

Supporting Information

Unprecedented associative exchange in CO₂-sourced cyclic S,O-acetals based covalent adaptable networks

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Instrumentation

Electrospray Ionization Mass Spectrometry (ESI-MS) and Liquid Chromatography Mass Spectrometry (LC-MS). An Agilent technologies 1100 series LC/MSD system equipped with a diode array detector and single quad MS detector (VL) with an electrospray source (ESI-MS) was used for classic reversed phase LCMS and MS analysis. Analytic reversed phase HPLC (high-performance liquid chromatography) was performed using a Cyano porous column with a flow rate of 1 mL min⁻¹ (5 μ m, 250 x 4.6 mm) using a solvent gradient of 50 \rightarrow 100 % acetonitrile in water over 15 minutes, unless otherwise stated. The eluting compounds were detected via UV-detection (λ = 214 nm). LCMS spectra were analyzed using ACD/Spectrus software and the purity of compounds was assessed by integrating the LC peaks (λ = 214 nm) using the in-software function.

Nuclear Magnetic Resonance (NMR) spectroscopy. NMR spectra were recorded on a Bruker Avance 300 (300 MHz) or Bruker Ascend 400 (400 MHz) FT-NMR spectrometer at 25 °C in either DMSO-*d*₆, D₂O, toluene-*d*₈ or CDCl₃, as indicated. Chemical shifts (δ) are expressed in parts per million (ppm) whereby the residual solvent peaks (CDCl₃: ¹H = 7.26 ppm and ¹³C = 77.16. DMSO-*d*₆: ¹H = 2.50 ppm and ¹³C = 39.52) served as an internal standard. Coupling constants (*J*) are reported in Hertz (Hz). The resonance multiplicities are abbreviated as follows: s (singlet), d (doublet), t (triplet), q (quadruplet), quint (quintet), sext (sextet) or m (multiplet).

Fourier-Transform Infrared spectroscopy (FTIR). Measurements were recorded on a Perkin Elmer FTIR SPECTRUM 1000 spectrometer with Attenuated Total Reflection (ATR) with a PIKE Miracle ATR unit in a frequency range from 4000 to 600 cm⁻¹.

Thermogravimetric Analysis (TGA). TGA were recorded on a Mettler Toledo TGA/SDTA 851 under nitrogen atmosphere at a heating rate of 10 K min⁻¹ starting from 25°C to 800°C. Isothermal measurements were conducted at 140°C for 80 minutes. Degradation temperatures are determined as onset temperature for 5% mass loss.

Differential Scanning Calorimetry (DSC). DSC analyses were performed using a Mettler Toledo instrument 1/700 in nitrogen atmosphere with a heating and cooling rate of 10 K min⁻¹ starting from -100°C to 150°C. Glass transition temperatures were deduced from the second heating run on all samples.

Rheology. Rheological measurements were performed on an Anton Paar MCR 302 in a parallel plate geometry using 8 mm sample disks that were obtained with a hollow puncher of Boehm. Amplitude sweep measurements were performed with a frequency of 1 Hz, a normal force of 1N and a shear strain which logarithmically increases from 0.01% to 10%. Stress relaxation experiments were conducted between 150 and 100°C with 10°C intervals, applying a constant shear strain of 0.75% (within the LVE of the samples) and a normal force of 1N. The obtained relaxation times (τ) were used to calculate the activation energies. Time sweep experiments were conducted at a constant strain of 1% and a constant angular frequency of 1 rad.s⁻¹. Temperature sweep experiments were performed with a constant strain of 0.5 %, a constant angular frequency of 1 rad.s⁻¹ and a constant normal force of 0.2 N

Solubility. Solubility measurements were performed in THF. Measurements on four samples were conducted using 6 mm sample disks. After 24 hours the samples were weighed and dried in a vacuum oven at 40°C overnight. The swelling degree and soluble fraction were calculated using equation (1) and (2) respectively, with m_i , the initial sample mass, m_s the mass of the swollen sample and m_d the mass of the dried sample.

$$\text{swelling degree (\%)} = \frac{m_s - m_i}{m_i} \quad (1)$$

$$\text{soluble fraction (\%)} = \frac{m_i - m_d}{m_i} \quad (2)$$

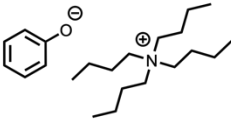

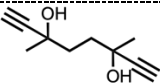
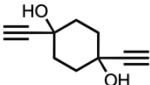
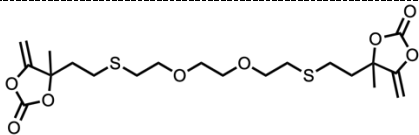
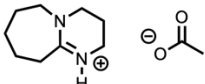
(Re)processing. The materials were (re)processed by compression molding at 120°C and 3 metric ton for 30 minutes. The networks were cut in pieces (2x2 mm) and put in a mold and compression molded. After 30 minutes the mold was taken out of the hot press and allowed to cool to room temperature.

Cross cut adhesion test. ASTM D3359-02 standards were followed to determine adhesion of the coatings to the aluminium substrate. An Elcometer 1542 Cross Hatch Adhesion Tester: cutter type 6 × 1mm was used. Next, 3M adhesion tape was used to determine possible coating failure.

Materials

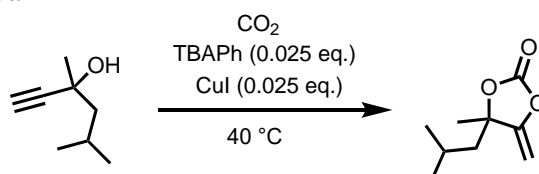
All reagents were purchased from commercial suppliers and used as received unless otherwise specified, all solvents were HPLC grade, deuterated solvents for NMR spectroscopy were purchased from Eurisotop. Benzyl mercaptan (99%, Sigma-Aldrich), diazabicyclo[5.4.0]undec-7-ene ($\geq 99\%$, TCI Europe), 2,2-dimethoxy-2-phenylacetophenone (99%, Sigma-Aldrich), hexane-1,6-dithiol (96%, TCI Europe), hydrochloric acid (36%, Chem-lab), magnesium sulfate monohydrate ($\geq 99\%$, Roth), sodium chloride ($\geq 99\%$, Sigma-Aldrich); sodium hydrogen bicarbonate ($\geq 99\%$, Roth); sodium sulfate (99%, Roth), thioacetic acid ($>95\%$, TCI Europe), 1,3,5-trimethoxybenzene ($\geq 99\%$, Sigma-Aldrich), 1,2,4-trivinylcyclohexane (mixture of isomers, 98%, Sigma-Aldrich). Copper iodide was dispersed in glacial acetic acid overnight, filtered, washed with methanol under nitrogen flow, and dried under vacuum.

The following compounds were synthesized according to previously reported procedures:

Compound	Name	Reference
	Tetrabutylammonium phenolate	1
	4,4-dimethyl-5-methylene-1,3-dioxolan-2-one	2
	3,6-dimethylocta-1,7-diyne-3,6-diol	3
	1,4-diethynylcyclohexane-1,4-diol	4
	Cross-linker 5a (mixture of isomers)	5
	DBU:acetate	6

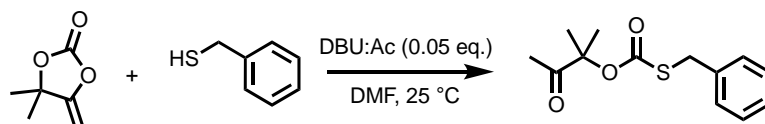
Synthetic procedures

Synthesis of *α*CC-branched



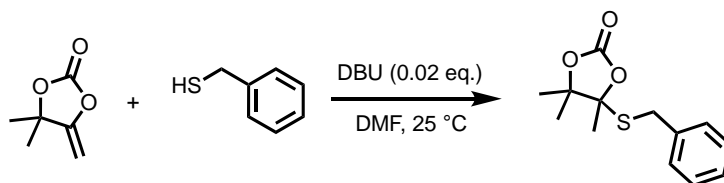
α CC-*branched* was synthesized by slightly modifying a previously reported procedure.¹ 3,5-Dimethyl-1-hexyn-3-ol (17.18 g, 0.136 mol, 1 eq.), CuI (650 mg, 3.4 mmol, 0.025 eq.), and tetrabutylammonium phenolate (1.15 g, 3.4 mmol, 0.025 eq.) were added in a 80 mL high pressure autoclave. The reactor was charged with 100 bars of CO₂ at 40 °C. After 24h, the reactor was depressurized. The product was distilled under vacuum and purified by silica gel chromatography using hexane/diethyl ether 98/2 as eluent. The pure product was isolated as a transparent liquid (11.3 g, isolated yield 49 %). ¹H NMR (400 MHz, DMSO-*d*₆) δ 4.84 (d, J = 4 Hz, 1H), 4.64 (d, J = 4 Hz, 1H), 1.86-1.68 (m, 3H), 1.57 (s, 3H), 0.91 (d, J = 6.8 Hz, 6H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 158.0, 151.5, 88.2, 86.5, 47.8, 26.7, 24.3, 24.1, 23.9.

Synthesis of **1a**



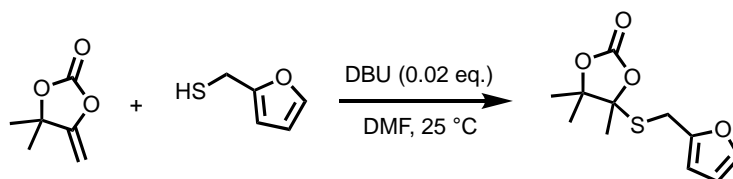
1b was synthesized by modifying a previously reported procedure.^{4,5} α CC (1.024 g, 8 mmol, 1 eq.), benzyl mercaptan (992 mg, 8 mmol, 1 eq.) and DMF (2 mL) were added in a reaction tube under N₂ atmosphere. DBU acetate (DBU:Ac) (84.8 mg, 0.4 mmol, 0.05 eq.) was added and the reaction medium was stirred at 25 °C for 1h and quenched with one drop of acetic acid. The mixture was then diluted with 100 mL of ethyl acetate and extracted 3 times with brine (3x100 mL). The organic phase was recovered, dried over MgSO₄ and filtered. The solvent was evaporated under vacuum at room temperature. The solid was then recrystallized in diethyl ether at -20 °C, filtered on a Büchner apparatus, and washed with cold diethyl ether. The pure product was isolated as white crystals (1.13 g, isolated yield 56 %). ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.31 (m, 5H), 4.14 (s, 2H), 2.08 (s, 3H), 1.45 (s, 6H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 205.9, 169.8, 137.8, 129.2, 129.0, 127.9, 87.3, 35.0, 24.2, 23.5.

Synthesis of **2a**



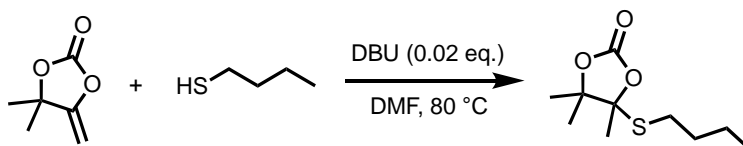
2a was synthesized by slightly modifying a previously reported procedure.⁴ α CC (1.024 g, 8 mmol, 1 eq.), benzyl mercaptan (992 mg, 8 mmol, 1 eq.) and DMF (2 mL) were added in a reaction tube under N₂ atmosphere. DBU (24.3 mg, 0.16 mmol, 0.02 eq.) was added and the reaction medium was stirred at 25 °C for 24h. The mixture was then diluted with 100 mL of ethyl acetate and extracted 3 times with brine (3x100 mL). The organic phase was recovered, dried over MgSO₄ and filtered. The solvent was evaporated under vacuum at room temperature. The solid was then recrystallized in ethanol, filtered on a Büchner apparatus, and washed with cold ethanol. The pure product was isolated as a white solid (1.41 g, isolated yield 70 %). ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.36 (m, 5H), 4.08 (d, J = 12 Hz, 1H), 3.96 (d, J = 12 Hz, 1H), 1.80 (s, 3H), 1.51 (s, 3H), 1.46 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 152.8, 137.2, 129.6, 129.1, 127.8, 96.9, 88.1, 33.0, 23.5, 21.8, 21.7.

Synthesis of **2b**



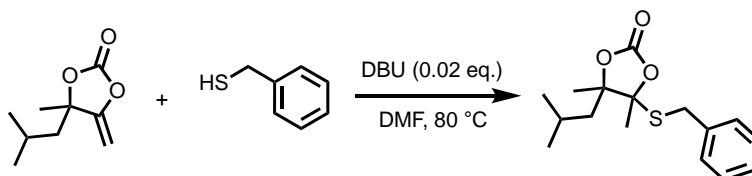
2b was synthesized by slightly modifying a previously reported procedure.⁴ α CC (1.024 g, 8 mmol, 1 eq.), 2-furanmethanethiol (912 mg, 8 mmol, 1 eq.) and DMF (2 mL) were added in a reaction tube under N₂ atmosphere. DBU (24.3 mg, 0.16 mmol, 0.02 eq.) was added and the reaction medium was stirred at 25 °C for 24h. The mixture was then diluted with 100 mL of ethyl acetate and extracted 3 times with brine (3x100 mL). The organic phase was recovered, dried over MgSO₄ and filtered. The solvent was evaporated under vacuum at room temperature. The product was diluted with diethyl ether (2 mL) and purified by silica gel chromatography using hexane/toluene/diethyl ether 50/30/20 as eluent. The pure product was isolated as viscous orange oil (1.32 g, isolated yield 68 %). ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.61 (m, 1H), 6.41 (m, 1H), 6.37 (m, 1H), 4.12 (d, *J* = 14.2 Hz, 1H), 4.03 (d, *J* = 14.2 Hz, 1H), 1.79 (s, 3H), 1.50 (s, 3H), 1.45 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 152.6, 150.6, 143.3, 111.3, 108.8, 96.7, 88.1, 25.4, 23.5, 21.6.

Synthesis of **2c**



α CC (1.024 g, 8 mmol, 1 eq.), 1-butanethiol (722 mg, 8 mmol, 1 eq.) and DMF (2 mL) were added in a reaction tube under N₂ atmosphere. DBU (24.3 mg, 0.16 mmol, 0.02 eq.) was added and the reaction medium was stirred at 80 °C for 24h. The mixture was then diluted with 100 mL of ethyl acetate and extracted 3 times with brine (3x100 mL). The organic phase was recovered, dried over MgSO₄ and filtered. The solvent was evaporated under vacuum at room temperature. The product was diluted with diethyl ether (2 mL) and purified by silica gel chromatography using hexane/diethyl ether 75/25 as eluent. The pure product was isolated as transparent oil (874 mg, isolated yield 50 %). ¹H NMR (400 MHz, DMSO-*d*₆) δ 2.73 (m, 2H), 1.73 (s, 3H), 1.54 (m, 2H), 1.50 (s, 3H), 1.43 (s, 3H), 1.37 (sext, *J* = 7.4 Hz, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 152.8, 96.8, 88.0, 31.6, 28.3, 23.5, 21.9, 21.8, 21.5, 13.9

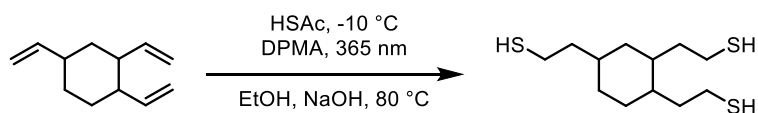
Synthesis of **2d**



2d was synthesized by slightly modifying a previously reported procedure.⁴ α CC-*branched* (1.36 g, 8 mmol, 1 eq.), benzyl mercaptan (992 mg, 8 mmol, 1 eq.) and DMF (2 mL) were added in a reaction tube under N₂ atmosphere. DBU (24.3 mg, 0.16 mmol, 0.02 eq.) was added and the reaction medium was stirred at 80 °C for 24h. The mixture was then diluted with 100 mL of chloroform and extracted 3 times with brine (3x100 mL). The organic phase was recovered, dried over MgSO₄ and filtered. The solvent was evaporated under vacuum at room temperature. The product was diluted with ethyl acetate (2 mL)

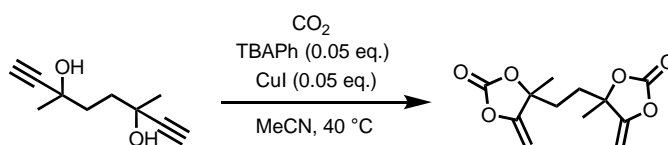
and purified by silica gel chromatography using hexane/ethyl acetate 98/2, 96/4, and then 90/10 as gradient of eluents. The pure product was isolated as a yellowish solid (1.32 g, isolated yield 56 %). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 (m, 5H), 4.03 (d, $J = 11.8$ Hz, 1H), 4.97 (d, $J = 11.8$ Hz, 1H), 1.90 (m, 2H), 1.78 (s, 3H), 1.62 (m, 1H), 1.47 (s, 3H), 1.01 (dd, $J = 6$ Hz, $J = 16$ Hz, 6H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 153.2, 136.3, 129.2, 128.8, 127.5, 96.8, 89.7, 42.2, 33.4, 24.7, 24.6, 22.6, 21.8, 20.2.

Synthesis of 1,2,4-tris(2-mercaptoethyl)cyclohexane (TVC-trithiol)



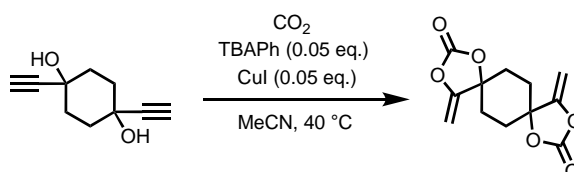
This compound was synthesized following a procedure reported in literature.⁷ 1,2,4-trivinylcyclohexane (mixture of isomers, 100 mL, 0.52 mol, 1 eq) was cooled in an ice-salt bath to -10°C in a 500 mL erlenmeyer flask. Thioacetic acid (124.3 mL, 1.586 mol, 3.05 eq) was added dropwise to the vigorously stirred mixture after which 2,2-dimethoxy-2-phenylacetophenone (1.5 g, 3.9 mmol) was added in one portion. The cooling bath was removed and a reflux condenser was fitted to the Erlenmeyer flask. After stirring for 30 minutes, the mixture was purged with argon, closed with a septum and irradiated for 1 hour in a photoreactor equipped with 4 X 36 W UV lamps (Philips CLEO Compact PL-L (2G11), $\lambda_{\text{max}} = 350$ nm, λ -range: 310-400 nm). Deprotection was achieved after mixing the trithioacetate mixture in a mixture of ethanol and water containing NaOH (62.4 g) (250 mL ethanol, 250 mL water). The mixture was heated to 100°C overnight. After cooling to room temperature, the mixture was neutralised with by slowly adding 1M HCl solution. Then the mixture was extracted with diethyl ether (2x100mL), the combined organic phases were washed with water (2x50 mL), dried over sodium sulfate, filtered and concentrated *in vacuo*, yielding a yellow coloured oil that was further purified by Kugelrohr distillation (116.9 g, isolated yield 85 %). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 2.70 – 2.34 (m, 6H), 1.91 – 0.62 (m, 18H).

Synthesis of crosslinker 5b



3,6-dimethyl-1,7-octadiyne-3,6-diol (20 g, 0.12 mol, 1 eq.), tetrabutylammonium phenolate (2 g, 6 mmol, 0.05 eq.), CuI (1.15 g, 6 mmol, 0.05 eq.), and acetonitrile (40 mL) were added in a 250 ml high pressure autoclave. The reactor was charged with 100 bar of CO_2 at 40°C . After 24h, the reactor was depressurized. The content of the autoclave was dissolved in dichloromethane (400 mL) and the mixture was purified by flash chromatography onto silica (eluent: dichloromethane). The solvent was evaporated and the obtained yellow solid was dried under vacuum. The solid was then dissolved in ethyl acetate and recrystallized at -20°C . The solid was filtered, washed with cold ethyl acetate, and dried under vacuum. The pure product was isolated as white crystals (23.2 g, isolated yield 76%). $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 4.87 (d, 2H), 4.72 (d, 2H), 1.90 (m, 4H), 1.61 (s, 6H). $^{13}\text{C NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 156.7, 151.2, 87.1, 87.0, 33.3, 26.0.

Synthesis of crosslinker 5c



1,4-diethynylcyclohexane-1,4-diol (20 g, 0.12 mol, 1 eq.), tetrabutylammonium phenolate (2 g, 6 mmol, 0.05 eq.), CuI (1.15 g, 6 mmol, 0.05 eq.), and acetonitrile (40 mL) were added in a 250 ml high pressure autoclave. The reactor was charged with 100 bar of CO₂ at 40°C. After 24h, the reactor was depressurized. The content of the autoclave was dissolved in dichloromethane (400 mL) and the mixture was purified by flash chromatography onto silica (eluent: dichloromethane). The solvent was evaporated and the obtained yellow solid was dried under vacuum. The solid was then dissolved in acetonitrile (300 mL) and recrystallized at -20°C. The solid was filtered, washed with cold acetonitrile, and dried under vacuum. The pure product was isolated as white crystals (23.9 g, isolated yield = 79%). ¹H NMR (400 MHz, DMSO-*d*₆) δ 4.87 (d, 2H), 4.80 (d, 2H), 2.08 (m, 8H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 157.1, 151.1, 87.1, 84.7, 31.6.

Synthesis of covalent adaptable networks

The bifunctional α -alkylidene cyclic carbonate (2.25 eq.) was dissolved in a minimal amount of THF and this mixture was slightly heated until all the solids were dissolved. Then, TVC-trithiol (1 eq.) and 1,6-hexanedithiol (1 eq.) were mixed in a minimal amount of THF together with a catalytic amount of DBU (1 mol% with respect to the total amount of thiol groups present in the mixture). The thiol mixture was added to the cyclic carbonate solution after which curing was triggered at 70°C overnight. The sample was removed from the container, brought in a polypropylene cup and the solvent was removed at 40°C in a vacuum oven. Uniform samples were obtained after hot pressing the material at 120°C for 1 hour under 2 metric tons.

Preparation of coatings

Based on literature,⁴ a prepolymer from **5c** (1 g, 3.96 mmol, 1 eq.) and 1,6-hexanedithiol (715.07 mg, 4.76 mmol, 1.2 eq.) with DBU (7.24 mg, 0.0476 mmol, 0.012 eq.) was prepared THF (1 mL) in a vial equipped with a stirring bar. The mixture was put in argon atmosphere and was stirred overnight at room temperature. Then 1,2,4-trivinylcyclohexane (8.36 mg, 0.05154 mmol, 0.013eq) was added together with 2,2'-dimethoxyphenylacetophenone (11.35 mg, 0.03965 mmol, 0.01 eq.). The substrate (glass or metal plates) were washed and degreased with water and detergent, rinsed with distilled water, acetone and isopropanol three times and were dried using a clean cloth. The above prepared solution was then put on the surface and evenly coated using an Elcometer 3560/6 for sided film applicator to create a film of uniform thickness (150 μ m). The samples were irradiated for 30 minutes after which the samples were dried overnight before coating tests were performed.

Experimental procedures

Thermal stability of compound 2a

Compound **2a** (126 mg, 0.5 mmol, 1 eq.) was dissolved in DMF (0.125 mL) and DBU (0.76 mg, 0.005 mmol, 0.01 eq.) was added to the mixture. The solution was stirred at 120 °C. An aliquot of the reaction medium was sampled, diluted with DMSO-*d*₆ and quenched with one drop of formic acid. The sample was analyzed by ¹H-NMR spectroscopy (**Figure S1**).

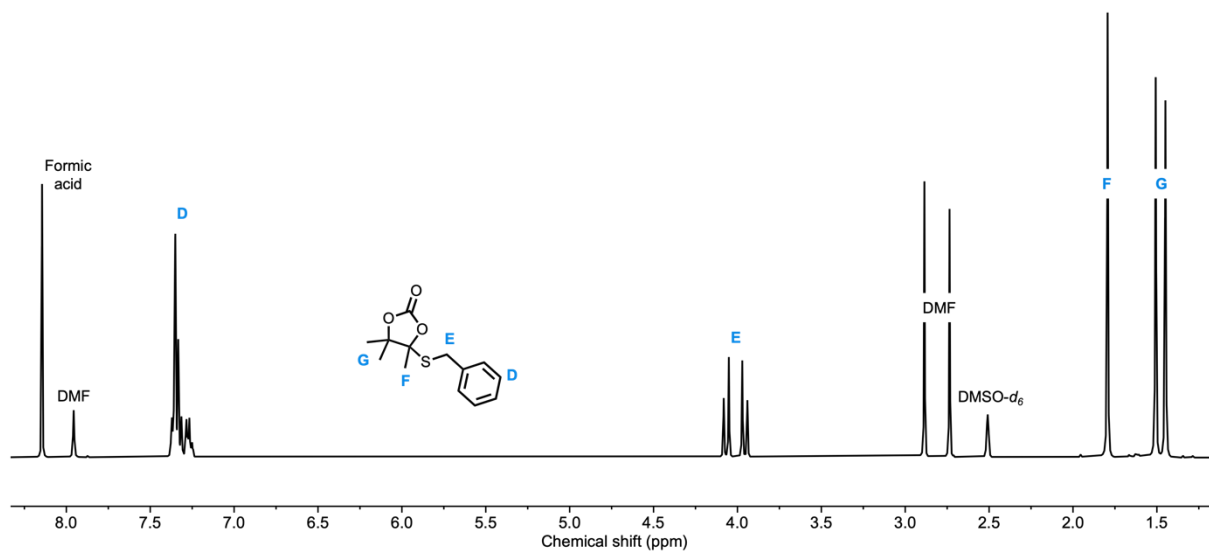


Figure S1. $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) spectrum of **2a** after 2 hours heating to 120°C in DMF with a catalytic amount of DBU (0.01 eq.).

Crossover exchange experiment between 2b and 2d

Compound **2a** (10 mg, 0.04127 mmol, 1 eq.) and compound **2d** (12.12 mg, 0.04127 mmol, 1 eq.) were dissolved in 1 mL DMF, DBU (0.06283 mg, 0.0004127 mmol, 0.01 eq.) was added and the mixture was stirred at 85°C overnight. The resulting mixture was subsequently analysed by LCMS-spectroscopy.

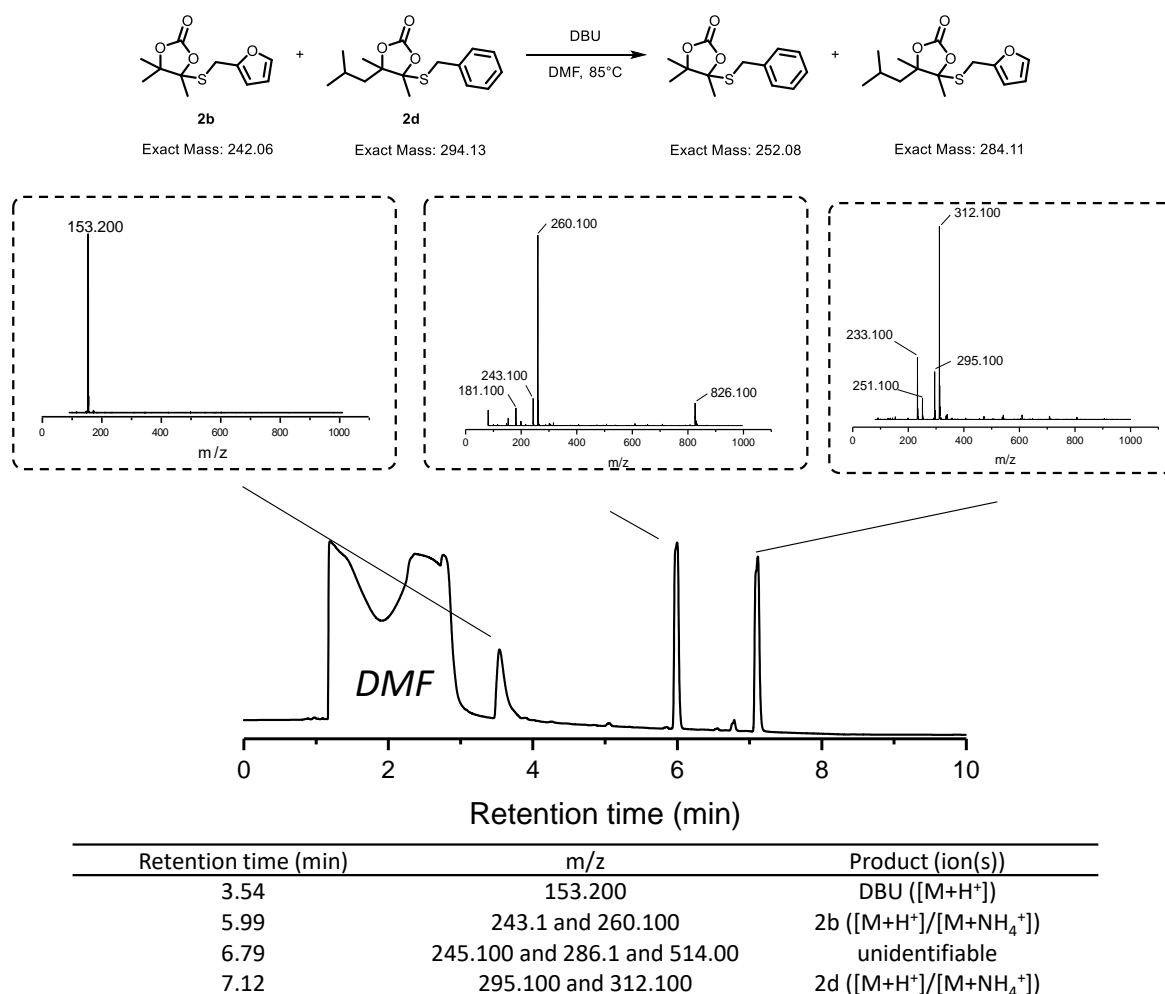


Figure S2. Crossover experiment between **2b** and **2d**. LC-MS analysis with UV detection at 214 nm after overnight reaction at 85 °C did not reveal any significant exchange product formation. A small unidentifiable peak is observed at a retention time of 6.79 min.

Reaction between 2a and 0.5 equivalents benzylmercaptan

To compound **2a** (252 mg, 1 mmol, 1 eq) in DMF (0.250 mL) was added benzylmercaptan (62 mg, 0.5 mmol, 0.5 eq) and DBU (1.52 mg, 0.01 mmol, 0.01 eq.). The mixture was stirred under nitrogen atmosphere at 85 °C for 1 hour. An aliquot of the reaction medium was sampled, diluted with DMSO-*d*₆ and quenched with one drop of formic acid. The sample was analyzed by ¹H-NMR spectroscopy (**Figure S3**), revealing the presence of the starting compound **2a** with a small amount of oxo-thiocarbonate **1a**. The crude reaction mixture spectrum was compared to spectra of pure **2a** and **1a**.

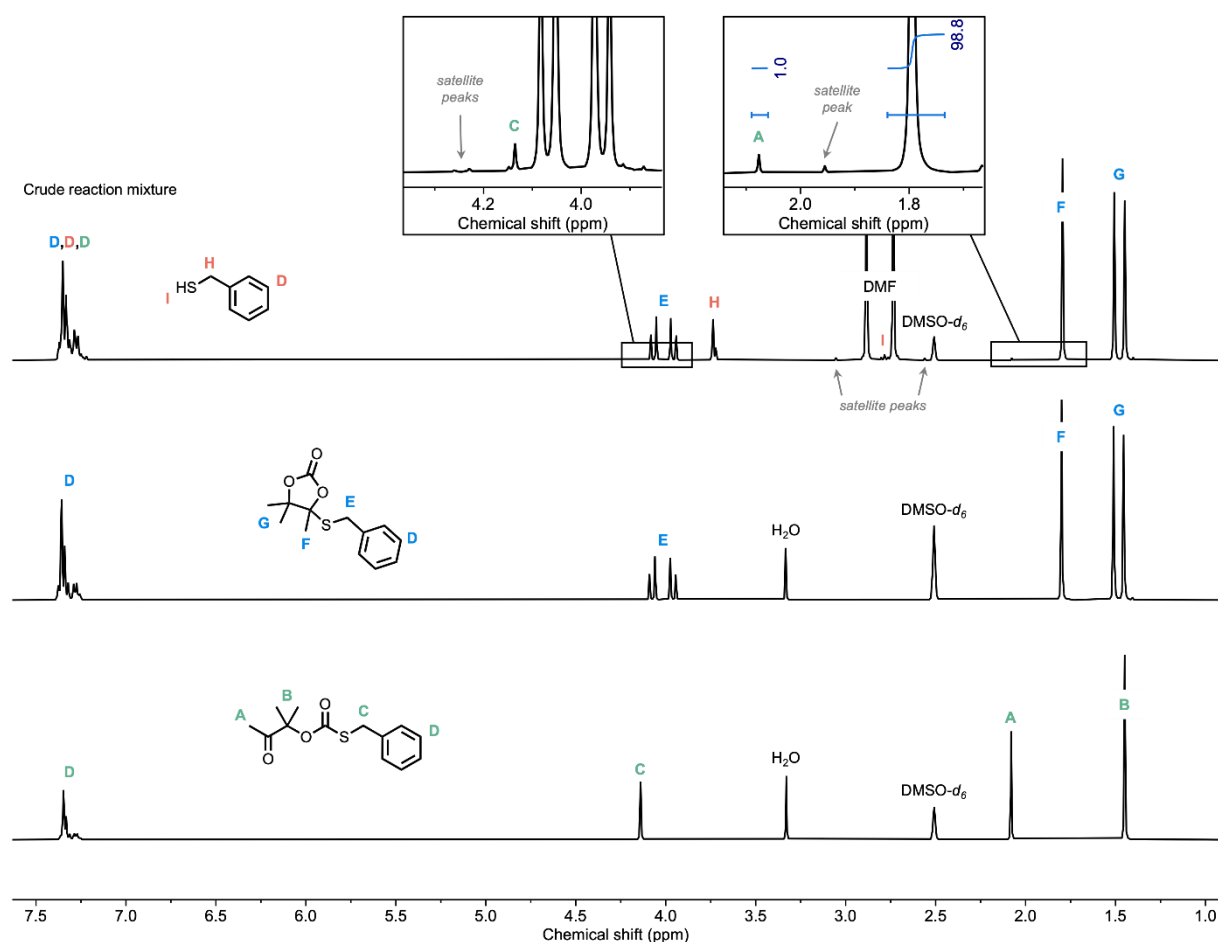


Figure S3. $^1\text{H-NMR}$ spectrum in $\text{DMSO-}d_6$ after reaction of **2a** with benzylmercaptan.

Exchange on 2b using excess benzylmercaptan

Compound **2b** (100 mg, 0.41243 mmol, 1 eq.) was weighed in a pressure tube equipped with a stirring bar. Benzyl mercaptan (256 mg, 2.06 mmol, 5 eq.) was dissolved in 10 mL acetonitrile containing DBU (0.00314 g, 0.02064 mmol, 0.05 eq) in a separate vial. This thiol solution was added to compound **2b** and heated at different temperatures (70, 75, 80, 85 and 95 °C). after which aliquots (0.1 mL) were sampled at regular time intervals, quenched with 0.01 mL acetic acid solution in acetonitrile (0.02 M) and diluted with 0.9 mL of an acetonitrile solution containing trimethoxybenzene (TMB) (10 mg in 9 mL). These solutions were analysed using LC-MS and the signal corresponding to **2b** was followed over time. The reaction rate constants were obtained from the initial part of the slope of the fraction of starting product as a function of time.

