157292

C,0,-0.4950896,5.2916324544,-3.464292958

H,0,-0.9919462595,4.2183563723,-1.6771211982

C,0,0.4760154525,6.0128840241,-4.1615213051

H,0,2.4870180658,6.7853000942,-4.1039476378

H,0,-1.4672372241,5.1155509357,-3.9150911063

H,0,0.26353603,6.4016679849,-5.1522282835

Int9

62

C,0,-1.6628210214,-1.4458253326,1.1623073257
C,0,-0.4168598954,1.0400937975,0.3713559736
C,0,1.5786780134,0.0028419949,1.2919779389
C,0,1.7053242566,0.8785049953,-0.9902966189
C,0,2.4112119654,0.5662195031,0.1756089499
O,0,0.3939603835,0.7774852505,1.4939226859
S,0,-2.0883559881,0.2483390144,0.6019520198
C,0,0.2283935273,0.585066905,-0.9573010019
C,0,2.3798994682,1.4165976392,-2.0836381091
C,0,3.7810556841,0.7988422708,0.2548973388
C,0,3.7553977588,1.6348278552,-2.0118165552
C,0,4.4564867255,1.3282042006,-0.8458821389
H,0,1.8282491764,1.6908043984,-2.9799701433
H,0,4.2767058487,2.0624747315,-2.8626597658
H,0,5.5252845774,1.5094499463,-0.7902296823
H,0,4.3192122551,0.5684195767,1.1710160009
H,0,0.0795671021,-0.495587804,-1.0708792959
H,0,-0.2993933399,1.0668298828,-1.7862387126
H,0,2.1039660066,0.0224995842,2.2488883456
H,0,1.3072610768,-1.039061643,1.069158092
C,0,-2.89274829,-1.934229809,1.9540154406
H,0,-3.0926306171,-1.1872588474,2.728976405
H,0,-3.7716918565,-1.9606466116,1.2964248793
C,0,-2.7958505809,-3.32515134,2.6386810047
C,0,-3.0530019219,-4.5018890916,1.6771179348
H,0,-2.3056275193,-4.5707189483,0.8866225057
H,0,-3.0568040474,-5.4424155853,2.2349333624
H,0,-4.0368820235,-4.3685851054,1.2160752622
C,0,-3.8382252423,-3.3753126936,3.772345466
H,0,-3.6485269612,-2.5999632606,4.5185280163
H,0,-4.8336678892,-3.2146639175,3.3463185849

H,0,-3.8253523148,-4.3493675542,4.2678054444

C,0,-1.4558966282,-3.4783399781,3.2420456531

N,0,-0.4031296367,-3.5857793667,3.7104986521

H,0,-0.831154761,-1.3310841902,1.8665473987

C,0,-1.2614362079,-2.3884061103,0.0468100755

C,0,-0.1293607788,-3.1964866929,0.1843840779

C,0,-2.0447277996,-2.5156665222,-1.1060714979

C,0,0.2131306434,-4.1169794941,-0.8075037366

H,0,0.4719515773,-3.1299473598,1.0874443847

C,0,-1.7094264628,-3.4378573724,-2.0926545044

H,0,-2.9137143242,-1.8748110611,-1.2321697843

C,0,-0.5773121685,-4.2425727482,-1.9468489049

H,0,1.095523628,-4.7367776117,-0.6833173721

H,0,-2.3280948862,-3.5263184514,-2.9804602168

H,0,-0.3135385948,-4.9580799927,-2.7191577113

C,0,-0.7333468969,2.5562845027,0.3866070381

C,0,0.4616992236,3.4013061658,0.1055098597

H,0,-1.5445719828,2.749813518,-0.3227088605

H,0,1.2124436049,3.4589846134,0.888865544

H,0,-1.1162278832,2.7735515444,1.3900269343

C,0,0.7499449406,4.0566097973,-1.1218149447

C,0,1.9869449245,4.7371320073,-1.2690154126

C,0,-0.113066417,4.028295142,-2.2473026244

C,0,2.3425615473,5.3371573164,-2.4648277876

H,0,2.6709960873,4.7583470449,-0.4245725313

C,0,0.2508812923,4.6331244735,-3.442437497

H,0,-1.0726750942,3.5249569518,-2.1830784592

C,0,1.4790875161,5.2886206337,-3.5652946656

H,0,3.3000030505,5.8425131522,-2.5489099824

H,0,-0.4283237886,4.5948157651,-4.2889353959

H,0,1.7583248324,5.7576293119,-4.5030285027

TS10

46

C,0,3.3370669593,1.3689464192,1.2934631262
C,0,3.5157722786,3.9712636709,0.3962122153
C,0,5.7021916805,3.8202011957,-0.8976290668
C,0,4.3438752488,5.9040299601,-0.9855197414
C,0,5.5801210669,5.2495353143,-1.1817728762
O,0,4.7232375413,3.7661144281,0.6929077257
S,0,2.3064642472,2.664362169,0.4958033296
C,0,3.1375832107,5.1411745737,-0.4921485995
C,0,4.2576010621,7.2786796596,-1.2076146701
C,0,6.6988209818,6.0082700512,-1.5594447152
C,0,5.3632998649,8.0120785866,-1.6299349835
C,0,6.5924527698,7.3728408435,-1.7976075795
H,0,3.3088322476,7.7828095333,-1.0394248896
H,0,5.2708020675,9.0783675871,-1.8093191946
H,0,7.465859094,7.9389840487,-2.1053152933
H,0,7.6560578195,5.507857436,-1.6789771822
H,0,2.5749713392,4.7404836261,-1.3467273401
H,0,2.453656871,5.8169701975,0.0354290188
H,0,6.6913312845,3.4397016314,-0.6582987973
H,0,5.0716385301,3.1065927224,-1.4246090773
C,0,2.3628721062,0.3273546306,1.8653809327
H,0,1.6600693178,0.8443243902,2.529747223
H,0,1.7718309318,-0.1133633941,1.0531588014
C,0,2.9918486064,-0.8177513406,2.6944868597
C,0,1.8504114789,-1.6104599333,3.3604644138
H,0,1.1388803174,-1.9731593973,2.6138122137
H,0,2.2458109083,-2.469673375,3.9076842266

