Supplementary Information

Rationalization of Asymmetric Amplification via Autocatalysis Triggered by Isotopically Chiral Molecules

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1. Materials and Instrumentation

A. Instrumentation

NMR Spectra were collected using a Bruker DRX-500 or Bruker AV-600 (500 and 600 MHz, respectively). Reaction calorimetry was performed using a Omnical Insight (eight port calorimeter) which was temperature controlled using circulated cooling bath with a Polyscience temperature controller. The nine-liter reservoir was filled with 25 to 30% ethylene glycol in water (Heat Capacity ~4.2 J/g/°C at -12°C).

Aliquot concentration analysis was performed using a Thermo-Fisher Ultimate 3000 High Performance Liquid Chromatography system, operating in reverse phase. Quantitative analysis was performed at 254 nm and 280 nm, depending on sample content. Enantiomeric excess was measured using an Agilent 1100 Series Liquid Chromatography System operating in normal phase. Quantitation was performed at 254 nm.

Purification was performed using a Biotage SP system with hand-packed columns from Thompson Scientific. Distillations performed using a Kugelrohr Distillation Apparatus with a Buchi B-580 Glass Oven.

B. Chemicals

Starting Aldehyde, 2-methyl-pyrimidine-5-carbaldehyde (CAS:90905-33-2) was purchased from Combi-Blocks (San Diego) and used after purification by column chromatography. (*R*) and (*S*) glycidyl methyl ether (CAS: 64491-70-9, 64491-68-5) were purchased from TCI America and used following distillation. Diisopropylzinc (CAS: 625-81-0) was purchased from Sigma-Aldrich as a 1M Solution in toluene, and was used after the concentration was determined via titration.[1] Toluene was purchased as an anhydrous solution (Sigma-Aldrich) and used directly from 100 mL Sure-Seal bottles kept under Ar. Chromatography was performed using HPLC grade water, acetonitrile, and hexanes purchased from Fisher Scientific and puriss ethanol purchased from Pharmco-Aaper. Dichloromethane, ethyl acetate, hexanes, sodium bicarbonate, sodium sulfate, and silica gel (60, Mesh 230-450) was purchased from Fisher Scientific. All deuterated solvents were purchased from Cambridge Isotopes Lab.

C. Analytical Methods

Normal Phase. Used for determination of product enantiomeric excess. Aliquots quenched in methanol (dilution factor ranged from 5x to 50x depending on reaction concentration) and filtered using Thompson 0.2μm PTFE Filter Vials.

Column: Lux-Amylose 1 (250mm x 4.6mm, 5μm)
Solvent: Hexanes (93%) and Ethanol (7%)
Flow Rate: 3.5 mL/min
Gradient: Isocratic – 11 minutes
Temperature: r.t.
Injection Volume: 2 – 40 μL depending on sample concentration
Detector Path Length: 10mm
Detection: 254 nm (unreferenced)

Retention Times:

Toluene/Biphenyl: 0.8 min
Product (*R*): 4.5 min
Product (S): 5.0 min
Aldehyde: 6.3 min
Reduction Product: 8.5 min