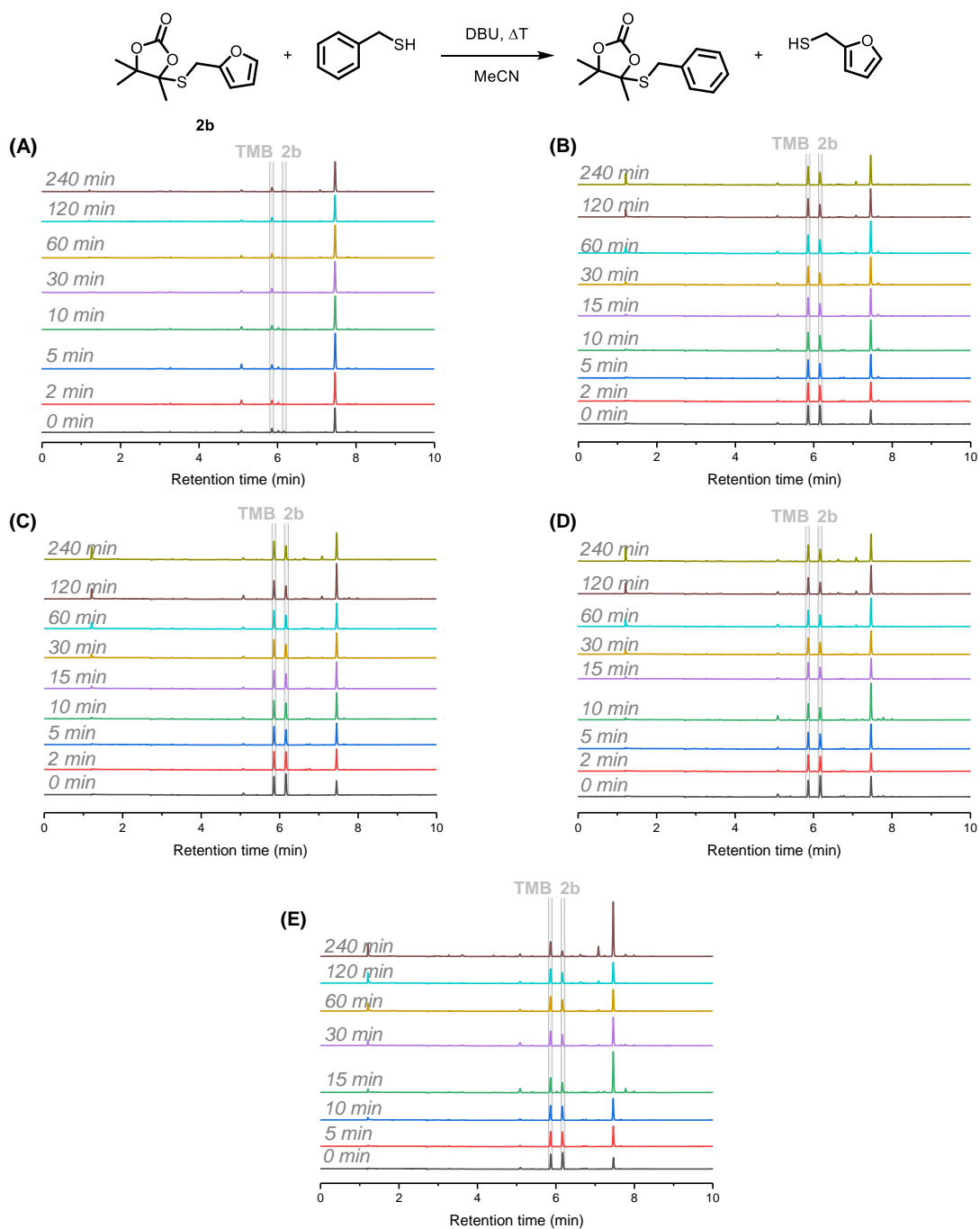


Figure S4. DBU catalysed associative exchange reaction between compound **2b** and benzylmercaptan at 70 °C (A), 75 °C (B), 80 °C (C), 85 °C (D) and 95 °C (E) with associated LC-MS spectra of aliquots withdrawn at regular time intervals.

Table S1. Summary of the reaction rate constants (k) as a function of temperature.

Temperature (°C)	Temperature (K)	1000/T	k (min ⁻¹)	ln(k)
70	343.15	2.914177	0.035	-3.33
75	348.15	2.872325	0.046	-3.08
80	353.15	2.831658	0.07	-2.66
85	358.15	2.792126	0.096	-2.34
95	368.15	2.716284	0.25	-1.36

Exchange on **2c** using excess dodecanethiol

Compound **2c** (100 mg, 0.4581 mmol, 1 eq.) was weighed in a pressure tube equipped with a stirring bar. Dodecanethiol (463.6 mg, 2.29 mmol, 5 eq.) was dissolved in 10 mL acetonitrile containing DBU (3.4868 mg, 0.0229 mmol, 0.05 eq) in a separate vial. This thiol solution was added to compound **2c** and heated 70 °C, after which aliquots (0.1 mL) were sampled at regular time intervals, quenched with 0.01 mL acetic acid solution in acetonitrile (0.02 M) and diluted with 0.9 mL of an acetonitrile solution containing trimethoxybenzene (TMB) (10 mg in 9 mL). These solutions were analysed using LC-MS and the signal corresponding to **2c** was followed over time. The reaction rate constants were obtained from the initial part of the slope of the fraction of starting product as a function of time.

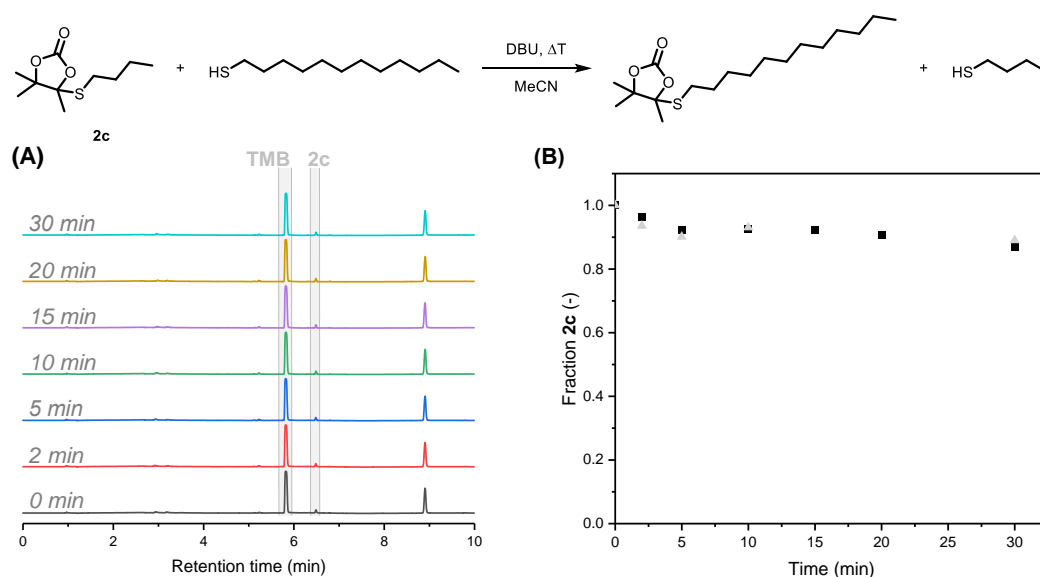


Figure S5. DBU catalysed associative exchange reaction between compound **2c** and dodecanethiol at 70 °C with (A) associated LC-MS spectra of aliquots withdrawn at regular time intervals and (B) Evolution of the fraction of **2c** over time using TMB as internal standard detected at 214 nm (a comparison with the exchange between **2b** and benzyl mercaptan is given in gray triangles).

Exchange on **2b** using 10 eq. benzylmercaptan

Compound **2b** (100 mg, 0.41243 mmol, 1 eq.) was weighed in a pressure tube equipped with a stirring bar. Benzyl mercaptan (512 mg, 4.12 mmol, 10 eq.) was dissolved in 10 mL acetonitrile containing DBU (0.00628 g, 0.04128 mmol, 0.1 eq) in a separate vial. This thiol solution was added to compound **2b** and heated at different temperatures (70, 75, 80, 85 and 95 °C). after which aliquots (0.1 mL) were sampled at regular time intervals, quenched with 0.01 mL acetic acid solution in acetonitrile (0.02 M) and diluted with 0.9 mL of an acetonitrile solution containing trimethoxybenzene (TMB) (10 mg in 9 mL). These solutions were analysed using LC-MS and the signal corresponding to **2b** was followed over time. The reaction rate constants were obtained from the initial part of the slope of the fraction of starting product as a function of time.

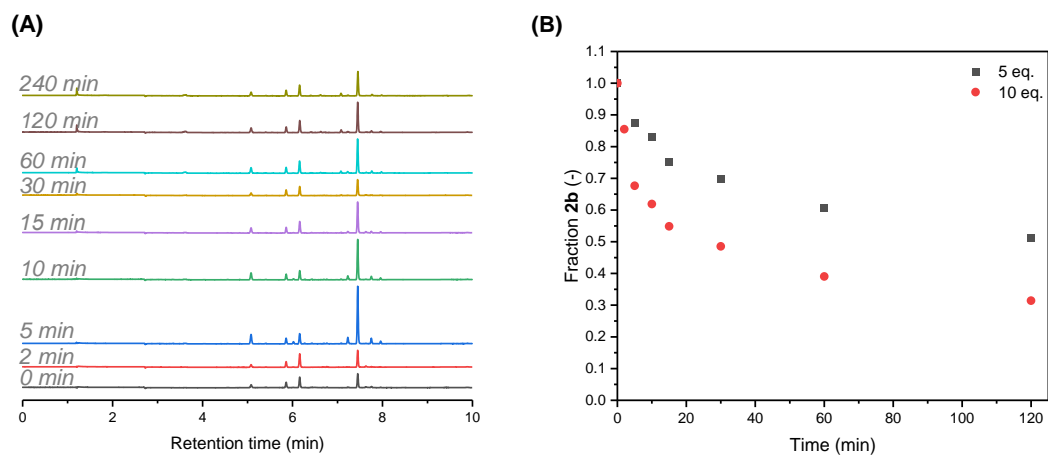


Figure S6. (A) LC-MS spectra measured at regular time intervals of the exchange reaction between compound **2b** and 10 equivalents benzyl mercaptan. (B) Evolution of the fraction **2b** over time compared to the exchange reaction with 5 equivalents benzyl mercaptan, an increase in reaction rate can be observed.

Density Functional Theory (DFT) calculations

Methodology

All calculations were performed using the quantum chemistry package Gaussian (version 16, Revision C.01).⁸ All structures were optimized using the range-separated hybrid functional wB97X-D,⁹ consistent with previously reported work on similar molecules.^{4,10} The 6-311++g(d,p) basis set was employed for all atoms and the conductor-like polarizable continuum model (CPCM)¹¹ was used with *N,N*-dimethylformamide as the solvent, providing implicit representation of the matrix environment. Confirmation of the stationary points, calculation of zero-point vibrational energies and thermal properties at standard conditions were performed by calculation of analytical normal modes. All transition states displayed one imaginary frequency and were further confirmed by Intrinsic Reaction Coordinate (IRC) calculations¹² leading to the pre- and post-reactive complexes. To consider enthalpic and entropic effects, the energies mentioned in this study correspond to the Gibbs free energy.

Results

The different reaction pathways are also discussed in the main manuscript. More detailed discussions are provided here with the corresponding Gibbs free energy profiles for all pathways including pre- and post-reactive complexes as determined by IRC calculations from the corresponding transition states. Because a divergent rheological behaviour was observed for the materials cross-linked with compound **5b** and **5c**, the calculations were conducted on both a dimethyl and a cyclohexyl model compound.

Pathway 1

Pathway 1 is a new pathway inspired by a mechanism reported in the alcoholysis of α CC to provide cyclic carbonate embedding *O,O*-acetal bonds, of similar structure to *S,O*-acetals studied in this work. However, thiols differ from alcohols in their pronounced acidity. While DBU loosely interacts with alcohols to facilitate reactions, thiols are prone to deprotonation by DBU to provide a thiolate and DBUH⁺.^{4,10} Therefore, a different mechanism can be expected, involving different transition states and intermediates.

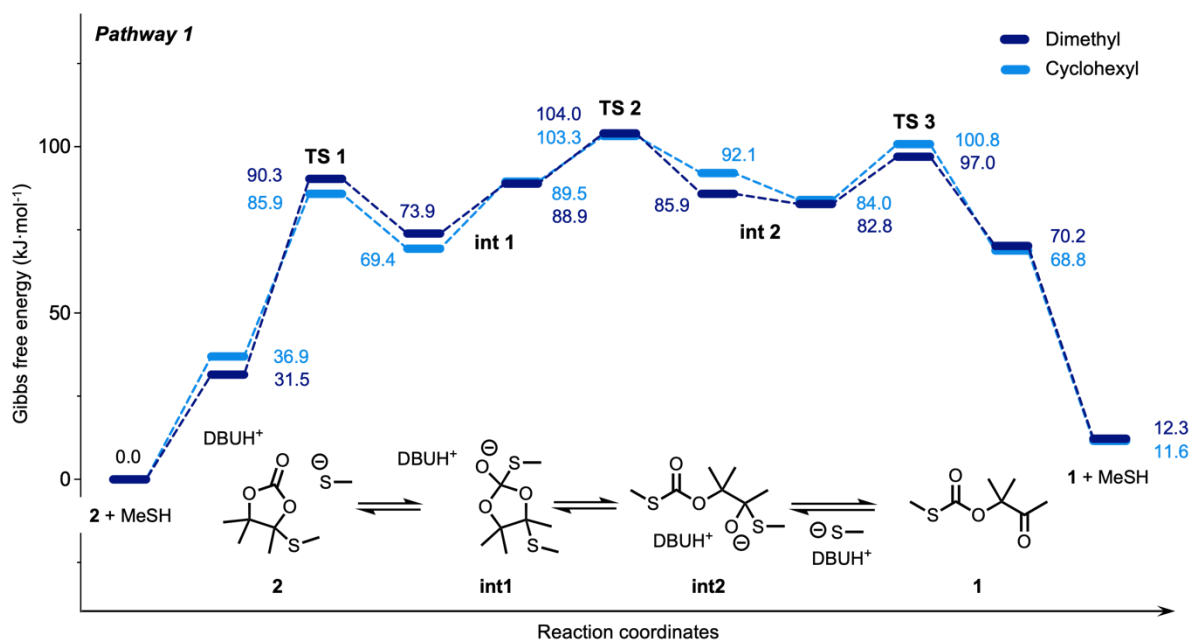


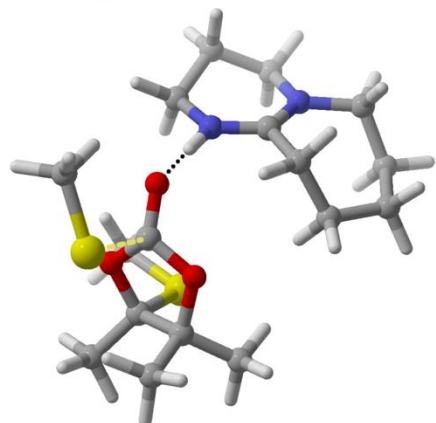
Figure S7. Gibbs free energy profile for pathway for the dimethyl- and cyclohexyl- α CC.

Pathway 1 consists of a three-step process starting from the cyclic carbonate embedding the *S,O*-acetal **2** to provide the thiocarbonate **1**. The reaction is triggered by the DBU-catalyzed addition of a thiol onto the ring. The first step involves an attack of the thiolate on the carbonate function (**TS1**, 90.3 kJ.mol⁻¹). Hereby, DBUH⁺ can act as a proton donor to render the carbonyl group more electrophilic and stabilize **TS1**. This step yields a tetrahedral intermediate **int1** which is highly destabilized (73.9 kJ.mol⁻¹) compared to the reactants. Subsequent rearrangement of DBUH to the oxygen atom of the *S,O*-acetal leads to another isomer of **int1** nearly as destabilized as **TS1** (88.9 kJ.mol⁻¹). This configuration leads to **TS2** (104.0 kJ.mol⁻¹) in which the ring is opened and the thiocarbonate group is formed. The formed alkoxide is stabilized by DBUH⁺, yielding a new tetrahedral intermediate **int2**. This step is rate-determining in Pathway 1. The last step involves the ejection of the thiolate (**TS3**, 97.0 kJ.mol⁻¹) to provide the thiocarbonate **1** which is a thermodynamically unfavored reaction. This result is in line with the experimentally observed spontaneous formation of **2** in the presence of DBU.

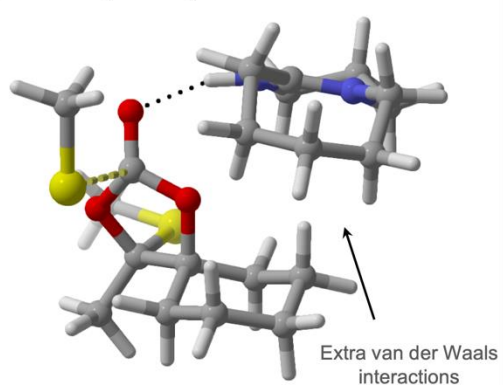
It must be noted that the backward reaction to yield **2** from **1** possesses an energy barrier of 91.7 kJ.mol⁻¹, of the rate-determining step which is 12.3 kJ.mol⁻¹ lower than the forward reaction. This rather small energy difference suggests reversibility and is therefore in line with the experimental observations.

The formation of **2** was previously studied and considered irreversible due to high energy barriers exceeding 150 kJ.mol⁻¹.⁴ In order to systematically compare the energy profile of the newly established pathways with the formerly proposed one, the latter was recalculated whereby DBU as the catalyst was included and the same thiol substrate was chosen (see Pathway 3). Since similar energy barriers as in the previous study were observed, we propose Pathway 1 to be more likely for the formation of compound **2** than the previously suggested mechanism (Pathway 3).

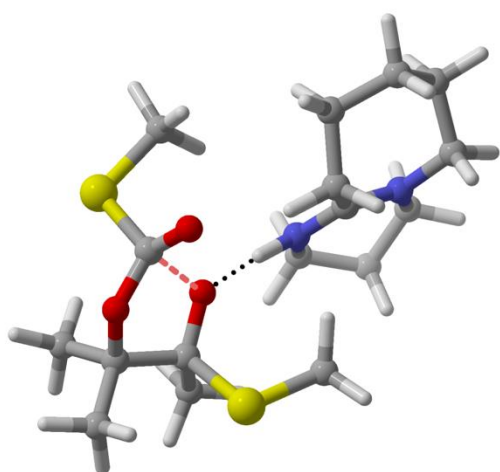
(A) TS1 – Dimethyl substituent



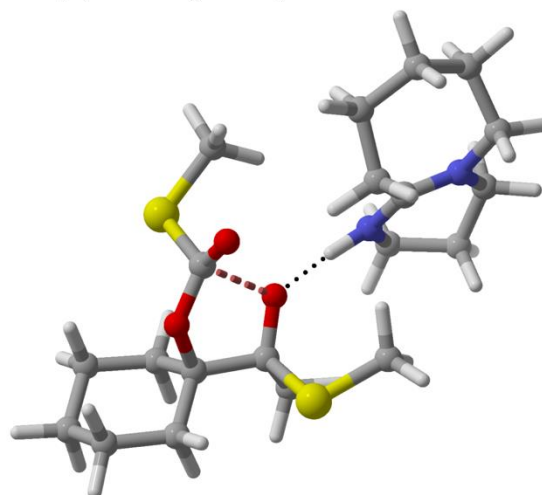
(B) TS1 – Cyclohexyl substituent



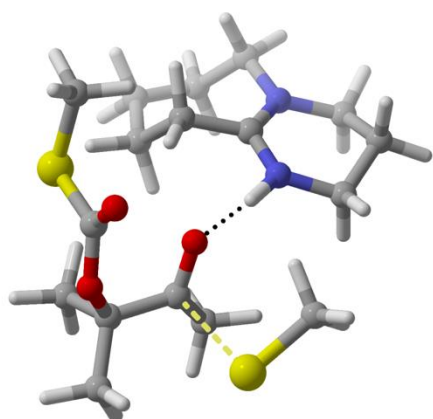
(C) TS2 – Dimethyl substituent



(D) TS2 – Cyclohexyl substituent



(E) TS3 – Dimethyl substituent



(F) TS3 – Cyclohexyl substituent

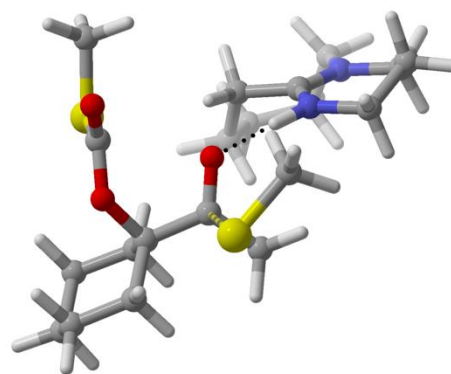


Figure S8. Optimized 3D structures for TS1, TS2 and TS3 in pathway 1 with both dimethyl and cyclohexyl substituents.

Pathway 2

Pathway 2 was modelled according to a previously reported pathway.⁴ However, DBU was not considered and one step of the process was therefore omitted. To be able to compare the herein proposed reaction pathways and their energetics, pathway 2 was thus modelled including DBU and using methanethiol as the thiol substrate.

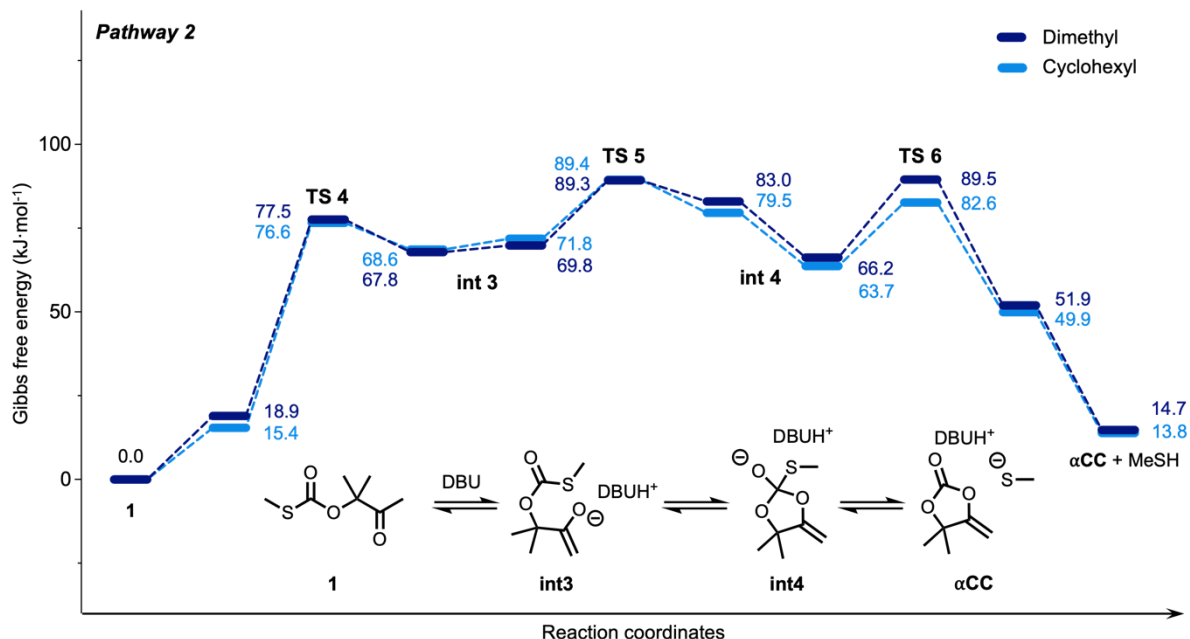
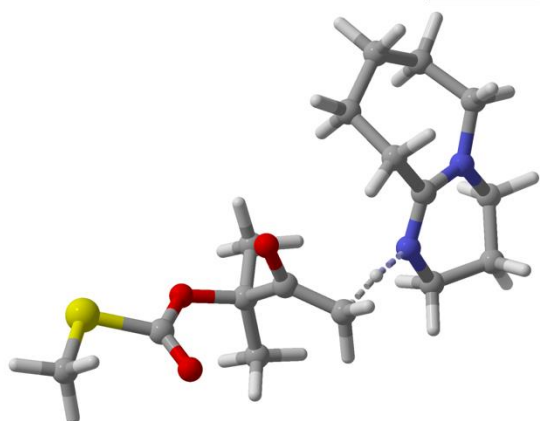


Figure S9. Gibbs free energy profile for pathway 2 for the dimethyl- and cyclohexyl- α CC.

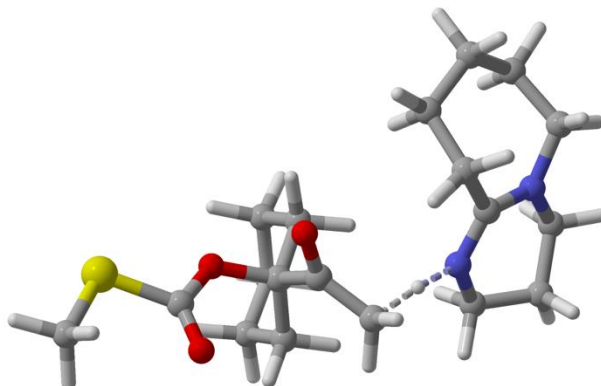
Since we are more interested in the dissociation, the thiocarbonate **1** and DBU were chosen as the starting reactants. However, the backward reaction energetics will be discussed and compared to previously reported values as well. Contrary to the previously reported pathway, the inclusion of DBU adds one step to the mechanism. Pathway 2 starts with the DBU-triggered H-abstraction from the ketone (**TS4**, 77.5 kJ.mol⁻¹) to provide an enolate **int3**. The transition state **TS5** (89.3 kJ.mol⁻¹) involving the attack of the oxygen of the enolate onto the carbonyl group of the thiocarbonate is further stabilized by DBUH⁺ and yields an unstable intermediate **int4** (83 kJ.mol⁻¹). **int4** becomes thermodynamically more stable through translation of DBUH⁺ to interact with the oxygen atom of the tetrahedral intermediate. The last step involves ejection of the thiolate and formation of α CC through **TS6** (89.5 kJ.mol⁻¹). The rate-determining step of this process is the last step involving **TS6** with an activation of 89.5 kJ.mol⁻¹. However, since **TS5** shows a very similar energy, the identification of the rate-determining step stays ambiguous. Overall, the reaction is thermodynamically unfavorable. This result is in line with the experimentally observed spontaneous formation of **1** in the presence of DBU.

The backward reaction from α CC to **1** has a lower energy barrier of 74.8 kJ.mol⁻¹, being 14.7 kJ.mol⁻¹ lower than the forward reaction. This small energy difference in energy suggests reversibility and is in line with the experimental observations. The previously reported energy barrier for the pathway (α CC to **1**) was 100.3 kJ.mol⁻¹. Our reported value is lower of 25.5 kJ.mol⁻¹ which can be rationalized by the fact that DBU was included in the calculations.

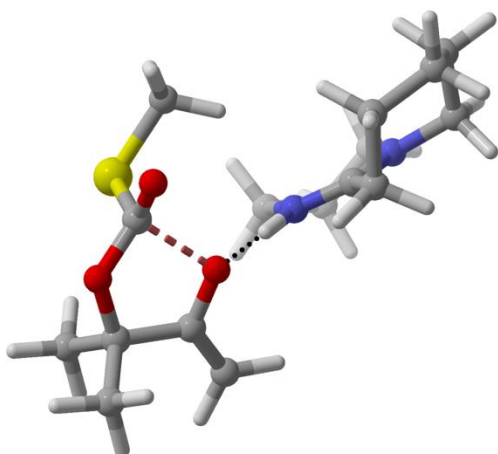
(A) TS4 – Dimethyl substituent



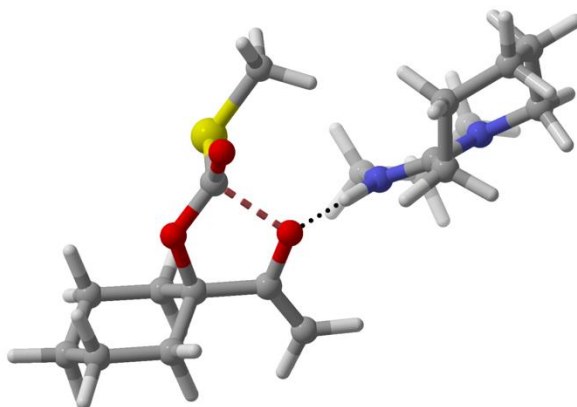
(B) TS4 – Cyclohexyl substituent



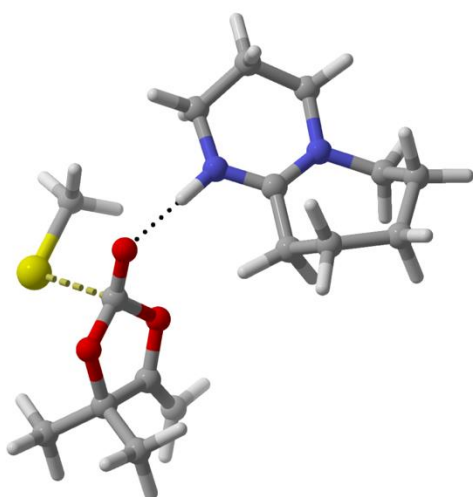
(C) TS5 – Dimethyl substituent



(D) TS5 – Cyclohexyl substituent



(E) TS6 – Dimethyl substituent



(F) TS6 – Cyclohexyl substituent

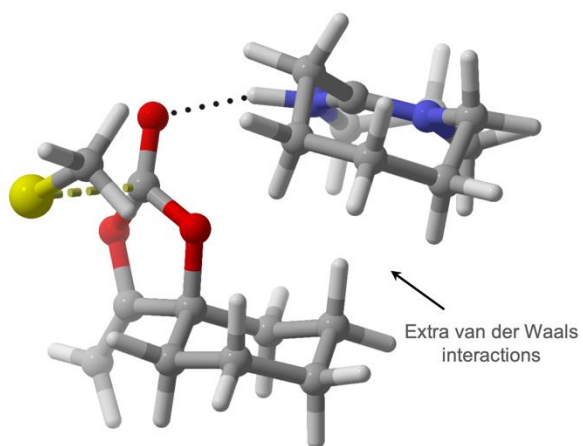


Figure S10. Optimized 3D structures for TS4, TS5 and TS6 in pathway 3 with both dimethyl and cyclohexyl substituents.

Pathway 3 (stepwise)

The stepwise Pathway 3 was modelled according to the previously reported pathway.⁴ However, since in former calculations DBU was not considered in the first step (only the second one) and the model included benzyl mercaptan, the same pathway was therefore reinvestigated with methanethiol as simple thiol and considering DBU in all steps.

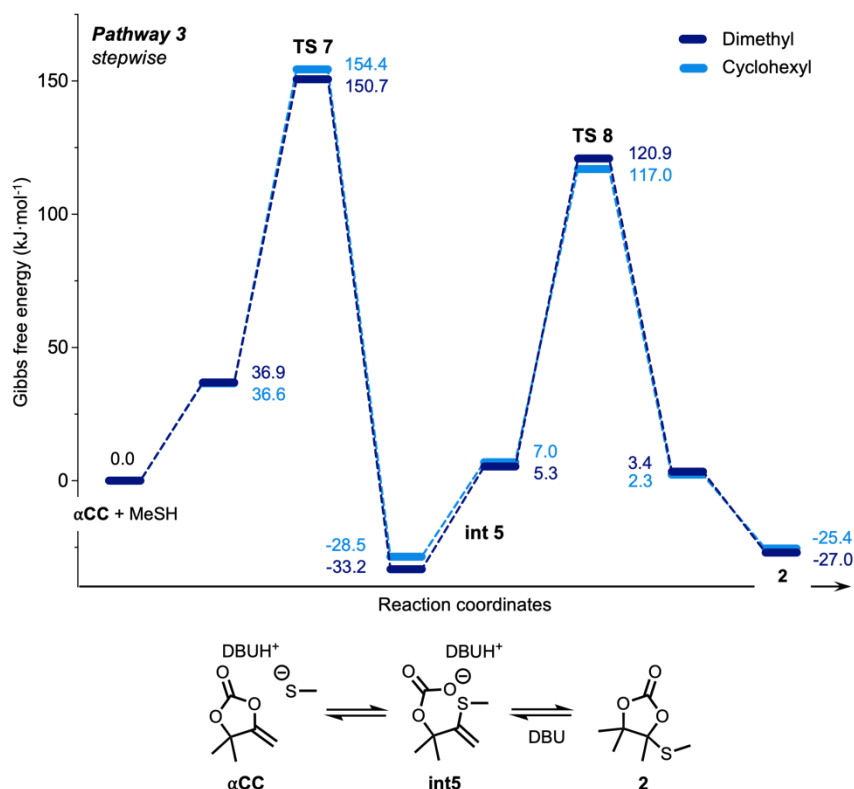
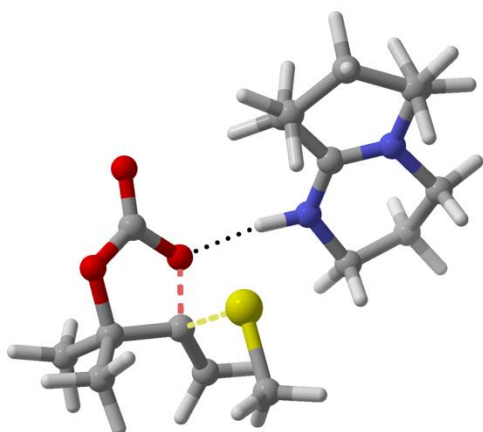


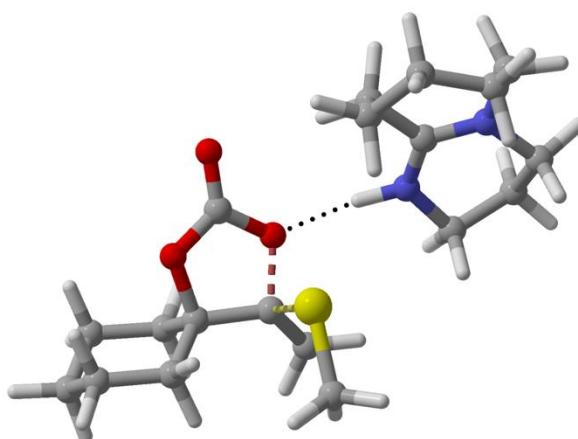
Figure S11. Gibbs free energy profile for pathway 3 (stepwise) for the dimethyl- and cyclohexyl- α CC are represented.