H,0,1.3210809009,-0.9602894625,4.0636756525

C,0,3.9496832169,-0.2843685173,3.7716607639

H,0,4.8392752517,0.1702045143,3.3308132785

H,0,3.4313065933,0.4666953697,4.3770420467

H,0,4.2732619937,-1.0977372104,4.4261046646

C,0,3.7277462963,-1.7680550872,1.8309663247

N,0,4.2798316552,-2.568222981,1.2037358272

H,0,3.8638185438,1.8747323198,2.1081434359

C,0,4.3536240489,0.7852731903,0.3370583763

C,0,5.7111772765,0.8129730624,0.6599977713

C,0,3.9538874428,0.1787413114,-0.8574962847

C,0,6.6526305685,0.2179615992,-0.1779981129

H,0,6.0331544184,1.3229363585,1.5647298511

C,0,4.8910503189,-0.4126873417,-1.6979867066

H,0,2.9014844789,0.1708146993,-1.1314224604

C,0,6.2437238561,-0.4008332499,-1.356726092

H,0,7.7044500864,0.2404104678,0.0901789052

H,0,4.5660936344,-0.8906122881,-2.6166301535

H,0,6.9736703664,-0.8699236795,-2.0086278377

TS10a

46

C,0,3.3488825213,1.3995237256,1.3453655876

C,0,3.5574856827,3.9910440755,0.427434527

C,0,5.6825076842,3.7834877545,-0.9589304434

C,0,4.3738237965,5.9011078694,-0.9921190665

C,0,5.5834277798,5.2152327288,-1.2407814595

O,0,4.7697164648,3.7526290699,0.6699656535

S,0,2.3187318717,2.7161992971,0.5846178922

C,0,3.1708601107,5.1713598845,-0.4428493361

C,0,4.3128528971,7.2772265904,-1.2137699475

C,0,6.7033174543,5.9450689858,-1.6685236992

C,0,5.4171234104,7.9818774865,-1.6857009912

C,0,6.6212588361,7.311525353,-1.9051315185

H,0,3.3857269908,7.8056402336,-1.004477188

H,0,5.3439772948,9.050057256,-1.8627185122

H,0,7.4947298881,7.8551080994,-2.250964144

H,0,7.6418329082,5.420680003,-1.8272045442

H,0,2.5573681447,4.7877072545,-1.2698440528

H,0,2.5321059713,5.8654576809,0.1165994701

H,0,6.6708720268,3.3796856656,-0.7575952999

H,0,5.0137458058,3.086329638,-1.460053375

C,0,2.3729086474,0.3769042837,1.9504796444

H,0,1.7051992434,0.920066011,2.6282165594

H,0,1.7464572082,-0.0597226086,1.1619134549

C,0,2.9986990059,-0.8048726319,2.7396882965

C,0,3.5516903263,-1.9237531219,1.835157122

H,0,4.395974685,-1.5944346735,1.229365705

H,0,3.8741753451,-2.7684218202,2.4500843561

H,0,2.7545683678,-2.2651685919,1.1668953052

C,0,1.9122960554,-1.3976302224,3.6569671973

H,0,1.5391271701,-0.6510279557,4.362246532

H,0,1.0772689955,-1.7456181308,3.0405172243

H,0,2.30418018,-2.2469901561,4.2218857115

C,0,4.0945599328,-0.2964715335,3.5904537941

N,0,4.9537337835,0.1072638493,4.2520289971

H,0,3.9112478621,1.8825017379,2.1507033278

C,0,4.3279012318,0.8087703801,0.3553397079

C,0,5.6857303613,0.7535547458,0.677139421

C,0,3.8943356988,0.2708507152,-0.8603868766

C,0,6.5939564871,0.1503101449,-0.1924191317

H,0,6.0277294024,1.1839518206,1.6145330369

C,0,4.7999261916,-0.3299205099,-1.7312984375

H,0,2.8423398757,0.3323557817,-1.1297584826

C,0,6.1535835946,-0.3953372028,-1.397230493

H,0,7.6460778831,0.109918149,0.0723687563

H,0,4.4507985465,-0.7447237792,-2.671879679

H,0,6.8600253784,-0.8632213328,-2.0756636015

Int10

46

C,0,-1.0897216389,-1.004632877,0.9739075654

C,0,-0.9080833123,1.6211859097,0.2055620416

C,0,0.7008308069,1.2522926418,-2.4076513957

C,0,0.0794326158,3.3853753872,-1.2783407906

C,0,0.9663861389,2.6001934915,-2.0771469458

O,0,0.0231818709,1.5977218836,0.966863607

S,0,-2.087242286,0.2672811379,0.0913990206

C,0,-1.1941756201,2.7780132996,-0.7460602866

C,0,0.4014914285,4.702271337,-0.9833057631

C,0,2.1581087054,3.2178959394,-2.5403068574

C,0,1.5780848855,5.2894540336,-1.4573515067

C,0,2.4572572895,4.5353523657,-2.2391495875

H,0,-0.2765468985,5.2861568348,-0.3662750707

H,0,1.8060626946,6.3215856101,-1.2131425305

H,0,3.3758580542,4.9798638931,-2.6089584408

H,0,2.8416625378,2.6287564268,-3.1454871856

H,0,-1.8425352566,2.4250461086,-1.5558747835

H,0,-1.756979735,3.5268030134,-0.1771209625

H,0,1.416049102,0.6841941242,-2.990459088

H,0,-0.2049426752,0.7378152649,-2.1104314318

C,0,-2.0431902073,-2.1217103944,1.4132616159
H,0,-2.8410023594,-1.6703259436,2.0154251998
H,0,-2.5228714291,-2.5817226959,0.5410413071
C,0,-1.4126296182,-3.2395040229,2.2794301686
C,0,-2.5510934083,-4.1035648733,2.854774871
H,0,-3.1880713714,-4.4931841793,2.0560470943
H,0,-2.1473944078,-4.9482067374,3.4183020012
H,0,-3.1631516734,-3.4942552231,3.5267663321
C,0,-0.562249065,-2.6662342635,3.4243682709
H,0,0.3304285392,-2.1608969098,3.0485658342
H,0,-1.1604317448,-1.9504810637,3.9981821905
H,0,-0.2416977532,-3.4684425666,4.0938262785
C,0,-0.5635610547,-4.1343404339,1.4624063668
N,0,0.0771814226,-4.8911813246,0.8666533173
H,0,-0.69124108,-0.4905375033,1.8524993968
C,0,0.0586558945,-1.449188863,0.0966244308
C,0,1.3716309717,-1.1534740872,0.4655456658
C,0,-0.1735070353,-2.1347026182,-1.1009924029
C,0,2.4395484551,-1.5566130416,-0.3364963278
H,0,1.5548941658,-0.5840687157,1.3727548432
C,0,0.888599819,-2.5392338954,-1.9001612511
H,0,-1.1927026091,-2.3546433265,-1.4105407512
C,0,2.2005218879,-2.2536781618,-1.5169297868
H,0,3.4558048979,-1.3197792893,-0.0379019104
H,0,0.6956566871,-3.0842599512,-2.8186883808
H,0,3.030380229,-2.5742037607,-2.1389546018