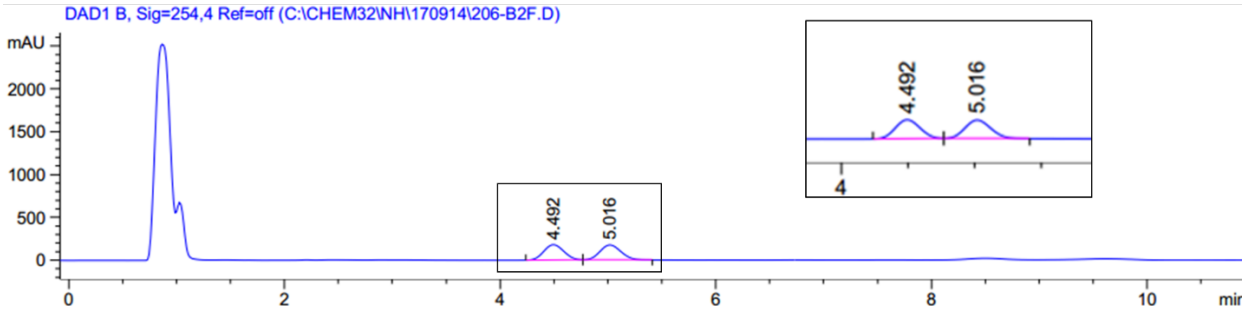

Figure S1. Normal phase LC chromatogram for separation of product enantiomers.
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Reverse Phase. Used for determination of [aldehyde], [product], and [reduction product]. Aliquots quenched in methanol (dilution factor ranged from 5x to 50x depending on reaction concentration) and filtered using Thompson 0.2μm PTFE Filter Vials. Reaction quantitated versus biphenyl internal standard. Calibration curves and quantitation method given on page 57. Two gradient methods were developed, high-throughput (fast) and high accuracy (slow).

Column: Waters XBridge C18 (250mm x 4.6mm, 5μm)
Solvent: Water (5mM Ammonium Acetate, pH 8.3 – 8.9) and Acetonitrile (gradient)
Flow Rate: 1.2 mL/min (slow), 3.0 mL/min (fast)
Gradient: Fast: 0.2 minutes – 3% ACN, 0.2 to 3 minutes – 95% ACN, 4 to 5.5 min - equilibrate
Slow: 0.5 minutes – 3% ACN, 0.5 to 12 minutes – 95% ACN, 13 to 17 min - equilibrate
Temperature: 60°C
Injection Volume: 2 or 5μL depending on sample concentration
Detector Path Length: 10mm
Detection: 254 and 280 nm (unreferenced)

Retention Times:

Reduction Product: 1.5 min (fast), 3.3 min (slow)
Aldehyde: 1.7 min (fast), 4.2 min (slow)
Product: 2.4 min (fast), 9.3 min (slow)
Toluene: 3.6 min (fast), 14.0 min (slow)
Biphenyl (IS): 3.8 min (fast), 14.6 min (slow)

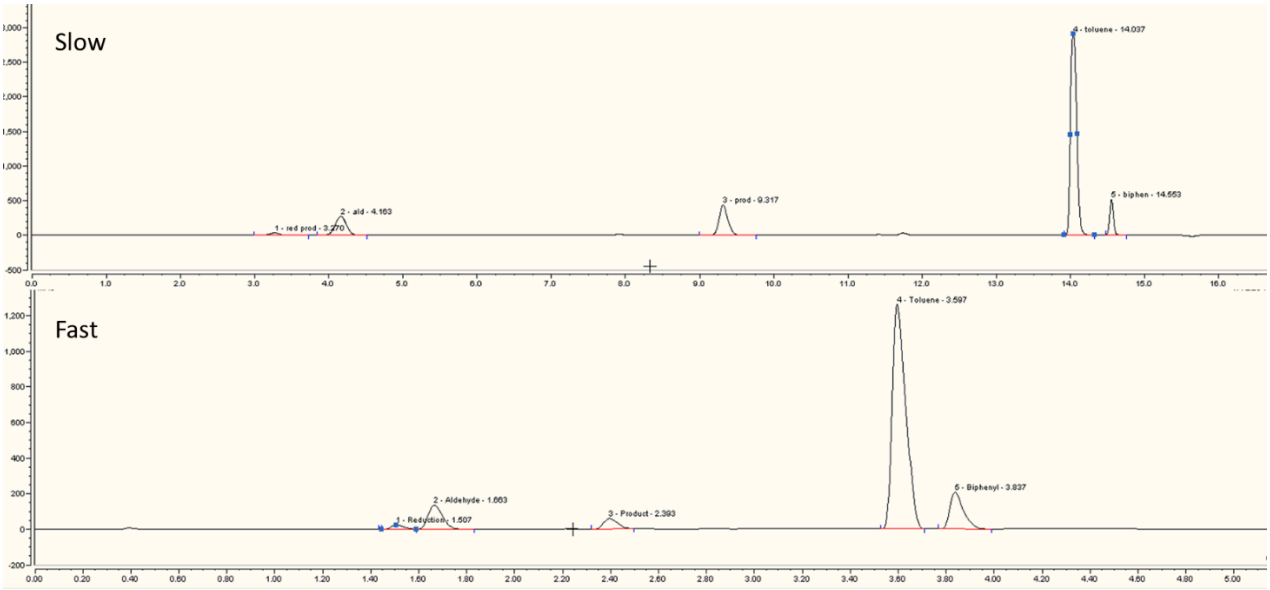
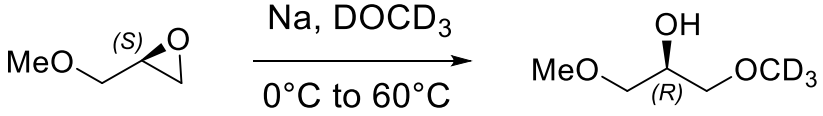