Similarly to the previous report, a two-step pathway was calculated resulting in similar transition state and intermediate structures. The first step involves the attack of the thiol onto the internal carbon of the exovinylene moiety with concomitant ring-opening of the ring through the C-O bond (**TS7**). The released carbonate group is stabilized by DBUH⁺. In a second step, the ring is closed assisted by proton transfer from DBUH⁺ to the external carbon of the alkene group (**TS8**). Despite the extra interaction by DBUH⁺ in **TS7** compared to the previous work, a very similar energy barrier was determined (150.7 kJ·mol⁻¹ in this work; 155.6 kJ·mol⁻¹ in the previous work) confirming that the role of DBU is negligible in the first step

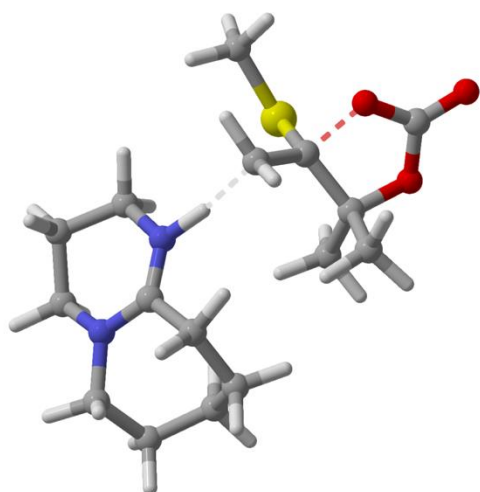
(A) TS7 – Dimethyl substituent



(B) TS7 – Cyclohexyl substituent



(C) TS8 – Dimethyl substituent



(D) TS8 – Cyclohexyl substituent

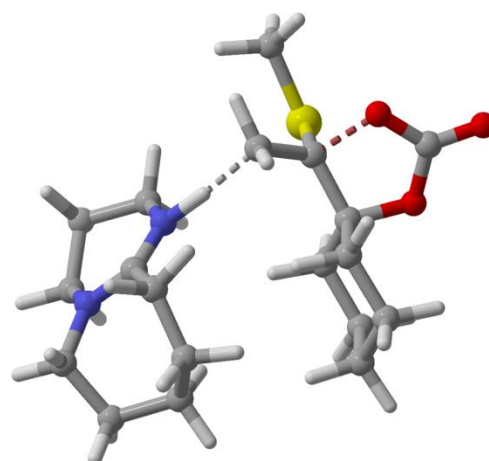


Figure S12. Optimized 3D structures for TS7 and TS8 in pathway 3 (stepwise) with both dimethyl and cyclohexyl substituents.

Pathway 3 (concerted)

The concerted pathway 3 was modelled according to the previously reported pathway in a similar fashion but again replacing benzyl mercaptan with methanethiol.

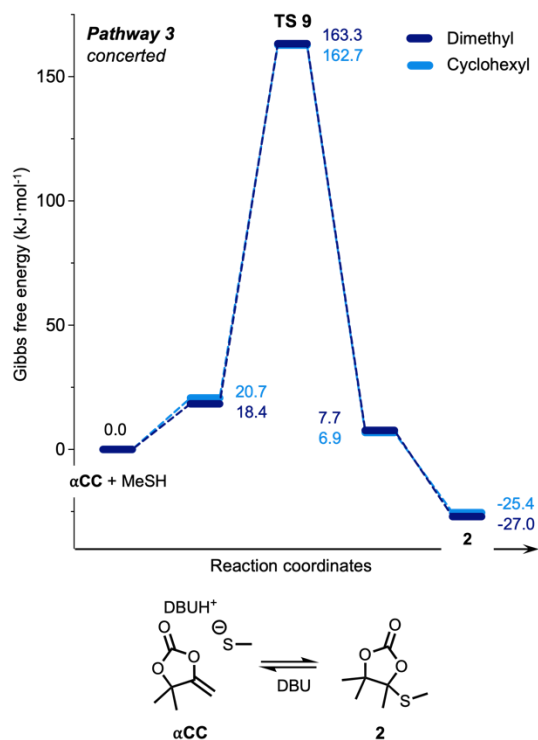
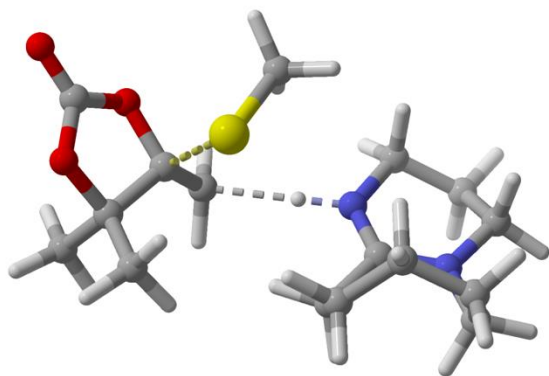


Figure S13. Gibbs free energy profile for pathway 3 (concerted) for the dimethyl- and cyclohexyl- α CC are represented.

The concerted pathway 3 involves only one step, namely the attack of the thiol onto the internal carbon of the exovinylene moiety with concomitant proton transfer from DBUH⁺ to the external carbon of the alkene group (TS9). The determined energy barrier agreed with the previously reported value (163.3 kJ·mol⁻¹ in this work; 168.1 kJ·mol⁻¹ in the previous work).

(A) TS9 – Dimethyl substituent



(B) TS9 – Cyclohexyl substituent

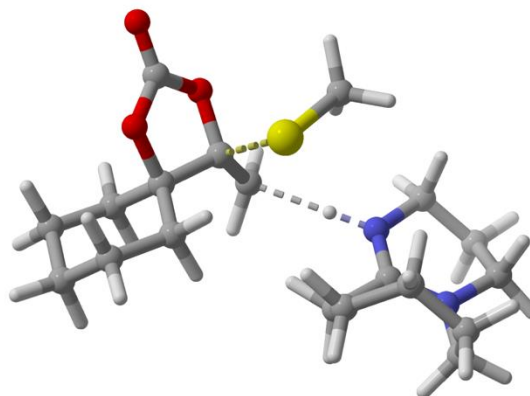


Figure S14. 3D structures for TS9 in pathway 3 (concerted) with both dimethyl and cyclohexyl substituents.

Effect of substituent

It was found that the introduction of the cyclohexyl substituent did not profoundly affect the reaction pathways, with only minor differences in the structures reflected in small changes in Gibbs free energy.

In pathway 1, **TS1** was characterized by a lowering of the TS energy (90.3 to 85.9 kJ.mol⁻¹, 4.4 kJ.mol⁻¹). This difference was ascribed to a change in DBU orientation within the TS to favor van der Waals interactions between the cyclohexyl ring and the cycloaliphatic ring on DBU (**Figure S8**). However, the rate-limiting step was only slightly altered by 0.7 kJ.mol⁻¹, suggesting no effect on the effective reaction rate. In pathway 2, a similar transition state stabilization was observed on **TS6** (89.5 to 82.6 kJ.mol⁻¹, 6.9 kJ.mol⁻¹). However, the other transition states of the pathway were only slightly impacted (< 1 kJ.mol⁻¹). Although the rate-determining step was difficult to identify for the dimethyl-substituent due to very close energies for **TS5** and **TS6**, the stabilization of **TS6** suggests **TS5** (89.4 kJ.mol⁻¹) to be the rate-determining step in this case. However, the overall energy barrier stays very similar in the case of both substituents. No significant changes were neither observed in Pathway 3 stepwise and Pathway 3 concerted. All 3D structures of transition states are displayed for each pathway in **Figure S8**, **Figure S10**, **Figure S12** and **Figure S14**.

Material characterisation

Thermal analysis of the covalent adaptable networks

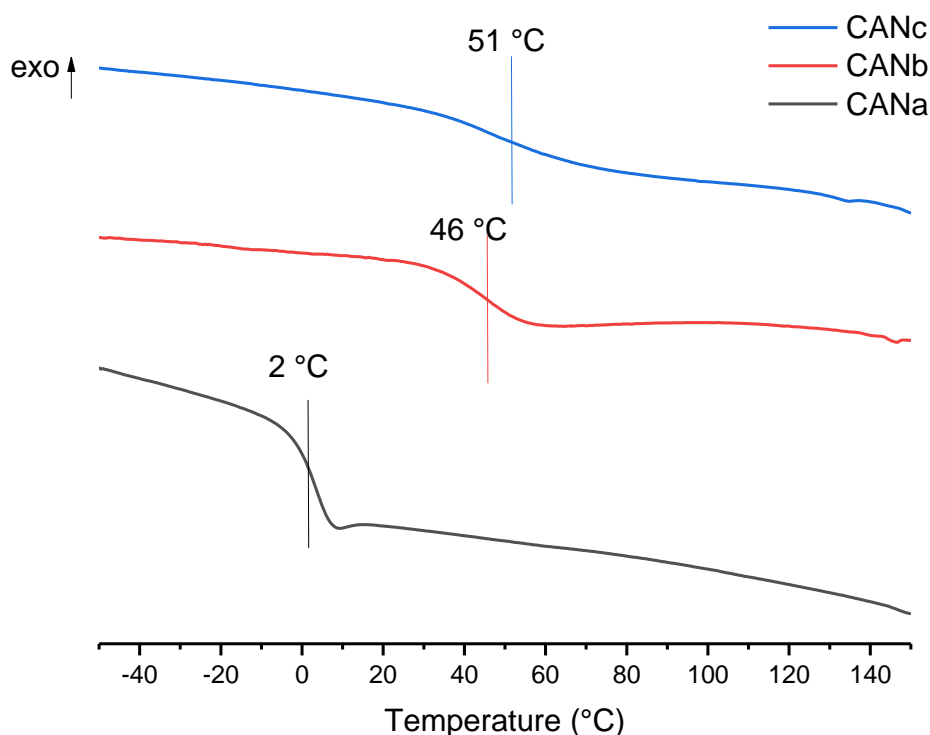


Figure S15. DSC thermograms of the second heating step for CANa-c, measured at a heating rate of 10 °C min⁻¹

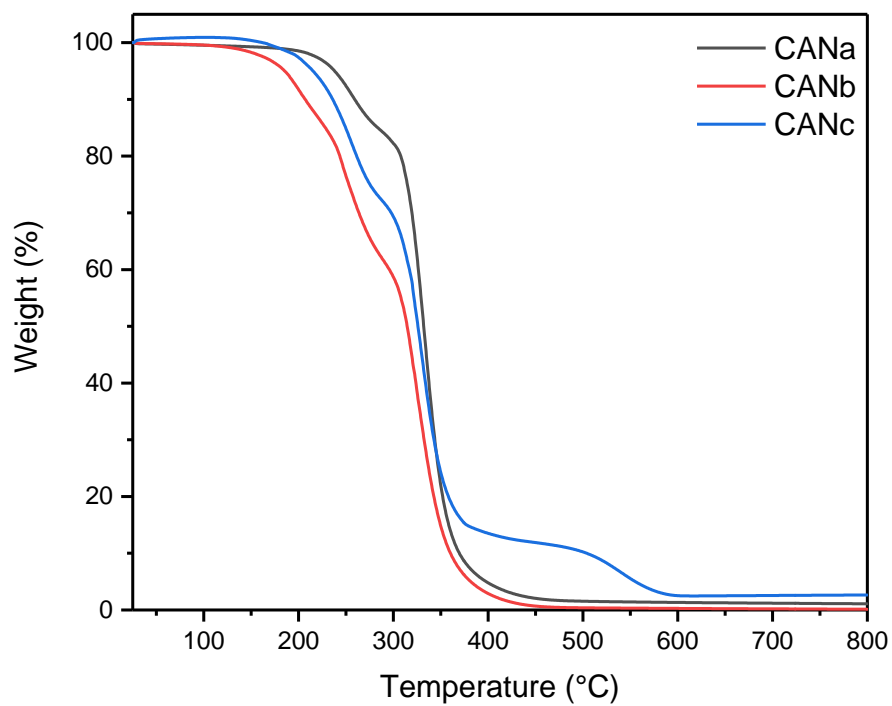


Figure S16. TGA thermogram for CANa-c measured with a temperature ramp of $10^{\circ}\text{C min}^{-1}$.

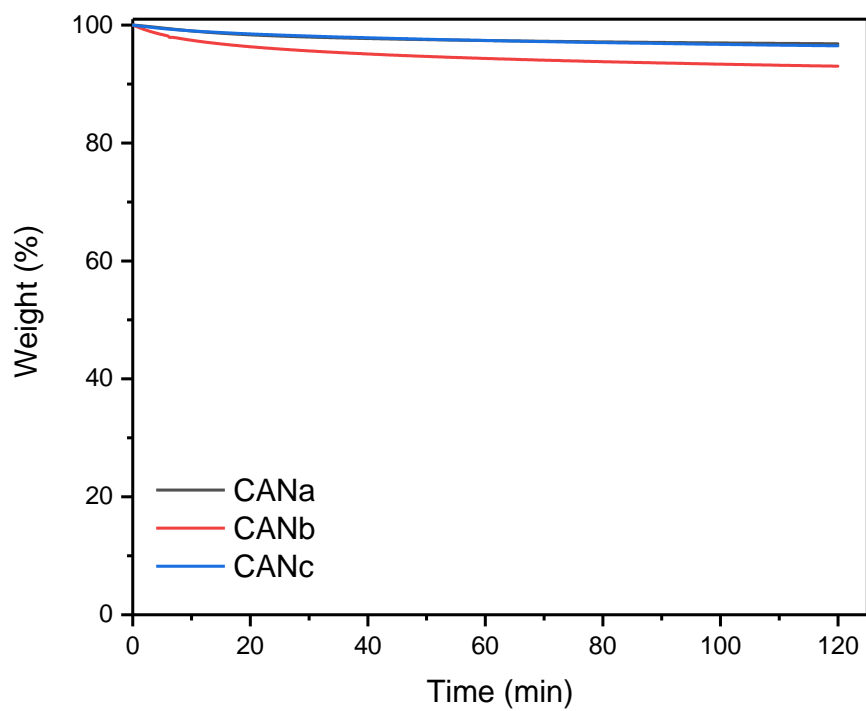


Figure S17. Isothermal TGA thermogram at 130°C for 120 minutes.

Rheological analysis of the Covalent Adaptable Networks

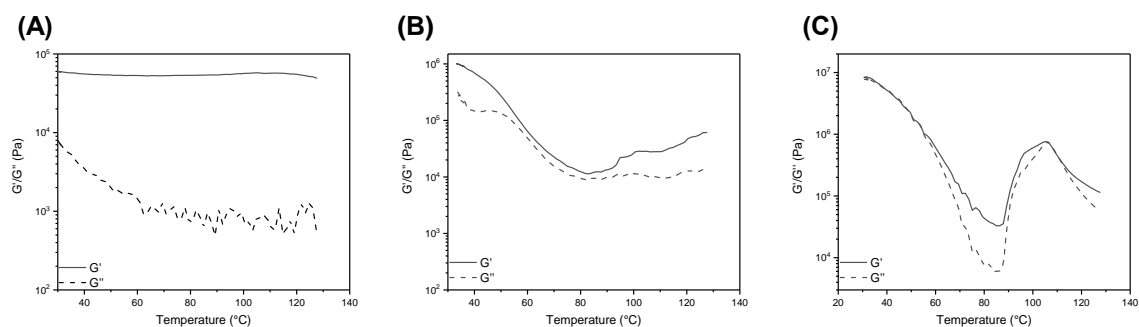


Figure S18. Temperature sweep rheological analysis of CAN-a (A), CAN-b (B) and CAN-c (C) between 30 and 130°C.

Stress-relaxation experiments were conducted at different temperatures for all materials. Fitting to single ($G(t) = G_0 e^{\frac{-t}{\tau_{single}}}$), stretched ($G(t) = G_0 e^{(\frac{-t}{\tau_{stretched}})^\beta}$), and multiple (n) single element ($G(t) = \sum_{i=1}^n G_{0,i} e^{\frac{-t}{\tau_i}}$) Maxwell models was conducted and specific care was taken to correctly assign the possible exchange chemistry with the correct relaxation mode.

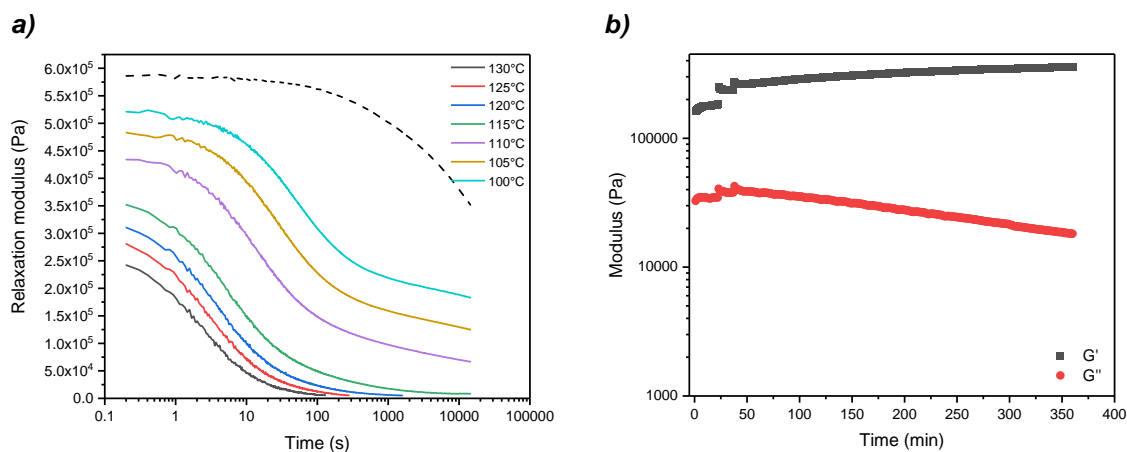


Figure S19. Rheological analysis of CAN-a (prepared using the bis(α CC) with a polyether backbone). a) Stress-relaxation profile of the CAN, the dashed line represents a cycling to the highest temperature after the final stress-relaxation measurement. b) Time-sweep experiments on CAN-a, an increase in storage modulus (G') and decrease in loss modulus (G'') can be observed, pointing towards additional cross-linking during the measurement.

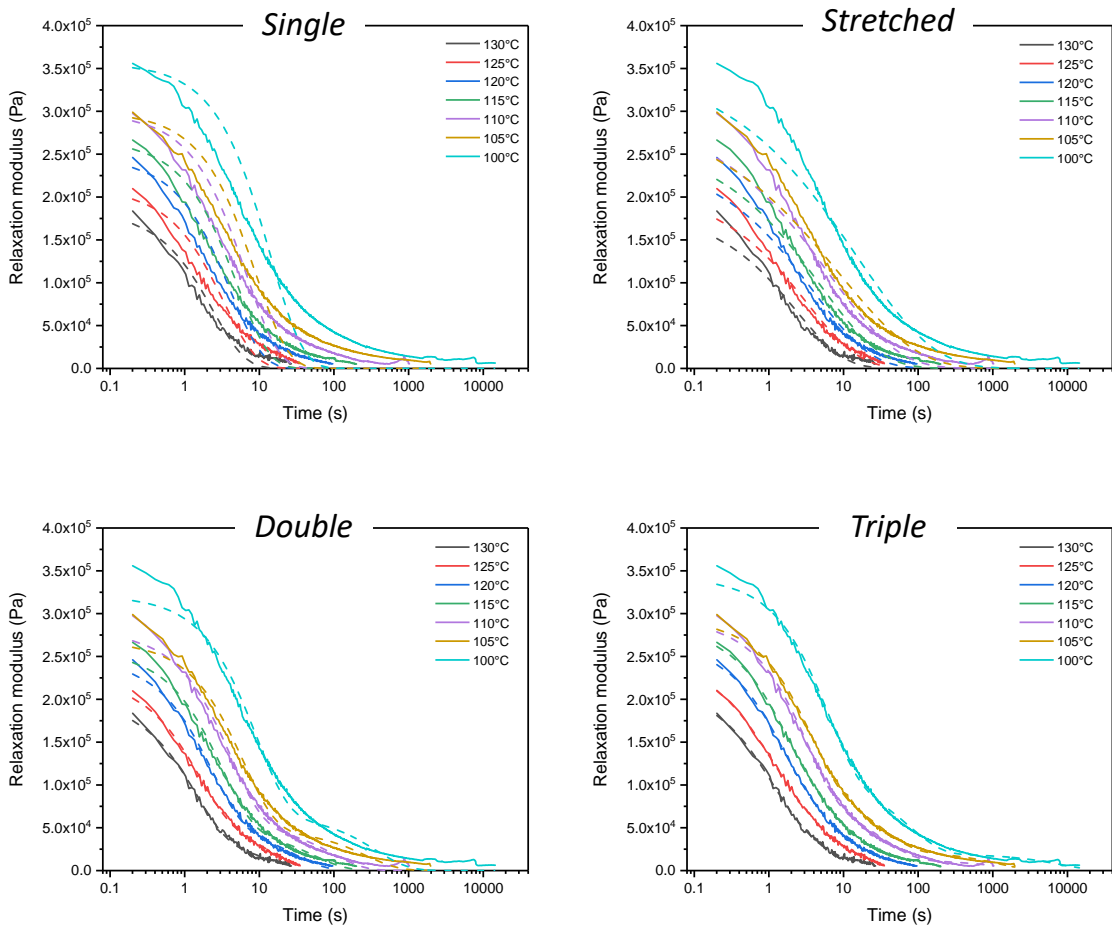


Figure S20. Non-normalized stress-relaxation profile of CAN-b, with fitting to a single Maxwell element, a stretched Maxwell element, a double Maxwell and triple Maxwell element presented in dashed lines.

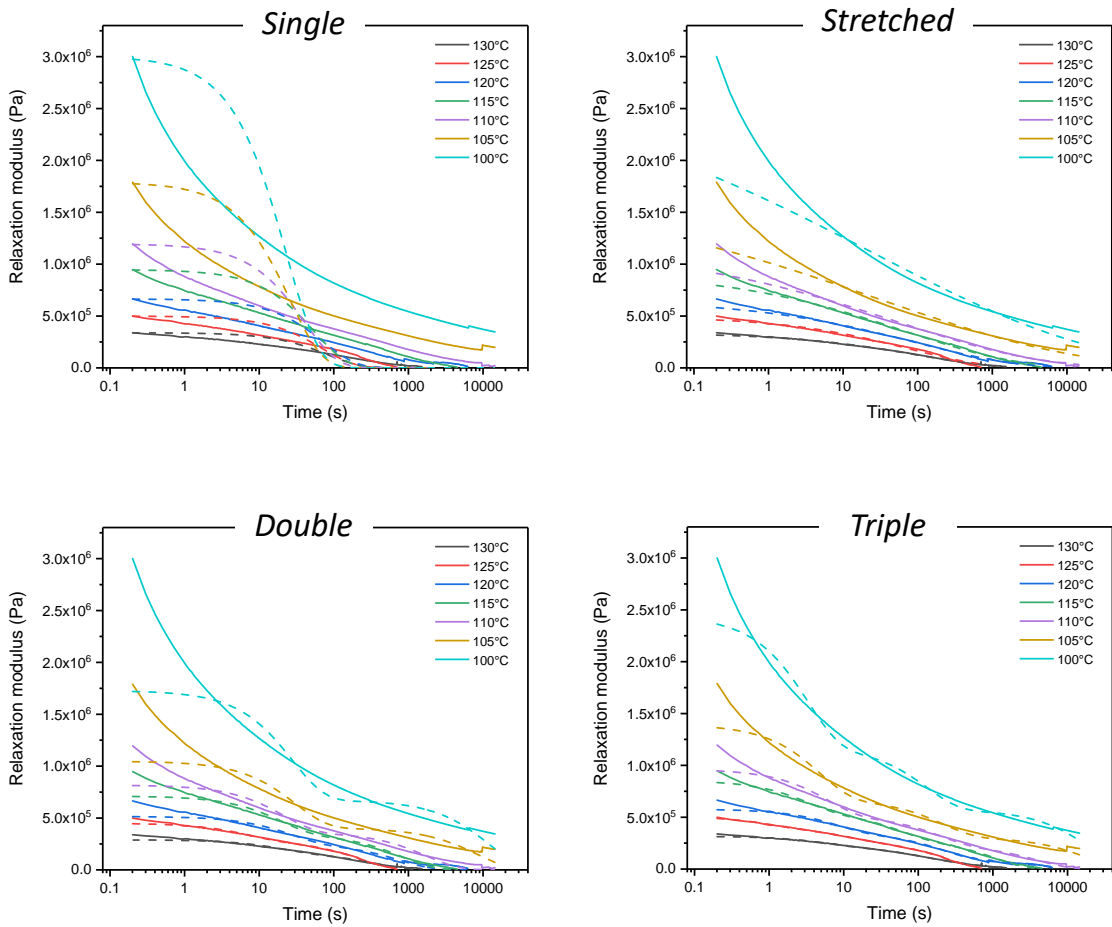


Figure S21. Non-normalized stress-relaxation profile of CAN-c, with fitting to a single Maxwell element, a stretched Maxwell element, a double Maxwell and triple Maxwell element presented in dashed lines.

Material properties after reprocessing of CAN-c

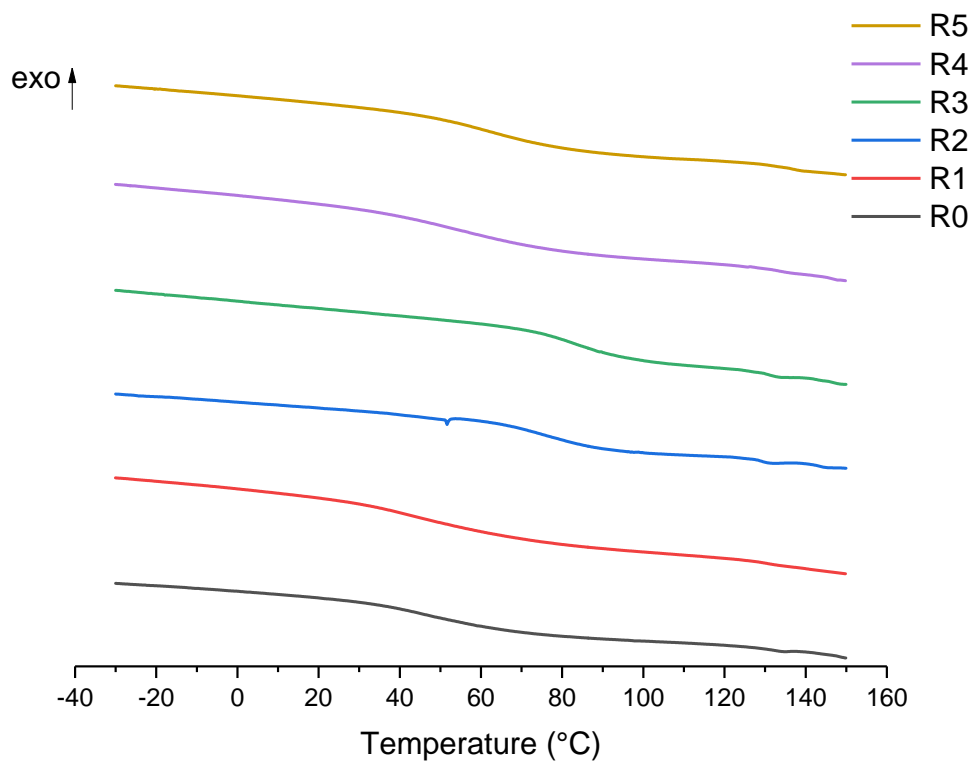


Figure S22. DSC thermograms of the second heating step for reprocessed samples of CAN-c, measured at a heating rate of $10\text{ }^{\circ}\text{C min}^{-1}$

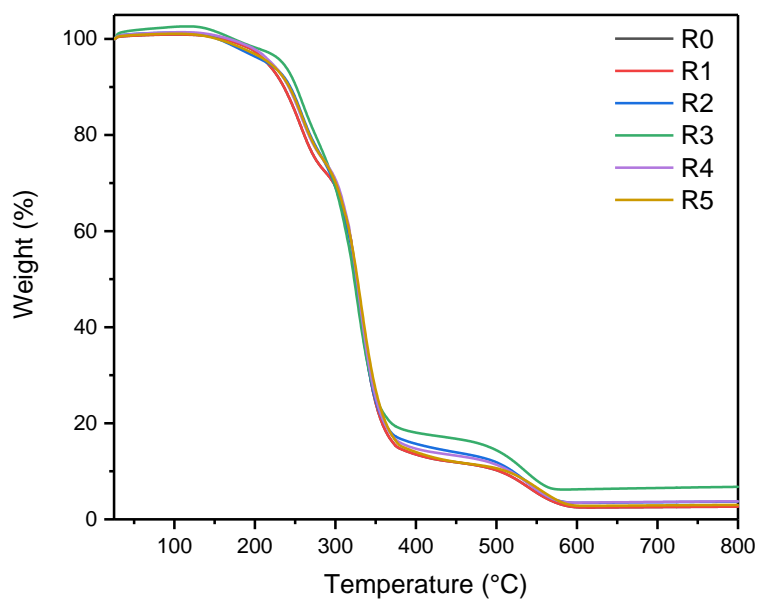


Figure S23. TGA thermograms for reprocessed sample of CAN-c measured with a temperature ramp of $10\text{ }^{\circ}\text{C min}^{-1}$.

Table S2. Summary of the glass transition temperatures and degradation temperatures over the different reprocessing cycles on CAN-c

	T _g (°C)	T _{deg,5%} (°C)
R0	51	215
R1	39	215
R2	72	215
R3	91	234
R4	66	221
R5	63	218

Properties of the coating

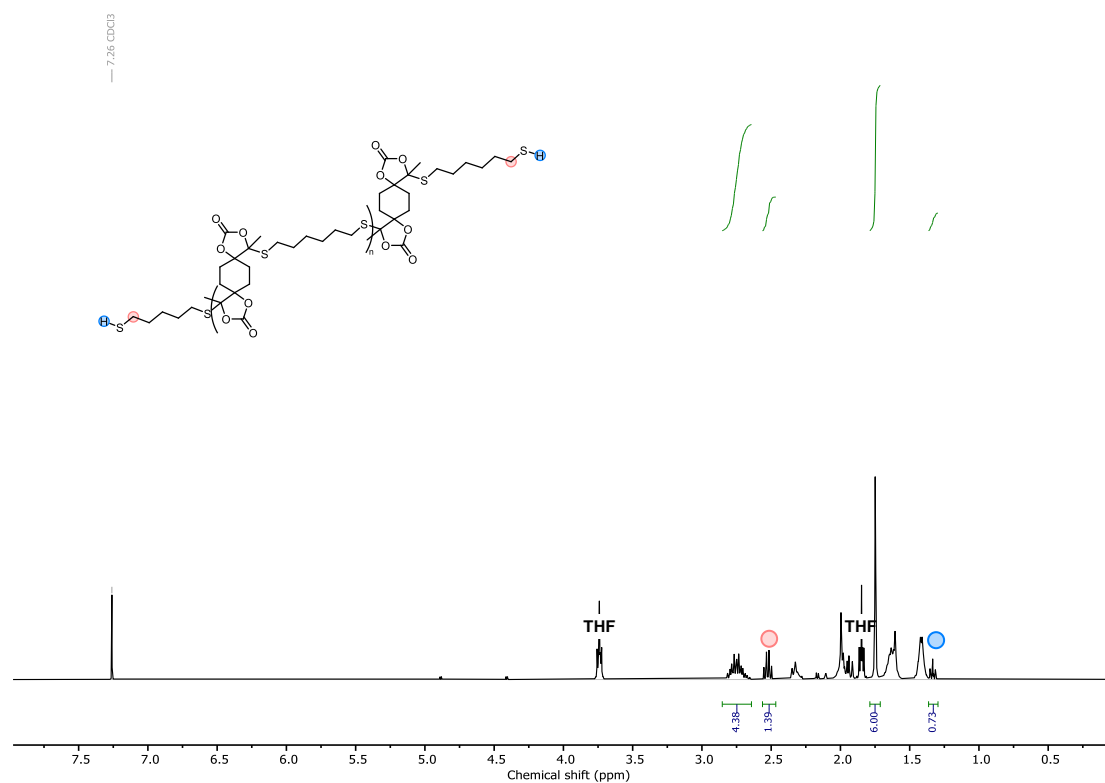


Figure S24. ¹H-NMR (400 MHz, CDCl₃) spectrum of the prepolymer obtained from 5c and 1,6-hexanedithiol, with indication of the -SH and -CH₂-SH signals.

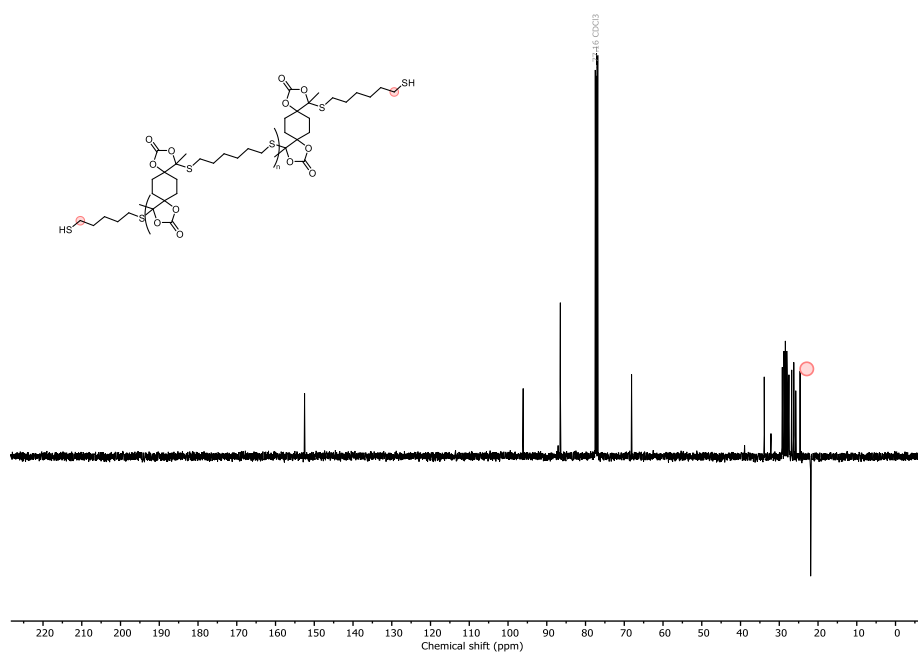


Figure S25. ^{13}C -APT NMR (400 MHz, CDCl_3) spectrum of the prepolymer obtained from 5c and 1,6-hexanedithiol, with indication of the $-\text{CH}_2\text{-SH}$ signal.

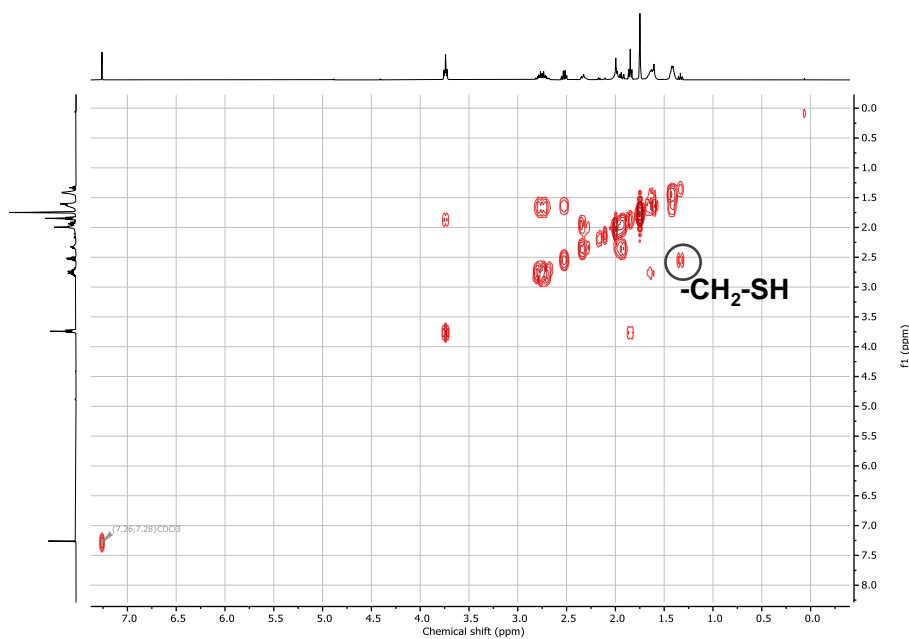


Figure S26. COSY NMR (400 MHz, CDCl_3) spectrum of the prepolymer obtained from 5c and 1,6-hexanedithiol a cross peak related to the thiol end-groups is visible.