TS10b
46

C,0,-0.985937884,-1.0223637504,0.6469502054

C,0,-0.9051569777,1.6378918944,-0.0332245558

C,0,1.1774593179,1.4917843011,-2.305396076

C,0,0.1263013978,3.543531123,-1.3342703651

C,0,1.2186714658,2.8845319115,-1.9623141769

O,0,-0.1054425786,1.6700571264,0.864700541

S,0,-1.9368245596,0.1976379311,-0.3533438557

C,0,-1.1374396709,2.7843611611,-1.0097004656

C,0,0.2153555006,4.9003276109,-1.0440611876

C,0,2.3512775708,3.6569850365,-2.3011014466

C,0,1.350712503,5.6426722336,-1.3745557776

C,0,2.4201323504,5.0120875226,-2.0115277368

H,0,-0.6202131858,5.3906000925,-0.5510014156

H,0,1.3965447893,6.7003730733,-1.1375192458

H,0,3.3083007927,5.5773993887,-2.2760738852

H,0,3.1885308465,3.162556106,-2.7873273512

H,0,-1.5997696565,2.3779641922,-1.9173614058

H,0,-1.8679803042,3.4559491667,-0.5439362289

H,0,2.0883723941,1.0124920973,-2.6523370427

H,0,0.464998946,0.8161043506,-1.8502703134

C,0,-1.900329366,-2.2257343711,0.9022918847

H,0,-2.8184977239,-1.8614461205,1.3789863361

H,0,-2.1943449796,-2.6901461981,-0.0465797097

C,0,-1.3224224449,-3.3205486802,1.831982312

C,0,-2.4611967508,-4.2910009347,2.199874455

H,0,-2.9311986996,-4.7008522244,1.3017360689

H,0,-2.0816588859,-5.1209322781,2.8008528797

H,0,-3.219026319,-3.7557480322,2.7801486546

C,0,-0.712589288,-2.7234046794,3.1103877144

H,0,0.1839485601,-2.1383268028,2.8930543402

H,0,-1.4499639396,-2.0761153256,3.5969648743

H,0,-0.4370847724,-3.5213134071,3.8046002331

C,0,-0.2846375201,-4.1170671793,1.1408158077

N,0,0.5012427208,-4.8022055046,0.6396105643

H,0,-0.7737907913,-0.5102878616,1.5893349398

C,0,0.3172554798,-1.3448082402,-0.0481231812

C,0,1.527759586,-0.9693953054,0.5367241085

C,0,0.3326289912,-1.988486098,-1.2910152603

C,0,2.7376572476,-1.2540436778,-0.0974742076

H,0,1.519543881,-0.4291025892,1.4796513468

C,0,1.5361907898,-2.2781226139,-1.9223264812

H,0,-0.602453131,-2.2616823531,-1.776395171

C,0,2.7432953048,-1.9130791831,-1.3234440262

H,0,3.6716343117,-0.9545332779,0.3675970391

H,0,1.5333461806,-2.7859026249,-2.8820442946

H,0,3.6826944851,-2.1395855152,-1.8186256257

C,0,-0.3970602983,0.2185506855,-4.4389210958

C,0,0.1353051547,1.4701356713,-4.321889706

H,0,-0.5065602048,2.3079793309,-4.0695521194

H,0,1.0788670475,1.7360418769,-4.7889460024

H,0,-1.4190129816,0.0584233785,-4.0983324064

C,0,0.3181483037,-0.9755530829,-4.8712728542

C,0,-0.3687635874,-2.2001905515,-4.9460598219

C,0,1.6878966292,-0.9679710111,-5.1924322679

C,0,0.2806156427,-3.3695140287,-5.3280004648

H,0,-1.4267297553,-2.2253175132,-4.6958886683

C,0,2.3372619264,-2.1361471337,-5.5745180343

H,0,2.2528086767,-0.0426085779,-5.13088168

C,0,1.6396077577,-3.3441564506,-5.6439687988

H,0,-0.2712595932,-4.3032180318,-5.3744588567

H,0,3.3960293336,-2.1077811156,-5.8137668582

H,0,2.1507819645,-4.2554039367,-5.9369811807

TS10b1

46

C,0,-1.0737736601,-0.9189957778,0.8976369266
C,0,-0.7466048342,1.7017374601,0.1470371701
C,0,1.007179171,1.2989628034,-2.3775799127
C,0,0.3366176181,3.4570388804,-1.2986158557
C,0,1.2716867563,2.663134499,-2.0166824244
O,0,0.1658557706,1.6280905587,0.9273352328
S,0,-1.9913569729,0.4044642177,0.0059476796
C,0,-0.962230814,2.8588363336,-0.8179966876
C,0,0.6172111943,4.7957531897,-1.0491012677
C,0,2.4704994036,3.2760582664,-2.4436829511
C,0,1.8002169289,5.3858423282,-1.4950080621
C,0,2.7327449811,4.6145554477,-2.1904973943
H,0,-0.1088340384,5.3944544869,-0.5051638425
H,0,1.9927550816,6.4349003386,-1.2950669935
H,0,3.6630973164,5.0581974071,-2.5319214876
H,0,3.1961533494,2.6735030866,-2.9852807762
H,0,-1.5699448153,2.5067871316,-1.6586552779
H,0,-1.5508353246,3.6175935505,-0.2887658294
H,0,1.8292237002,0.6975697181,-2.7553510604
H,0,0.206433643,0.734654925,-1.9139397847
C,0,-2.0874179916,-1.9892722421,1.3179655578
H,0,-2.869948527,-1.5013347764,1.9115467353
H,0,-2.5771920844,-2.4203598017,0.4365690997
C,0,-1.5251971261,-3.1412741078,2.1861797215
C,0,-2.7125609156,-3.9528620095,2.7386451519
H,0,-3.3549756011,-4.3073176731,1.9279913191
H,0,-2.3585982389,-4.8188004055,3.3032816154
H,0,-3.3051553895,-3.3184140871,3.4047861282