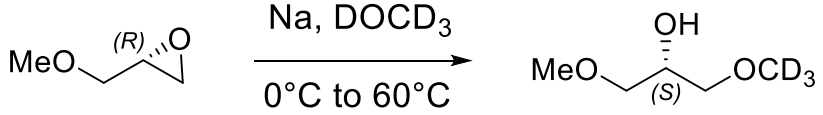
Figure S2. Reverse phased LC chromatogram of quenched reaction mixture.

2. Experimental Methods

A. Synthesis and Characterization

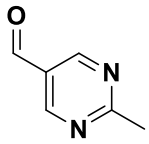


(*R*)-1-methoxy -($^2H_3$)-3-methoxy propanol. Methanol-*d4* (6.0 mL, 0.147 mol, ~16M) was added dropwise to an argon flushed flask at 0°C containing sodium metal (1.1g, 48 mmol, 5.4M) with an affixed balloon for venting offgas. Solution was warmed to room temperature and stirred until all metal was dissolved. Flask was cooled to 0°C and (*S*)-glycidyl methyl ether (3.0 mL, distilled, 33 mmol, 3.7M) was added dropwise under argon. Solution turned pale yellow (precipitation of white solids indicates that the epoxide was not dry). After stirring for five minutes, solution was heated to 60°C for 2-12 hours. Reaction was cooled once starting material consumption was complete by thin-layer chromatography (visualized by I_2 stain). Resulting reaction mixture was orange (brown reaction mixture indicative of impure/low yielding reaction). Ether (10 mL) was added to the reaction mixture, and remaining base was quenched by dropwise addition of HCl until bubbling ceased. Solution was decanted, dried over magnesium sulfate and filtered. Methanol and ether was removed via distillation or in-vacuo at 0°C. Product was purified by column chromatography (0-35% ether in petroleum ether). Solvent was removed in vacuo, and product was purified further twice by bulb-to-bulb distillation to give 2.37g (20.8 mmol, 63% yield, 4.06 g expected) of product as a clear oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.78 (CH, ttd, J = 6.4, 4.3, 0.7 Hz, 1H), 3.40 (CH_2, mult, 4H), 3.36 (CH_3, s, 3H), (OH, br s, 1H); ^{1}H NMR (500 MHz, Toluene-d_8) δ 3.85 (CH, pd, J = 5.5, 4.4 Hz, 1H), 3.24 (CH_2, d(2x), J = 5.2 Hz, 4H), 3.05 (CH_3,s, 3H), 2.21 – 2.15 (OH, br tr, 1H); ^{2}H NMR (77 Mhz, Toluene-d_8) 3.04 (CD_3, s); ^{13}C NMR (151 MHz, $CDCl_3$) δ 73.92, 73.92, 73.81, 69.33, 59.26, 58.38 (mult, weak); HRMS (ESI-TOF, CH_3OH) *m/z* calc for $C_5H_{10}D_3O_3(M+H)^+$ 124.1048 found 124.1043.