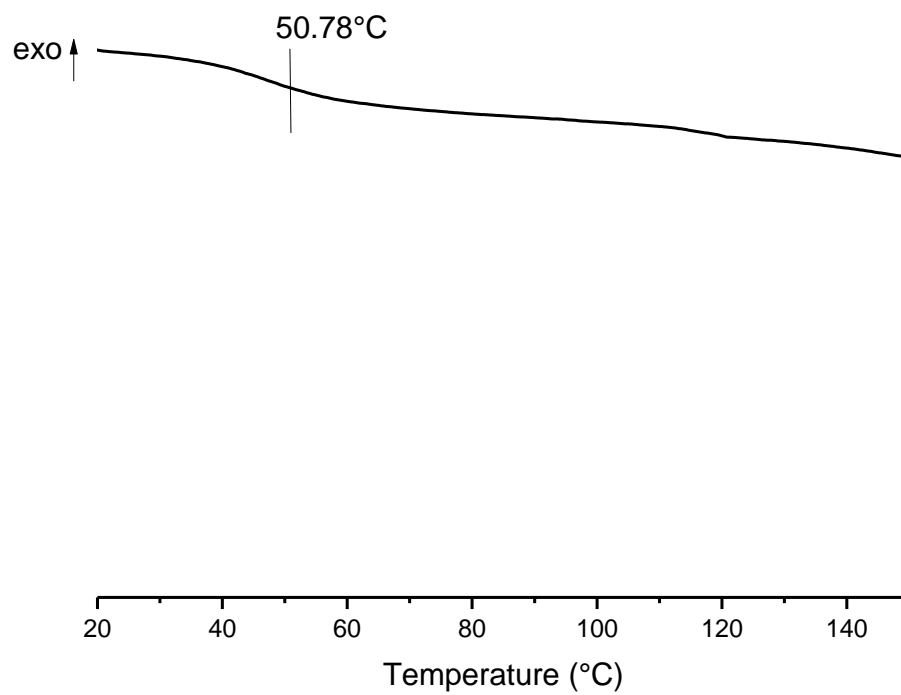


Figure S27. DSC-thermogram of the coating sample prepared from **5c**, 1,6-hexanedithiol and 1,2,4-trivinylcyclohexane, measured with a temperature ramp of 10 °C min⁻¹.

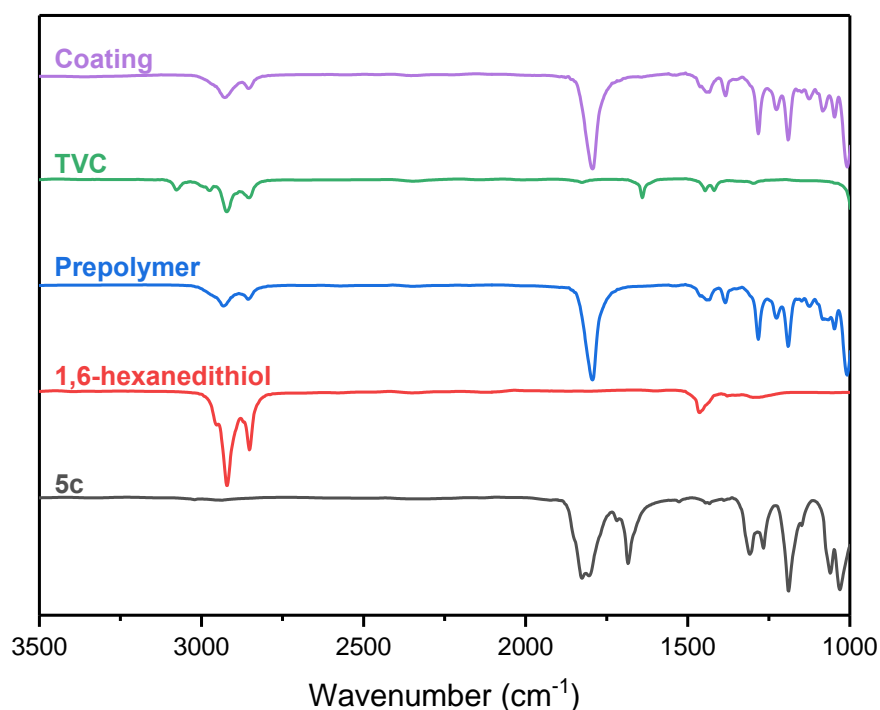


Figure S28. FTIR spectrum of the coating sample prepared from **5c**, 1,6-hexanedithiol and 1,2,4-trivinylcyclohexane.

DFT XYZ-coordinates

aCC (dimethyl)

C	-0.72127000	-0.48869300	0.00001500
C	1.54529400	-0.11585600	-0.00075000
O	2.72552200	-0.29523900	0.00018200
O	0.61939800	-1.06544500	-0.00046500
O	0.97808300	1.11255700	0.00018100
C	-0.39830300	0.99170800	-0.00002200
C	-1.19983100	2.03972800	-0.00009400
H	-0.80618300	3.04737600	0.00001500
H	-2.27189200	1.89526300	-0.00026500
C	-1.43114100	-0.93682100	1.26734500
H	-2.42167600	-0.47979600	1.30943700
H	-1.54710500	-2.02225900	1.26493000
H	-0.87055500	-0.63572500	2.15368700
C	-1.43205600	-0.93697600	-1.26670800
H	-1.54832400	-2.02238100	-1.26391500
H	-2.42250200	-0.47972600	-1.30831500
H	-0.87194000	-0.63627900	-2.15347600

aCC (cyclohexyl)

C	-1.86510500	-0.99922800	0.00158900
O	-2.60213500	-1.93869800	0.00099800
O	-0.54079500	-1.05655200	0.00228300
O	-2.29420500	0.28357800	-0.00108100

C	-1.20795700	1.13817500	-0.00061400
C	-1.34392100	2.45085700	-0.00123700
H	-2.32143400	2.91433700	-0.00206500
H	-0.46431700	3.08036400	-0.00077000
C	0.03836700	0.28425600	0.00013800
C	0.87515900	0.44706300	-1.26877100
C	0.87648300	0.45075600	1.26760600
C	2.11066700	-0.45353100	-1.25972100
H	1.17881500	1.49839300	-1.31889800
H	0.24535100	0.25158100	-2.14065500
C	2.11205300	-0.44977500	1.25995600
H	1.18018200	1.50224200	1.31424500
H	0.24760400	0.25788100	2.14073700
C	2.94985900	-0.23374000	-0.00067200
H	2.70299300	-0.25428800	-2.15637300
H	1.79584700	-1.50128300	-1.31253100
H	2.70533800	-0.24777400	2.15535000
H	1.79736300	-1.49738600	1.31628700
H	3.80968000	-0.90891600	-0.00015600
H	3.34603400	0.78923300	-0.00241500

DBU

C	0.34308900	-0.72037900	-0.30970300
C	1.53639200	1.37008900	0.12880400
H	1.61221400	2.30628700	-0.42993600
H	1.42344900	1.62922100	1.19063000
C	2.78019300	0.52490200	-0.07817700
H	2.97817600	0.42642600	-1.15058600
H	3.64455500	1.01355600	0.37729400
C	2.54526400	-0.85110600	0.52937700
H	3.38195000	-1.51701900	0.29886400
H	2.51167200	-0.76659300	1.62441100
C	-1.92703600	1.28229800	0.50803100
H	-2.56497500	2.17152300	0.48468200
H	-1.44480100	1.26326100	1.49245600
C	-0.84671000	1.44145600	-0.56647900
H	-1.26885000	1.21899600	-1.55310200
H	-0.52287000	2.48250400	-0.60114100
C	-2.05289100	-1.28428300	0.33490600
H	-1.61724600	-1.45573800	1.32649800
H	-2.77230100	-2.09138400	0.16846000
C	-0.94127700	-1.40295500	-0.72133800
H	-0.68763200	-2.45246900	-0.86700800
H	-1.29759300	-1.01527100	-1.68194900
N	0.35990000	0.64945500	-0.34548400
C	-2.80466000	0.04618700	0.31652500
H	-3.57861800	0.02965500	1.09032700
H	-3.32807000	0.13929100	-0.64390500
N	1.31677900	-1.48081200	0.06295800

DBUH+

C	0.30029700	-0.65324600	-0.29807600
C	1.51266600	1.40695100	0.14696900
H	1.53905200	2.33391800	-0.42494700
H	1.41210400	1.66365700	1.20575300

C	2.77086300	0.59649000	-0.10728900
H	2.94117800	0.50674300	-1.18303700
H	3.62703600	1.11115400	0.32819100
C	2.62494900	-0.78332200	0.50659200
H	3.42848200	-1.44751200	0.19153200
H	2.62771300	-0.73212300	1.59858900
C	-2.00918600	1.27286600	0.48022500
H	-2.66629700	2.14388700	0.41167400
H	-1.56720000	1.28823300	1.48237200
C	-0.89776600	1.45857500	-0.55166100
H	-1.25437400	1.22937800	-1.55986200
H	-0.57313900	2.49734100	-0.56072300
C	-2.05954700	-1.29692800	0.34951300
H	-1.63794400	-1.43625700	1.35060000
H	-2.74389600	-2.13093000	0.18009800
C	-0.93386500	-1.40741100	-0.69465100
H	-0.65735000	-2.45301700	-0.83245000
H	-1.27834100	-1.04154400	-1.66602300
N	0.31266200	0.66626400	-0.27327600
C	-2.84527200	0.01056400	0.27763000
H	-3.63986500	-0.01478800	1.02812600
H	-3.34046400	0.07038800	-0.69910500
N	1.36206900	-1.35953200	0.05588800
H	1.28135000	-2.36289100	0.01541700

Methanethiol

C	-1.15763200	0.01952200	0.00000200
H	-1.52800200	-1.00497000	-0.00019300
H	-1.51695500	0.52751800	-0.89335400
H	-1.51698800	0.52720300	0.89352300
S	0.66209400	-0.08739000	0.00000100
H	0.91423300	1.23136000	-0.00000100

Methanethiolate-

C	0.00000000	0.00000000	-1.13053900
H	0.00000000	1.01889700	-1.52724500
H	-0.88239000	-0.50944800	-1.52724500
H	0.88239000	-0.50944800	-1.52724500
S	0.00000000	0.00000000	0.71031000

Thiocarbonate 1 (dimethyl)

O	-0.81814900	0.96993300	0.84596400
C	-1.00381800	-0.01348900	0.17783100
O	-0.07205000	-0.87163800	-0.23506200
S	-2.57879800	-0.56287100	-0.41959800
C	-3.62842500	0.73704500	0.27838700
H	-4.64441700	0.49970700	-0.03586800
H	-3.34061400	1.71032700	-0.11438600
H	-3.56987700	0.73193500	1.36509600
C	1.31497100	-0.62070400	0.10638600
C	1.72824000	0.75943800	-0.44976400
C	1.52840400	-0.79495300	1.60668600
H	2.59468100	-0.78744600	1.83761600
H	1.03776100	-0.01225400	2.18359200
H	1.12638600	-1.76421000	1.90825000

C	2.09083500	-1.67291800	-0.68505300
H	1.87328500	-1.58552100	-1.75066100
H	1.80666300	-2.66901300	-0.34070700
H	3.16419600	-1.54773100	-0.53032200
O	1.16635800	1.21594300	-1.41792700
C	2.88621000	1.44918100	0.21207500
H	2.58792200	1.77120700	1.21384000
H	3.18398200	2.31463600	-0.37708000
H	3.73303300	0.76879900	0.33110400

Thiocarbonate 1 (cyclohexyl)

O	-1.53124400	0.79732400	1.04875000
C	-1.42240900	0.02957000	0.12839200
O	-0.29882400	-0.27532000	-0.51583200
S	-2.75023800	-0.89604600	-0.59418800
C	-4.11391600	-0.31664400	0.44653200
H	-5.00402900	-0.83023500	0.08432500
H	-4.24237600	0.75889600	0.34114800
H	-3.93680100	-0.57916000	1.48772700
C	0.94265500	0.35676900	-0.11292900
C	0.79111600	1.88390800	-0.25703400
C	1.96020100	-0.10108600	-1.17144200
C	1.36546000	-0.12555700	1.28080000
O	0.00612900	2.34003200	-1.05650200
C	1.69349500	2.75603300	0.56783200
H	1.41432000	2.66822600	1.62175700
H	1.59378700	3.79166800	0.24781000
H	2.73531500	2.43768600	0.48217600
C	1.57482500	-1.64027000	1.31536700
H	0.63276000	0.18821000	2.02517300
H	2.31065100	0.36576100	1.52997900
C	2.60044000	-2.07977500	0.27033600
H	0.62195300	-2.14994500	1.13442100
H	1.90202800	-1.92975500	2.31728800
C	2.19515500	-1.61222400	-1.12723600
H	2.71278100	-3.16732100	0.28403400
H	3.57902300	-1.65427200	0.52625400
H	2.90251400	0.42384900	-0.98167800
H	1.60390500	0.21068200	-2.15650700
H	1.28006800	-2.12792700	-1.43512700
H	2.96728100	-1.87027400	-1.85681200

Cyclic acetal 2 (dimethyl)

C	-0.89161000	1.55708700	-0.04620900
O	-1.48825300	0.58178500	-0.72870100
O	-1.15237000	2.72081600	-0.14257100
O	0.04542500	1.06216000	0.78028000
C	-1.07601500	-0.71189000	-0.19191800
C	0.29028500	-0.31943500	0.44371200
C	-1.02628200	-1.71091300	-1.32984100
H	-0.42262300	-1.34825000	-2.16154900
H	-2.03830800	-1.89926500	-1.69175200
H	-0.60923700	-2.65467600	-0.97241000
C	0.67569200	-1.06592100	1.70165500
H	-0.08077300	-0.93422700	2.47551700

H	1.62441700	-0.69760800	2.09082900
H	0.78079700	-2.12883200	1.47914700
C	-2.11363200	-1.11501800	0.84956500
H	-2.17401800	-0.39250800	1.66601100
H	-1.87724500	-2.09586800	1.26510400
H	-3.08958100	-1.17185400	0.36526300
S	1.62088700	-0.37200100	-0.83372300
C	2.96920800	0.44901600	0.05963700
H	3.71847700	0.69374400	-0.69293300
H	3.41631600	-0.20528500	0.80662700
H	2.61329500	1.37101200	0.51804800

Cyclic acetal 2 (cyclohexyl)

O	-1.33053300	1.16271000	0.52687900
O	0.46952400	1.10174400	-0.74248700
C	-0.57192200	1.83341500	-0.35561600
O	-0.80750700	2.94482700	-0.73243700
C	-0.92418900	-0.22242800	0.54451000
C	-1.15438200	-0.77175000	1.93548000
H	-2.21864200	-0.78722700	2.16855700
H	-0.65573800	-0.15330200	2.68192700
S	-1.91120700	-1.12298700	-0.72985300
H	-0.77059600	-1.79100600	1.99781500
C	-3.59409200	-0.80401900	-0.13236200
H	-4.25676800	-1.07933800	-0.95261800
H	-3.83610300	-1.41119700	0.73873100
H	-3.72381300	0.25502000	0.08774800
C	0.55943500	-0.09893500	0.08543800
C	1.50746900	0.21311100	1.24917200
C	1.10287400	-1.23543000	-0.77037700
C	2.93372600	0.48556400	0.77020300
H	1.51366500	-0.65235100	1.91887000
H	1.12689800	1.06342000	1.82224800
C	2.54394000	-0.98601100	-1.22460400
H	1.05533100	-2.14929300	-0.16796400
H	0.46348600	-1.38450400	-1.64207000
C	3.47012300	-0.68681100	-0.04810100
H	3.56849100	0.67200900	1.64010300
H	2.94862100	1.39672300	0.16304300
H	2.89314800	-1.86130600	-1.77802700
H	2.55803700	-0.14255800	-1.92323200
H	4.47864900	-0.46805600	-0.40914700
H	3.54488600	-1.57373000	0.59356400

Pathway 1 Pre-reaction TS1 (dimethyl)

C	2.78018200	-1.85985500	-0.25894200
O	1.16274000	-0.20629500	-0.27200100
O	2.00284800	-1.82516500	-1.50252600
C	1.18725700	-0.78566300	-1.47732600
O	0.54090700	-0.38781300	-2.41196000
C	3.02854100	-3.30801200	0.10705600
H	3.69846400	-3.75821100	-0.62706000
H	3.50934700	-3.35996200	1.08604200
H	2.10378700	-3.88436600	0.13349100
C	4.08360600	-1.12173700	-0.53293100

H	4.73011100	-1.15899200	0.34536600
H	4.59648900	-1.61418600	-1.36049300
H	3.91790000	-0.07366100	-0.79325600
C	1.82861900	-1.06259700	0.68229500
C	2.49918000	-0.19770900	1.72583300
H	1.75473800	0.35189100	2.30182200
H	3.16762700	0.52908100	1.26009600
S	0.55580000	-2.18512900	1.40731100
H	3.06902200	-0.82923400	2.40920400
C	-0.60017600	-0.96394400	2.08412900
H	-1.49657200	-1.52189000	2.35417900
H	-0.20525600	-0.47579900	2.97354000
H	-0.85398000	-0.22577200	1.32316700
C	2.65670200	2.94020300	-0.06821900
H	2.28545700	3.84664200	-0.55473600
H	2.35524900	2.08599600	-0.67972800
H	2.14568500	2.84655300	0.89440100
S	4.48103500	3.00146800	0.15044200
C	-2.54403100	0.77987100	-0.84667300
C	-3.02868500	2.30641400	0.98233500
H	-3.94494700	2.84650900	1.21923100
H	-2.63601000	1.88490000	1.91320100
C	-2.02103800	3.23875700	0.33200200
H	-2.49933300	3.78533500	-0.48455500
H	-1.67430000	3.96546000	1.06650300
C	-0.84941800	2.43799400	-0.20324700
H	-0.19819100	3.04673400	-0.82973100
H	-0.24087600	2.02732500	0.60791100
C	-4.49042300	-0.89860400	0.90785500
H	-5.42813100	-1.16820500	1.40119100
H	-3.72318100	-0.87100300	1.68863700
C	-4.66072800	0.50916900	0.33879600
H	-5.25643300	0.49262300	-0.57812500
H	-5.19733400	1.13292100	1.05152700
C	-2.88868600	-1.72273800	-0.94095600
H	-2.00784300	-1.77075200	-0.29199200
H	-2.77484400	-2.52789000	-1.67025600
C	-2.87593800	-0.39499200	-1.71826200
H	-2.12934000	-0.43881600	-2.51076100
H	-3.84389400	-0.22472400	-2.19790200
N	-3.38848400	1.20217000	0.07923800
C	-4.16620000	-1.96400300	-0.13872200
H	-4.09281300	-2.93668000	0.35531800
H	-5.00870800	-2.03236800	-0.83750300
N	-1.36312600	1.34436100	-1.01740600
H	-0.73452700	0.90226500	-1.68383300

Pathway 1 TS1 (dimethyl)

C	2.41324400	-1.51827800	-0.32979700
O	2.19872400	0.45201600	0.86747200
O	1.76757900	-0.49192900	-1.10918100
C	1.78964800	0.69676900	-0.43671100
O	0.95436400	1.56786000	-0.67276200
C	1.71748800	-2.83706500	-0.62151800
H	1.92355200	-3.13342600	-1.65200000

H	2.10283600	-3.61619400	0.04018000
H	0.63831300	-2.76371600	-0.49545000
C	3.88684900	-1.61811700	-0.72119900
H	4.35984400	-2.45168500	-0.19761300
H	3.94854100	-1.80722600	-1.79463500
H	4.43467200	-0.70246200	-0.49988600
C	2.21548100	-0.94464200	1.10519900
C	3.30478100	-1.27233200	2.10601500
H	3.08076500	-0.82965200	3.07688000
H	4.26323900	-0.87663100	1.76759100
S	0.54428900	-1.45778200	1.76196200
H	3.38578500	-2.35376400	2.22913200
C	0.37348500	-0.28694000	3.13354600
H	-0.65623400	-0.37525100	3.48107500
H	1.04362000	-0.52461500	3.95948300
H	0.55155400	0.72900500	2.78192600
C	3.21223200	3.41242900	-1.40594300
H	3.45642100	3.86470100	-2.36975700
H	2.12454900	3.40933900	-1.28685700
H	3.64940600	4.02595900	-0.61449500
S	3.79462000	1.68944400	-1.32417200
C	-2.47192700	0.68327600	-0.47108600
C	-4.32610700	1.19461300	1.01585900
H	-5.36110300	1.44920900	0.78882000
H	-4.32733800	0.47591100	1.84144300
C	-3.54465600	2.44490300	1.38020500
H	-3.69759200	3.21057700	0.61526400
H	-3.90920600	2.83791200	2.32927900
C	-2.06899100	2.10754400	1.48288700
H	-1.45664700	3.00477100	1.57075900
H	-1.87530500	1.47783000	2.35562100
C	-4.30786800	-1.80780700	-0.86877700
H	-5.20640200	-2.36663900	-1.14481000
H	-4.08758400	-2.05700800	0.17504900
C	-4.64751300	-0.32066700	-0.95973900
H	-4.65381300	0.01351700	-2.00147100
H	-5.64867100	-0.14810900	-0.56842000
C	-1.83280000	-1.53748900	-1.50350100
H	-1.47670500	-1.77562600	-0.49598400
H	-1.07872400	-1.91504700	-2.19801200
C	-1.87839900	-0.00850000	-1.66347000
H	-0.86645500	0.37561800	-1.79101000
H	-2.44930000	0.26466100	-2.55618500
N	-3.75702400	0.54914200	-0.17591700
C	-3.15986700	-2.23925100	-1.77928300
H	-3.01539100	-3.31917200	-1.68436500
H	-3.44900500	-2.05349700	-2.82106900
N	-1.65863300	1.40096300	0.27755200
H	-0.67638800	1.45913400	-0.01691900

Pathway 1 Post-reaction TS1 (dimethyl)

C	2.38289200	-1.56925100	-0.19429800
O	2.55966900	0.57416900	0.62491800
O	1.72710000	-0.66889900	-1.08973700
C	1.93339200	0.69304600	-0.69197200

O	0.90098100	1.43194100	-0.72484700
C	1.58420900	-2.86109100	-0.12961900
H	1.62012300	-3.36109400	-1.10040100
H	2.01667900	-3.53542900	0.61428900
H	0.54149800	-2.67512300	0.12277700
C	3.79851200	-1.87210600	-0.69607100
H	4.28481900	-2.62032800	-0.06590300
H	3.72769200	-2.27226000	-1.71023700
H	4.41580300	-0.97351800	-0.72315300
C	2.40685200	-0.72278600	1.10885500
C	3.52634000	-1.03837800	2.08441800
H	3.43720000	-0.42166900	2.98031700
H	4.49696700	-0.83708400	1.62752800
S	0.75359700	-0.89949000	2.00639600
H	3.48223700	-2.08738600	2.38421600
C	0.72843300	0.68531900	2.87848100
H	-0.19615100	0.70722400	3.45651400
H	1.57210600	0.78564900	3.56277600
H	0.73560100	1.50264000	2.15827300
C	3.25848900	3.09873500	-1.45286900
H	3.86306500	3.63481000	-2.18577800
H	2.22818700	3.45042700	-1.50261600
H	3.66225200	3.28025700	-0.45564500
S	3.31241000	1.33649300	-1.87114500
C	-2.45188100	0.46511100	-0.45697900
C	-4.32209300	1.51589200	0.69178800
H	-5.30494500	1.80323200	0.31801900
H	-4.45815500	1.04319500	1.66995000
C	-3.42281300	2.73542100	0.79594100
H	-3.44160200	3.28801100	-0.14716500
H	-3.79268200	3.39477900	1.58144400
C	-2.00500900	2.28955200	1.10220300
H	-1.29669400	3.11443700	1.02006900
H	-1.93763300	1.88887700	2.11796800
C	-4.53572800	-1.86208700	-0.38036900
H	-5.47641400	-2.38398800	-0.57770100
H	-4.39421800	-1.86237700	0.70607800
C	-4.70063100	-0.41959900	-0.85653200
H	-4.61593200	-0.36064800	-1.94600800
H	-5.69605900	-0.06084600	-0.59972100
C	-2.01775300	-1.99769900	-0.87498800
H	-1.73640700	-2.02244400	0.18347400
H	-1.28276500	-2.60680900	-1.40655900
C	-1.87546700	-0.55699000	-1.39401200
H	-0.81763400	-0.32096700	-1.51627200
H	-2.35465500	-0.45798900	-2.37312800
N	-3.76243800	0.53024200	-0.24254400
C	-3.40048000	-2.61330500	-1.07195200
H	-3.38223100	-3.64593200	-0.71176000
H	-3.61583300	-2.66174800	-2.14663000
N	-1.60481500	1.26375700	0.15159000
H	-0.59512800	1.20765200	-0.11716500

Pathway 1 Pre-reaction TS2 (dimethyl)

C	3.69049000	-0.02325100	0.02864000
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O	1.39796600	-0.03652900	0.19642500
O	3.18263800	1.20497800	-0.49299200
C	1.77080300	1.33051500	-0.29057600
O	1.09033300	1.73710200	-1.25588200
C	4.87547900	-0.45248300	-0.82380500
H	5.70215000	0.24535600	-0.67262600
H	5.21629600	-1.44809300	-0.52759100
H	4.62430000	-0.46261200	-1.88447500
C	4.15147200	0.16659400	1.47771800
H	4.63044700	-0.73911300	1.85688500
H	4.88316400	0.97730100	1.50366300
H	3.32177300	0.43098300	2.13403800
C	2.43325600	-0.93739600	-0.05408100
C	2.38337700	-2.07585000	0.95026100
H	1.51342800	-2.71072800	0.77225200
H	2.32325000	-1.68449900	1.96761500
S	2.29072800	-1.65939500	-1.78862300
H	3.27596200	-2.69787000	0.85920900
C	0.50992700	-1.97045800	-1.84225600
H	0.31276300	-2.48352200	-2.78396000
H	0.18100400	-2.60849700	-1.02063600
H	-0.03058100	-1.02650500	-1.82575000
C	-0.13773700	2.88843200	1.17882400
H	-0.76912400	2.09726800	1.58789400
H	-0.31055100	3.80713200	1.74068800
H	-0.38457000	3.05197400	0.12898600
S	1.61934600	2.46729900	1.28999600
C	-2.29672600	-0.35167500	0.02611600
C	-3.67890400	-1.92028800	1.27542400
H	-4.37445900	-2.67242900	0.90371800
H	-4.15046900	-1.41287800	2.12253200
C	-2.37123600	-2.57319900	1.68636900
H	-2.01432900	-3.22385900	0.88363200
H	-2.53540200	-3.18706500	2.57196100
C	-1.33966900	-1.49784200	1.97058200
H	-0.34475000	-1.91916500	2.11107300
H	-1.59853300	-0.93509000	2.87196500
C	-5.15600700	0.80096000	-0.48504600
H	-6.19134200	0.81050000	-0.83680400
H	-5.18119400	1.04932000	0.58163200
C	-4.63211700	-0.62431400	-0.64785300
H	-4.38423200	-0.83109200	-1.69333700
H	-5.40682800	-1.33351200	-0.36175400
C	-2.89033100	1.94330100	-0.86499600
H	-2.80376300	2.25838300	0.17994000
H	-2.40939200	2.72073200	-1.46364800
C	-2.08458300	0.64750000	-1.07226100
H	-1.01931300	0.89261200	-1.10863300
H	-2.35109900	0.18955200	-2.03018700
N	-3.46911600	-0.94302900	0.19632000
C	-4.36015900	1.84602300	-1.26314100
H	-4.82851800	2.82515100	-1.12937400
H	-4.42348300	1.61285100	-2.33306600
N	-1.28049300	-0.58699800	0.83550800
H	-0.35803400	-0.23270800	0.56948000

Pathway 1 TS2 (dimethyl)

C	3.55293700	-0.15322200	0.04933300
O	1.22369700	-0.16478700	0.24384100
O	3.19654800	1.10225100	-0.57217100
C	1.95624700	1.63729200	-0.35970200
O	1.26992200	2.00040500	-1.29184100
C	4.72972100	-0.68397200	-0.75716400
H	5.60670000	-0.05381300	-0.58952200
H	4.97675800	-1.69872400	-0.43647300
H	4.51062000	-0.69381500	-1.82502000
C	4.00177600	0.06273900	1.49730400
H	4.47991300	-0.84270100	1.87736100
H	4.73664100	0.87112100	1.52500500
H	3.17022500	0.32275900	2.14967600
C	2.23528500	-1.00312200	-0.00729700
C	2.26962200	-2.20616100	0.93839900
H	1.40317700	-2.84651500	0.76071400
H	2.22664900	-1.86126900	1.97459700
S	2.11509500	-1.74093100	-1.80260500
H	3.17032300	-2.80880100	0.79954900
C	0.35076300	-2.13735300	-1.82569200
H	0.14857300	-2.64982900	-2.76706100
H	0.07175300	-2.79747500	-1.00211400
H	-0.24259800	-1.22694000	-1.78148200
C	0.09466600	2.90898400	1.25027200
H	-0.47545000	1.99159300	1.39942100
H	-0.08516000	3.58611200	2.08565000
H	-0.20109000	3.38801700	0.31871100
S	1.86263000	2.53932700	1.23523900
C	-2.26716100	-0.34446300	0.05612300
C	-3.80822100	-1.86754800	1.16784200
H	-4.55172500	-2.53784900	0.73649800
H	-4.25935900	-1.37748700	2.03648400
C	-2.56638500	-2.64592200	1.56462000
H	-2.23912600	-3.26978900	0.72842000
H	-2.80063900	-3.30081200	2.40411300
C	-1.46414500	-1.67243900	1.93889100
H	-0.50827800	-2.17840800	2.07686900
H	-1.70579700	-1.15216300	2.87060200
C	-5.01497900	1.05579500	-0.48250900
H	-6.03471700	1.16419200	-0.86239600
H	-5.05448200	1.25391200	0.59426100
C	-4.59635500	-0.39655100	-0.70244100
H	-4.33202400	-0.56806400	-1.75058900
H	-5.43370200	-1.05516000	-0.47804400
C	-2.65779200	2.03432900	-0.73579300
H	-2.58745500	2.29052100	0.32637900
H	-2.09888400	2.80104000	-1.27771500
C	-1.94672000	0.69151500	-0.98319800
H	-0.86638700	0.84823500	-0.97265000
H	-2.21373900	0.30542200	-1.97230700
N	-3.49178500	-0.84875000	0.15683700
C	-4.11589400	2.07082800	-1.18389100

H	-4.51222100	3.07642000	-1.01717500
H	-4.15978600	1.89305400	-2.26542500
N	-1.29604900	-0.69707200	0.87167800
H	-0.30898700	-0.43368800	0.62270000

Pathway 1 Post-reaction TS2 (dimethyl)

C	-3.36708200	-0.46442200	-0.23673100
O	-0.99409000	-0.39235900	-0.24267400
O	-3.26136000	0.77106900	0.53543700
C	-2.31079200	1.70699500	0.42664800
O	-1.74206100	2.13476600	1.39939900
C	-4.58862300	-1.14428000	0.36820900
H	-5.48693600	-0.57028400	0.12752900
H	-4.70658000	-2.14736300	-0.04550200
H	-4.50591600	-1.21865500	1.45272600
C	-3.63387500	-0.18624300	-1.71676400
H	-3.99300500	-1.09986100	-2.19469600
H	-4.41508200	0.57111700	-1.81583700
H	-2.73911800	0.14754600	-2.23998300
C	-2.00336300	-1.22507200	-0.06399700
C	-1.94046000	-2.46971400	-0.96431700
H	-1.06864500	-3.06961700	-0.69475200
H	-1.82176000	-2.15750800	-2.00590600
S	-2.01527800	-1.93519000	1.78080200
H	-2.82555600	-3.10415600	-0.88044400
C	-0.24198100	-2.25351700	1.94603200
H	-0.07910800	-2.68796900	2.93335100
H	0.11609600	-2.95706000	1.19130000
H	0.31925500	-1.32437500	1.86758500
C	-1.00152900	3.83311900	-0.73267400
H	-0.05019700	3.38079400	-0.46089000
H	-0.87528900	4.43164000	-1.63523300
H	-1.36522300	4.46082300	0.07841000
S	-2.20977500	2.55473200	-1.15132100
C	2.36932400	-0.34611000	-0.03052000
C	4.15215000	-1.71655400	-0.96573100
H	4.99128100	-2.20225200	-0.46681100
H	4.52551000	-1.26710400	-1.89185800
C	3.05569000	-2.72661300	-1.25515900
H	2.82507400	-3.29065800	-0.34709600
H	3.39976600	-3.43118100	-2.01283200
C	1.81385100	-1.99444500	-1.73014700
H	0.95663900	-2.66466600	-1.80342700
H	1.97830100	-1.55589100	-2.71951700
C	4.82322800	1.55738500	0.24925700
H	5.81147100	1.89670600	0.57239500
H	4.81304600	1.60632300	-0.84522200
C	4.67312100	0.09861200	0.67927600
H	4.45066600	0.03214100	1.74901600
H	5.61401300	-0.42670000	0.52212600
C	2.32833600	2.14359800	0.46494800
H	2.17970500	2.25874800	-0.61481400
H	1.66200900	2.85957500	0.95271300
C	1.87473300	0.73647300	0.88798600

H	0.78445900	0.68769000	0.87883500
H	2.20998900	0.52557900	1.90858400
N	3.66418800	-0.65323900	-0.07848200
C	3.76742300	2.48846900	0.84076400
H	3.97846200	3.51509800	0.52806400
H	3.85822900	2.47061900	1.93390000
N	1.47605700	-0.94269800	-0.78433600
H	0.43676100	-0.74411200	-0.59344600

Pathway 1 Pre-reaction TS3 (dimethyl)