C,0,-0.6662864221,-2.6163801365,3.3478644227

H,0,0.2563046497,-2.1536539021,2.9899050026

H,0,-1.2377866463,-1.8747496225,3.9159732925

H,0,-0.3966279482,-3.4366867671,4.0178315574

C,0,-0.7075375021,-4.0707066262,1.375753166

N,0,-0.0944562234,-4.8525076481,0.7831037332

H,0,-0.6615047436,-0.4297481894,1.7840529938

C,0,0.0627195672,-1.4176149568,0.0336397491

C,0,1.3840359388,-1.1968000932,0.4242206765

C,0,-0.1878553947,-2.075373055,-1.1761485497

C,0,2.4409099256,-1.6477121826,-0.367432824

H,0,1.5842241826,-0.6474077796,1.3401804434

C,0,0.8629413211,-2.5257761622,-1.9659328409

H,0,-1.2128122854,-2.2357393857,-1.5026724483

C,0,2.1826909672,-2.3162318838,-1.5602389076

H,0,3.463767819,-1.4693517304,-0.0512225307

H,0,0.6548710235,-3.049213506,-2.8938144219

H,0,3.0033684959,-2.6734839075,-2.1744499737

C,0,-1.1457930533,2.2000077504,-4.2464030252

C,0,-0.0072894596,1.4576741943,-4.3918891668

H,0,0.9080483288,1.9029776556,-4.7703151332

H,0,-0.0807354599,0.3778999758,-4.4749338483

H,0,-2.0743517702,1.6754699388,-4.0232262124

C,0,-1.2186624504,3.6549371036,-4.2213713926

C,0,-2.4239760772,4.2752863637,-3.8425073488

C,0,-0.1170193607,4.4804118505,-4.5156293264

C,0,-2.5198927641,5.6587547264,-3.7369306742

H,0,-3.2885975003,3.6541186941,-3.6188147318

C,0,-0.2138715482,5.8610102114,-4.41147236

H,0,0.8299224462,4.0370401746,-4.8065921892

C,0,-1.4127521069,6.4599240968,-4.0166322136

H,0,-3.4592162722,6.1132327353,-3.4365605876

H,0,0.6547335898,6.4752273343,-4.6289430005

H,0,-1.4830238471,7.5396599813,-3.9316210602

TS10b2

46

C,0,-1.1205332178,-0.9608813181,0.8198811268

C,0,-0.8741455688,1.6649138331,0.0755517838

C,0,0.9344123547,1.3361119602,-2.4313300284

C,0,0.1543666332,3.4676545953,-1.3594920315

C,0,1.1218576734,2.7182040718,-2.0803608062

O,0,0.0357179984,1.6267962207,0.8636243933

S,0,-2.0646585866,0.3301310925,-0.0915504305

C,0,-1.1245478823,2.8216662959,-0.8838989718

C,0,0.3935921174,4.8101946587,-1.0817792125

C,0,2.2935831651,3.3825955848,-2.5027976425

C,0,1.5585726233,5.4483339198,-1.5091105565

C,0,2.5121486932,4.7241604565,-2.2253327777

H,0,-0.3460189282,5.3704125332,-0.5153525011

H,0,1.7199985547,6.4964758487,-1.2798957435

H,0,3.4258832125,5.2048450907,-2.5606174994

H,0,3.0395191273,2.8152944723,-3.0542179777

H,0,-1.7242532341,2.4514715345,-1.7219976148

H,0,-1.7350777324,3.5555428506,-0.3445632305

H,0,1.7996245719,0.7816633428,-2.7832731133

H,0,0.1618135905,0.7298753308,-1.9699199644

C,0,-2.1095589845,-2.0729653566,1.1876992877

H,0,-2.9209062363,-1.6230412009,1.7726420089

H,0,-2.5661107014,-2.491922327,0.2822993851

C,0,-1.5361432038,-3.2304814292,2.0408725453

C,0,-2.7134143473,-4.0795876859,2.5575177312

H,0,-3.3360257937,-4.4293734932,1.7295171649

H,0,-2.3492916274,-4.9501935661,3.1084155952

H,0,-3.3293887111,-3.4727198495,3.228125214

C,0,-0.7069792717,-2.7115139574,3.2265230252

H,0,0.2084023559,-2.2178696792,2.8919446706

H,0,-1.3048827664,-1.9972746143,3.8024730116

H,0,-0.4263976,-3.5398542144,3.8820354307

C,0,-0.6866952044,-4.1257288065,1.2246683626

N,0,-0.050596998,-4.8833744798,0.6248519215

H,0,-0.755854109,-0.4706404771,1.7265072397

C,0,0.0603175243,-1.402617049,-0.0155117104

C,0,1.3612136261,-1.1163393087,0.4010321112

C,0,-0.1321443567,-2.0685192344,-1.2311130035

C,0,2.4545909892,-1.5063470622,-0.3735218525

H,0,1.5153901099,-0.5621725149,1.3229134367

C,0,0.9547375331,-2.4571608908,-2.0048711938

H,0,-1.1418471346,-2.2790214365,-1.5740543042

C,0,2.2541531193,-2.1791488663,-1.5753299681

H,0,3.4607373733,-1.2766446599,-0.0373564569

H,0,0.791368233,-2.9886550369,-2.9377543148

H,0,3.1038063424,-2.4882831082,-2.1761801641

C,0,-1.3873835519,1.670948809,-4.2390900888

C,0,-0.0824468573,1.3247391153,-4.4447706094

H,0,0.6081815343,2.0553204204,-4.852918065

H,0,0.2138229505,0.2837269716,-4.5370025265

H,0,-1.6566357784,2.7245133937,-4.3013398625

C,0,-2.4427409605,0.7692781792,-3.787723876

C,0,-3.6747944843,1.3056000834,-3.371494807

C,0,-2.2735081784,-0.6247011959,-3.7095403476

C,0,-4.6897421474,0.4899660419,-2.8825564372

H,0,-3.8273565114,2.3811298673,-3.4303636389

C,0,-3.2911555142,-1.4405954494,-3.2296608452

H,0,-1.3368924736,-1.0746341184,-4.0256754166

C,0,-4.5022142748,-0.8898177284,-2.8064074762

H,0,-5.6280790663,0.9308661484,-2.5604318917

H,0,-3.1415915268,-2.5162303068,-3.1866094901

H,0,-5.2930944852,-1.5303923014,-2.4292519965

TS10b3

46

C,0,-1.0802249719,-0.5723021803,1.0320735618

C,0,-0.4215667595,2.0048174764,0.3788569605

C,0,1.2731107878,1.6451566455,-2.2103485241

C,0,0.748352728,3.7695900327,-0.9889894069

C,0,1.6224654942,2.9683507069,-1.769072327

O,0,0.5853221988,1.7118910889,0.9683333192

S,0,-1.9009216098,0.9739106937,0.4626035822

C,0,-0.577130317,3.224219358,-0.5205962978

C,0,1.132383378,5.0601323928,-0.635849852

C,0,2.8556132055,3.5252866388,-2.1670893423

C,0,2.3548563405,5.5947558229,-1.0434406928

C,0,3.2198778581,4.8166776944,-1.8136774453

H,0,0.4623884167,5.6608690965,-0.025834879

H,0,2.6294497689,6.6046378209,-0.7570030192

H,0,4.1772361081,5.2164300401,-2.1332159038

H,0,3.5305031931,2.9166523725,-2.7642973029

H,0,-1.2215635107,2.9429073009,-1.3620257219

H,0,-1.1222902607,3.9836099812,0.0532149866

H,0,2.065398352,0.9983707137,-2.5737379947

H,0,0.4083795999,1.1268174077,-1.806962831

C,0,-2.1810104535,-1.5211356796,1.5213880938

H,0,-2.7490785338,-1.0070964629,2.3062538194

H,0,-2.884507932,-1.738723768,0.7084852327

C,0,-1.6962578014,-2.8605048259,2.1274712966

C,0,-2.8999457257,-3.5522488095,2.7953703686

H,0,-3.7210597193,-3.6806170785,2.0849198254

H,0,-2.616463014,-4.5358275205,3.1776986473

H,0,-3.2509704189,-2.9392191418,3.631070291

C,0,-0.5766050116,-2.6506285095,3.1593974009

H,0,0.3401911805,-2.2863051151,2.6904843862

H,0,-0.9050514992,-1.9224136861,3.9084809619

H,0,-0.3481495266,-3.5922974282,3.6649262484

C,0,-1.2036726146,-3.773786799,1.0725940631

N,0,-0.8466687497,-4.5414940425,0.2842129814

H,0,-0.4420217577,-0.2784938898,1.8693326363

C,0,-0.2183307908,-1.1222629524,-0.0828483109

C,0,1.1645939537,-1.2106396091,0.0785140301

C,0,-0.7863959904,-1.5206974434,-1.2985569452

C,0,1.967080634,-1.7109673511,-0.9477601911

H,0,1.6168293712,-0.860414132,1.0025552365