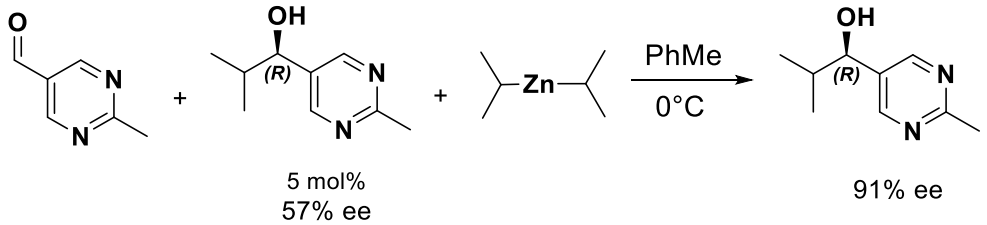


(*S*)-1-methoxy -($^2H_3$)-3-methoxy propanol. Methanol-*d4* (6.0 mL, 0.147 mol, ~16M) was added dropwise to an argon flushed flask at 0°C containing sodium metal (1.1g, 48 mmol, 5.4M) with an affixed balloon for venting offgas. Solution warmed to room temperature and stirred until all metal was dissolved. Flask was cooled to 0°C and (*R*)-glycidyl methyl ether (3.0 mL, distilled, 33 mmol, 3.7M) was added dropwise under argon. Solution turned pale yellow (precipitation of white solids indicates that the epoxide was not dry). After stirring for five minutes, solution was heated to 60°C for 2-12 hours. Reaction was cooled once starting material consumption was complete by thin-layer chromatography (visualized by I_2 stain). Resulting reaction mixture was orange (brown reaction mixture indicative of impure/low yielding reaction). Ether (10 mL) was added to the reaction mixture, and remaining base was quenched by dropwise addition of HCl until bubbling ceased. Solution was decanted, dried over magnesium

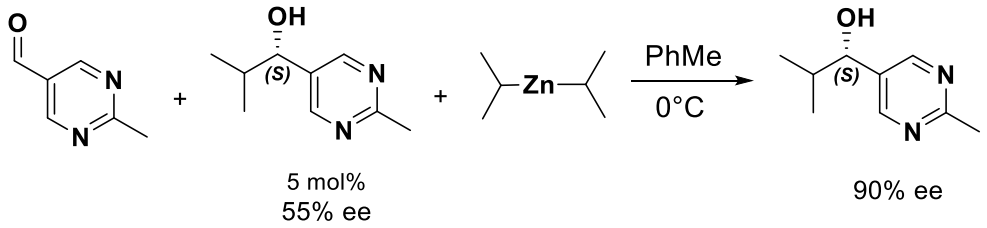
sulfate and filtered. Methanol and ether was removed via distillation or in-vacuo at 0°C. Product was purified by column chromatography (0-35% ether in petroleum ether). Solvent was removed in vacuo, and product was purified further twice by bulb-to-bulb distillation to give 2.07g (20.8 mmol, 51% yield, 4.06 g expected) of product as a clear oil. ^{1}H NMR (500 MHz, Toluene-d_8) δ 3.88 (CH, hept, J = 5.3 Hz, 1H), 3.24 (CH_2, d (2x), J = 5.5 Hz, 4H), 3.03 (s, 3H), 2.56 – 2.45 (OH, br t, 1H); ^{2}H NMR (77 Mhz, Toluene-d_8) 3.02 (CD_3, s); ^{13}C NMR (126 MHz, Toluene-d_8) δ 74.61, 74.49, 69.84, 59.12; HRMS (ESI-TOF, CH_3OH) m/z calc for $C_5H_{10}D_2O_3(M+H)^+$ 124.1048 found 124.1042.