C	-2.65910100	-0.21904100	1.19901100
O	-1.01483800	0.54439600	-0.34988700
O	-3.26496900	-0.89407100	0.05067900
C	-2.62753900	-1.39126400	-1.01418600
O	-2.96751200	-1.11612300	-2.13670100
C	-3.86943400	0.18664300	2.02997300
H	-4.35705100	-0.70630700	2.42898900
H	-3.56026700	0.80844200	2.87181200
H	-4.59575300	0.73865200	1.43311400
C	-1.78430200	-1.16954400	2.01658400
H	-1.60389100	-0.73472300	3.00170400
H	-2.30312000	-2.12010300	2.16154100
H	-0.82447500	-1.35231100	1.53710400
C	-1.78730800	0.96083500	0.63891000
C	-1.00626900	1.65836100	1.76685200
H	-0.53942500	2.56497200	1.37596700
H	-0.20671800	0.99990500	2.11957900
S	-3.06739400	2.31560600	-0.01411100
H	-1.63651400	1.93886500	2.61296400
C	-1.90822300	3.25350700	-1.03863100
H	-2.48421300	3.85840000	-1.73970800
H	-1.27482700	3.91207200	-0.44013800
H	-1.28693500	2.54609400	-1.59147800
C	-0.88081200	-3.03346400	-2.36347500
H	-0.37173600	-2.14099800	-2.72614600
H	-0.16626000	-3.85296800	-2.28346500
H	-1.68670200	-3.30932300	-3.04047600
S	-1.50792100	-2.75342200	-0.69056100
C	2.35116800	0.23690600	-0.35289900
C	4.21202100	1.80365700	-0.41703300
H	5.15760500	1.75407800	-0.95800900
H	4.42304200	2.15804400	0.59760700
C	3.24719500	2.73617500	-1.12926500
H	3.19400100	2.46984000	-2.18840100
H	3.61142400	3.76140000	-1.05793900
C	1.86973700	2.61644500	-0.50240000
H	1.11748900	3.14397900	-1.08969000
H	1.86452600	3.04349100	0.50610400
C	4.53417400	-1.28472600	1.26335800
H	5.48867700	-1.78101700	1.46066600
H	4.43157300	-0.48770400	2.00824400
C	4.62079800	-0.65162000	-0.12600700
H	4.49342700	-1.40979500	-0.90474300
H	5.60951500	-0.21822700	-0.26993100

C	2.00621900	-1.75785600	1.16684300
H	1.75346000	-1.00638500	1.92390300
H	1.28273700	-2.56963000	1.28187100
C	1.79744900	-1.15313100	-0.23077600
H	0.72903600	-1.09157400	-0.43827300
H	2.24955700	-1.79538100	-0.99287900
N	3.66694800	0.44282100	-0.34696200
C	3.40945700	-2.30837500	1.41181400
H	3.45142800	-2.74273000	2.41478700
H	3.59048000	-3.13049200	0.70817000
N	1.48281300	1.21628200	-0.43543000
H	0.43381400	0.96808200	-0.39610100

Pathway 1 TS3 (dimethyl)

C	-2.73832400	-0.27930400	1.16669000
O	-1.04522300	0.48331600	-0.32574500
O	-3.32496900	-0.85974700	-0.02706600
C	-2.69331700	-1.42994400	-1.06158800
O	-3.01823600	-1.17545100	-2.19170000
C	-3.93608300	0.30525000	1.89882500
H	-4.57018700	-0.50998500	2.25590200
H	-3.60955000	0.88536000	2.76257200
H	-4.51102500	0.94985300	1.23741800
C	-2.06551300	-1.32758800	2.06918000
H	-1.90694400	-0.89495600	3.05875700
H	-2.72753100	-2.18892700	2.17868000
H	-1.10227800	-1.66073500	1.68458100
C	-1.63719300	0.71880700	0.73568700
C	-0.91713200	1.45986800	1.84034500
H	-0.41565500	2.33331200	1.42567200
H	-0.15288600	0.78912300	2.25199900
S	-3.08122500	2.82879700	0.03209300
H	-1.57815200	1.77594600	2.64443800
C	-1.69493700	3.41169900	-0.99763900
H	-2.04923400	4.02474400	-1.82938600
H	-0.98298000	4.00662200	-0.41749100
H	-1.16503600	2.54815900	-1.41455700
C	-0.98035400	-3.13783700	-2.35781800
H	-0.50155800	-2.26161800	-2.79262800
H	-0.24732600	-3.93641500	-2.24316100
H	-1.80014600	-3.47407000	-2.98901200
S	-1.56560500	-2.76482000	-0.68734600
C	2.43064500	0.21446400	-0.40319800
C	4.33414800	1.72370400	-0.32578600
H	5.31636000	1.64051700	-0.79084900
H	4.47500000	2.06686700	0.70409900
C	3.46077300	2.68798400	-1.10969900
H	3.47925700	2.42221600	-2.16981200
H	3.85511300	3.69906700	-1.00884300
C	2.03611800	2.62522500	-0.59084100
H	1.34926200	3.16763700	-1.24043300
H	1.96558800	3.05710000	0.41236300
C	4.42966300	-1.37842100	1.36098800
H	5.34943500	-1.90776900	1.62461900

H	4.30211200	-0.57912900	2.09931500
C	4.64159300	-0.74809800	-0.01595000
H	4.54602500	-1.49737700	-0.80725400
H	5.65082300	-0.34544800	-0.08455000
C	1.90018600	-1.76504200	1.08158800
H	1.61790500	-1.00686100	1.82071800
H	1.14336400	-2.55168500	1.13674400
C	1.81967000	-1.15352900	-0.32641000
H	0.77452700	-1.06623600	-0.62147400
H	2.31078500	-1.80775300	-1.05281500
N	3.74104600	0.37927400	-0.30113900
C	3.26266300	-2.36287800	1.42537300
H	3.21681600	-2.79698000	2.42797400
H	3.46533700	-3.19136700	0.73555800
N	1.60820700	1.23392700	-0.54895800
H	0.59907100	1.02363400	-0.54679900

Pathway 1 Post-reaction TS3 (dimethyl)

C	-3.16749200	-0.30645900	-0.00922600
O	-1.02494000	0.18946600	-0.91280500
O	-3.22626200	-1.37975700	-0.98431300
C	-2.42022800	-2.44378100	-1.02478300
O	-2.35902200	-3.10913800	-2.02423000
C	-3.98072500	0.81983200	-0.65223200
H	-5.02353200	0.50785600	-0.73467200
H	-3.92889100	1.72300300	-0.03548500
H	-3.59053200	1.04151900	-1.64653700
C	-3.80138700	-0.71995900	1.31416600
H	-3.92787300	0.15953400	1.94788500
H	-4.78896900	-1.13787600	1.11220100
H	-3.21614200	-1.45641000	1.86400600
C	-1.72403800	0.22775500	0.08192600
C	-1.29499100	0.86674900	1.35969700
H	-0.27399900	1.23560100	1.27642900
H	-1.36930800	0.15092500	2.18174200
S	-2.99678200	4.17023500	1.15577300
H	-1.96578900	1.70882300	1.58586200
C	-1.75144700	3.85803600	-0.15950700
H	-1.61126400	4.74004500	-0.78942000
H	-0.77915400	3.59725600	0.26773700
H	-2.05776500	3.03430200	-0.81173900
C	-0.42715500	-4.14156000	-0.21692400
H	0.21638700	-3.72863400	-0.99185600
H	0.17630900	-4.48692100	0.62230600
H	-1.01813600	-4.96517900	-0.61082300
S	-1.51140700	-2.85763800	0.45567300
C	2.55333300	0.22023800	-0.52363400
C	4.32368100	1.88455300	-0.61766500
H	5.32656000	1.80967000	-1.03756900
H	4.39813900	2.39234600	0.34894900
C	3.41163600	2.64176600	-1.56721000
H	3.49685800	2.22302800	-2.57314500
H	3.72007900	3.68624500	-1.60922300
C	1.97534500	2.53675300	-1.08899100

H	1.27531400	2.91908600	-1.83133900
H	1.82816800	3.09832200	-0.16169900
C	4.58199000	-0.89149100	1.55103200
H	5.52594100	-1.29364900	1.92873000
H	4.35708600	0.00015400	2.14636200
C	4.81166300	-0.46949900	0.10011800
H	4.81802000	-1.33816400	-0.56452600
H	5.78613500	0.00637800	0.00461400
C	2.10743000	-1.52971100	1.24305700
H	1.73221100	-0.68657100	1.83293600
H	1.41135800	-2.35472700	1.40818100
C	2.05179500	-1.16806100	-0.25143900
H	1.02209900	-1.22245900	-0.60549000
H	2.63356400	-1.88408000	-0.83879100
N	3.83636400	0.51514700	-0.39492200
C	3.49297400	-1.94828800	1.72957200
H	3.42876300	-2.21899400	2.78694100
H	3.79355400	-2.85616100	1.19259400
N	1.66034400	1.13298800	-0.85630900
H	0.68636900	0.83141400	-0.92665100

Pathway 1 Pre-reaction TS1 (cyclohexyl)

O	-2.66249000	0.62000900	-0.95903600
O	-0.72500800	0.12346200	-0.04242600
C	-1.34087100	0.53912400	-1.14258400
O	-0.78525200	0.79513100	-2.17644500
C	-3.01240100	-0.10875000	0.24143700
C	-4.23478000	0.53812800	0.85346400
H	-5.09221600	0.43575900	0.18892700
H	-4.06456000	1.60138300	1.02302600
S	-3.31695600	-1.86519600	-0.23831200
H	-4.47082900	0.05479300	1.80244900
C	-4.65070600	-1.65462600	-1.44916600
H	-4.73153700	-2.60944600	-1.96834100
H	-5.60107700	-1.43084500	-0.96699100
H	-4.39066500	-0.87970300	-2.16912400
C	0.86480400	3.93758200	-2.06864400
H	1.93324200	4.17030700	-2.04208200
H	0.75455700	2.85325800	-2.14659200
H	0.45215400	4.38047500	-2.97927500
S	0.00593000	4.57783600	-0.57180100
C	2.35165400	-0.93354900	-1.17863200
C	2.40028700	-3.05874100	0.00253000
H	3.24104600	-3.71126100	0.23571400
H	1.77261800	-2.98449400	0.89613700
C	1.61543900	-3.61221000	-1.17404200
H	2.29922800	-3.85518000	-1.99118300
H	1.11124700	-4.53012800	-0.87244900
C	0.59868700	-2.58935700	-1.64311400
H	0.14414800	-2.88250600	-2.58906500
H	-0.20045400	-2.45603000	-0.90775300
C	3.81572300	-0.18487800	1.48820600
H	4.62866600	-0.18667800	2.21951900
H	2.90531900	-0.44781100	2.03551000

C	4.11830400	-1.28363200	0.47080100
H	4.90590500	-0.96952100	-0.21982600
H	4.48558100	-2.17019100	0.98462500
C	2.64869400	1.37222900	-0.20732300
H	1.64319500	1.19899100	0.18663400
H	2.66189000	2.40357900	-0.56372200
C	2.85502800	0.45692200	-1.42463700
H	2.31613400	0.85922300	-2.28288200
H	3.91190800	0.41402600	-1.70339000
N	2.94567300	-1.72637100	-0.30312800
C	3.70185100	1.21460700	0.88653100
H	3.48518500	1.92813600	1.68668700
H	4.67758800	1.49731200	0.47315900
N	1.27757500	-1.31657500	-1.84485400
H	0.79093000	-0.59924200	-2.36889300
C	-1.68609400	-0.00090000	1.05442700
C	-1.61109000	1.27677700	1.89531400
C	-1.28780500	-1.21837400	1.87847700
C	-0.24965400	1.45644200	2.56814700
H	-2.38651600	1.21088700	2.66457500
H	-1.84064600	2.14594600	1.27265900
C	0.08667800	-1.03343300	2.52289300
H	-2.05024500	-1.36265400	2.65116500
H	-1.28350700	-2.11241300	1.25257000
C	0.14719800	0.22682700	3.38213300
H	-0.28888600	2.34339400	3.20536100
H	0.50912900	1.65626500	1.80638800
H	0.32631100	-1.91971600	3.11546200
H	0.83697700	-0.96931500	1.72715800
H	1.15246900	0.35623300	3.79318000
H	-0.53427200	0.11561800	4.23429100

Pathway 1 TS1 (cyclohexyl)

O	-2.73939400	0.39331400	-0.81586900
O	-0.67362000	0.27618400	0.01553400
C	-1.39426300	0.56658900	-1.10675800
O	-0.93891000	0.29447000	-2.21654500
C	-2.86469200	-0.31900700	0.40564600
C	-4.15556900	0.09249200	1.08396200
H	-5.01468900	-0.20450000	0.48202400
H	-4.19116900	1.17521100	1.20962700
S	-2.87578700	-2.14845100	0.03226100
H	-4.23486700	-0.38630200	2.06139700
C	-4.22886100	-2.21804400	-1.17222900
H	-4.16460600	-3.19765600	-1.64604000
H	-5.20376700	-2.11845900	-0.69568300
H	-4.09360300	-1.44585200	-1.92883800
C	-0.30700400	3.21035400	-2.57278100
H	0.67610700	3.59227400	-2.28571200
H	-0.17749200	2.23696100	-3.05689300
H	-0.74715200	3.90114800	-3.29558500
S	-1.39071200	2.97740000	-1.13028100
C	2.39938900	-0.58313900	-1.14073000
C	3.02742900	-2.55597700	0.12871600

H	3.99731300	-3.02224700	0.29871100
H	2.49936300	-2.51396700	1.08719600
C	2.23319900	-3.34556400	-0.89716300
H	2.84798000	-3.51564400	-1.78485300
H	1.96608200	-4.31723900	-0.48151600
C	0.98195600	-2.57663700	-1.27385200
H	0.48411400	-3.02156900	-2.13575100
H	0.26513200	-2.55282400	-0.44813800
C	4.05016600	0.60852300	1.24147900
H	4.93540800	0.80581400	1.85256000
H	3.28541400	0.21146200	1.91729000
C	4.42361200	-0.46997900	0.22536900
H	5.01894000	-0.04631600	-0.58844400
H	5.03985200	-1.23079300	0.70163600
C	2.37945400	1.80509800	-0.31734800
H	1.48953200	1.48415600	0.22821400
H	2.14979500	2.79551800	-0.71687900
C	2.56866500	0.86025700	-1.51415800
H	1.82426900	1.08919100	-2.27691500
H	3.55340000	1.00051900	-1.97045800
N	3.26853000	-1.18352700	-0.33969200
C	3.58797900	1.91971400	0.60837800
H	3.35336200	2.63459400	1.40251200
H	4.42550700	2.34647800	0.04272900
N	1.34529200	-1.21079200	-1.62053200
H	0.60722400	-0.62818200	-2.03268000
C	-1.54439400	0.06121400	1.14208900
C	-1.68269600	1.35089400	1.96431700
C	-0.90488000	-1.02507300	2.00407800
C	-0.34377300	1.81424000	2.53727700
H	-2.37762900	1.14820800	2.78613900
H	-2.11600000	2.14172100	1.34972700
C	0.45427700	-0.57652900	2.54384200
H	-1.58405800	-1.24691000	2.83469900
H	-0.78329700	-1.94285700	1.42696800
C	0.34405700	0.71682600	3.34882000
H	-0.51055200	2.69776200	3.16004900
H	0.30212600	2.12945800	1.71401100
H	0.88221400	-1.37523600	3.15594500
H	1.13201000	-0.42677300	1.69597600
H	1.33670300	1.04925300	3.66776200
H	-0.23464700	0.52140900	4.26039600

Pathway 1 Post-reaction TS1 (cyclohexyl)

O	2.81064500	-0.28344200	-0.77178800
O	0.68751200	-0.46568700	-0.00120800
C	1.45588400	-0.62609800	-1.19019600
O	0.97850200	0.00143100	-2.18650500
C	2.79670200	0.34369300	0.47722200
C	4.10149500	0.04630400	1.19634100
H	4.94190400	0.49156700	0.66232600
H	4.26965500	-1.03050200	1.24832000
S	2.63183500	2.20770600	0.26436200
H	4.07920900	0.45541100	2.20827100

C	3.96472500	2.49502700	-0.92925300
H	3.80862800	3.49369200	-1.33789600
H	4.94898200	2.45404100	-0.46204900
H	3.89912400	1.76325700	-1.73410200
C	0.46303300	-2.79519100	-2.84756200
H	-0.49272100	-3.11995400	-2.43477200
H	0.33595100	-1.85317500	-3.38438900
H	0.83220700	-3.55789200	-3.53419600
S	1.70656800	-2.52439800	-1.55988200
C	-2.31289700	0.64531400	-1.03080400
C	-3.11106500	2.47568100	0.34167500
H	-4.10470000	2.88242300	0.52517400
H	-2.60398700	2.37117200	1.30716600
C	-2.32701400	3.38422600	-0.58924100
H	-2.91509100	3.57513500	-1.49093000
H	-2.14044300	4.34060600	-0.10015000
C	-1.01383400	2.71858300	-0.95088800
H	-0.51709400	3.23711700	-1.77230400
H	-0.32528500	2.71510300	-0.10233100
C	-4.16824200	-0.80639800	1.05066400
H	-5.10297200	-1.06764700	1.55494800
H	-3.47216100	-0.47606900	1.82896800
C	-4.45998900	0.36534400	0.11425900
H	-4.96305600	0.01600000	-0.79236200
H	-5.13843800	1.06605000	0.59825500
C	-2.33889300	-1.83215500	-0.44667200
H	-1.51143800	-1.58330100	0.22031500
H	-2.07087200	-2.77661000	-0.92734200
C	-2.40389300	-0.76225600	-1.54679600
H	-1.57136300	-0.90062800	-2.23573900
H	-3.32622700	-0.86272000	-2.12871800
N	-3.27344800	1.14626200	-0.26003700
C	-3.63471300	-2.04387600	0.33232500
H	-3.47644600	-2.84167400	1.06393400
H	-4.40741600	-2.40358800	-0.35862300
N	-1.25395100	1.34596800	-1.37063700
H	-0.43947900	0.82738400	-1.76596600
C	1.50801100	-0.23330400	1.13893900
C	1.77792700	-1.55766500	1.87727900
C	0.75793100	0.71225500	2.07779200
C	0.47957300	-2.20092700	2.36411700
H	2.42433500	-1.35272300	2.73745700
H	2.31251000	-2.24780300	1.22082400
C	-0.55053500	0.09678500	2.57400700
H	1.41015400	0.94128200	2.92881500
H	0.54328700	1.65200100	1.56725400
C	-0.32366600	-1.25227000	3.25526700
H	0.71414400	-3.12042400	2.90863100
H	-0.11869300	-2.49291000	1.49614100
H	-1.04266500	0.79231800	3.26031100
H	-1.22022500	-0.02674700	1.71699200
H	-1.28303800	-1.70564500	3.52373600
H	0.22455600	-1.08993400	4.19221400

Pathway 1 Pre-reaction TS2 (cyclohexyl)

O	0.79882900	-0.17113100	0.11912900
O	2.62029400	0.94755300	-0.66753000
C	1.22724600	1.15295000	-0.43261700
O	0.54035800	1.55934200	-1.39402700
C	1.78529100	-1.13297900	-0.10530400
C	1.69930000	-2.21414200	0.95852300
H	0.79309100	-2.80935600	0.83236400
H	1.68171900	-1.76813100	1.95468900
S	1.55896700	-1.93631600	-1.79528300
H	2.55567300	-2.88704700	0.88299600
C	-0.23104200	-2.19765800	-1.77120300
H	-0.47530400	-2.74899000	-2.67965800
H	-0.54832100	-2.78639700	-0.90928500
H	-0.74705100	-1.24002400	-1.78246500
C	-0.55584900	2.87654600	1.01562600
H	-1.22090000	2.14513300	1.47909900
H	-0.66129500	3.83103600	1.53275800
H	-0.81985500	3.00044200	-0.03546200
S	1.17692000	2.35970900	1.10560300
C	-2.90617300	-0.28283500	0.06573200
C	-4.34482900	-1.66103700	1.46502400
H	-5.10657500	-2.38372400	1.17364800
H	-4.74428600	-1.06207300	2.28918000
C	-3.07113000	-2.37765500	1.87667300
H	-2.79045000	-3.10340600	1.10884600
H	-3.24400200	-2.91846500	2.80709200
C	-1.95791700	-1.36239500	2.05290800
H	-0.98945900	-1.84369400	2.18616600
H	-2.14201100	-0.72624900	2.92326800
C	-5.70153800	1.01868900	-0.45136700
H	-6.74484000	1.07105400	-0.77462800
H	-5.67650300	1.34526700	0.59400300
C	-5.27516400	-0.44610800	-0.52217300
H	-5.07441900	-0.74234300	-1.55609300
H	-6.08418600	-1.08036400	-0.16415300
C	-3.38112300	1.97866900	-0.97411000
H	-3.24389100	2.36123700	0.04242300
H	-2.86988300	2.67842500	-1.63974200
C	-2.66470100	0.62202100	-1.10614800
H	-1.58779100	0.79662700	-1.18507200
H	-2.98638700	0.11552700	-2.02195200
N	-4.10869100	-0.78017800	0.31106300
C	-4.86541000	1.94928100	-1.32647600
H	-5.26636700	2.96420400	-1.25479500
H	-4.97593900	1.64263700	-2.37381800
N	-1.88060800	-0.53241600	0.85858100
H	-0.94691600	-0.25428000	0.54449300
C	3.08677200	-0.27784300	-0.10080400
C	3.60502200	-0.05200300	1.33258800
C	4.23133400	-0.79987500	-0.96956500
C	4.79285600	0.90882700	1.35677900
H	3.92280300	-1.01683700	1.74224400
H	2.79641900	0.32185200	1.96394500
C	5.45057700	0.12617500	-0.93817000

H	4.51381400	-1.79306400	-0.59970000
H	3.88833900	-0.91589000	-1.99935500
C	5.93503600	0.38612000	0.48709600
H	5.12835100	1.04500000	2.38915000
H	4.47130700	1.89023800	0.99191600
H	6.25050000	-0.31401700	-1.54062800
H	5.18407200	1.07817400	-1.40980300
H	6.76771700	1.09589200	0.47976200
H	6.31652400	-0.54913400	0.91729300

Pathway 1 TS2 (cyclohexyl)

O	0.63338500	-0.24648100	0.15724200
O	2.63164600	0.91018400	-0.74577600
C	1.42573800	1.50739100	-0.52384200
O	0.73007000	1.86804500	-1.45033900
C	1.60498200	-1.13352800	-0.08264500
C	1.60301400	-2.30447300	0.90321400
H	0.70944300	-2.91453200	0.75588000
H	1.58505000	-1.92336800	1.92747000
S	1.40555800	-1.93472300	-1.84802100
H	2.47725500	-2.94742300	0.77561500
C	-0.37459400	-2.25224700	-1.80847000
H	-0.62798100	-2.77810500	-2.72989200
H	-0.65847700	-2.87824000	-0.96021500
H	-0.92529400	-1.31519100	-1.77043200
C	-0.34102600	2.91162900	1.08610700
H	-0.94295100	2.02482800	1.28646700
H	-0.47006300	3.62722800	1.89850700
H	-0.64260300	3.36629300	0.14423600
S	1.40934700	2.46868700	1.03939900
C	-2.86185100	-0.29114200	0.10022400
C	-4.41993000	-1.70420800	1.32802300
H	-5.20252800	-2.36220800	0.95012600
H	-4.82222500	-1.16183000	2.18956200
C	-3.19537000	-2.51371500	1.71628200
H	-2.92158800	-3.18484500	0.89754800
H	-3.42473600	-3.12279100	2.59090300
C	-2.04410500	-1.56980400	2.01009500
H	-1.10420600	-2.10714500	2.13835200
H	-2.23258900	-1.00067400	2.92541800
C	-5.57042700	1.19676800	-0.40267100
H	-6.59864200	1.33061300	-0.75026100
H	-5.56157800	1.44222000	0.66501500
C	-5.21815900	-0.27962200	-0.57308400
H	-5.00103900	-0.50648800	-1.62151500
H	-6.07197900	-0.89282800	-0.28977000
C	-3.18805000	2.06664000	-0.78109900
H	-3.06989800	2.36522000	0.26563300
H	-2.61962000	2.78627500	-1.37519800
C	-2.53867500	0.68707000	-0.99307500
H	-1.45341000	0.80098800	-1.02448400
H	-2.85400300	0.27071100	-1.95530100
N	-4.10094500	-0.74060000	0.26492300
C	-4.65879800	2.14286500	-1.17998100

H	-5.00919800	3.17005900	-1.04504800
H	-4.74891900	1.91992300	-2.25025600
N	-1.87620100	-0.64882300	0.89573800
H	-0.88827100	-0.43767600	0.60095500
C	2.95831900	-0.33691700	-0.08898900
C	3.45850800	-0.10017500	1.34716900
C	4.10054500	-0.93724400	-0.91065500
C	4.69294200	0.79954800	1.38790100
H	3.72770200	-1.07521600	1.76561900
H	2.65527800	0.30480900	1.96236600
C	5.37191300	-0.08353500	-0.86585900
H	4.31204000	-1.93503300	-0.50930300
H	3.78305200	-1.06194500	-1.94743600
C	5.82969500	0.19492600	0.56488200
H	5.00513900	0.93973800	2.42711400
H	4.44063600	1.79075200	0.99497500
H	6.16258700	-0.58898600	-1.42825500
H	5.17814400	0.86647800	-1.37538500
H	6.69819500	0.86049300	0.56101300
H	6.15000100	-0.74493600	1.03311500

Pathway 1 Post-reaction TS2 (cyclohexyl)

O	-0.45206500	-0.36409100	-0.08764100
O	-2.69786700	0.76889000	0.77288800
C	-1.74157700	1.69633100	0.66070800
O	-1.15541500	2.11028300	1.63007000
C	-1.44015200	-1.21215500	0.12936300
C	-1.38094100	-2.46379900	-0.76126000
H	-0.50187100	-3.05549500	-0.49757600
H	-1.27816500	-2.16030500	-1.80708300
S	-1.35862200	-1.92176500	1.98022600
H	-2.26051800	-3.10341700	-0.65952700
C	0.42931200	-2.18386300	2.06653600
H	0.65473900	-2.58315100	3.05639000
H	0.77257400	-2.89764700	1.31430600
H	0.95401200	-1.23991000	1.93237400
C	-0.41756100	3.81794900	-0.49478100
H	0.52717400	3.34314200	-0.23927200
H	-0.29031700	4.42082500	-1.39431600
H	-0.75664100	4.44670400	0.32609200
S	-1.65702200	2.56821000	-0.90606200
C	2.93065000	-0.34906900	-0.10556400
C	4.61777100	-1.75671700	-1.15879800
H	5.46962800	-2.26986200	-0.71155000
H	4.95109300	-1.30962100	-2.10113600
C	3.47895600	-2.73332100	-1.39250800
H	3.28710300	-3.30204800	-0.47835900
H	3.75795400	-3.43758400	-2.17674500
C	2.23160600	-1.96248500	-1.78432300
H	1.35474800	-2.60943900	-1.81728400
H	2.35028800	-1.51252200	-2.77513100
C	5.44728300	1.48909400	0.03283900
H	6.46274200	1.79961900	0.29464400
H	5.36852600	1.54840300	-1.05831600

C	5.28559500	0.03119600	0.46079800
H	5.12841200	-0.03894800	1.54181300
H	6.20055200	-0.51701500	0.24141700
C	2.98763300	2.13701400	0.41209100
H	2.77281000	2.26880900	-0.65449600
H	2.37462700	2.86513400	0.94934500
C	2.52309200	0.73783600	0.85018600
H	1.43337300	0.71822900	0.90747600
H	2.91336500	0.50797700	1.84688000
N	4.21176900	-0.68719400	-0.23803700
C	4.45622400	2.44080100	0.69822100
H	4.67332400	3.46489600	0.38145500
H	4.61582700	2.40952000	1.78309800
N	1.97677700	-0.91706200	-0.80581800
H	0.95628500	-0.70788000	-0.54053100
C	-2.82391500	-0.47410000	0.01294300
C	-3.16763800	-0.21206700	-1.46136000
C	-4.01163900	-1.17400300	0.68046100
C	-4.46722600	0.57363700	-1.64073700
H	-3.29441600	-1.19000100	-1.93567400
H	-2.32942900	0.27162500	-1.96351300
C	-5.33220400	-0.42113700	0.49545200
H	-4.09886000	-2.17396800	0.24296100
H	-3.80947700	-1.30186000	1.74530000
C	-5.63575700	-0.15300000	-0.97717100
H	-4.65790100	0.71350000	-2.70894800
H	-4.36424100	1.57288300	-1.20449700
H	-6.13986700	-0.99946500	0.95374000
H	-5.27886100	0.53130300	1.03367700
H	-6.55548200	0.43151800	-1.07473700
H	-5.80694000	-1.10677100	-1.49303300

Pathway 1 Pre-reaction TS3 (cyclohexyl)

O	0.46394800	0.96142000	0.49211200
O	2.91780300	-0.10762400	0.70848200
C	2.23797000	-0.28749100	1.84454000
O	2.42973700	0.40649000	2.81122000
C	1.26259800	1.18086300	-0.53788300
C	0.50642600	1.35905700	-1.86631500
H	-0.10881100	2.25972800	-1.81407700
H	-0.16514000	0.51025200	-2.02471000
S	2.24339200	2.88645100	-0.29111900
H	1.17282700	1.45201700	-2.72612700
C	0.84999400	3.86103600	0.32688500
H	1.24638400	4.74681400	0.82442400
H	0.18237100	4.17597300	-0.47829800
H	0.29750900	3.25409700	1.04672700
C	0.53667800	-1.57598300	3.58445500
H	-0.11556400	-0.70418100	3.54040600
H	-0.06056800	-2.46888200	3.77055800
H	1.27626700	-1.45445200	4.37317300
S	1.33567300	-1.83291100	1.98282600
C	-2.79448400	0.06293300	0.20504500
C	-4.83649800	1.26300600	-0.35056900

H	-5.84652800	1.16578400	0.04852000
H	-4.91222700	1.35412100	-1.43937300
C	-4.14772900	2.47642200	0.24983500
H	-4.24196600	2.45011600	1.33884300
H	-4.63211700	3.38540000	-0.10795700
C	-2.67995800	2.46931400	-0.13699800
H	-2.12024900	3.22813800	0.41058400
H	-2.55957600	2.67446000	-1.20614400
C	-4.45075300	-2.11635500	-1.28121500
H	-5.28209000	-2.79879200	-1.47968400
H	-4.33727900	-1.48805200	-2.17171100
C	-4.85051500	-1.23043200	-0.10063900
H	-4.74737500	-1.77504300	0.84287600
H	-5.90009400	-0.95318900	-0.18859300
C	-1.93205200	-2.12067700	-0.74781900
H	-1.65926500	-1.51714500	-1.62113400
H	-1.09784500	-2.80566800	-0.57364400
C	-2.04007900	-1.20537700	0.48260500
H	-1.03969300	-0.91817200	0.80741100
H	-2.51721700	-1.73909600	1.31040100
N	-4.10666000	0.03309600	-0.02101300
C	-3.18740600	-2.94051100	-1.03820100
H	-3.00241100	-3.57719500	-1.90813400
H	-3.36849800	-3.61439500	-0.19160500
N	-2.09732300	1.17350300	0.17338600
H	-1.02960900	1.10752800	0.30728000
C	2.36057100	0.06132800	-0.63533700
C	1.73904200	-1.24079500	-1.16042100
C	3.59059900	0.40183400	-1.48088800
C	2.73317200	-2.40088400	-1.20563700
H	1.39969700	-1.04337400	-2.18172100
H	0.85373400	-1.49063500	-0.57746800
C	4.59453900	-0.75197500	-1.56312500
H	3.24470200	0.65478200	-2.48836300
H	4.08144800	1.28780100	-1.07390400
C	3.94531000	-2.04121400	-2.06354300
H	2.23144700	-3.28917100	-1.60100900
H	3.06529800	-2.65102600	-0.19211500
H	5.42048000	-0.46060300	-2.21861900
H	5.02304500	-0.92397900	-0.56998000
H	4.67324900	-2.85800200	-2.06009000
H	3.62207600	-1.90566500	-3.10383500

Pathway 1 TS3 (cyclohexyl)

O	0.45918500	0.83916200	0.49528600
O	2.91033000	-0.15640800	0.77297900
C	2.20884500	-0.52335400	1.85192900
O	2.33434800	0.06109000	2.89662900
C	1.17308700	0.95640800	-0.51294300
C	0.53057500	1.35625300	-1.82378400
H	-0.10999000	2.22242600	-1.66280600
H	-0.09899300	0.52335800	-2.15973800
S	2.23227500	3.32222300	-0.11460100
H	1.25467800	1.58778000	-2.60216600

C	0.66838200	3.88598100	0.63101800
H	0.84193200	4.67685800	1.36405700
H	-0.02593000	4.26798400	-0.12346400
H	0.19127200	3.04429500	1.14525200
C	0.53205300	-2.08224600	3.37253600
H	-0.11565800	-1.21311800	3.47902400
H	-0.06753300	-2.99195600	3.40613000
H	1.27689300	-2.09916800	4.16529100
S	1.32359100	-2.07343100	1.74628000
C	-2.91571300	0.04680000	0.20953200
C	-4.97987800	1.21014600	-0.33610900
H	-5.99149100	1.05429700	0.03881600
H	-5.03898500	1.35211000	-1.41984000
C	-4.34867600	2.41479700	0.34053600
H	-4.46518300	2.33098600	1.42416100
H	-4.85875800	3.32182900	0.01624200
C	-2.87399900	2.48532400	-0.01089800
H	-2.35411400	3.23029400	0.59136400
H	-2.73429700	2.74522800	-1.06487500
C	-4.42950300	-2.09752700	-1.44630000
H	-5.22674400	-2.79741700	-1.71142100
H	-4.31140100	-1.41616000	-2.29604600
C	-4.90651500	-1.29607000	-0.23468100
H	-4.81762800	-1.88565100	0.68250200
H	-5.96088500	-1.04945900	-0.34854400
C	-1.93102000	-2.04163500	-0.82668200
H	-1.65295500	-1.37952900	-1.65427800
H	-1.07711600	-2.70240200	-0.65640500
C	-2.12291600	-1.20451700	0.44837700
H	-1.14815300	-0.90957600	0.83559100
H	-2.61547000	-1.79999800	1.22271700
N	-4.21192600	-0.01172300	-0.05855100
C	-3.14403300	-2.88834900	-1.20612400
H	-2.90694000	-3.46538300	-2.10424200
H	-3.32606300	-3.61661800	-0.40633200
N	-2.26257600	1.19039200	0.25236200
H	-1.24252700	1.14181600	0.40176500
C	2.42960600	0.05766900	-0.58177000
C	2.00483300	-1.25281300	-1.28140800
C	3.64675100	0.63234300	-1.30765900
C	3.14206300	-2.27081700	-1.35329000
H	1.71025100	-0.98438500	-2.30095800
H	1.11984500	-1.67268200	-0.80216000
C	4.79314300	-0.37649000	-1.41401800
H	3.33089100	0.93278900	-2.31111700
H	3.97205400	1.53123200	-0.78514600
C	4.35242000	-1.68157100	-2.07538000
H	2.78451000	-3.16761300	-1.86695500
H	3.42970200	-2.57830300	-0.34192800
H	5.61277100	0.07853800	-1.97724800
H	5.17812000	-0.58905700	-0.41100700
H	5.17722500	-2.39986200	-2.08386900
H	4.08639500	-1.48757700	-3.12234200

Pathway 1 Post-reaction TS3 (cyclohexyl)