C,0,0.0104933326,-2.01441296,-2.3247187097

H,0,-1.8620406031,-1.4402013524,-1.4423847616

C,0,1.3926652206,-2.1149493566,-2.1491760794

H,0,3.0415969603,-1.7743722208,-0.8075366745

H,0,-0.4453469191,-2.3322790188,-3.257660104

H,0,2.0147779697,-2.506961948,-2.9477377926

C,0,-0.5946234466,2.7867807337,-4.255395872

C,0,0.4082513913,1.8616070977,-4.2905861894

H,0,1.3743513799,2.144591151,-4.695271386

H,0,0.194432864,0.7962599622,-4.2610828583

H,0,-0.3507690048,3.824750979,-4.4740417158

C,0,-1.9694668029,2.5273237545,-3.8437387121

C,0,-2.930579958,3.5487359538,-3.9478146756

C,0,-2.3707790539,1.2955295288,-3.2949730381

C,0,-4.2437245898,3.3441840848,-3.5388042997

H,0,-2.6332115633,4.510948116,-4.3570476488

C,0,-3.6832061903,1.093844433,-2.8835071242

H,0,-1.6430430864,0.4989205035,-3.1628439529

C,0,-4.6283145691,2.1130882766,-3.0054139506

H,0,-4.9690092161,4.1466348076,-3.6326870269

H,0,-3.9674898655,0.140048622,-2.4481880382

H,0,-5.6510928497,1.9528599932,-2.6798873315

Int10

46

C,0,-1.2938561962,-0.6718064616,0.3432907995

C,0,-0.5852185634,1.9371052978,-0.1501667499

C,0,1.1887590338,1.561652156,-2.7119095498

C,0,0.604407204,3.7612627613,-1.4762077444

C,0,1.4569248517,2.9901552657,-2.2885130795

O,0,0.362409546,1.6216244679,0.5222445267

S,0,-2.0292892621,0.876077928,-0.3260177524

C,0,-0.703602512,3.2383815837,-0.9211514721

C,0,0.9357771472,5.0936612767,-1.210338744

C,0,2.6147426854,3.5937263793,-2.7950742082

C,0,2.0803491803,5.6830277005,-1.7372032276

C,0,2.9300834703,4.9237350643,-2.5369369998

H,0,0.2731298301,5.6838782867,-0.5827653691

H,0,2.3084880411,6.7210075668,-1.5170541161

H,0,3.8348033351,5.3591521729,-2.9496509126

H,0,3.280841308,2.9967283296,-3.4147235783

H,0,-1.444470387,3.1178557775,-1.7185322555

H,0,-1.1148957294,3.9714634268,-0.2164213412

H,0,2.1458893098,1.0294010395,-2.7554261147

H,0,0.5777036531,1.0134088419,-1.9915813366

C,0,-2.4478782387,-1.6258841115,0.6743056504

H,0,-3.1257805089,-1.114047857,1.368148117

H,0,-3.025843038,-1.8507218371,-0.2302372587

C,0,-2.046069372,-2.9599183821,1.3488038835

C,0,-3.3291184547,-3.6597559386,1.8363364727

H,0,-4.0364354971,-3.797165458,1.0140046248

H,0,-3.0967632396,-4.6397649637,2.2600665221

H,0,-3.8034057,-3.0473109027,2.6092405444

C,0,-1.0911840523,-2.7380836659,2.5326028763

H,0,-0.1181259439,-2.3681540453,2.2017597517

H,0,-1.531372606,-2.0103535832,3.2225211141

H,0,-0.9323526164,-3.6763711808,3.0700532033

C,0,-1.3975332499,-3.8723781296,0.3811065275

N,0,-0.9229401779,-4.6407237076,-0.3418847337

H,0,-0.7791629155,-0.3740094362,1.260912987

C,0,-0.2818726894,-1.2192013642,-0.6381072663

C,0,1.0630493307,-1.3093841631,-0.2783721847

C,0,-0.670322343,-1.615780186,-1.9229763806

C,0,2.0046873242,-1.8084945104,-1.1788232434

H,0,1.377252587,-0.9604899362,0.7017282072

C,0,0.2654252436,-2.1131819047,-2.8216155319

H,0,-1.7125674457,-1.5309498394,-2.2226802255

C,0,1.6079815786,-2.2130450285,-2.449995561

H,0,3.0480195004,-1.8721644924,-0.8863097114

H,0,-0.0511044803,-2.4297218949,-3.8107160637

H,0,2.3384144569,-2.6044784906,-3.1510718941

C,0,-0.9270410036,1.8398219705,-4.08924427

C,0,0.5158793817,1.4584915087,-4.1069227087

H,0,1.0809296106,2.0675927761,-4.8228677157

H,0,0.601060811,0.4151109642,-4.4310639276

H,0,-1.6361111687,1.0595308827,-3.8196519553

C,0,-1.4528459295,3.1401434196,-4.3162743729

C,0,-2.855058025,3.3540873599,-4.225608995

C,0,-0.6386510838,4.2690850277,-4.5963350939

C,0,-3.4052751676,4.6127465337,-4.4024713687

H,0,-3.4980387727,2.504299977,-4.0086888481

C,0,-1.1998449319,5.5256657837,-4.7704046709

H,0,0.4395824717,4.1560564435,-4.6514647766

C,0,-2.5822132935,5.7111547278,-4.6764391787

H,0,-4.4803271814,4.74571122,-4.3270328493

H,0,-0.5523503011,6.373274711,-4.9740023753

H,0,-3.0130468744,6.6976452926,-4.8126717145

TS11

81

C,0,-1.3172822349,-0.6944339639,0.5941158386

C,0,-0.1375785935,1.8536856317,0.0455903424

C,0,1.9828411446,0.7443656558,0.5190565662

C,0,1.7608311875,1.972075448,-1.5860216464

C,0,2.6329634206,1.5321436302,-0.5841955881

O,0,0.8055770405,1.3927801837,0.9984547958

S,0,-1.7797385709,1.0714399697,0.3967726481

C,0,0.3198944104,1.5765849413,-1.403216499

C,0,2.2590963003,2.7136378763,-2.6562912805

C,0,3.9914296302,1.8318329132,-0.650797527

C,0,3.6210892626,3.0146962004,-2.7266084714

C,0,4.4863989251,2.5723914404,-1.7262456712

H,0,1.5846369095,3.0446071073,-3.4428447137

H,0,4.0050668101,3.6071511403,-3.5522213512

H,0,5.542923741,2.8162187332,-1.7791897668

H,0,4.6607054521,1.4928222759,0.136021543

H,0,0.2133909187,0.5057800622,-1.613808952

H,0,-0.3451625552,2.0997088182,-2.0951057792

H,0,2.6340154436,0.6423243092,1.3894754323

H,0,1.7322682726,-0.2646696907,0.1577047336

C,0,-2.4169990083,-1.3032920111,1.4868846115

H,0,-2.4653882453,-0.694922865,2.3957308248

H,0,-3.3916297136,-1.2158844384,0.9887592693

C,0,-2.2533009397,-2.7890765619,1.9087549553

C,0,-2.6985338076,-3.7878982598,0.8226811978

H,0,-2.0902683311,-3.7269060282,-0.0798401624

H,0,-2.6423345817,-4.8083737527,1.2116011523

H,0,-3.7389315119,-3.5751040977,0.5569276094

C,0,-3.0991389075,-3.0245616654,3.1749356864

H,0,-2.7680330048,-2.3844317981,3.9962322637

H,0,-4.1450627741,-2.7923857407,2.9506560231

H,0,-3.0354650542,-4.0674917271,3.4954673695

C,0,-0.8381816478,-3.0451457394,2.2483196748

N,0,0.2735058603,-3.2324870117,2.509953004

H,0,-0.3784466582,-0.7019180073,1.1588164303

C,0,-1.1318361601,-1.4384031872,-0.711547485

C,0,-0.0133713762,-2.2548388306,-0.9021312524

C,0,-2.0969256508,-1.3692181227,-1.7229175345

C,0,0.1370490639,-2.9930674562,-2.077375526

H,0,0.7302403389,-2.3383469328,-0.1134766718

C,0,-1.9525257494,-2.1097230412,-2.8921564533

H,0,-2.9575745345,-0.717947249,-1.5927577233

C,0,-0.8333859946,-2.9252081925,-3.0739520728

H,0,1.0109659149,-3.6236871831,-2.2076189028

H,0,-2.7110477286,-2.0478497276,-3.6665348976

H,0,-0.7194661302,-3.4995593574,-3.9878518327

C,0,-0.2959925807,3.3682621032,0.3174684701

C,0,-1.3857430016,4.0772091267,-0.43261545

H,0,-0.4020221419,3.4934164926,1.3979021239

H,0,-1.3156179254,4.0264150067,-1.5185057023

H,0,0.6765785904,3.8040268496,0.0544023969

C,0,-2.7431970361,4.2290175658,0.0651467568