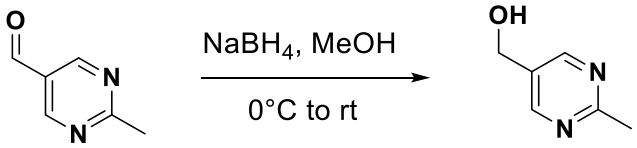
2-methyl-5-pyrimidine-carboxaldehyde. Original material was purchased from Combi-Blocks (San Diego) as an orange sticky solid. Solid was purified by column chromatography (0 to 50% ethyl acetate in hexanes) to give a fluffy white solid.



(*R*)-2-methyl-1(2-methyl-pyrimidin-5-yl)-propan-1-ol. A sample of 57% ee (*R*) catalyst (product) was isolated from previous experiments. Product alcohol (33.2 mg, 0.2 mmol, 5 mol%) and aldehyde (0.4885 g, 4 mmol) was added to a screw top vial. Vial was backfilled with argon, and 33 mL of toluene were added. Solution was cooled to 0°C and 7.0 mL of diisopropyl zinc in toluene (0.85M stock, 6.4 mmol) was added to initiate the reaction. Aldehyde was no longer visible by TLC after 3.0 hours, and reaction mixture was quenched with 30 mL of HCl. After stirring for several minutes, saturated sodium bicarbonate was added until the aqueous phase was pH 8.0 or greater. Aqueous phase was extracted (4x) with 30 mL of ethyl acetate. Organic phase was dried over sodium sulfate, filtered, and purified by column chromatography (0 to 100% ethyl acetate in hexanes), giving a white powder. No yield was taken. ee = 91% (LC-DAD) ^{1}H NMR (500 MHz, Toluene-d_8) δ 8.33 (s, 1H), 3.83 (dd, J = 6.4, 2.6 Hz, 0H), 2.65 (s, 1H), 1.57 (h, J = 6.7 Hz, 0H), 0.79 (d, J = 6.7 Hz, 1H), 0.61 (d, J = 6.8 Hz, 1H). ^{13}C NMR (126 MHz, Toluene-d_8) δ 166.95, 155.24, 133.49, 74.67, 34.94, 25.25, 18.27, 17.37.



(*S*)-2-methyl-1(2-methyl-pyrimidin-5-yl)-propan-1-ol. A sample of 55% ee (*S*) catalyst (product) was isolated from previous experiments. Product alcohol (33 mg, 0.2 mmol, 5 mol%) and aldehyde (0.4885 g, 4 mmol) was added to a screw top vial. Vial was backfilled with argon, and 33 mL of toluene were added. Solution was cooled to 0°C and 7.0 mL of diisopropyl zinc in toluene (0.85M stock, 6.4 mmol) was added to initiate the reaction. Aldehyde was no longer visible by TLC after 3.0 hours, and reaction mixture was quenched with 30 mL of HCl. After stirring for several minutes, saturated sodium bicarbonate was added until the aqueous phase was pH 8.0 or greater. Aqueous phase was extracted (4x) with 30 mL of ethyl acetate. Organic phase was dried over sodium sulfate, filtered, and purified by column chromatography (0 to 100% ethyl acetate in hexanes), giving a white powder. No yield was taken. ee = 90% (LC-DAD) ^{1}H NMR (500 MHz, Toluene-d_8) δ 8.33 (s, 1H), 3.83 (dd, J = 6.4, 2.6 Hz, 0H), 2.65 (s, 1H), 1.57 (h, J = 6.7 Hz, 0H), 0.79 (d, J = 6.7 Hz, 1H), 0.61 (d, J = 6.8 Hz, 1H). ^{13}C NMR (126 MHz, Toluene-d_8) δ 166.95, 155.24, 133.49, 74.67, 34.94, 25.25, 18.27, 17.37.