O	0.44332500	0.22900000	0.94935900
O	2.65512900	-1.30104700	1.07450100
C	1.87062100	-2.37878100	1.11210600
O	1.79762700	-3.03110900	2.11983800
C	1.15625000	0.26896200	-0.03641300
C	0.72604200	0.88512400	-1.32546600
H	-0.30178400	1.23694900	-1.25260200
H	0.81592100	0.15777700	-2.13610500
S	2.40996600	4.21854000	-1.16102400
H	1.38348600	1.73450900	-1.56083000
C	1.15117000	3.91601700	0.14354000
H	0.99334100	4.80744200	0.75578600
H	0.18740400	3.63679900	-0.29134200
H	1.45808900	3.10741600	0.81405800
C	-0.06987200	-4.12769900	0.28503600
H	-0.73828400	-3.71700500	1.03985700
H	-0.64788600	-4.49649700	-0.56214700
H	0.52813600	-4.93388500	0.70367500
S	1.00340100	-2.83163200	-0.38207200
C	-3.12567700	0.19731600	0.50503600
C	-4.92185400	1.83613700	0.54642500
H	-5.93067700	1.75153700	0.95000100
H	-4.98719600	2.33031000	-0.42788400
C	-4.03785700	2.61924800	1.50147000
H	-4.13500400	2.21276000	2.51133600
H	-4.36211500	3.65954000	1.52382800
C	-2.59181600	2.52892000	1.05034200
H	-1.91094200	2.93181800	1.79957900
H	-2.43609200	3.07987100	0.11807200
C	-5.09867400	-0.96636000	-1.59423400
H	-6.02942300	-1.38622200	-1.98521500
H	-4.87554400	-0.07768500	-2.19464500
C	-5.36136100	-0.53308600	-0.15226200
H	-5.36620400	-1.39499000	0.52112100
H	-6.34469000	-0.07168300	-0.07920500
C	-2.62125800	-1.56512000	-1.23344800
H	-2.24681200	-0.72325600	-1.82567100
H	-1.91054900	-2.38181500	-1.37605500
C	-2.59886300	-1.18638200	0.25777300
H	-1.57518000	-1.22148100	0.63125500
H	-3.18080200	-1.90460400	0.84225800
N	-4.41039900	0.47151800	0.34973200
C	-3.99127800	-2.00882400	-1.74122900
H	-3.90327100	-2.28956200	-2.79426300
H	-4.28877900	-2.91536800	-1.20030800
N	-2.25233900	1.12692700	0.84288600
H	-1.27498200	0.84082400	0.93289300
C	2.60298400	-0.24200400	0.08348800
C	3.27334200	-0.65524200	-1.23213500
C	3.39434000	0.91124900	0.72998500
C	4.74191100	-1.02817400	-1.02835800
H	3.21792700	0.20484900	-1.90648500
H	2.73128300	-1.46915600	-1.71613100
C	4.87246900	0.56592400	0.91424300

H	3.29431000	1.79110700	0.08160700
H	2.92799800	1.14958400	1.68906400
C	5.51836700	0.12793900	-0.39918100
H	5.17404500	-1.29919600	-1.99488500
H	4.81177300	-1.91465300	-0.38862900
H	5.38610900	1.44117900	1.32098800
H	4.96887900	-0.23428300	1.65512300
H	6.55866900	-0.16228800	-0.22896900
H	5.53157700	0.97399400	-1.09780700

Pathway 2 Pre-reaction TS4 (dimethyl)

C	-1.81741400	-0.05960100	-0.23301700
O	-2.33919900	0.83871600	1.91960600
O	-3.08698700	0.50321600	-0.66226800
C	-4.21450200	-0.04581100	-0.21932900
O	-4.30413000	-0.99916800	0.51025400
C	-1.61380700	-1.43861600	-0.85022100
H	-2.30917400	-2.17557600	-0.44977600
H	-1.75504100	-1.36569000	-1.93070000
H	-0.59138100	-1.77027000	-0.66289800
C	-0.76555400	0.91839700	-0.74842400
H	-0.82590500	0.97479300	-1.83751400
H	-0.92155100	1.91365400	-0.32805500
H	0.22504300	0.55005600	-0.47252300
C	-1.74598500	-0.02326100	1.30978600
C	-0.85230900	-1.02428800	1.97238400
H	-1.28438800	-2.02284500	1.85412300
H	-0.75746200	-0.79009200	3.03192800
C	2.97154000	-0.25526300	0.39482500
C	4.61833400	-1.69108200	-0.69485700
H	5.64606300	-1.96521600	-0.44492300
H	4.58232300	-1.49928800	-1.77611900
C	3.66448700	-2.81410600	-0.32641500
H	3.83561800	-3.10763600	0.71435300
H	3.85418100	-3.68701900	-0.95505300
C	2.23428900	-2.31921200	-0.49139400
H	1.52686000	-3.06225200	-0.10871400
H	2.00579900	-2.19877100	-1.55937100
C	5.04832700	1.76147900	-0.80789300
H	6.00871000	2.25382900	-0.99062300
H	4.69026700	1.39466800	-1.77700600
C	5.29470500	0.56176800	0.11255200
H	5.41422700	0.90504400	1.14636600
H	6.23611200	0.08333800	-0.16077100
C	2.67625800	2.24922000	0.06715100
H	2.18650600	1.94667300	-0.86584000
H	2.07126800	3.05879000	0.48576500
C	2.64722400	1.06711100	1.05087500
H	1.64446900	0.95975200	1.46425600
H	3.32416100	1.26360600	1.88911500
N	4.27533800	-0.48175600	0.04598100
C	4.07469100	2.78845100	-0.23065500
H	3.99129200	3.63371600	-0.92093600
H	4.50210400	3.18721000	0.69840900

N	1.98344900	-1.05977800	0.19261700
H	0.13120500	-1.03728200	1.48155700
C	-6.94703600	-0.07908900	-0.15286300
H	-7.86153000	0.39982000	-0.50176800
H	-6.92267600	-1.11322300	-0.49110500
H	-6.90001000	-0.03230700	0.93340400
S	-5.58472200	0.86091000	-0.88697000

Pathway 2 TS4 (dimethyl)

C	1.72112800	-0.57097200	0.62990900
O	1.43362300	0.87345200	-1.24586600
O	2.97759700	0.13735700	0.87902400
C	4.01266100	-0.07063500	0.07963600
O	4.07398800	-0.84766500	-0.83787000
C	1.89714900	-2.03862500	0.99560000
H	2.55918900	-2.55393600	0.30001200
H	2.31218000	-2.11103500	2.00375200
H	0.92696000	-2.53883400	0.99385500
C	0.73637400	0.10824700	1.57497700
H	1.05002000	-0.03191100	2.61206400
H	0.68220300	1.17560400	1.35568500
H	-0.25663700	-0.32733800	1.44511300
C	1.25932300	-0.28081500	-0.82881700
C	0.50386900	-1.28404700	-1.49443000
H	0.75596800	-2.32002200	-1.28224300
H	0.32728400	-1.07783400	-2.54995400
C	-2.76437100	-0.15979500	-0.52056900
C	-4.61384100	-1.38110800	0.49488800
H	-5.66392600	-1.44530500	0.20535200
H	-4.57378600	-1.27822300	1.58539400
C	-3.86664000	-2.62483400	0.04411100
H	-4.07218400	-2.81318300	-1.01357600
H	-4.21436800	-3.48813000	0.61346500
C	-2.37603100	-2.40813900	0.24410000
H	-1.79207400	-3.21938500	-0.19853700
H	-2.13581000	-2.38210100	1.31370800
C	-4.45986900	2.13723300	0.76295800
H	-5.32731500	2.77778500	0.94766100
H	-4.17478000	1.70277400	1.72781800
C	-4.90259200	1.01050300	-0.17179100
H	-4.97779200	1.37558400	-1.20138500
H	-5.89956700	0.67428300	0.11139400
C	-2.03844000	2.23278800	-0.09924500
H	-1.61842900	1.82034800	0.82424300
H	-1.29716300	2.93427900	-0.49025700
C	-2.20029100	1.09872500	-1.12653300
H	-1.22531500	0.84875000	-1.54336000
H	-2.83475100	1.42929800	-1.95477500
N	-4.04956200	-0.18118700	-0.12934200
C	-3.32617400	2.99550300	0.20466700
H	-3.10399500	3.79995800	0.91204800
H	-3.67494100	3.47859100	-0.71671300
N	-1.95008700	-1.16627600	-0.37570500
H	-0.78313300	-1.16006600	-0.88577800

C	6.60350500	0.50206300	-0.60547200
H	7.48166800	1.10711600	-0.38115200
H	6.84581600	-0.55252900	-0.48816700
H	6.26884300	0.70416900	-1.62119100
S	5.33857200	1.00011500	0.59028900

Pathway 2 Post-reaction TS4 (dimethyl)

C	-1.79104400	-0.75490900	-0.70323200
O	-1.33801900	0.57480300	1.23531100
O	-3.00036000	0.06793100	-0.86602900
C	-4.03168300	-0.08558200	-0.05688500
O	-4.19456200	-0.93803500	0.77728200
C	-2.10392800	-2.17151300	-1.16625100
H	-2.77374400	-2.68356500	-0.47615300
H	-2.56780200	-2.13620400	-2.15547700
H	-1.17943900	-2.74577700	-1.25034000
C	-0.80323100	-0.08452500	-1.65123600
H	-1.18963300	-0.08815500	-2.67368300
H	-0.62593700	0.94505100	-1.33776700
H	0.14547500	-0.62542100	-1.63681300
C	-1.26812600	-0.59858400	0.75515500
C	-0.66922700	-1.68576900	1.35176900
H	-0.73411800	-2.68335100	0.93730200
H	-0.28324800	-1.58220500	2.36222800
C	2.77106200	-0.11235700	0.46344200
C	4.81914800	-1.14978200	-0.33824900
H	5.83902500	-1.07978300	0.03908100
H	4.85572800	-1.06540100	-1.42899200
C	4.19102600	-2.46578200	0.08699800
H	4.31878800	-2.60309300	1.16387600
H	4.69374100	-3.28901800	-0.42073700
C	2.71334500	-2.45553600	-0.25803600
H	2.18796300	-3.29829400	0.19230600
H	2.56484400	-2.50356200	-1.34081400
C	4.35953300	2.35050400	-0.62958200
H	5.17368100	3.07784500	-0.69354900
H	4.25242300	1.90595200	-1.62511800
C	4.79206900	1.26306300	0.35234100
H	4.69717500	1.61231300	1.38472800
H	5.84296800	1.02478700	0.19709100
C	1.85354700	2.17614200	-0.09246600
H	1.61373600	1.72297500	-1.06013900
H	0.99116700	2.78614800	0.18607800
C	1.98730200	1.06491500	0.96503500
H	0.98946500	0.71949700	1.24436900
H	2.46520700	1.45766900	1.86787700
N	4.06712000	-0.00804200	0.20198000
C	3.07900100	3.07689800	-0.22363600
H	2.86558900	3.86103400	-0.95555600
H	3.25016200	3.58262000	0.73462900
N	2.11188700	-1.23386500	0.25603000
H	1.12141000	-1.28047600	0.56031200
C	-6.52446600	0.74971700	0.74212600
H	-7.31591200	1.48611500	0.60362300

H	-6.90631900	-0.24423600	0.51599400
H	-6.16121200	0.79153200	1.76730900
S	-5.21041700	1.20558500	-0.41650000

Pathway 2 Pre-reaction TS5 (dimethyl)

O	-1.41364800	0.25887400	-1.55627600
O	-2.83850300	-1.34220200	0.08671500
C	-1.78002100	-1.32899800	0.88070300
O	-1.07813500	-2.30768400	0.97566500
C	-2.46964700	0.81742200	-1.05590100
C	-2.74045400	2.14773900	-1.04680100
C	0.07218000	-0.35171300	2.64595800
H	0.33399700	0.46310600	3.32120200
H	-0.01825600	-1.28068800	3.20453300
H	0.83609300	-0.44791300	1.87564500
S	-1.51033200	0.11197800	1.90196400
C	1.92484100	0.42976500	-0.77842700
C	3.28564700	1.91641300	0.58015700
H	4.30357300	2.27932400	0.43814000
H	3.17311700	1.62797200	1.63069400
C	2.28291300	2.99210600	0.20117400
H	2.51704000	3.37682200	-0.79509800
H	2.35144800	3.82021100	0.90698700
C	0.88463100	2.40353500	0.21309200
H	0.15405800	3.08568000	-0.22154300
H	0.56420300	2.18490600	1.23609100
C	4.11791800	-1.51319100	0.28494300
H	5.12124300	-1.91675900	0.44834400
H	3.67797500	-1.34963300	1.27509300
C	4.27280700	-0.16382500	-0.41622700
H	4.48817400	-0.30423400	-1.47997300
H	5.11946000	0.37478200	0.00651600
C	1.86606900	-2.11091700	-0.80984800
H	1.28534300	-2.02370100	0.11350600
H	1.38519500	-2.89925900	-1.39452000
C	1.73878600	-0.80574300	-1.61291700
H	0.74383700	-0.74422800	-2.05285900
H	2.46383400	-0.79238800	-2.43284000
N	3.11527700	0.72798400	-0.26537600
C	3.30249200	-2.53196400	-0.50900500
H	3.28577500	-3.47986600	0.03648100
H	3.81894100	-2.72745200	-1.45710200
N	0.86430300	1.17632200	-0.56987500
H	-0.05412300	0.85364500	-0.98593100
C	-3.52015000	-0.17551900	-0.50256700
H	-2.04826000	2.83741800	-1.51995800
H	-3.62437900	2.55841400	-0.57822200
C	-4.51474600	0.38023900	0.50999000
H	-5.11454900	-0.43859100	0.91446300
H	-4.02701000	0.90250200	1.33332400
H	-5.19120400	1.08040300	0.01728200
C	-4.26482500	-0.80227400	-1.67937600
H	-4.93739300	-1.58966300	-1.32948400
H	-4.85430200	-0.03511100	-2.18499200

H -3.55392900 -1.22785000 -2.38897100

Pathway 2 TS5 (dimethyl)

O -1.41032000 -0.25072200 -0.83405100
O -3.53066500 -1.02135000 -0.00959000
C -2.27221600 -1.38526700 0.41520700
O -1.87327600 -2.51993400 0.24084800
C -2.29275200 0.68468800 -1.09282000
C -2.04171900 1.86082700 -1.69681200
C -0.27475500 -1.33160000 2.37887300
H 0.03414300 -0.98098900 3.36421700
H -0.40319400 -2.41237100 2.39692800
H 0.48578600 -1.05988400 1.64688800
S -1.84627900 -0.51883000 2.00384900
C 2.05379400 0.42857500 -0.50968000
C 3.30585300 2.04020000 0.81039400
H 4.16997500 2.64717900 0.53982800
H 3.48013700 1.63069700 1.81055100
C 2.04038400 2.88031900 0.77692400
H 1.98204600 3.42008800 -0.17198300
H 2.07210900 3.61534700 1.58129000
C 0.82741200 1.98121700 0.93024400
H -0.10214000 2.51551700 0.73232700
H 0.77016800 1.56656800 1.94152800
C 4.72084800 -1.08873600 -0.03387900
H 5.79533400 -1.28795000 -0.07389600
H 4.43438300 -1.10891600 1.02347700
C 4.49444300 0.32156200 -0.57897800
H 4.55072100 0.33022100 -1.67151700
H 5.27888100 0.98526400 -0.21891800
C 2.46977800 -2.04626900 -0.83758200
H 2.06121400 -2.14741000 0.17381800
H 2.05045500 -2.86727600 -1.42368300
C 1.96816300 -0.73115800 -1.45892300
H 0.92202700 -0.83351100 -1.74799000
H 2.53632200 -0.49886700 -2.36438600
N 3.22709400 0.93079800 -0.15023900
C 3.99070300 -2.18317800 -0.81111600
H 4.25049700 -3.15644900 -0.38557700
H 4.36087700 -2.18556600 -1.84370500
N 0.91973000 0.89225800 -0.03074300
H 0.04047100 0.44238100 -0.35182600
C -3.69663300 0.27194000 -0.62164200
H -1.04083100 2.10807000 -2.03225600
H -2.83652600 2.57270700 -1.88062900
C -4.30511100 1.25764000 0.37330100
H -5.26425100 0.87659400 0.73356800
H -3.64353500 1.42127800 1.22529300
H -4.47725800 2.21920700 -0.11480000
C -4.63453400 0.05071800 -1.80535300
H -5.58892900 -0.35335600 -1.45737900
H -4.82267400 0.99744600 -2.31558700
H -4.19137700 -0.64894600 -2.51691800

Pathway 2 Post-reaction TS5 (dimethyl)

O	-1.53035300	-0.26879300	-0.76898600
O	-3.51770000	-1.03278500	0.04330300
C	-2.12683300	-1.28952600	0.19035500
O	-1.72477200	-2.44299900	-0.01511900
C	-2.42284200	0.71047900	-1.00536900
C	-2.11473900	1.86717000	-1.58883600
C	-0.11894400	-1.42503500	2.27115700
H	-0.03946600	-1.66764500	3.33104200
H	-0.11791800	-2.34712100	1.68623100
H	0.72859200	-0.80173500	1.98149300
S	-1.70261500	-0.59532500	1.97864300
C	2.02553600	0.43009300	-0.49337700
C	3.32965900	2.10347800	0.69079200
H	4.18634500	2.68932900	0.35829400
H	3.53846800	1.74192200	1.70250900
C	2.06901300	2.95084700	0.66158100
H	1.97813700	3.44249100	-0.31050200
H	2.13581200	3.72493100	1.42595500
C	0.85628400	2.07245100	0.90693600
H	-0.07528300	2.60392700	0.71192000
H	0.83055200	1.71129000	1.93956300
C	4.71695700	-1.06157800	-0.05728100
H	5.78885400	-1.26093400	-0.14053900
H	4.48386300	-1.02560200	1.01258600
C	4.45900600	0.31689700	-0.66519700
H	4.46057900	0.26772700	-1.75794400
H	5.25651600	1.00078600	-0.37980500
C	2.43221800	-2.06006900	-0.69507900
H	2.07509800	-2.10065100	0.33912400
H	1.98475000	-2.91257300	-1.21105800
C	1.89649200	-0.78339000	-1.36660500
H	0.83883300	-0.90543900	-1.60049000
H	2.41833200	-0.60305600	-2.31097800
N	3.21014300	0.94637100	-0.20885600
C	3.95265400	-2.19612000	-0.73783600
H	4.23507300	-3.14486500	-0.27329400
H	4.27171300	-2.25472000	-1.78565000
N	0.91244000	0.93338100	0.00236000
H	0.03739400	0.46726400	-0.24564400
C	-3.79106500	0.25038500	-0.52368700
H	-1.10190400	2.08671500	-1.90450800
H	-2.88658800	2.60187200	-1.77719000
C	-4.38659600	1.18903500	0.52365200
H	-5.32960300	0.77760300	0.89213100
H	-3.70258200	1.31906100	1.36413300
H	-4.58501300	2.16867200	0.08236900
C	-4.75371100	0.04901600	-1.69182500
H	-5.68578100	-0.39250600	-1.32998100
H	-4.98305400	1.00708400	-2.16389500
H	-4.31386800	-0.61508300	-2.43857700

Pathway 2 Pre-reaction TS6 (dimethyl)

C	2.69035900	-1.66595000	0.04828400
O	1.44089000	0.20485600	0.67208300
O	2.60922700	-0.73831300	-1.03744900
C	2.06482200	0.51192500	-0.63139000
O	1.25032000	1.04440900	-1.44324900
C	2.05181800	-2.97692700	-0.40247200
H	2.07712600	-3.70954400	0.40730300
H	1.01305300	-2.81819300	-0.69790100
H	2.60303100	-3.38261400	-1.25456200
C	4.14384100	-1.87988100	0.46732100
H	4.60155900	-0.93657800	0.76953100
H	4.19384100	-2.57733700	1.30693300
H	4.70997300	-2.29978200	-0.36804300
C	1.87305800	-0.97990500	1.13304800
C	1.57961300	-1.45120200	2.34360300
H	0.98425100	-0.87523000	3.04089900
H	1.92933600	-2.43086600	2.64205800
C	2.69248900	3.12137600	0.23639300
H	3.42699300	3.91373800	0.38461800
H	2.13828200	2.96669200	1.16305400
S	3.58327600	1.61510200	-0.23676900
C	-1.90495400	0.31514100	-0.07899200
C	-3.68742800	1.69292400	0.85941000
H	-3.48652700	1.95431600	1.90318700
H	-4.76533700	1.56728900	0.74552800
C	-3.18061100	2.77218500	-0.08131700
H	-3.53220900	3.74561700	0.26098700
H	-3.57685800	2.60396900	-1.08626200
C	-1.66314300	2.73751300	-0.12174500
H	-1.23988900	3.04069000	0.84141900
H	-1.26729400	3.40405300	-0.88786500
C	-4.39789500	-1.63776200	-0.04346500
H	-5.17375400	-2.25876500	0.41301100
H	-4.90043500	-0.96920300	-0.75113800
C	-3.76247000	-0.79681400	1.06130600
H	-3.07358000	-1.39970000	1.65966400
H	-4.52839700	-0.43082600	1.74430000
C	-2.23723600	-1.81040200	-1.43193700
H	-2.60637500	-1.13495800	-2.21154600
H	-1.60465600	-2.54663900	-1.93439000
C	-1.33887000	-1.02080400	-0.46545600
H	-0.37415000	-0.83026300	-0.93275400
H	-1.14144800	-1.60148100	0.44206000
N	-3.06050200	0.39608700	0.56958000
C	-3.40281300	-2.54185800	-0.76833100
H	-3.93404300	-3.12251300	-1.52780700
H	-2.99827300	-3.26510100	-0.04942400
N	-1.23245100	1.38539100	-0.43924600
H	-0.28838200	1.24894400	-0.86315900
H	2.00545400	3.40734000	-0.56039200

Pathway 2 TS6 (dimethyl)

C	3.61967300	-1.23070400	-0.13426500
O	1.60366500	-0.27626300	0.53361500

O	3.01864500	-0.44108300	-1.18542400
C	1.94375000	0.23908400	-0.71514000
O	1.05554500	0.64238400	-1.45573300
C	3.61475700	-2.68574100	-0.59072100
H	4.04090200	-3.31891800	0.19046000
H	2.59667100	-3.02136100	-0.79784300
H	4.21722300	-2.79332200	-1.49559300
C	5.02741200	-0.72811200	0.15142400
H	5.00931200	0.32338000	0.43927500
H	5.46658000	-1.30923900	0.96549700
H	5.65099100	-0.85183300	-0.73683100
C	2.65306900	-1.00148400	1.01383700
C	2.72405300	-1.42861700	2.26521800
H	1.94786300	-1.19456800	2.98215500
H	3.56476400	-2.03149300	2.58190000
C	1.44243500	3.10107900	0.37459700
H	1.61324900	4.10318200	0.77338800
H	0.83996400	2.54194600	1.09600600
S	3.02463900	2.25278900	0.06378200
C	-2.18306900	0.09878400	0.06216000
C	-4.07150300	1.54566000	0.59810700
H	-3.97572400	1.96700400	1.60336100
H	-5.13058600	1.37005800	0.40511800
C	-3.49300100	2.48150300	-0.44774200
H	-3.89904100	3.48270000	-0.30411400
H	-3.77703100	2.14070700	-1.44691400
C	-1.98010300	2.50296000	-0.32712900
H	-1.66743800	2.98143700	0.60568500
H	-1.52132000	3.04406600	-1.15401400
C	-4.65938300	-1.86130100	0.03780500
H	-5.48078600	-2.44028700	0.46880800
H	-5.08112500	-1.27643500	-0.78704800
C	-4.15170400	-0.90082900	1.11111400
H	-3.53362800	-1.42568100	1.84448800
H	-4.98795100	-0.47041600	1.66075700
C	-2.35198800	-2.15830600	-1.07148300
H	-2.62325800	-1.57047600	-1.95512900
H	-1.66686200	-2.93700900	-1.41471900
C	-1.57442800	-1.26434400	-0.08926700
H	-0.55152700	-1.12974400	-0.43556500
H	-1.51323600	-1.74083000	0.89397000
N	-3.39873100	0.23923700	0.56870400
C	-3.59069300	-2.82548400	-0.47477800
H	-4.03456900	-3.48277200	-1.22765200
H	-3.27469600	-3.47031700	0.35437100
N	-1.48485200	1.13339700	-0.36141800
H	-0.54907600	0.95818400	-0.75059000
H	0.87269800	3.19377300	-0.55282400

Pathway 2 Post-reaction TS6 (dimethyl)

C	3.75351700	-1.30852100	-0.14998200
O	1.62178500	-0.50701500	0.35678100
O	3.08511700	-0.66670200	-1.28384300
C	1.88538200	-0.24735200	-0.93683400

O	1.08540400	0.26523800	-1.67330000
C	3.93748300	-2.77958500	-0.49120900
H	4.40255400	-3.28979200	0.35447300
H	2.97772800	-3.25536200	-0.70092100
H	4.58790300	-2.88048100	-1.36212600
C	5.06418100	-0.58744000	0.10588900
H	4.87722000	0.47056400	0.29658300
H	5.55324200	-1.03001800	0.97628300
H	5.72401200	-0.69992300	-0.75677500
C	2.72780300	-1.09387800	0.94414400
C	2.76735800	-1.38871100	2.22886400
H	1.92969300	-1.17363500	2.87876800
H	3.65088400	-1.85234500	2.64624600
C	1.31002500	2.94370100	0.38701400
H	0.95151200	3.82528500	0.92609800
H	0.84989200	2.06201400	0.84216800
S	3.14293700	2.82339300	0.42678500
C	-2.24018700	0.08552900	-0.00732700
C	-4.01209200	1.68613900	0.48532500
H	-3.83559400	2.19110200	1.43965400
H	-5.08812100	1.55485700	0.36565600
C	-3.44587200	2.48625900	-0.67350500
H	-3.78853300	3.51838800	-0.60279200
H	-3.80477000	2.07369100	-1.62001200
C	-1.92988700	2.43162000	-0.63347700
H	-1.53950600	2.96866800	0.23556200
H	-1.48842600	2.86871100	-1.52831700
C	-4.81327500	-1.71958600	0.29705400
H	-5.63620100	-2.20533200	0.82848600
H	-5.25303700	-1.19347900	-0.55730800
C	-4.19148700	-0.69207900	1.24014300
H	-3.55818400	-1.17891800	1.98642200
H	-4.96831200	-0.16181100	1.78953000
C	-2.59600700	-2.25600300	-0.90197400
H	-2.88808800	-1.74081100	-1.82335900
H	-1.97424300	-3.10238200	-1.20244800
C	-1.71462800	-1.31852600	-0.05723100
H	-0.71062400	-1.28073100	-0.47459200
H	-1.61591500	-1.70097100	0.96315200
N	-3.41282100	0.34487100	0.54625400
C	-3.82968700	-2.78927600	-0.17474400
H	-4.35164500	-3.48840300	-0.83384200
H	-3.49888900	-3.36930300	0.69536400
N	-1.51502200	1.03576900	-0.56702200
H	-0.61776700	0.77372400	-0.97344900
H	0.94691700	3.01201500	-0.64169500

Pathway 2 Pre-reaction TS4 (cyclohexyl)

C	-1.71877000	-0.06046400	-0.33628300
O	-2.65845700	-0.07659400	-2.53178800
O	-2.97404900	-0.66141100	0.07826200
C	-4.08156300	0.07261500	0.07037200
O	-4.17299100	1.22957300	-0.24865400
C	-1.85231200	0.43725200	-1.78788200

C	-0.90056200	1.50485700	-2.23844300
H	-1.20974900	2.45496200	-1.78955300
H	-0.93485300	1.59220300	-3.32360300
C	3.11171800	0.46209200	-0.61460400
C	4.39601600	1.66941500	1.07999000
H	5.44221700	1.98103500	1.12804300
H	4.11934500	1.29048600	2.07333100
C	3.50981700	2.84149600	0.69751400
H	3.90643400	3.31873600	-0.20444900
H	3.50867400	3.58584400	1.49695100
C	2.10481700	2.32270800	0.42944000
H	1.46467400	3.12433100	0.04719800
H	1.65242700	1.99346400	1.37609400
C	4.95658200	-1.75144900	0.65365800
H	5.87536500	-2.26509400	0.95395400
H	4.37237700	-1.58465500	1.56633900
C	5.34143300	-0.39254800	0.06095600
H	5.71309300	-0.52514400	-0.96150800
H	6.16849000	0.02926700	0.63350400
C	2.87117300	-2.05763200	-0.81689800
H	2.18554900	-1.92347100	0.02668100
H	2.39720300	-2.77607100	-1.49207200
C	3.01245800	-0.71575100	-1.55523100
H	2.12713000	-0.53554700	-2.16502400
H	3.87269400	-0.75059600	-2.23236500
N	4.28006100	0.61005400	0.08321800
C	4.18809500	-2.64757000	-0.31625900
H	3.98769600	-3.61047500	0.16400200
H	4.83138700	-2.85872700	-1.18017400
N	2.07273600	1.22149100	-0.52197400
H	0.11968900	1.30750700	-1.88722300
C	-6.76892800	0.27131200	0.53819800
H	-7.66746000	-0.25418400	0.86050900
H	-6.57146000	1.10550000	1.20874400
H	-6.89746300	0.62570500	-0.48276400
S	-5.42803400	-0.94230900	0.62332700
C	-0.72252200	-1.23019100	-0.36371200
C	-1.26439900	1.00534700	0.66593900
C	-1.00805200	0.42175800	2.05616200
H	-1.99147800	1.81735400	0.70733000
H	-0.32859300	1.41533000	0.28380700
C	-0.00199300	-0.72853700	1.99860700
H	-1.94884700	0.06538900	2.49146000
H	-0.64056600	1.21836100	2.70932800
C	-0.47752800	-1.80970000	1.02964300
H	0.14759100	-1.15206600	2.99572600
H	0.96777600	-0.34334300	1.65837800
H	0.21832300	-0.84138800	-0.76527800
H	-1.09621900	-1.99501400	-1.04954400
H	-1.40099600	-2.26215700	1.40566800
H	0.25961500	-2.61400800	0.95500200

Pathway 2 TS4 (cyclohexyl)

C	-1.53511700	0.35559900	0.03934100
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O	-1.16957900	-1.73938700	-1.03219900
O	-2.80369100	-0.19296500	0.52289800
C	-3.82413600	-0.32094200	-0.30816100
O	-3.85929200	-0.00491100	-1.46953300
C	-1.04131300	-0.51167700	-1.15482500
C	-0.31635700	0.13179500	-2.19388500
H	-0.62250500	1.13976700	-2.46300400
H	-0.10488000	-0.50984200	-3.04909100
C	2.95859500	-0.19819500	-0.74389700
C	4.60635800	1.49933800	-0.15600600
H	5.67503700	1.55442200	-0.36917900
H	4.45609500	1.81718400	0.88211400
C	3.83313900	2.39439400	-1.10981500
H	4.13932700	2.18542700	-2.13882900
H	4.06036100	3.44001400	-0.89682200
C	2.34695900	2.12023100	-0.95365100
H	1.76314000	2.63727000	-1.71975200
H	1.99401200	2.48005100	0.02069600
C	4.66304800	-1.63862200	1.45464100
H	5.54804000	-2.06851000	1.93300300
H	4.25576700	-0.89545700	2.14948100
C	5.12067500	-0.92373200	0.18250500
H	5.31812700	-1.64944400	-0.61320800
H	6.06158200	-0.40839000	0.37277700
C	2.35127500	-2.29928800	0.54108700
H	1.81482800	-1.60566300	1.19693700
H	1.69984600	-3.16703800	0.41034700
C	2.53862800	-1.64199500	-0.83766200
H	1.59400000	-1.66763900	-1.37999300
H	3.26939000	-2.20456400	-1.42698200
N	4.19131300	0.10121100	-0.30246500
C	3.64915700	-2.75363700	1.20537500
H	3.40995100	-3.23993900	2.15572400
H	4.11908700	-3.51815300	0.57395600
N	2.07263200	0.69963100	-1.06950300
H	0.95216200	0.37918100	-1.57012100
C	-6.42264600	-1.08449800	-0.73229800
H	-7.31581100	-1.52494200	-0.28975900
H	-6.64391800	-0.07616300	-1.07719000
H	-6.08144400	-1.70262400	-1.56058400
S	-5.18131500	-1.04754200	0.58500600
C	-0.57403900	0.13333900	1.21302000
C	-1.69640600	1.85332000	-0.23311200
C	-2.12089300	2.62794500	1.01587600
H	-2.39745100	2.01323300	-1.05409000
H	-0.72260500	2.22892900	-0.56196900
C	-1.13178500	2.40970100	2.16111600
H	-3.12137200	2.30825800	1.32873000
H	-2.19192400	3.69128700	0.77052100
C	-0.96740200	0.92053800	2.46353600
H	-1.46252900	2.94356300	3.05677700
H	-0.15846000	2.83230800	1.87942300
H	0.42119200	0.44412500	0.87787400
H	-0.52673600	-0.93802800	1.42111600
H	-1.90765300	0.52428600	2.86113600

H -0.20716800 0.76828600 3.23520200

Pathway 2 Post-reaction TS4 (cyclohexyl)

C -1.59673100 0.51931400 0.05575800
O -1.05224300 -1.31360400 -1.37982000
O -2.81316600 -0.23271300 0.40611800
C -3.83982100 -0.28358600 -0.41809900
O -3.97917600 0.29836600 -1.46289800
C -1.02979600 -0.04751200 -1.27791500
C -0.44805500 0.82257800 -2.17373300
H -0.56013400 1.89620000 -2.09984900
H -0.03748800 0.42095800 -3.09635300
C 3.00525700 -0.14109400 -0.66160400
C 4.93859200 1.24833600 -0.16564600
H 5.98288800 1.12808300 -0.45285100
H 4.90938700 1.53673400 0.88987600
C 4.27215500 2.29851700 -1.03772700
H 4.46488300 2.07807700 -2.09086600
H 4.69592100 3.27766400 -0.81431400
C 2.77685400 2.29707800 -0.77889200
H 2.23998400 2.90291400 -1.50951000
H 2.55144300 2.68957900 0.21723500
C 4.64366400 -1.97444100 1.27631200
H 5.48863300 -2.57847500 1.61851200
H 4.44833700 -1.23101900 2.05695600
C 5.08259300 -1.25109500 0.00446200
H 5.07503700 -1.93248800 -0.85143400
H 6.10685200 -0.89946500 0.11691700
C 2.17364200 -2.16577100 0.60265600
H 1.85280500 -1.43005800 1.34725700
H 1.36104800 -2.89064100 0.51435100
C 2.31758700 -1.47116500 -0.76447700
H 1.32457200 -1.31051200 -1.18959800
H 2.87248700 -2.11152400 -1.45698000
N 4.28373200 -0.05885400 -0.31871000
C 3.43193000 -2.88350300 1.08347900
H 3.21152900 -3.39039300 2.02719300
H 3.69084300 -3.66720800 0.36097200
N 2.27739200 0.93427400 -0.88204800
H 1.30875000 0.80639900 -1.23305800
C -6.35725700 -1.23868600 -0.96431300
H -7.17327500 -1.87661400 -0.62529600
H -6.70458500 -0.20987600 -1.04033100
H -5.99633500 -1.58847300 -1.92975600
S -5.05842800 -1.38030900 0.28902000
C -0.63559000 0.15600000 1.19265800
C -1.90690100 2.01782700 0.09298400
C -2.42347000 2.47331700 1.45962300
H -2.61080200 2.27417100 -0.70020200
H -0.97170200 2.54569600 -0.11811600
C -1.43449100 2.11752100 2.57050500
H -3.39160300 2.00286000 1.66636900
H -2.59706300 3.55311700 1.43642300
C -1.12192800 0.62102900 2.56584700