C,0,-3.7764505209,4.5239950535,-0.8466652078

C,0,-3.0710606207,4.1578689895,1.4331881586

C,0,-5.0830201525,4.7142591927,-0.4167004399

H,0,-3.5361709986,4.6000640782,-1.9043064782

C,0,-4.3791419291,4.3494412262,1.8603512137

H,0,-2.2986265985,3.9469071912,2.1651582254

C,0,-5.3934113014,4.6251655864,0.9415271625

H,0,-5.8619602251,4.9346691339,-1.1402148809

H,0,-4.6101111872,4.2853592412,2.9192869691

H,0,-6.413408947,4.7741392082,1.2811119769

C,0,0.9551776083,6.2308227392,-0.7281886672

C,0,3.1172368999,5.4392433604,-0.1054748971

C,0,2.8971130333,6.4714480331,-2.3316583922

C,0,3.7530730164,6.0926333314,-1.2967888095

O,0,1.8702493972,6.057540298,0.2460199214

S,0,-0.645110868,6.3402551816,-0.3250557049

C,0,1.4313578065,6.1750172082,-2.161155625

C,0,3.4239087138,7.0597481299,-3.4806805014

C,0,5.1267986829,6.292458996,-1.4094581502

C,0,4.800128866,7.246867615,-3.602450521

C,0,5.653150192,6.8609341499,-2.5682280907

H,0,2.7573073582,7.3683141075,-4.281963277

H,0,5.2065283739,7.7019593786,-4.5001398705

H,0,6.7235686,7.0152211375,-2.6593734996

H,0,5.7839086875,6.0012098553,-0.5937129906

H,0,1.2356925217,5.151542888,-2.5235015711

H,0,0.806002831,6.838469568,-2.7629097523

H,0,3.740512124,5.5180085811,0.7863759339

H,0,2.9241895495,4.3744459582,-0.3062415007

TS11a

81

C,0,-1.3740713823,-0.8098610075,0.6848001303

C,0,-0.1337464271,1.6781939905,0.0118719603

C,0,1.9984836263,0.558569763,0.3845976966

C,0,1.6586094184,1.7838649637,-1.706809006

C,0,2.5828949759,1.3612516976,-0.7447199683

O,0,0.8310662357,1.1853555541,0.9237642757

S,0,-1.7858878423,0.9650746586,0.459643702

C,0,0.2389080005,1.3593556602,-1.4499018699

C,0,2.0800439589,2.572027017,-2.7736713446

C,0,3.9247063359,1.710274658,-0.8570440458

C,0,3.4286218731,2.9125472477,-2.8941275293

C,0,4.3494829662,2.4801914163,-1.9413176543

H,0,1.3582725753,2.9213045883,-3.5076907448

H,0,3.7582841055,3.5254447653,-3.7270775334

H,0,5.3955145405,2.7545189749,-2.0337568741

H,0,4.6356457148,1.3897501937,-0.0997632332

H,0,0.1416619013,0.2797218912,-1.6143713768

H,0,-0.4724689348,1.8462355517,-2.1206310827

H,0,2.6911015487,0.4661926124,1.2233783177

H,0,1.7427835514,-0.4534504715,0.0353938488

C,0,-2.4605503405,-1.3620472741,1.6288008373

H,0,-2.4551760026,-0.7346589049,2.5260173363

H,0,-3.4491746938,-1.250989526,1.1639069743

C,0,-2.3339247623,-2.8438133697,2.0764495437

C,0,-2.8461670859,-3.8490957431,1.026373483

H,0,-2.2610204982,-3.8317665867,0.1068921101

H,0,-2.8171001147,-4.8618443668,1.4379013669

H,0,-3.8848665446,-3.6033115323,0.7832324494

C,0,-3.1478146065,-3.0242564883,3.3723141096

H,0,-2.7707035083,-2.3786377302,4.1691522406

H,0,-4.1920807319,-2.7622326439,3.1744967648

H,0,-3.1084451031,-4.0617594033,3.7136736277

C,0,-0.9190034743,-3.143141735,2.3792391311

N,0,0.191692594,-3.3679861321,2.6139296873

H,0,-0.4149978317,-0.8323827475,1.2139702493

C,0,-1.2581450839,-1.5893097503,-0.6076326219

C,0,-0.1701960721,-2.4417480237,-0.8157216585

C,0,-2.2564614225,-1.5174589591,-1.585700039

C,0,-0.0834504162,-3.2145803004,-1.974965138

H,0,0.600116062,-2.5232040708,-0.0528709645

C,0,-2.1753857338,-2.2919091571,-2.7388947344

H,0,-3.0924618157,-0.8373192791,-1.4430390038

C,0,-1.0873291217,-3.1446426078,-2.9377260155

H,0,0.76758549,-3.8727198079,-2.11969899

H,0,-2.9586771372,-2.2273665867,-3.48800056

H,0,-1.0225480374,-3.7452558649,-3.8394597864

C,0,-0.2173152643,3.2034809185,0.2608526025

C,0,-1.2514940917,3.9482985855,-0.5345785128

H,0,-0.3466082692,3.3518545528,1.3360990276

H,0,-1.1300689718,3.904132273,-1.6149134921

H,0,0.7797642477,3.5890103451,0.0116106987

C,0,-2.6207570309,4.1548408987,-0.0950311617
C,0,-3.5839220305,4.5620644013,-1.0397354761
C,0,-3.0148464346,4.0852736241,1.2563608345
C,0,-4.8851857338,4.8710664048,-0.657043163
H,0,-3.2929150922,4.6350068441,-2.0853323602
C,0,-4.3145759034,4.3972454812,1.6365671098
H,0,-2.2986292918,3.7819286912,2.0127827516
C,0,-5.2583973435,4.7964619431,0.6862589426
H,0,-5.6122198477,5.1690409031,-1.4075817918
H,0,-4.5950569172,4.3324821005,2.6835501958
H,0,-6.2721978337,5.038764992,0.9884140751
C,0,-1.6767227126,7.1075804877,-0.5563291365
C,0,-3.2930979363,8.1431568722,-1.9711327297
C,0,-2.9882710264,9.037245198,0.2897829769
C,0,-3.3774548817,9.3056669821,-1.0244680711
O,0,-2.0598432782,7.4232503937,-1.8086732138
S,0,-0.3587415723,6.1270607178,-0.3505715799
C,0,-2.540058197,7.6247441277,0.5680107488
C,0,-3.0218479133,10.0532074346,1.2409897475
C,0,-3.8044103018,10.5785607414,-1.3903705778
C,0,-3.4637601259,11.3265913396,0.8805537702
C,0,-3.8563746073,11.5898751576,-0.4310740067
H,0,-2.7040581736,9.8505846578,2.2600790471
H,0,-3.4934453522,12.1173536789,1.6234885467
H,0,-4.1906680294,12.5840525906,-0.7094811941
H,0,-4.0918249603,10.7821183432,-2.4186920144
H,0,-3.4269059942,6.9689267298,0.6408998649
H,0,-1.9958850223,7.5341499068,1.5085012647
H,0,-3.3098681434,8.4562262992,-3.0157135963
H,0,-4.1166227121,7.4356432482,-1.7944831942

TS11b

81

C,0,-1.7470689132,-0.807195755,0.9482886032
C,0,-0.8581225023,1.9032777308,0.6958842022
C,0,1.3661941103,1.321974577,1.5226041127
C,0,1.1653539081,2.6113634768,-0.5639724222
C,0,1.9107837002,2.3809830985,0.5995799628
O,0,-0.0397216051,1.4344687543,1.7575907038
S,0,-2.4028009882,0.8860388858,0.6749212212
C,0,-0.12463316,1.8432875904,-0.6586705258
C,0,1.6296925164,3.5182943644,-1.5131420383
C,0,3.0951439361,3.0780962992,0.8245170023
C,0,2.838038437,4.1896252345,-1.3051192001
C,0,3.5636396927,3.9806808852,-0.1335121727
H,0,1.048801062,3.7013209088,-2.4138577028
H,0,3.1999402721,4.8936162653,-2.0482845858
H,0,4.4832792958,4.5290539594,0.0453306614
H,0,3.6570025436,2.9173268208,1.7418758497
H,0,0.0866586719,0.7942321636,-0.8974779864
H,0,-0.7811114002,2.2260203368,-1.4440983044
H,0,1.8348138434,1.3664675514,2.5090924809
H,0,1.5759655051,0.3322611389,1.0890721555
C,0,-2.9650126465,-1.6469668738,1.3768715005
H,0,-3.4237842183,-1.1391422476,2.2318958869
H,0,-3.7121484199,-1.6628186902,0.5725896626
C,0,-2.700256461,-3.1233555632,1.7800000606
C,0,-2.5614588616,-4.0729046167,0.5737117614
H,0,-1.6918865785,-3.8441733258,-0.0426499486
H,0,-2.4772843175,-5.1055834106,0.9233857277
H,0,-3.4601315238,-3.988410559,-0.0456582249