H	-1.83071200	2.41948100	3.54464900
H	-0.50510600	2.68130700	2.41552900
H	0.32490600	0.63204900	0.96710200
H	-0.47583700	-0.92397200	1.17425700
H	-2.02138400	0.06069300	2.84177400
H	-0.36001300	0.38736100	3.31566200

Pathway 2 Pre-reaction TS5 (cyclohexyl)

O	-0.74243400	0.39654300	-1.56336400
O	-2.28761700	-0.96873900	0.14647900
C	-1.23828900	-1.02310600	0.94645500
O	-0.63680800	-2.06123300	1.09230200
C	-1.73726600	1.08316800	-1.09618100
C	-1.86919800	2.43302200	-1.16527100
C	0.71102600	-0.14807900	2.66283900
H	1.04370600	0.66147600	3.31285400
H	0.53633100	-1.04654800	3.25049300
H	1.46534200	-0.33709200	1.90001400
S	-0.82245600	0.43176800	1.89767600
C	2.59855300	0.28495900	-0.79832400
C	4.11070500	1.71718900	0.45500600
H	5.15596500	1.97325100	0.28213500
H	3.98665100	1.50632300	1.52253400
C	3.20828400	2.85752500	0.01716200
H	3.46445000	3.15680400	-1.00274700
H	3.36344600	3.71713600	0.66955200
C	1.76124800	2.40553800	0.07505200
H	1.09240200	3.12565800	-0.39616800
H	1.43397700	2.28119000	1.11169800
C	4.61150200	-1.78920400	0.36796200
H	5.57433000	-2.27398800	0.55279800
H	4.19664200	-1.52574100	1.34729900
C	4.88467700	-0.50500500	-0.41465900
H	5.07393600	-0.72868100	-1.46913500
H	5.78306600	-0.02479400	-0.03000200
C	2.30319400	-2.23797900	-0.67647000
H	1.74418100	-2.04359000	0.24386200
H	1.74416100	-3.01084200	-1.21007600
C	2.28632800	-0.97562800	-1.55449400
H	1.29450800	-0.84731800	-1.98741000
H	2.99709300	-1.07839000	-2.38064800
N	3.81808100	0.49976800	-0.31217000
C	3.69762100	-2.77285500	-0.35988800
H	3.59905500	-3.68143500	0.24109500
H	4.18356100	-3.07096300	-1.29737300
N	1.61604600	1.14039400	-0.63031900
H	0.66707100	0.88435500	-1.02529300
C	-2.87076200	0.22878300	-0.48100700
C	-3.79673300	0.93110200	0.51768200
C	-3.71213800	-0.37245200	-1.61753500
C	-4.89067500	0.00272800	1.04865400
H	-4.27110700	1.76277500	-0.01120100
H	-3.22379700	1.36862100	1.33750200
C	-4.82751100	-1.29096600	-1.11518200

H	-4.14514500	0.46866200	-2.16921400
H	-3.04461700	-0.90326300	-2.30033400
C	-5.71989700	-0.58304600	-0.09515400
H	-5.53271700	0.56104500	1.73605700
H	-4.43624400	-0.80887000	1.62764000
H	-5.42178500	-1.63459200	-1.96712900
H	-4.38486400	-2.18127100	-0.65682400
H	-6.47152800	-1.27523100	0.29595500
H	-6.26407600	0.22968100	-0.59364900
H	-1.10987700	3.01651200	-1.67685100
H	-2.70286600	2.96295800	-0.72604700

Pathway 2 TS5 (cyclohexyl)

O	-0.71448300	-0.43814200	-0.79511300
O	-2.83003300	-1.13271600	0.11009200
C	-1.57395700	-1.48384600	0.54087600
O	-1.18741000	-2.63109000	0.42981500
C	-1.60763200	0.45397700	-1.15163000
C	-1.37073100	1.54014000	-1.91141600
C	0.46596900	-1.32052500	2.45340200
H	0.78974100	-0.92458600	3.41656300
H	0.34193100	-2.39983600	2.52229300
H	1.21302200	-1.07890500	1.69704300
S	-1.11417200	-0.52995600	2.06733800
C	2.70755600	0.43202700	-0.53266800
C	3.88597700	2.16192200	0.70182400
H	4.71294700	2.80305900	0.39629400
H	4.09283800	1.80242300	1.71500800
C	2.57647600	2.93074000	0.65169600
H	2.47778500	3.42606400	-0.31793900
H	2.57776400	3.69973100	1.42432900
C	1.41616200	1.97494800	0.85973900
H	0.45664300	2.44914600	0.65216300
H	1.39260100	1.60235000	1.88840300
C	5.46094500	-0.91461500	-0.03755100
H	6.54415100	-1.05633700	-0.08598300
H	5.19005300	-0.90525600	1.02405300
C	5.14919800	0.45667100	-0.63729600
H	5.18952200	0.42168200	-1.73005900
H	5.90059400	1.17721800	-0.31822900
C	3.25575200	-2.02729200	-0.76601100
H	2.86662200	-2.10823100	0.25489000
H	2.87525600	-2.89401600	-1.31141500
C	2.67372000	-0.76877700	-1.43276200
H	1.63094200	-0.94000000	-1.70079000
H	3.21608700	-0.54314500	-2.35557900
N	3.85620100	1.01287300	-0.21348600
C	4.78216700	-2.07940100	-0.75704800
H	5.10093100	-3.01806200	-0.29537000
H	5.13845100	-2.10547800	-1.79420300
N	1.55644100	0.85139800	-0.05437500
H	0.69892800	0.34238900	-0.34550700
C	-2.99383000	0.11933700	-0.58396500

C	-3.52380500	1.20497200	0.36449600
C	-4.01981400	-0.14956600	-1.69181300
C	-4.89594500	0.84752400	0.93574700
H	-3.59511200	2.13417600	-0.21103400
H	-2.79964700	1.38373200	1.16257600
C	-5.39848100	-0.50508400	-1.13267500
H	-4.09415200	0.75631800	-2.30231900
H	-3.63965400	-0.94634000	-2.33736100
C	-5.90733100	0.57718100	-0.17921600
H	-5.24598300	1.65984300	1.57949700
H	-4.80177500	-0.04240300	1.56824900
H	-6.10087400	-0.64580400	-1.95954500
H	-5.33755000	-1.46044800	-0.60044500
H	-6.87169800	0.28353600	0.24606800
H	-6.07677300	1.50399900	-0.74277900
H	-0.37669000	1.73875500	-2.29601900
H	-2.16762700	2.22741800	-2.16594400

Pathway 2 Post-reaction TS5 (cyclohexyl)

O	-0.82510200	-0.33649700	-0.74532400
O	-2.77994100	-1.09992200	0.13575000
C	-1.38359200	-1.30062000	0.28948400
O	-0.94551000	-2.45325700	0.16827600
C	-1.75154800	0.59087600	-1.05216200
C	-1.48293500	1.70092200	-1.73759200
C	0.62887500	-1.24406200	2.37546000
H	0.71113500	-1.40645600	3.45045700
H	0.64507800	-2.20662100	1.85989600
H	1.46702900	-0.63057500	2.04032300
S	-0.96723700	-0.46361400	2.02199900
C	2.70858900	0.41683000	-0.53906000
C	4.01987600	2.15708800	0.53405700
H	4.88281700	2.71403200	0.16964300
H	4.21997100	1.86042300	1.56843000
C	2.76573900	3.00953600	0.44169900
H	2.68269400	3.43372000	-0.56229700
H	2.83514200	3.83385500	1.15132700
C	1.54556200	2.15873700	0.74153700
H	0.61894200	2.68193600	0.50463700
H	1.51155900	1.87131300	1.79685000
C	5.39438500	-1.05302100	-0.00151700
H	6.46543600	-1.26200900	-0.07087200
H	5.16157000	-0.94262800	1.06333400
C	5.14136900	0.28117900	-0.70306300
H	5.14077000	0.15603300	-1.78975300
H	5.94207400	0.98011400	-0.46738900
C	3.10536300	-2.08314800	-0.57117200
H	2.74726500	-2.05236100	0.46283400
H	2.65478900	-2.96687200	-1.02867600
C	2.57453300	-0.85282000	-1.32769900
H	1.51634200	-0.98643000	-1.55231400
H	3.09682000	-0.73899600	-2.28212700
N	3.89576500	0.94562300	-0.28980300
C	4.62524300	-2.22825300	-0.60307000

H	4.90314200	-3.14417200	-0.07433400
H	4.94482000	-2.35983200	-1.64407700
N	1.59765500	0.95854900	-0.08049000
H	0.72202200	0.47385000	-0.28789200
C	-3.09470400	0.13737100	-0.50891500
C	-3.69617500	1.13993300	0.48662600
C	-4.09531100	-0.15565300	-1.63477500
C	-5.03771300	0.65506600	1.03569400
H	-3.83325300	2.09193700	-0.03903300
H	-2.98316700	1.31904500	1.29530000
C	-5.43886400	-0.64116900	-1.08955400
H	-4.24137000	0.76867000	-2.20488900
H	-3.65633000	-0.89254500	-2.31324100
C	-6.02673400	0.35879100	-0.09266600
H	-5.44766400	1.40786000	1.71524700
H	-4.87494700	-0.25327900	1.62659100
H	-6.13131500	-0.80481300	-1.92039500
H	-5.29849200	-1.60896600	-0.59587500
H	-6.96579700	-0.02421100	0.31766700
H	-6.26585600	1.29316500	-0.61706900
H	-0.47975700	1.91985200	-2.08332300
H	-2.27695900	2.39548900	-1.97840200

Pathway 2 Pre-reaction TS6 (cyclohexyl)

O	2.79545000	1.49838800	-0.72802300
O	1.19764000	0.00783600	-0.12131800
C	1.88095000	0.48139400	-1.27127800
O	1.11696100	0.89703800	-2.19316000
C	2.99690800	1.25473900	0.58465400
C	3.97811300	1.80488800	1.29566800
C	1.93398400	-2.22401800	-2.06781700
H	1.51752300	-2.51448400	-1.10300400
H	1.12977100	-1.91351400	-2.73715700
H	2.45783400	-3.07278400	-2.50863600
S	3.12362900	-0.87649600	-1.85139000
C	-2.16035700	0.38913800	-1.00827700
C	-3.52819600	1.72083800	0.49158900
H	-4.60899900	1.79739000	0.60742200
H	-3.08482200	1.65085200	1.49079200
C	-2.98974000	2.92518200	-0.26065600
H	-3.55201900	3.05816000	-1.18874700
H	-3.11945800	3.82311100	0.34374100
C	-1.52116600	2.70806900	-0.57044000
H	-1.14281300	3.45943900	-1.26430900
H	-0.92286600	2.76520900	0.34327000
C	-3.45372000	-1.78684300	0.81299700
H	-4.24703100	-2.37565700	1.28196400
H	-2.86909200	-1.34089000	1.62528800
C	-4.11869000	-0.66981400	0.00874700
H	-4.50022000	-1.05343800	-0.94234500
H	-4.97542600	-0.27925700	0.55545400
C	-1.42778000	-2.03724100	-0.75871200
H	-0.69296900	-1.64809600	-0.05084600
H	-0.90740300	-2.78827500	-1.35785900

C	-1.82408100	-0.89740300	-1.70833600
H	-0.99077700	-0.68355100	-2.37772200
H	-2.67689600	-1.19166700	-2.32879900
N	-3.24501700	0.48303200	-0.24591300
C	-2.58685800	-2.71580100	-0.03389100
H	-2.18380300	-3.50888000	0.60283900
H	-3.22872900	-3.20795000	-0.77519100
N	-1.34055700	1.40139000	-1.18334500
H	-0.41879400	1.20656200	-1.63739000
C	1.90402800	0.32334000	1.07838800
C	2.42420800	-0.95307500	1.74831500
C	0.93741600	1.05309500	2.02082600
C	1.27433500	-1.86488800	2.18249400
H	3.01830700	-0.65960800	2.62135300
H	3.09027100	-1.47260200	1.05559700
C	-0.23588100	0.15937800	2.41497700
H	1.49565400	1.35127500	2.91521500
H	0.59427300	1.96973000	1.53500100
C	0.25625000	-1.13617700	3.06422900
H	1.67808300	-2.73166800	2.71373400
H	0.77458200	-2.25253800	1.28905800
H	-0.90021100	0.69823400	3.09699200
H	-0.82093400	-0.07143900	1.51856800
H	-0.59016700	-1.79523100	3.28116000
H	0.72416100	-0.89344200	4.02688800
H	4.70003200	2.46929000	0.83755800
H	4.05514600	1.60378600	2.35631600

Pathway 2 TS6 (cyclohexyl)

O	-2.76789900	-1.53494800	-0.80390700
O	-1.18193800	-0.10932700	-0.14542600
C	-1.80791100	-0.62747600	-1.23442900
O	-1.19763500	-0.81386900	-2.27928300
C	-3.01140200	-1.31820000	0.52283100
C	-4.04604100	-1.84253900	1.16212200
C	-2.01235700	2.42795700	-1.71103700
H	-1.64580000	2.59099800	-0.69459600
H	-1.17307000	2.08784600	-2.32461700
H	-2.36598000	3.38098000	-2.11039600
S	-3.34298000	1.18365600	-1.72097500
C	2.23500500	-0.26023000	-1.10312600
C	3.53423000	-1.69770500	0.36152700
H	4.61004200	-1.77380300	0.51581800
H	3.05029900	-1.70461000	1.34384900
C	3.04171400	-2.84604100	-0.50125300
H	3.65179600	-2.91303100	-1.40560500
H	3.14478200	-3.78331500	0.04536100
C	1.59000000	-2.61545600	-0.87381500
H	1.25619800	-3.31716400	-1.63801300
H	0.94099800	-2.73222200	-0.00150600
C	3.36625800	1.75596400	0.98582100
H	4.11865900	2.32097700	1.54276300
H	2.76129900	1.22261800	1.72722500
C	4.10270300	0.73467800	0.11985500

H	4.52443600	1.21122500	-0.76971200
H	4.93728400	0.30956500	0.67474200
C	1.41600100	2.09725600	-0.66668200
H	0.66364600	1.60918300	-0.04333500
H	0.89366300	2.88641900	-1.21177500
C	1.90998200	1.07665200	-1.70311700
H	1.13352900	0.91641300	-2.45176200
H	2.79249200	1.45337100	-2.22913700
N	3.26942800	-0.40620200	-0.28814300
C	2.50950200	2.73512400	0.18592500
H	2.04379400	3.44652000	0.87407000
H	3.16924800	3.31968700	-0.46694800
N	1.44204000	-1.26837900	-1.40609600
H	0.57185800	-1.05179000	-1.90318500
C	-1.88386500	-0.46592500	1.06458800
C	-2.33919200	0.79471800	1.79784200
C	-0.92339000	-1.28645100	1.93264400
C	-1.15643500	1.62818000	2.29667300
H	-2.95314000	0.47447600	2.64714000
H	-2.97511400	1.37551900	1.12661800
C	0.28227700	-0.45431800	2.36327800
H	-1.47962300	-1.62453400	2.81358400
H	-0.61847300	-2.18143900	1.38402400
C	-0.16102900	0.80220700	3.11480200
H	-1.53344100	2.46301800	2.89374300
H	-0.64463400	2.07112000	1.43695100
H	0.94421000	-1.06037000	2.98799500
H	0.85521600	-0.17186000	1.47266200
H	0.70806700	1.41451700	3.37356800
H	-0.63044900	0.50172600	4.05981500
H	-4.77331200	-2.45501700	0.64520400
H	-4.16759700	-1.66864500	2.22297900

Pathway 2 Post-reaction TS6 (cyclohexyl)

O	-2.65108400	-1.51029700	-1.27131800
O	-1.06795200	-0.35801000	-0.26131900
C	-1.59282100	-0.69560000	-1.42682100
O	-1.16353500	-0.36150500	-2.49695800
C	-2.88347000	-1.71270800	0.07789700
C	-3.90942000	-2.41589400	0.51752200
C	-2.21646600	2.72023100	-0.81121600
H	-1.84768700	2.48665500	0.19138000
H	-1.53632400	2.24912200	-1.52559900
H	-2.14801700	3.80304800	-0.94566200
S	-3.94010200	2.12755500	-1.04464700
C	2.35802300	0.21324100	-1.16413900
C	3.68056000	-1.46739200	-0.00209300
H	4.75281300	-1.49262500	0.19040800
H	3.16587900	-1.77132000	0.91478600
C	3.33254000	-2.38616000	-1.15969500
H	3.99700400	-2.18527200	-2.00357400
H	3.47724900	-3.42244400	-0.85519200
C	1.89232600	-2.16100900	-1.57809100

H	1.65798900	-2.67963900	-2.50684100
H	1.20182500	-2.51417400	-0.80658900
C	3.07359500	1.67089500	1.48610400
H	3.70872000	2.12692800	2.25017800
H	2.46764100	0.91397100	1.99535000
C	3.99143600	0.97469800	0.48232500
H	4.45091900	1.69806900	-0.19687500
H	4.80346600	0.47550400	1.00794300
C	1.25531900	2.28616800	-0.23851600
H	0.51083300	1.58240200	0.14181800
H	0.69636900	3.14531700	-0.61560400
C	1.96363200	1.63416200	-1.43626300
H	1.29759100	1.63298700	-2.29959300
H	2.85273500	2.20454500	-1.72002500
N	3.32038500	-0.07332800	-0.30450900
C	2.18860300	2.75570500	0.87446700
H	1.58657900	3.21098300	1.66610500
H	2.83392300	3.54942100	0.47911300
N	1.68747900	-0.73492400	-1.79358500
H	0.88400500	-0.44739200	-2.34171400
C	-1.77232000	-1.02279600	0.83377000
C	-2.26637000	0.02878000	1.82226300
C	-0.79377500	-2.00227900	1.48147300
C	-1.11916800	0.73388100	2.54820200
H	-2.89617200	-0.49733800	2.54809900
H	-2.90463600	0.73821800	1.28772100
C	0.37197700	-1.26363700	2.13677200
H	-1.35069900	-2.57074400	2.23333200
H	-0.44741700	-2.72036000	0.73301600
C	-0.13026700	-0.25392900	3.16951200
H	-1.53658200	1.38816300	3.31773200
H	-0.59153600	1.38548700	1.84505800
H	1.04750700	-1.98672300	2.60051200
H	0.94535600	-0.74245800	1.36025100
H	0.71153100	0.28806900	3.60976300
H	-0.62049600	-0.79609500	3.98722900
H	-4.61913400	-2.86099300	-0.16693600
H	-4.04767700	-2.55408100	1.58134300

Pathway 3 stepwise Pre-reaction TS7 (dimethyl)

C	3.59807000	-0.17825500	0.28986900
O	1.94173100	-0.50159800	-1.32529500
O	3.08351700	-1.54725700	0.24738200
C	2.16248400	-1.68221900	-0.69008100
O	1.58227300	-2.68704800	-0.96973800
C	3.34746300	0.38282000	1.67802100
H	3.90149200	-0.19945300	2.41716400
H	3.69842700	1.41626000	1.71536200
H	2.28090200	0.37060800	1.91625600
C	5.07256700	-0.21954600	-0.08027900
H	5.46730700	0.79807600	-0.09903700
H	5.62593500	-0.79559700	0.66368300
H	5.21721100	-0.66800900	-1.06476400
C	2.75106700	0.48106100	-0.77899900

C	2.72525000	1.73149000	-1.19625500
H	2.06953200	2.05016300	-1.99492200
H	3.37692500	2.46102600	-0.73493100
S	-0.46802700	1.25069700	2.07640200
C	0.65333500	2.70353400	1.95246100
H	0.09143400	3.64165700	1.96994100
H	1.37259000	2.72967200	2.77610000
H	1.22557100	2.67306600	1.02024300
C	-1.92747600	-0.33497700	-1.02573200
C	-3.22607600	1.66596100	-0.57740500
H	-4.29117100	1.86395400	-0.69751100
H	-2.89833100	2.04076600	0.39740800
C	-2.43693900	2.31593900	-1.70019200
H	-2.87662200	2.05375700	-2.66616100
H	-2.48269100	3.39987700	-1.59285900
C	-0.99410400	1.84940000	-1.64488200
H	-0.44304500	2.16011200	-2.53244200
H	-0.49386000	2.23511800	-0.75152300
C	-3.56352200	-1.11775400	1.49079000
H	-4.44655400	-1.33130500	2.09973100
H	-3.00237700	-0.32491800	1.99718300
C	-4.05048800	-0.58501200	0.14334900
H	-4.39645500	-1.39986500	-0.49913800
H	-4.89966900	0.08027100	0.29108300
C	-1.44089600	-2.23409500	0.56139900
H	-0.77389600	-1.50600200	1.03558000
H	-0.91169400	-3.18920200	0.53835700
C	-1.68235600	-1.80854200	-0.89793600
H	-0.80724800	-2.05838100	-1.49813200
H	-2.52968700	-2.35437700	-1.32285000
N	-3.04436400	0.20816700	-0.57924400
C	-2.71900100	-2.38690700	1.38358100
H	-2.45182200	-2.72307600	2.38955900
H	-3.33266200	-3.18206500	0.94159700
N	-0.97873800	0.39390600	-1.58982600
H	-0.11583100	-0.07796800	-1.81895600

Pathway 3 stepwise TS7 (dimethyl)

C	3.65605200	-0.21936300	-0.17912500
O	1.47766800	-0.10942700	-1.03671400
O	3.10671900	-1.51596400	-0.57090300
C	1.90906700	-1.35995000	-1.13094600
O	1.30115300	-2.25376500	-1.66686200
C	4.41563200	-0.40383200	1.12005800
H	5.30100700	-1.02044300	0.95023900
H	4.74042900	0.57230400	1.48686500
H	3.78618300	-0.87288200	1.87461000
C	4.59653700	0.20972900	-1.30307500
H	5.07793000	1.15552100	-1.05151900
H	5.37112900	-0.55011000	-1.43278400
H	4.05764500	0.33636500	-2.24308900
C	2.39461200	0.66279200	-0.09333500
C	2.49168400	2.02895500	-0.27432000
H	1.61664600	2.66254800	-0.19414700

H	3.46379000	2.50099700	-0.21620000
S	1.25284500	0.09283800	1.59572300
C	1.97209100	1.25084900	2.77695400
H	1.19456100	1.65697100	3.42517000
H	2.75066000	0.79069500	3.38906300
H	2.40719500	2.06984600	2.18610600
C	-2.21966800	0.10497900	-0.71574300
C	-3.67954100	1.93818900	-0.06474800
H	-4.71688900	2.13670200	-0.33380800
H	-3.56746200	2.11989500	1.00880500
C	-2.74812800	2.82637200	-0.87150000
H	-3.00715600	2.76494400	-1.93161400
H	-2.87054500	3.86197500	-0.55457600
C	-1.31174100	2.38197700	-0.66855700
H	-0.63612700	2.88210100	-1.36242300
H	-0.97045900	2.59073000	0.35015100
C	-4.19812800	-1.29126500	1.22998400
H	-5.15553000	-1.65782700	1.61037300
H	-3.77121500	-0.65209700	2.01064700
C	-4.49075800	-0.43460000	-0.00211500
H	-4.69980000	-1.06182900	-0.87338700
H	-5.37973300	0.16990400	0.17025700
C	-1.90483100	-2.13266600	0.41454600
H	-1.33483400	-1.55898300	1.15330100
H	-1.34522800	-3.05429000	0.23825100
C	-1.93149900	-1.35315300	-0.91163900
H	-0.96378800	-1.44309400	-1.40568600
H	-2.67871900	-1.77794700	-1.58844400
N	-3.41794700	0.51632600	-0.33233300
C	-3.28807100	-2.48810700	0.95576800
H	-3.17012600	-3.06410600	1.87783800
H	-3.78769500	-3.14927300	0.23696000
N	-1.22682300	0.94990400	-0.91360000
H	-0.30817500	0.55019300	-1.08840800

Pathway 3 stepwise Post-reaction TS7 (dimethyl)

C	3.45554900	0.12969300	0.02682500
O	1.42432300	0.07132200	-1.80761600
O	3.08820000	-1.03412500	-0.73647500
C	2.03172600	-1.01040000	-1.64251100
O	1.82765300	-2.10290600	-2.18485200
C	4.61359400	-0.36777100	0.90075600
H	5.44223700	-0.68492900	0.26330900
H	4.95833300	0.43598800	1.55449200
H	4.30283700	-1.21316800	1.51700500
C	3.96214500	1.24723700	-0.88489100
H	4.47722200	2.01386000	-0.30226300
H	4.68457300	0.81803500	-1.58325900
H	3.15012100	1.70164900	-1.44832200
C	2.30473000	0.56791500	0.93843700
C	2.06856400	1.83807800	1.26268800
H	1.30832800	2.13115800	1.97413800
H	2.64423200	2.63770700	0.81422400
S	1.40676500	-0.81253100	1.60942800

C	0.18180400	-0.01697800	2.67050500
H	-0.40144600	-0.82518800	3.11256600
H	0.65427700	0.55705600	3.46827800
H	-0.48184400	0.62207800	2.08577800
C	-1.92717000	0.23843800	-0.69118200
C	-3.34706400	2.07336900	0.03463000
H	-4.36100100	2.33843600	-0.26439600
H	-3.27829500	2.17102300	1.12279200
C	-2.34019700	2.97345200	-0.65944300
H	-2.53304500	2.98094000	-1.73544200
H	-2.44688200	3.99313100	-0.28932800
C	-0.93934100	2.45864400	-0.38829500
H	-0.19363200	2.96703900	-0.99942200
H	-0.66909000	2.61054400	0.66007100
C	-4.13055400	-1.29696800	0.88313500
H	-5.13512900	-1.63866200	1.14754100
H	-3.71153900	-0.82095100	1.77667800
C	-4.27905300	-0.24288500	-0.21327300
H	-4.47222400	-0.71447500	-1.18176200
H	-5.13659700	0.39167100	0.00377400
C	-1.84920100	-2.17606100	0.09774300
H	-1.31390800	-1.77561100	0.96318400
H	-1.33463300	-3.09824400	-0.18273600
C	-1.70538700	-1.19539700	-1.07803400
H	-0.70197900	-1.26851500	-1.49792700
H	-2.40898600	-1.45675400	-1.87473600
N	-3.13063900	0.66754900	-0.33414300
C	-3.29127900	-2.50511200	0.47299700
H	-3.28683000	-3.23166500	1.29042400
H	-3.77668000	-2.99682000	-0.37902900
N	-0.88035500	1.03820700	-0.70504300
H	0.01570200	0.64900600	-1.04116400

Pathway 3 stepwise Pre-reaction TS8 (dimethyl)

O	4.64596800	-0.76319700	0.62408900
O	3.19552100	-0.73855600	-1.12711600
C	4.50366500	-0.65849100	-0.60218100
O	5.34951000	-0.48282000	-1.49435500
C	1.87476000	0.16137800	0.71870600
C	1.38795800	-0.00826500	1.95094800
H	1.21384600	0.81166200	2.63607000
H	1.18557000	-1.00338100	2.32669100
S	2.25499900	1.74800700	0.01581300
C	-2.41707100	0.30383400	0.54201800
C	-3.75445500	1.44129900	-1.13621400
H	-4.79719400	1.75728100	-1.12512400
H	-3.55432200	0.96008900	-2.09875500
C	-2.83206800	2.62784400	-0.91430600
H	-3.15111500	3.18070600	-0.02733100
H	-2.89126200	3.30005800	-1.76992800
C	-1.40397000	2.14489500	-0.73485000
H	-0.75368300	2.94716100	-0.38824900
H	-0.99578800	1.75774400	-1.67232300
C	-4.36668500	-1.86691300	-0.55321500

H	-5.00574600	-2.62373800	-0.08950700
H	-4.66052900	-1.80052700	-1.60406300
C	-4.64916400	-0.53364700	0.15025100
H	-4.77435300	-0.67979900	1.22323700
H	-5.57425000	-0.08930600	-0.21397600
C	-2.27184900	-2.21012900	0.92009200
H	-1.24601500	-2.57997800	0.85535800
H	-2.80098000	-2.87737000	1.60448600
C	-2.23854600	-0.79089800	1.55185900
H	-1.29267100	-0.63061400	2.06844800
H	-3.02149700	-0.68088300	2.30406900
N	-3.58176400	0.45093600	-0.06644200
C	-2.89810400	-2.29159100	-0.47549400
H	-2.80657100	-3.31778700	-0.83854900
H	-2.31084600	-1.67955300	-1.17022400
N	-1.38657900	1.08269100	0.26607200
H	-0.51442100	0.86532200	0.73426500
C	1.83898400	2.88999500	1.35305900
H	2.05445300	3.88606000	0.96683600
H	0.78278500	2.83816600	1.62473500
H	2.45734000	2.70560100	2.23218000
C	2.06591200	-0.98508200	-0.28371800
C	2.16077400	-2.35638900	0.38627600
C	0.88401000	-0.99340200	-1.26218700
H	1.20390300	-2.63913400	0.83092000
H	2.93517000	-2.37296500	1.14996700
H	-0.04749100	-1.18671800	-0.72812100
H	0.79970300	-0.04055100	-1.78795200
H	2.40086500	-3.09505700	-0.38202200
H	1.03063000	-1.78603400	-1.99876600

Pathway 3 stepwise TS8 (dimethyl)

O	3.71756600	0.05084700	0.81471800
O	3.30697900	-1.40983900	-0.78466900
C	4.24183200	-0.77099900	-0.04588600
O	5.42346400	-0.98292700	-0.21754100
C	2.10902100	0.23549900	0.41193500
C	1.26130600	0.54011200	1.52747500
H	1.42252700	1.53112000	1.95198300
H	1.28059200	-0.22002200	2.30960500
S	2.19224400	1.53148200	-0.88156400
C	-2.29872800	0.17936200	0.66424600
C	-3.77452500	1.71163200	-0.51523600
H	-4.80650300	2.01345200	-0.33138100
H	-3.66573400	1.51916100	-1.58867900
C	-2.80810700	2.79348500	-0.06158600
H	-3.03469800	3.07617300	0.97022600
H	-2.92691500	3.67911100	-0.68689900
C	-1.38648000	2.26556600	-0.15408900
H	-0.67685100	2.94350500	0.32471800
H	-1.07862100	2.15793700	-1.19877200
C	-4.37247500	-1.61957200	-0.82959000
H	-5.01013700	-2.47106300	-0.57284400
H	-4.71105800	-1.24859100	-1.80117700

C	-4.58143500	-0.54295200	0.24155500
H	-4.62526100	-0.99557400	1.23326100
H	-5.53206500	-0.03071300	0.09388800
C	-2.22501600	-2.36167600	0.39116700
H	-1.22962400	-2.75651600	0.17608600
H	-2.76540900	-3.15424000	0.91565100
C	-2.07910500	-1.14391400	1.34626900
H	-1.08474200	-1.12100900	1.79066500
H	-2.78521700	-1.21845300	2.17547500
N	-3.53116500	0.47625500	0.23074100
C	-2.91284400	-2.06675400	-0.94565600
H	-2.86329700	-2.96183500	-1.57074500
H	-2.34223900	-1.29893300	-1.48134300
N	-1.27642400	0.97512300	0.50868300
H	-0.24206700	0.70505400	0.93106100
C	2.56824100	2.99965500	0.10664900
H	2.82520700	3.78476900	-0.60495900
H	1.70852500	3.31983900	0.69440700
H	3.42197500	2.80848700	0.75617800
C	1.98610200	-1.16286000	-0.23928400
C	1.71557700	-2.25859000	0.78768200
C	0.98656500	-1.23342400	-1.38182300
H	0.71026600	-2.16638700	1.19722200
H	2.42808700	-2.21785100	1.61346100
H	0.00816000	-0.90029300	-1.03130900
H	1.28819600	-0.60136200	-2.21764700
H	1.80146700	-3.22896500	0.29495500
H	0.89901100	-2.26222800	-1.73705100

Pathway 3 stepwise Post-reaction TS8 (dimethyl)

O	3.81791700	-0.16540800	0.58540100
O	2.91000000	-1.74129200	-0.65973100
C	4.04496500	-1.25781200	-0.16075600
O	5.12973300	-1.73194900	-0.34134800
C	2.46018200	0.28337600	0.37497800
C	1.94039300	0.89622600	1.65581600
H	2.43757100	1.84273200	1.86546100
H	2.12438200	0.22509800	2.49588100
S	2.46751500	1.48226600	-1.02713700
C	-2.56561900	0.18924900	0.85458900
C	-3.57829500	1.81429400	-0.64945800
H	-4.58638200	2.20753500	-0.80063900
H	-3.16063800	1.58447700	-1.64030000
C	-2.70114600	2.82617300	0.06774400
H	-3.19929400	3.14294800	0.98961100
H	-2.55811800	3.71186100	-0.55553700
C	-1.36399400	2.17442800	0.39558500
H	-0.78095700	2.81936600	1.06096900
H	-0.76637800	2.06976500	-0.52024000
C	-4.34040100	-1.37280400	-1.23803700
H	-5.05246300	-2.20312500	-1.18423600
H	-4.43563900	-0.93843700	-2.23820300
C	-4.73741100	-0.33624000	-0.17597900
H	-5.06174000	-0.84358700	0.73389500

H	-5.59461300	0.24678000	-0.51885300
C	-2.54693600	-2.31548000	0.36897500
H	-1.52056100	-2.69183200	0.35021600
H	-3.17899200	-3.15644100	0.67081500
C	-2.63937500	-1.19914400	1.44424000
H	-1.81354500	-1.28886300	2.14894700
H	-3.55943600	-1.30360400	2.02384700
N	-3.67543600	0.60566300	0.15705900
C	-2.90989800	-1.88392900	-1.05645100
H	-2.74111000	-2.72617000	-1.73377900
H	-2.21446800	-1.10016100	-1.37573900
N	-1.48007200	0.86252900	1.02161300
H	0.86445400	1.05828500	1.56358000
C	3.58533300	2.75203700	-0.37400400
H	3.85742700	3.37533800	-1.22564500
H	3.09798500	3.37149900	0.37764500
H	4.48646500	2.29267400	0.03089600
C	1.77348300	-1.04450600	-0.06256700
C	1.29891500	-1.87404300	1.12363500
C	0.67881300	-0.92242700	-1.10082600
H	0.42930500	-1.39537700	1.57755100
H	2.07659900	-1.99358700	1.88057000
H	-0.13298100	-0.32419300	-0.68123100
H	1.03666300	-0.46454700	-2.02280900
H	1.00961200	-2.86388600	0.76651900
H	0.28990100	-1.91535600	-1.33519200

Pathway 3 stepwise Pre-reaction TS7 (cyclohexyl)