C,0,-3.8754644015,-3.600738996,2.6543886422

H,0,-3.9655438353,-2.9959958177,3.5600061042

H,0,-4.8034679238,-3.5115970583,2.0806867155

H,0,-3.7444464106,-4.6466669575,2.9430198601

C,0,-1.4655886946,-3.1972433934,2.5884347453

N,0,-0.4956796869,-3.2491696671,3.2175480399

H,0,-1.0592013249,-0.7297359817,1.7959236589

C,0,-1.0081183156,-1.384740939,-0.2373575016

C,0,0.2553394035,-1.9531127788,-0.0569320465

C,0,-1.5831010629,-1.4019144241,-1.5133598065

C,0,0.9335942996,-2.5333435733,-1.1306244544

H,0,0.6980024308,-1.9636301978,0.9362881899

C,0,-0.9114433655,-1.9844126497,-2.5834616986

H,0,-2.5545202761,-0.9376488327,-1.6654784736

C,0,0.3511713588,-2.5523356257,-2.3955443828

H,0,1.9136855662,-2.9730644057,-0.9739529716

H,0,-1.368764232,-1.9916866212,-3.5681720788

H,0,0.8759816347,-3.0029212729,-3.2319656637

C,0,-1.2596449371,3.346916181,1.0858652071

C,0,-2.002823682,4.1654834954,0.0732999

H,0,-1.7854003135,3.2995719897,2.0439511174

H,0,-1.4430825039,4.3843284191,-0.8358496791

H,0,-0.3025007511,3.8372579883,1.2906030908

C,0,-3.4440131954,4.1114847737,-0.109247802

C,0,-3.9984237992,4.5281021559,-1.3356490742

C,0,-4.3269148536,3.7169445806,0.9152779518

C,0,-5.3723088859,4.5251389754,-1.5415242857

H,0,-3.3309432339,4.8539583346,-2.1297795401

C,0,-5.6999769568,3.7149227194,0.706130745

H,0,-3.9330929853,3.4108620535,1.8790441793

C,0,-6.2320872366,4.1144353726,-0.5216777492

H,0,-5.7749105249,4.8450457666,-2.497761764

H,0,-6.3623814945,3.4031979858,1.5078955387

H,0,-7.3059293725,4.1115655537,-0.6790217188

C,0,-0.1993293064,6.221603016,1.663858417

C,0,1.1936251256,5.2606341984,3.3480097067

C,0,2.2808853432,6.6808814163,1.6567614197

C,0,2.360699748,6.1055328544,2.9258349994

O,0,-0.0603737694,5.8326784421,2.9487863198

S,0,-1.7180382316,6.3240618336,1.009738178

C,0,1.0569053953,6.367149192,0.8414908069

C,0,3.3299734895,7.4708123559,1.1907735771

C,0,3.4849352716,6.3077453437,3.7226011757

C,0,4.4625210382,7.6644080604,1.9809994396

C,0,4.5430600418,7.0804252556,3.2450944965

H,0,3.2624518272,7.9294327201,0.2075040698

H,0,5.2793538358,8.278016093,1.6141051781

H,0,5.420935675,7.2388158173,3.8631461214

H,0,3.5332980045,5.8662070351,4.7148989391

H,0,1.2216845897,5.4041577532,0.3271390718

H,0,0.8824603909,7.104678493,0.0550267801

H,0,1.1322249999,5.1583000541,4.4322530422

H,0,1.2611423151,4.2545748832,2.9030496727

Int11

81

C,0,-0.2365517286,-3.7080967362,0.5478175824

C,0,1.023471986,-1.1293191137,0.7160617937

C,0,3.1116037395,-2.3739224058,0.829502709

C,0,2.917930328,-0.5600188915,-0.8013762837

C,0,3.777385507,-1.2962669969,0.0210103329

O,0,1.9397656899,-1.8830244806,1.4855048847

S,0,-0.6490055247,-1.9438426292,0.8343162036

C,0,1.4708954102,-0.9732464129,-0.7507905477

C,0,3.4244259169,0.4773057054,-1.5802508617

C,0,5.1371900645,-1.0043607638,0.0619899084

C,0,4.7906609328,0.7617351755,-1.5504358103

C,0,5.645804097,0.0234076066,-0.73348773

H,0,2.7518203702,1.063124921,-2.2004306041

H,0,5.1864471096,1.5682473435,-2.1597581595

H,0,6.7060617132,0.2544842463,-0.7072057977

H,0,5.796479539,-1.5735444429,0.7124673645

H,0,1.3472784805,-1.9332739903,-1.2664947637

H,0,0.8213809874,-0.2516511144,-1.2541649867

H,0,3.7554176678,-2.7468104327,1.6284718324

H,0,2.8424467133,-3.2201966858,0.1797831425

C,0,-1.3745661656,-4.5049444115,1.216280633

H,0,-1.4335510003,-4.1695048496,2.2567467837

H,0,-2.3326349202,-4.2550145545,0.7415105778

C,0,-1.2588221872,-6.0537437552,1.2149579759

C,0,-1.695381228,-6.7011062255,-0.1139141705

H,0,-1.0577395554,-6.4157600025,-0.9506808391

H,0,-1.6775154171,-7.7903525818,-0.0188482289

H,0,-2.7212026495,-6.3893785991,-0.3350799864

C,0,-2.1480580901,-6.6014158752,2.3479365183

H,0,-1.8263132818,-6.2229052962,3.3211521598

H,0,-3.1809126097,-6.2836787487,2.1731980539

H,0,-2.1194424219,-7.693742864,2.369567373

C,0,0.1381702883,-6.4392783077,1.5028596868

N,0,1.2348411698,-6.7312949163,1.7293450589

H,0,0.687039665,-3.8943057955,1.1070668855

C,0,-0.0311138344,-4.0700589717,-0.907887001

C,0,1.0723779725,-4.8387698037,-1.2883184487

C,0,-0.9635384807,-3.6985883435,-1.8830388803

C,0,1.2394328837,-5.2351760343,-2.6162622562

H,0,1.7907066882,-5.1549291316,-0.5361193743

C,0,-0.8024920921,-4.0980418857,-3.2061305021

H,0,-1.8106846512,-3.0790103806,-1.5999835748

C,0,0.3010990747,-4.8688632689,-3.5778947684

H,0,2.1018605369,-5.8329863201,-2.89397392

H,0,-1.5345834826,-3.802742179,-3.9515318509

H,0,0.4289037321,-5.1758116449,-4.6110733769

C,0,0.8833372491,0.2235189899,1.4320653404

C,0,-0.1802580479,1.1698068776,0.8442673794

H,0,0.6452862847,0.0029372657,2.4769049878

H,0,-0.8331045793,0.6278284068,0.1531477173

H,0,1.8778850013,0.6887950086,1.4238826219

C,0,-1.0402701777,1.8632760643,1.8647168344

C,0,-2.424303217,1.9132903252,1.6860668292

C,0,-0.4749420467,2.5361113495,2.9543206279

C,0,-3.2325746904,2.6280399964,2.571369455

H,0,-2.8666383373,1.3902295833,0.8410417723

C,0,-1.2779801578,3.2461811458,3.841221247

H,0,0.6036982064,2.5192654046,3.0912027034

C,0,-2.6604651497,3.3006971373,3.6485612487

H,0,-4.3074644941,2.6578477399,2.4189291869

H,0,-0.8261758925,3.7655764867,4.6807362812

H,0,-3.2851432757,3.8607480123,4.3371336738

C,0,-0.5825925171,3.5618242092,-0.5769528495

C,0,-2.8047070118,3.798533487,-1.3892019256

C,0,-1.5660513582,5.8146881819,-0.7110807939

C,0,-2.5652529812,5.2764307307,-1.5277297646

O,0,-1.5792379757,3.0551547976,-1.3582395043

S,0,0.6990580038,2.4621418452,-0.1991424863

C,0,-0.8385170933,4.8359813304,0.1774094822

C,0,-1.2882314125,7.1776804883,-0.7705837839

C,0,-3.2848987387,6.0945375928,-2.3938592965

C,0,-2.0181608015,8.001668995,-1.6278920047

C,0,-3.0161131132,7.4626198642,-2.4382343404

H,0,-0.5018316117,7.5954517003,-0.1475595293

H,0,-1.8012242505,9.064456742,-1.6696366828

H,0,-3.5764748505,8.1037726263,-3.1110835408

H,0,-4.0512657448,5.6659300278,-3.0347847617

H,0,-1.4528846468,4.6286795958,1.0757089437

H,0,0.1112114357,5.2405501316,0.5348446592

H,0,-3.3735561689,3.3953371962,-2.2286642093

H,0,-3.3499529113,3.5893471998,-0.4564070251

TS12

97

C,0,-5.0102217717,-0.6388693427,-1.0939862821

C,0,-2.7775041733,1.1400524556,-1.1463706806

C,0,-1.4275994479,-0.7262269646,-1.9503702271

C,0,-1.3913792673,1.3928963232,-3.1814888355

C,0,-0.6692582299,0.255010058,-2.8025235926

O,0,-2.1105770578,-0.083249668,-0.8697624908

S,0,-4.4924207894,1.0022121728,-0.454702647

C,0,-2.7995113125,1.4446607454,-2.6566074327

C,0,-0.7771039619,2.3829990968,-3.942355914

C,0,0.6559439907,0.1009780045,-3.196085545

C,0,0.54966153,2.2237993154,-4.3471101958

C,0,1.2634318436,1.0849875448,-3.9784239225

H,0,-1.3309694294,3.2771405478,-4.2187471393

H,0,1.0288316112,2.9945992458,-4.9423584344

H,0,2.2971226032,0.9686996433,-4.288041655

H,0,1.21561816,-0.7791463961,-2.8899333519

H,0,-3.4106071355,0.6865809945,-3.1600994835

H,0,-3.2861471526,2.4065497012,-2.8329115052

H,0,-0.7655080878,-1.4570362872,-1.4818693736

H,0,-2.158707098,-1.2716284429,-2.5674138751

C,0,-6.0844019171,-1.1380099424,-0.107550824

H,0,-5.6362708229,-1.1182419612,0.8911414731

H,0,-6.9324448884,-0.4404278882,-0.0945030047

C,0,-6.6684269613,-2.5573656412,-0.3452527001

C,0,-7.7622030437,-2.5975312914,-1.4303827653

H,0,-7.3856737579,-2.3287694073,-2.4173911505

H,0,-8.1940153719,-3.6007529961,-1.4844020998

H,0,-8.5542291026,-1.8935321848,-1.1556687812

C,0,-7.2697540566,-3.0572361448,0.9824372628

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H,0,-8.0502176565,-2.3597950864,1.3029374857

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H,0,-4.1339691064,-1.2898928108,-1.0053899059

C,0,-5.484309877,-0.6174077232,-2.5314695597

C,0,-5.0223410159,-1.579586607,-3.4340312692

C,0,-6.4233270392,0.3238467148,-2.9685652325

C,0,-5.4971440408,-1.6098159011,-4.7463523028

H,0,-4.3061260956,-2.3265351568,-3.1004262042

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H,0,-5.1296733066,-2.3653141917,-5.433780508