O	1.16831600	-0.47404000	-1.86748900
O	2.52504000	-1.38934900	-0.38743100
C	1.54815800	-1.62077800	-1.24395800
O	1.03887300	-2.67766600	-1.46516400
C	1.93867600	0.58263300	-1.40808700
C	1.77367300	1.81626100	-1.84466400
H	1.03221200	2.05881800	-2.59364900
H	2.39663200	2.60884500	-1.45293700
S	-0.96509500	1.50955000	1.99115600
C	0.13490200	2.91906500	1.55971300
H	-0.39125300	3.87428500	1.64150600
H	1.00973300	2.96242200	2.21467100
H	0.50207900	2.82499100	0.53303700
C	-2.57138900	-0.45853800	-0.86081800
C	-3.98923700	1.42808300	-0.28974700
H	-5.07591900	1.50903900	-0.25635500
H	-3.56398200	1.88851800	0.60757200
C	-3.44831200	2.08877300	-1.54534300
H	-3.99538400	1.73130600	-2.42178600
H	-3.59253800	3.16719000	-1.47575700
C	-1.97162500	1.77158200	-1.69444600
H	-1.59642500	2.08616000	-2.66823400
H	-1.38766700	2.25548100	-0.90642200
C	-3.66721900	-1.26015000	1.91662500
H	-4.40517300	-1.52076300	2.68058000
H	-3.10791200	-0.39389600	2.28592400

C	-4.43350800	-0.84409900	0.66072200
H	-4.80773900	-1.71817200	0.11993600
H	-5.30310300	-0.25010800	0.93725500
C	-1.63677100	-2.23244000	0.66796100
H	-0.96582500	-1.43004000	0.99301400
H	-1.03598700	-3.14043000	0.58104000
C	-2.17048500	-1.89759600	-0.73589100
H	-1.39869800	-2.10022800	-1.47874800
H	-3.02548200	-2.53330200	-0.98279300
N	-3.65234400	-0.00160400	-0.25805600
C	-2.73324700	-2.45229200	1.70852300
H	-2.26578200	-2.70859500	2.66356600
H	-3.33324000	-3.32185500	1.41165200
N	-1.79454900	0.32958900	-1.58556400
H	-0.95024700	-0.07891200	-1.96036100
C	2.91435300	0.02250900	-0.40006000
C	4.36836200	0.10922600	-0.86296900
C	2.72140900	0.59598500	0.99997200
C	5.32835600	-0.50505300	0.15692900
H	4.59651900	1.17167400	-0.99953800
H	4.46599500	-0.37055000	-1.84059200
C	3.68857000	-0.02091700	2.00946300
H	2.90114400	1.67393800	0.92439300
H	1.67799000	0.47349100	1.30567000
C	5.13917500	0.11079500	1.54394600
H	6.35504000	-0.36341700	-0.19002500
H	5.15737600	-1.58581200	0.20952800
H	3.54992900	0.46628200	2.97810200
H	3.44245900	-1.07939400	2.14931700
H	5.81093000	-0.36826300	2.26136800
H	5.41321500	1.17274000	1.50936500

Pathway 3 stepwise TS7 (cyclohexyl)

O	0.81090500	0.14536700	-0.92335600
O	2.55881300	-1.16908200	-0.67940600
C	1.34309100	-1.03641000	-1.20216900
O	0.80035800	-1.89234400	-1.85771500
C	1.67695400	0.84520500	0.12490900
C	1.64386600	2.22722200	0.15336600
H	0.71618400	2.75178800	0.34964400
H	2.56725100	2.77530600	0.28661700
S	0.61569200	-0.06966700	1.70452600
C	1.25172300	0.94701600	3.05239400
H	0.45216700	1.17571700	3.75811600
H	2.07658300	0.46559700	3.58195300
H	1.60577100	1.88356600	2.59868900
C	-2.89994700	0.10585600	-0.69302000
C	-4.51294900	1.81472500	-0.06396200
H	-5.53396300	1.97146000	-0.41167600
H	-4.50263800	1.93964700	1.02328200
C	-3.57167500	2.79828300	-0.73720000
H	-3.73515100	2.78507500	-1.81782000
H	-3.78179700	3.80520600	-0.37681600
C	-2.13434200	2.42041700	-0.43232400

H	-1.43100900	2.99802800	-1.03183200
H	-1.89760000	2.58564300	0.62346500
C	-4.93411700	-1.52397100	0.99223300
H	-5.89478500	-1.96425900	1.27326900
H	-4.60102200	-0.92107100	1.84420500
C	-5.18530400	-0.59747600	-0.19754600
H	-5.29944400	-1.16999200	-1.12252200
H	-6.11567200	-0.05164800	-0.04922600
C	-2.54382500	-2.18999100	0.30354200
H	-2.06213300	-1.64525900	1.12254200
H	-1.92350000	-3.06803600	0.10838900
C	-2.51443700	-1.31768500	-0.96344600
H	-1.50941200	-1.32005400	-1.38628300
H	-3.18261600	-1.73048100	-1.72516000
N	-4.14613000	0.42726200	-0.38319900
C	-3.94214400	-2.65146500	0.70881100
H	-3.86218500	-3.28619000	1.59571600
H	-4.34966000	-3.28274500	-0.09043400
N	-1.94457300	1.01287500	-0.75093100
H	-0.99570900	0.68013100	-0.90754400
C	3.00620000	0.10107300	-0.10720500
C	3.88048200	0.78470000	-1.16877700
C	3.81520000	-0.20498700	1.14706000
C	5.15570800	-0.00339200	-1.47039600
H	4.14896800	1.77462400	-0.79064500
H	3.29043700	0.94178300	-2.07544800
C	5.11156000	-0.96145400	0.84890700
H	4.04344800	0.75668500	1.62013600
H	3.19169000	-0.77079400	1.83974400
C	5.96426600	-0.24604800	-0.19718500
H	5.75045000	0.54683700	-2.20503700
H	4.89538300	-0.96441100	-1.92741800
H	5.67100400	-1.08819300	1.78004900
H	4.86630800	-1.96703400	0.48883500
H	6.86096800	-0.83158600	-0.42015800
H	6.30306600	0.71714200	0.20572700

Pathway 3 stepwise Post-reaction TS7 (cyclohexyl)

O	0.87195100	0.17317500	-1.66457000
O	2.45409400	-1.01276500	-0.55431100
C	1.46331000	-0.92141200	-1.52499000
O	1.29018200	-1.97647900	-2.14760500
C	1.59261300	0.46653200	1.18019700
C	1.33122800	1.70465200	1.59730300
H	0.52631400	1.93290800	2.28293000
H	1.92666900	2.54218100	1.25831200
S	0.65134500	-0.95978400	1.67756000
C	-0.63590900	-0.24813400	2.72411500
H	-1.24466400	-1.08762600	3.06103400
H	-0.21426600	0.25601800	3.59437800
H	-1.26360400	0.43955100	2.15492200
C	-2.52646900	0.30373700	-0.71943200
C	-3.97313700	2.08314300	0.08603700
H	-4.96909200	2.38430600	-0.23805800

H	-3.95868700	2.08276100	1.18073800
C	-2.92674500	3.03050200	-0.47368900
H	-3.06317000	3.13336200	-1.55339200
H	-3.04730800	4.01515800	-0.02190800
C	-1.54476300	2.48098900	-0.17558700
H	-0.76553900	3.03147400	-0.70268300
H	-1.32834900	2.54199600	0.89417700
C	-4.82951000	-1.33532800	0.58870400
H	-5.85022900	-1.68717300	0.76249300
H	-4.46272900	-0.94127000	1.54307800
C	-4.90497700	-0.19111100	-0.42145800
H	-5.04133200	-0.57785000	-1.43608600
H	-5.77061900	0.43229300	-0.20418200
C	-2.51024700	-2.16856100	-0.13261600
H	-2.02581000	-1.84692000	0.79357400
H	-1.98447600	-3.06934900	-0.45819400
C	-2.29090900	-1.09508700	-1.21178600
H	-1.26476200	-1.14399800	-1.57647200
H	-2.94761700	-1.28141000	-2.06739300
N	-3.74611200	0.71368400	-0.39586500
C	-3.97383500	-2.51324800	0.12775200
H	-4.02203300	-3.30630300	0.87930900
H	-4.41022600	-2.92609000	-0.79017100
N	-1.47623600	1.09119400	-0.60655300
H	-0.56448200	0.72052600	-0.92041100
C	2.78952400	0.09285800	0.30278900
C	3.35442100	1.27885500	-0.49548100
C	3.91032500	-0.46918300	1.20309800
C	4.57058100	0.86941500	-1.32681200
H	3.67121800	2.04688300	0.21729300
H	2.57078500	1.70305000	-1.12115500
C	5.15793900	-0.86036200	0.40889600
H	4.16136500	0.30639300	1.93485100
H	3.52847300	-1.32935800	1.75891600
C	5.67755600	0.30095000	-0.43822800
H	4.93652100	1.73966800	-1.87962400
H	4.27418300	0.12204700	-2.07094300
H	5.93163600	-1.20096000	1.10370300
H	4.91800600	-1.70710500	-0.24164100
H	6.52694000	-0.02493900	-1.04625000
H	6.04603000	1.09547900	0.22383100

Pathway 3 stepwise Pre-reaction TS8 (cyclohexyl)

O	-4.48941200	0.01990500	-0.86846100
O	-3.02477500	-0.34762600	0.83260000
C	-4.33119500	-0.12567100	0.35223900
O	-5.16452300	-0.10403300	1.27332200
C	-1.66402800	0.87344000	-0.77439800
C	-1.19394000	0.97451200	-2.02164900
H	-0.99685500	1.92454000	-2.50166800
H	-1.03592800	0.08972100	-2.62452200
S	-1.97762000	2.27465200	0.27244600
C	2.62543600	0.53958400	-0.59876000
C	3.97204800	1.24494800	1.29718000

H	5.04427800	1.41885400	1.38389500
H	3.64897400	0.66648800	2.16826500
C	3.22164300	2.56282900	1.20552000
H	3.66945200	3.18826000	0.42931300
H	3.30123600	3.09363400	2.15390200
C	1.76191500	2.30316700	0.87962900
H	1.24212500	3.22636100	0.62587800
H	1.24220400	1.84101200	1.72344900
C	4.22174100	-1.99921600	0.27606000
H	4.81526200	-2.76008800	-0.23872200
H	4.42639200	-2.10234900	1.34490300
C	4.70489800	-0.63139400	-0.21752400
H	4.87817700	-0.64714700	-1.29384900
H	5.65215800	-0.36174100	0.24719600
C	2.24772200	-1.86683100	-1.37927800
H	1.19470500	-2.14370300	-1.46175000
H	2.78483100	-2.46489700	-2.11923200
C	2.38511200	-0.36774700	-1.76992200
H	1.48572900	-0.02989300	-2.28460400
H	3.20960100	-0.22371200	-2.47093200
N	3.75150400	0.44252000	0.08747200
C	2.72941800	-2.23189200	0.02794800
H	2.49788600	-3.28352600	0.21339900
H	2.14971400	-1.66863700	0.76813600
N	1.68690200	1.40934100	-0.27134700
H	0.82630100	1.37605600	-0.80643300
C	-1.52886400	3.67331000	-0.77895000
H	-1.70170900	4.56345300	-0.17431700
H	-0.47812300	3.64530600	-1.07317800
H	-2.16108400	3.71554000	-1.66653500
C	-1.90360500	-0.45619200	-0.04855700
C	-2.03874600	-1.65116200	-1.00675000
C	-0.71519300	-0.72608800	0.89812700
C	-2.22218300	-2.96503900	-0.24668100
H	-1.12030900	-1.72271600	-1.59867800
H	-2.86523800	-1.47216900	-1.69276400
C	-0.85147100	-2.04561100	1.65708600
H	0.18937000	-0.75366700	0.28540200
H	-0.61024600	0.10759100	1.59712400
C	-1.05357900	-3.22348200	0.70498100
H	-2.31460800	-3.78459800	-0.96525700
H	-3.15835000	-2.93253600	0.32089200
H	0.04313500	-2.19897700	2.26883000
H	-1.70128100	-1.97858400	2.34283600
H	-1.21880600	-4.14404900	1.27254700
H	-0.13900200	-3.37604900	0.11698300

Pathway 3 stepwise TS8 (cyclohexyl)

O	-3.55868400	0.47854900	-1.08629100
O	-3.24373800	-0.96394600	0.54961100
C	-4.12672500	-0.36508100	-0.28073300
O	-5.31014600	-0.62989900	-0.22195800
C	-1.98795200	0.72697100	-0.52298600
C	-1.06604900	1.06359500	-1.56662700

H	-1.20219700	2.06185100	-1.98076300
H	-1.02727700	0.32058900	-2.36425500
S	-2.25003600	2.01708400	0.74680800
C	2.46121000	0.59446600	-0.69754600
C	3.82796900	1.70543300	0.97938300
H	4.86281500	2.05000100	0.96941900
H	3.65264600	1.19171200	1.93167300
C	2.86914400	2.87258900	0.81278200
H	3.15398900	3.45511100	-0.06780600
H	2.92929200	3.52730300	1.68295800
C	1.45628600	2.34003700	0.64725900
H	0.76372700	3.12709000	0.34274800
H	1.08255400	1.92973200	1.59116600
C	4.50863500	-1.53556400	0.32446500
H	5.20906400	-2.26028200	-0.10192900
H	4.74865600	-1.44513200	1.38770900
C	4.73861100	-0.19600300	-0.38073100
H	4.83216300	-0.34403100	-1.45784400
H	5.66951800	0.26374100	-0.04876300
C	2.52000800	-1.91321000	-1.25681500
H	1.56119800	-2.43403600	-1.30076100
H	3.18514300	-2.43738500	-1.94857800
C	2.31198000	-0.45793800	-1.76512000
H	1.31838100	-0.34426500	-2.19641400
H	3.02218000	-0.22481200	-2.56191300
N	3.66186000	0.76059400	-0.12554900
C	3.07007100	-2.03607100	0.16743300
H	3.01972500	-3.08271600	0.47871500
H	2.41474100	-1.48867600	0.85577800
N	1.41391900	1.30061400	-0.37080300
H	0.39318100	1.13980000	-0.88672300
C	-2.50057000	3.49093900	-0.27199600
H	-2.87292900	4.26235600	0.40273800
H	-1.56780100	3.83056200	-0.72143000
H	-3.24570500	3.29709600	-1.04316000
C	-1.88453100	-0.66870500	0.14050000
C	-1.44839800	-1.74786400	-0.85855800
C	-0.99897000	-0.71649200	1.38504700
C	-1.42427300	-3.14134700	-0.23100400
H	-0.44574500	-1.48860500	-1.20648400
H	-2.10511700	-1.72817600	-1.73233900
C	-0.94700800	-2.11145100	2.01321500
H	0.00555000	-0.40509400	1.07951900
H	-1.35153800	0.00724600	2.12230200
C	-0.52642200	-3.17775500	1.00427700
H	-1.07758500	-3.86234600	-0.97694600
H	-2.44210500	-3.43513800	0.04648700
H	-0.25526000	-2.09262000	2.86010300
H	-1.93476300	-2.36053200	2.41553400
H	-0.55639700	-4.16835300	1.46708900
H	0.51248300	-3.00073900	0.70332700

Pathway 3 stepwise Post-reaction TS8 (cyclohexyl)

O	3.67779200	0.11642100	1.10844900
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O	3.24845900	-1.26146800	-0.55629600
C	4.16272700	-0.85367700	0.31851900
O	5.27433100	-1.29269500	0.40310800
C	2.42052200	0.58675600	0.57047900
C	1.52810300	1.01922700	1.71152700
H	1.92967200	1.90760000	2.19874300
H	1.46064200	0.22857800	2.46045400
S	2.78651500	1.97812300	-0.58837800
C	-2.56309700	0.68046700	0.64410400
C	-4.06634100	1.72747600	-0.96034300
H	-5.05887100	2.18146800	-0.90724400
H	-4.04802000	1.07445500	-1.84483500
C	-2.98644700	2.79026600	-1.07113000
H	-3.10247600	3.50737800	-0.25216300
H	-3.08941100	3.33739500	-2.01099400
C	-1.62333600	2.11577200	-0.98303200
H	-0.83072100	2.86527400	-0.89352000
H	-1.42379100	1.57218500	-1.91670300
C	-4.93612500	-1.30390200	0.08649200
H	-5.59776300	-1.94169000	0.68227000
H	-5.35078400	-1.27495100	-0.92606200
C	-4.95231400	0.10315200	0.70097500
H	-4.92864500	0.03190700	1.78978400
H	-5.88385000	0.61497800	0.45093700
C	-2.72482600	-1.77632300	1.33017200
H	-1.78113100	-2.31135900	1.19275600
H	-3.25355700	-2.28929000	2.13954300
C	-2.40976600	-0.31893300	1.76691000
H	-1.38144700	-0.24348600	2.11850800
H	-3.04777100	-0.02593600	2.60401400
N	-3.85412800	0.95145800	0.25360300
C	-3.52858400	-1.90267200	0.03114400
H	-3.59660300	-2.95905800	-0.24416300
H	-2.96995300	-1.41676000	-0.77747000
N	-1.49540100	1.18774400	0.13385100
H	0.52904600	1.23214800	1.31887600
C	3.61810400	3.13485300	0.53414500
H	4.09688800	3.87675700	-0.10481000
H	2.91164100	3.63732100	1.19340200
H	4.38335400	2.61844400	1.11264300
C	1.95320700	-0.66621500	-0.22812400
C	1.18905500	-1.66172300	0.65026400
C	1.19362000	-0.39971000	-1.51884100
C	0.85568600	-2.95385700	-0.09523800
H	0.25998900	-1.17075200	0.95277000
H	1.75893600	-1.87800200	1.55839700
C	0.83367600	-1.68828000	-2.26275300
H	0.28189100	0.13364800	-1.23147900
H	1.77800600	0.25116900	-2.17154700
C	0.06850100	-2.66242800	-1.37051100
H	0.28444700	-3.60816700	0.56931600
H	1.78064100	-3.48457000	-0.34454800
H	0.24151100	-1.42960800	-3.14455600
H	1.75009100	-2.16685800	-2.62529600
H	-0.13797200	-3.59036500	-1.91087200

H -0.90036800 -2.22379500 -1.10493100

Pathway 3 concerted Pre-reaction TS9 (dimethyl)

C -2.58038300 -1.07271100 1.12231300
O -1.70395600 -1.41068400 -1.01331000
O -3.35865000 -0.42992100 0.06732800
C -2.80628700 -0.63022100 -1.11940600
O -3.20350600 -0.19811900 -2.15897100
C -2.03653900 0.01187000 2.03737400
H -1.38874800 -0.44122100 2.79067900
H -1.46197400 0.75141900 1.47508800
H -2.86059400 0.51836800 2.54412400
C -3.48101000 -2.06219300 1.84227700
H -2.90583300 -2.58097100 2.61160100
H -4.30583500 -1.53227100 2.32224500
H -3.88167200 -2.80188700 1.14740300
C -1.49614900 -1.74900900 0.30850600
C -0.50473200 -2.53282100 0.68813300
H 0.19187400 -2.94333300 -0.03071000
H -0.38383400 -2.77556200 1.73540500
C -2.26869000 2.92250400 -0.23498100
H -2.93254600 2.44631100 0.49007800
H -2.07167400 2.19603000 -1.02856600
S -0.70582200 3.47979100 0.55525400
C 1.52411600 0.18258300 -0.05429600
C 2.30078100 -0.92956300 -2.06967100
H 2.44571700 -1.98363700 -2.30732000
H 3.18226500 -0.37990200 -2.41703700
C 1.03447600 -0.40400200 -2.72506300
H 0.19987200 -1.06590400 -2.48852400
H 1.16228900 -0.39114300 -3.80769700
C 0.73391200 0.99752800 -2.22177400
H -0.27049600 1.31246000 -2.50784900
H 1.44248800 1.72245700 -2.63291300
C 4.37955100 -0.90592400 0.61237100
H 4.81558400 -1.44279500 1.46006200
H 5.10532200 -0.95502300 -0.20409700
C 3.09447600 -1.63971700 0.21022000
H 2.54540300 -1.96725200 1.09384700
H 3.32178000 -2.53742800 -0.36392200
C 2.97766300 0.80415100 1.94681000
H 2.94184600 1.87280700 2.16909000
H 3.17150100 0.29172300 2.89279200
C 1.57672400 0.37097200 1.43419800
H 0.83231000 1.12108700 1.70142700
H 1.26206300 -0.56514100 1.89929400
N 2.20833400 -0.81165400 -0.61147100
C 4.13929300 0.56091200 0.97812300
H 5.05239600 0.97012700 1.41738900
H 3.96600300 1.13764900 0.06210100
N 0.81597200 1.02897700 -0.76673100
H 0.35648800 1.82557800 -0.26882100
H -2.80329300 3.76317700 -0.68300600

Pathway 3 concerted TS9 (dimethyl)

C	2.93100300	-0.83777100	0.83044400
O	3.23400800	1.23589500	-0.15121000
O	4.03034700	-0.81934500	-0.13347500
C	4.19603800	0.42086600	-0.58968900
O	5.10872000	0.76804100	-1.29040700
C	2.19881400	-2.15625700	0.70132100
H	1.32744100	-2.15399700	1.35927700
H	1.86880100	-2.33954700	-0.31994300
H	2.85420200	-2.97202200	1.01375300
C	3.55760300	-0.69610700	2.21513700
H	2.78657900	-0.76796900	2.98327900
H	4.27981300	-1.50146000	2.36744700
H	4.06355600	0.26470100	2.32580500
C	2.17229000	0.44288500	0.42031100
C	1.33057000	1.14437400	1.30781500
H	1.48169400	2.21624700	1.37889900
H	1.08811200	0.64004500	2.23853100
C	0.67353400	1.54896000	-1.83500400
H	1.38861800	2.05751100	-2.48287400
H	0.56367800	2.11944300	-0.90494900
S	1.21163500	-0.12526800	-1.41725400
C	-2.25709400	0.08668100	0.64179200
C	-4.24261700	1.35231000	0.03738500
H	-5.27335100	1.29050500	0.38731000
H	-4.26035600	1.43601900	-1.05457700
C	-3.53430700	2.54377000	0.66140000
H	-3.65753000	2.51546200	1.74724700
H	-3.98002500	3.46883900	0.29520200
C	-2.05870100	2.49496500	0.30536600
H	-1.48155900	3.22118600	0.87993200
H	-1.90958700	2.71468100	-0.75605400
C	-4.03230800	-1.86713200	-1.02078300
H	-4.43198600	-2.88215600	-0.93357200
H	-4.57498400	-1.37799500	-1.83479100
C	-4.31283800	-1.14870000	0.30086100
H	-4.05479100	-1.78837300	1.14662900
H	-5.37161100	-0.91096900	0.40043500
C	-1.64696100	-2.27987700	-0.16380000
H	-0.63218800	-2.42934800	-0.53386000
H	-1.98065600	-3.22967100	0.26389600
C	-1.58020500	-1.21528800	0.96615800
H	-0.54167500	-0.98053900	1.19282000
H	-2.02999300	-1.59591500	1.88686100
N	-3.56939100	0.10776200	0.41747900
C	-2.53784800	-1.91392400	-1.35373000
H	-2.37408100	-2.63808300	-2.15573300
H	-2.21530100	-0.94602600	-1.75468500
N	-1.52495900	1.17335600	0.59960900
H	-0.48693300	1.10192000	0.80119600
H	-0.29803500	1.50874000	-2.33020200

Pathway 3 concerted Post-reaction TS9 (dimethyl)

C	2.79107600	-0.15569200	1.11935500
O	3.47996800	0.73727700	-0.90312900
O	4.01770700	-0.76728300	0.61606400
C	4.41548300	-0.12790500	-0.48335300
O	5.46929100	-0.29391300	-1.02687300
C	1.93211800	-1.23642600	1.74427500
H	0.95346000	-0.82146900	1.99482500
H	1.79480800	-2.08413700	1.07333000
H	2.40205800	-1.59178000	2.66268500
C	3.19988300	0.88350700	2.15660900
H	2.31644100	1.35152900	2.59396300
H	3.75534400	0.38325500	2.95135300
H	3.83437400	1.66158300	1.72758900
C	2.24520000	0.48387700	-0.19199800
C	1.49856000	1.78691100	-0.02907700
H	1.21936300	2.19166500	-1.00172800
H	2.12343200	2.52695600	0.47129900
C	0.84351400	0.16624900	-2.62588400
H	1.71734800	0.67364500	-3.03425600
H	0.04039400	0.87592300	-2.43047100
S	1.28050300	-0.76853900	-1.13623400
C	-2.56631500	0.26862300	0.92599800
C	-4.01763600	1.33287500	-0.71707900
H	-5.09751200	1.38516400	-0.87574800
H	-3.54963600	1.12966900	-1.69123400
C	-3.48733600	2.63494600	-0.14256200
H	-4.05668000	2.88986000	0.75700400
H	-3.61757100	3.44697600	-0.86162000
C	-2.01597600	2.45197100	0.20566000
H	-1.64594900	3.31693700	0.76458100
H	-1.42517000	2.41296400	-0.71948200
C	-3.76048700	-1.96531900	-0.95140100
H	-4.21176100	-2.95586100	-0.82898500
H	-3.94157000	-1.66009300	-1.98699600
C	-4.46521100	-1.00072700	0.01160700
H	-4.61847200	-1.48734900	0.97649700
H	-5.45966700	-0.74847700	-0.36252100
C	-1.84859300	-2.18654600	0.76567000
H	-0.76355800	-2.30965100	0.79774200
H	-2.28078600	-3.10740600	1.17029200
C	-2.23410200	-0.99453200	1.68605500
H	-1.40600600	-0.75009300	2.35039300
H	-3.07869500	-1.26423200	2.32522900
N	-3.74557800	0.25010400	0.21748100
C	-2.25188000	-2.03225300	-0.70470000
H	-1.82943700	-2.86344600	-1.27703100
H	-1.78030200	-1.12642700	-1.10166400
N	-1.73616900	1.25200900	0.98635000
H	0.58886900	1.61346500	0.55132900
H	0.49555200	-0.57334000	-3.34698800

Pathway 3 concerted Pre-reaction TS9 (cyclohexyl)

O	1.05851200	-0.93138300	2.03935800
O	2.81720900	-0.05128000	1.04120400

C	2.07782000	-0.04501600	2.13887600
O	2.26041600	0.63695900	3.10185500
C	1.10896000	-1.56584700	0.81434800
C	0.24515000	-2.50288000	0.47077500
H	-0.54324700	-2.81176400	1.14410100
H	0.32948600	-2.98074300	-0.49615300
C	1.34510400	3.12807700	0.23161100
H	2.33883400	2.88733100	-0.15213800
H	1.01947100	2.28120100	0.84409900
S	0.15848400	3.44473900	-1.13461500
C	-2.01292300	0.16055400	-0.17223400
C	-3.06951300	-0.51021800	1.91350000
H	-3.09056000	-1.47382100	2.42377700
H	-4.08235500	-0.09423900	1.93383600
C	-2.07974600	0.42660800	2.58654200
H	-1.11953800	-0.07811600	2.70631900
H	-2.44887500	0.69417400	3.57683900
C	-1.89668600	1.67563800	1.74191900
H	-1.05939300	2.27757500	2.09681300
H	-2.79373700	2.30130400	1.76606800
C	-4.45462200	-1.59386700	-1.02144500
H	-4.59747500	-2.41899000	-1.72553300
H	-5.34915700	-1.55106700	-0.39409700
C	-3.23151100	-1.92934100	-0.15963900
H	-2.44559000	-2.38165300	-0.76598200
H	-3.48690300	-2.65784000	0.60915300
C	-2.98418800	-0.08675100	-2.51728400
H	-3.02370100	0.86512500	-3.05098900
H	-2.87143800	-0.86794800	-3.27362300
C	-1.71496600	-0.08664000	-1.62213900
H	-1.01794900	0.68277100	-1.95485200
H	-1.18769000	-1.03975000	-1.69360200
N	-2.68051100	-0.75485300	0.52133800
C	-4.31245800	-0.26971900	-1.77623600
H	-5.12928800	-0.18433800	-2.49715100
H	-4.44739100	0.56189000	-1.07509400
N	-1.61953400	1.29402300	0.36277500
H	-1.11699200	1.98141700	-0.24191200
H	1.43417600	3.99657600	0.88830100
C	2.27892500	-0.98481100	0.05464200
C	3.35335900	-2.01967400	-0.27264400
C	1.85170200	-0.19132900	-1.17788900
C	4.53950400	-1.40140800	-1.01364000
H	2.87927700	-2.78289600	-0.89910800
H	3.67150100	-2.51141000	0.65021500
C	3.04586400	0.41632600	-1.91168800
H	1.32522700	-0.88836400	-1.83907700
H	1.13786200	0.58424200	-0.88628800
C	4.08481200	-0.64811200	-2.26447200
H	5.24666800	-2.19224100	-1.27623100
H	5.06665800	-0.71338900	-0.34368700
H	2.68844800	0.92433400	-2.81111000
H	3.50742200	1.18138500	-1.27819500
H	4.94432400	-0.18623000	-2.75759700
H	3.64988900	-1.35846200	-2.97879100

Pathway 3 concerted TS9 (cyclohexyl)

O	2.48750900	-2.08455400	-0.00407600
O	3.57375200	-0.30163600	0.70061800
C	3.50573600	-1.63029800	0.72972800
O	4.27681300	-2.33488600	1.32511600
C	1.62060500	-0.97795600	-0.33597000
C	0.77437500	-1.21191500	-1.44239000
H	0.77929000	-2.21721500	-1.85075200
H	0.71253100	-0.41240000	-2.17462400
C	-0.24096900	-2.46535300	1.35389100
H	0.33301100	-3.26802900	1.81856800
H	-0.35468400	-2.67843500	0.28425200
S	0.57313900	-0.86134500	1.53206500
C	-2.64160300	0.22849700	-0.65838500
C	-4.85886000	-0.76716200	-0.59339400
H	-5.82111300	-0.41176700	-0.96306100
H	-5.01115900	-1.17040700	0.41357300
C	-4.28536000	-1.82602200	-1.52111800
H	-4.28179700	-1.45022900	-2.54771100
H	-4.91080000	-2.71840400	-1.49072500
C	-2.86924200	-2.16155900	-1.08694400
H	-2.35605900	-2.77738300	-1.82729800
H	-2.87527600	-2.71216800	-0.14143800
C	-4.25155300	1.88511100	1.43871800
H	-4.46844700	2.93576300	1.65504800
H	-4.95292000	1.28549000	2.02596000
C	-4.49802800	1.66356200	-0.05531300
H	-4.05082700	2.46879500	-0.64061300
H	-5.56405700	1.66817600	-0.28113100
C	-1.75016100	2.07984700	0.88906900
H	-0.77227100	1.91242000	1.34163200
H	-1.87296600	3.16026800	0.77048900
C	-1.73413600	1.41795500	-0.51661800
H	-0.72835100	1.07491200	-0.75208200
H	-2.01556900	2.13770700	-1.28967100
N	-3.95724100	0.38549700	-0.52318700
C	-2.81570600	1.54567500	1.84958200
H	-2.62660700	1.94664200	2.84852600
H	-2.70156800	0.45896100	1.93685100
N	-2.10138400	-0.93634400	-0.92196600
H	-1.04777100	-1.00181600	-1.03940300
H	-1.23392400	-2.42307600	1.80439000
C	2.60284200	0.21067300	-0.26724700
C	3.34823600	0.39979400	-1.59584200
C	2.06487900	1.54023200	0.23852700
C	4.44308100	1.46244300	-1.49995000
H	2.61160000	0.70194000	-2.34533900
H	3.75648400	-0.56006100	-1.92418200
C	3.14636700	2.62121800	0.31291300
H	1.28134900	1.85566200	-0.45913900
H	1.59699300	1.40686000	1.21406400
C	3.87024000	2.79545900	-1.02102100
H	4.91707000	1.57727300	-2.47867400

H	5.22171600	1.12706100	-0.80638100
H	2.68569200	3.56197400	0.62643000
H	3.87160100	2.35001200	1.08797300
H	4.66551000	3.54011300	-0.92482400
H	3.16443400	3.17622000	-1.77036000

Pathway 3 concerted Post-reaction TS9 (cyclohexyl)

O	-3.31118200	-1.60493600	-0.05661400
O	-3.27338800	0.46093000	-0.82366500
C	-3.92968700	-0.69552700	-0.82715300
O	-4.94290000	-0.90750500	-1.42936300
C	-1.99933900	-1.11546200	0.29802600
C	-1.64759800	-1.63164100	1.67565800
H	-1.49054500	-2.70953900	1.65894400
H	-2.45151500	-1.41855600	2.38044000
C	-0.98472800	-3.48883700	-0.82969300
H	-2.03768200	-3.76757800	-0.80134500
H	-0.46103100	-3.86906000	0.04635700
S	-0.80872400	-1.69111100	-0.98925100
C	2.72686800	0.65854700	0.68131600
C	4.01548800	-1.41277800	0.77145600
H	5.08160400	-1.65258300	0.75518400
H	3.50836600	-2.11385400	0.09312600
C	3.44929400	-1.53966500	2.17433000
H	4.05207300	-0.93981300	2.86373800
H	3.49379900	-2.57886700	2.50810300
C	2.01244700	-1.03601800	2.16246200
H	1.61732300	-0.98522600	3.18175600
H	1.38258800	-1.75707400	1.62368800
C	3.86118000	0.05346300	-2.18593400
H	4.40436900	0.54807500	-2.99853500
H	3.87953500	-1.02036700	-2.39747500
C	4.60223600	0.34567600	-0.87732400
H	4.84274200	1.40950100	-0.81783100
H	5.55635300	-0.18496100	-0.85106500
C	2.26158400	1.93731300	-1.51730600
H	1.24538400	2.28713400	-1.70727000
H	2.92578300	2.63787800	-2.03376800
C	2.53153700	2.00381900	0.01428900
H	1.69197400	2.47637000	0.52382000
H	3.40911100	2.62501700	0.21558800
N	3.85104000	-0.04163000	0.30929700
C	2.41182700	0.54688600	-2.14243600
H	2.00430600	0.56195200	-3.15733000
H	1.79593300	-0.16365300	-1.57991000
N	1.85067500	0.27527800	1.54492000
H	-0.73199900	-1.14931500	2.01881300
H	-0.53061400	-3.91199700	-1.72562400
C	-2.21401100	0.42320100	0.18382700
C	-2.78179100	1.02487000	1.47481100
C	-1.02702100	1.22888000	-0.32243200
C	-3.11007400	2.50972400	1.32608500
H	-2.02801300	0.90535000	2.25878400
H	-3.66748900	0.46471900	1.78815200

C	-1.33495900	2.72508000	-0.42862700
H	-0.19872000	1.05633100	0.37553600
H	-0.71321600	0.84838900	-1.29693100
C	-1.87906600	3.29347800	0.87912100
H	-3.48409300	2.88642800	2.28149800
H	-3.91506700	2.63809600	0.59467600
H	-0.42441900	3.25450500	-0.72178100
H	-2.06517400	2.88925400	-1.22870400
H	-2.12390300	4.35210300	0.75718400
H	-1.10554300	3.22961700	1.65495800

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