H,0,-7.6339435979,1.0253690852,-4.5990268234

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C,0,-4.5835777279,4.6206053199,-1.3176829882

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C,0,-5.5463262928,4.4195979413,1.2816413239

H,0,-3.6001755747,3.6493492417,1.7792469114

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H,0,-6.521770659,5.4146315517,-1.8182669422

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H,0,-7.3857927203,5.2354073354,0.504751252

C,0,-1.5362468978,6.3425505794,-0.1749172678

C,0,-2.6486990357,7.5139367176,-1.9466423755

C,0,-2.497114234,8.5664690328,0.276066043

C,0,-2.5686752909,8.7583145474,-1.1069617434

O,0,-1.7314485613,6.4930885578,-1.5217003199

S,0,-1.0878355102,4.68561532,0.270390838

C,0,-2.4353304274,7.1365313717,0.7434522497

C,0,-2.4439154076,9.6718159067,1.1215522304

C,0,-2.5846971065,10.0441125436,-1.6411337365

C,0,-2.4775704598,10.9612875325,0.5896431802

C,0,-2.5465238138,11.1487312952,-0.7901969074

H,0,-2.3723588252,9.5224995528,2.1961239538

H,0,-2.4391708174,11.8203216572,1.252145767

H,0,-2.5604663338,12.1522133528,-1.203251993

H,0,-2.6249775958,10.1842558981,-2.7184831821

H,0,-3.4467735802,6.6945380035,0.7427128501

H,0,-2.0438701464,7.0597084954,1.7620379242

H,0,-2.4029098423,7.7124462831,-2.9917562952

H,0,-3.6637374557,7.0947777102,-1.8943904994

C,0,0.467346737,7.3777579136,0.1324853499

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H,0,0.959738186,6.5039968334,-0.2848112277

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H,0,0.1423562031,8.1228154831,-0.587414389

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C,0,1.7198729349,5.6377357018,2.2860352554

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C,0,2.2514908179,4.8967701304,3.3343735177

H,0,1.694691415,5.2066630656,1.2899095167

C,0,2.2923114393,5.4231870877,4.6271929404

H,0,1.8197723756,7.1264935435,5.8596283108

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H,0,2.7084025915,4.8404106653,5.4427812711

TS12a

97

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C,0,-0.9151543858,1.5334418794,-2.4043092402

C,0,-0.2703728547,0.4330034913,-1.8266926421

O,0,-2.0552157448,0.1743032998,-0.1863796528
S,0,-4.4650870203,1.2784298034,-0.2739771684
C,0,-2.3968623571,1.5913321884,-2.15466101
C,0,-0.1743532037,2.4893173809,-3.093148047
C,0,1.1066290653,0.2810223408,-1.9515099923
C,0,1.2061733049,2.3302837124,-3.2293130997
C,0,1.844930689,1.22834111,-2.6636143936
H,0,-0.6706771432,3.3572299196,-3.5212344928
H,0,1.7840327689,3.0726677457,-3.7709730277
H,0,2.9193742972,1.1128038173,-2.7644862974
H,0,1.6042296309,-0.5688316344,-1.4913382138
H,0,-2.899766871,0.7935027469,-2.7133630942
H,0,-2.8485204395,2.5324812144,-2.4764587946
H,0,-0.6018803948,-1.201498718,-0.447669644
H,0,-1.7632593735,-1.1063833241,-1.7885310535
C,0,-6.1537317291,-0.8020014919,-0.0761090438
H,0,-5.9475294872,-0.6707837151,0.9912044955
H,0,-6.9605159342,-0.1041775592,-0.3368653403
C,0,-6.7103002787,-2.2366321129,-0.2856540838
C,0,-7.5213584553,-2.3968339395,-1.5864893484
H,0,-6.9153373446,-2.2493205221,-2.4804597742
H,0,-7.9628514293,-3.396478959,-1.6268873493
H,0,-8.3308248068,-1.6598363902,-1.5884314796
C,0,-7.6200404184,-2.5774759145,0.9102851295
H,0,-7.0648024364,-2.5456255664,1.8508521121
H,0,-8.4320192167,-1.8449072082,0.9584675088
H,0,-8.0562962982,-3.5728122544,0.7942948087
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C,0,-4.9980671011,-0.5634683442,-2.3367717736

C,0,-4.3613794994,-1.6190845654,-2.9953819655

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H,0,-3.7611821789,-2.3222419556,-2.4231616775

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H,0,-6.2640530958,1.1592360851,-2.580117154

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H,0,-4.0174421065,-2.6230278601,-4.8668439609

H,0,-6.5703132185,0.8302422127,-5.0162132949

H,0,-5.4394864335,-1.0567030527,-6.1717775178

C,0,-2.0380059445,2.5068016874,0.2101788157

C,0,-2.2934022658,3.9458590441,-0.2503843873

H,0,-2.3658403303,2.3601666207,1.2448599265

H,0,-1.9301343519,4.0715181147,-1.2735058588

H,0,-0.9562929959,2.3331908519,0.191290561

C,0,-3.7258748501,4.4099815275,-0.1778649007

C,0,-4.3524292072,4.9087439982,-1.3207720227

C,0,-4.4384907657,4.3850551749,1.0263616363

C,0,-5.6683610329,5.369861296,-1.2715897705

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H,0,-3.9535395667,4.0176453302,1.927224108

C,0,-6.3713561779,5.3356561103,-0.069844364

H,0,-6.1406776332,5.7564007628,-2.1697588233

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C,0,-2.1642489826,7.6601791298,-1.9942398989

C,0,-2.5797522333,8.8646268078,0.1521474924

C,0,-2.3662081751,8.9372836403,-1.224650685

O,0,-1.5235682677,6.607598197,-1.2613198435

S,0,-1.1801477516,5.0177334822,0.7711575712

C,0,-2.5563198525,7.4962625824,0.7794343569

C,0,-2.7776016534,10.0382137089,0.881515076

C,0,-2.3789871908,10.1738990152,-1.8705872674

C,0,-2.7920670183,11.2727997262,0.236913048

C,0,-2.5987739371,11.3406577257,-1.1440602176

H,0,-2.9205618582,9.9810114956,1.9576302477

H,0,-2.9477564409,12.181427901,0.8099246387

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H,0,-2.1954714395,10.2211591936,-2.9413066605

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H,0,-0.0365618441,8.6062879739,0.6859369183

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Int12

97

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C,0,1.2011739299,-1.001735888,-1.3713928555
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S,0,-1.869789404,-2.3366815244,1.0726446675
C,0,-0.2138967459,-1.329863767,-0.9823271609
C,0,1.6394152072,0.2371672495,-1.8279277768
C,0,3.4848851801,-1.7958554199,-1.3196469953
C,0,2.9998768425,0.4638999176,-2.0386159557
C,0,3.9191759233,-0.553832426,-1.7892695411
H,0,0.9212379812,1.036927358,-1.9931890185
H,0,3.3444615039,1.440306432,-2.3696090959
H,0,4.9785148249,-0.368942921,-1.9398213024
H,0,4.2043429981,-2.5810960691,-1.1009182908
H,0,-0.6345177209,-2.0924345726,-1.6477783739
H,0,-0.876249185,-0.4628456147,-1.0300477756
H,0,2.315792195,-3.9463404006,-0.1480152344
H,0,1.0264395649,-3.8385156354,-1.3668179118
C,0,-3.3444147309,-4.5816062803,1.0703257372
H,0,-3.1141106124,-4.5476684259,2.1406909087
H,0,-4.2284228779,-3.9502524567,0.9110989577
C,0,-3.7551323218,-6.0360388131,0.712981547
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H,0,-4.0203540318,-5.8396797704,-1.466332217
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C,0,3.74134454,4.1766990121,-1.077769023

C,0,5.9416882314,2.6404637723,-1.8528838205

H,0,5.8634125668,1.7916823239,0.1174056769

C,0,4.2667912453,4.3058755201,-2.3548961093

H,0,2.8837084393,4.7775726709,-0.7911301485

C,0,5.3663187673,3.5397465296,-2.757456997

H,0,6.7988081128,2.0443428459,-2.1526674046

H,0,3.8178208148,5.0118658904,-3.0478966526

H,0,5.7709645699,3.6450267086,-3.758711