5-(hydroxymethyl)=2-methylpyrimidine. Aldehyde (199.2mg, 1.6 mmol) was dissolved in 8.0 mL of Methanol in a round bottom flask and cooled to 0°C. Sodium borohydride was added, the solution was capped, and a vent balloon was attached. After 2 hours, TLC (EtOAC, R_{fprod} = 0.04, R_{fsm} = 0.53) revealed aldehyde consumption. The reaction was quenched with 5.0 mL of ammonium chloride (aq, saturated), and aqueous phase was extracted (4x) with 10mL dichloromethane. Organic phase was dried over sodium sulfate and filtered. Solvent was removed in vacuo to give 159.1 mg (1.28 mmol, 80% yield) of product as a white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.66 (s, 1H), 4.74 (d, J = 4.2 Hz, 2H), 2.75 (s, 3H), 2.12 (s, 1H). Spectra matches previously reported characterization.[2]

B. Reaction Calorimetry Experiments

Typical Experimental Procedure. Calorimeter was put under a steady flow of dry N_2 (to prevent icing and maintain an inert atmosphere) and the instrument was cooled to -12°C over one hour. Dry ice was added to the chiller reservoir to maintain a stable temperature. All stock solutions and vials prepared gravimetrically. A stock solution containing (*S*) initiator (115.9 mg, 0.93 mmol, 46.3 mM), biphenyl (as internal standard, 65.2 mg, 0.42 mmol, 21 mM) and toluene (20 mL) was prepared. Under argon atmosphere, 3.0 mL of the initiator stock solution and 3.0 mL of $Zn(iPr)_2$ (0.74M solution in toluene, titrated) were weighed into a flame dried calorimetry vial ([initiator] = 17.4 mM, [biphenyl] = 7.9 mM). Vial was placed in the calorimeter for at least one hour to equilibrate to temperature. An aldehyde stock solution (0.44M, 4.4 mmol in 10 mL) was prepared and loaded into 1.0mL syringes. Syringes were weighed, the tip was capped with a small rubber septa, and the syringe was placed fully in a calorimeter port to equilibrate. Once the syringe and vial had equilibrated to temperature (at least one hour), the syringes were removed and 2.0 mL of aldehyde solution was injected into the reaction vessel from two syringes. Syringes were weighed after injection to determine the $[aldehyde]_0$. Calorimeter was maintained at temperature during the reaction, and once heat returned to baseline, a 50 μL aliquot was taken and diluted in 0.5 mL of methanol. Once the heat returned to baseline, the internal heater was switched on for 20 minutes in order to perform a Tau correction. Aliquot sample was filtered and analyzed by reverse phase liquid chromatography to determine final concentrations.

C. LC Reaction Monitoring

Typical Experimental Procedure. Reactions were performed inside the calorimeter using the procedure mentioned above. At regular time intervals 50 – 100 μL aliquots were removed, dissolved in 500 μL of MeOH, filtered and analyzed by reverse phase liquid chromatography.

D. NMR Experiments

Titration: Typical Experimental Procedure. A screw-top NMR tube was flamed dried under vacuum and backflushed with Argon. An initiator stock solution (0.5 M in toluene) was prepared gravimetrically. The initiator solution (120 μL, 0.060 mmol), diisopropylzinc solution (700 μL, 0.60 mmol), and toluene-*d*8 (150 μL, for locking) were weighed into the NMR tube. Sample was inserted into the machine, cooled to 273K, locked and shimmed, a qualitative ^{1}H spectra was performed under the given conditions:

Dummy Scans (ds) = 4
Number of Scans (ns) = 16
Relaxation Delay (d1) = 2 seconds
Temperature = 273K (0 °C)

A quantitative ^{2}H NMR spectra was taken under the following conditions. The pulse time (p1) was optimized to give the optimal 90-degree pulse angle, and T_1 was determined to be ~2 seconds for the benzylic ^{2}H signal in toluene-*d*8. This was used as the T_1, as toluene-*d*8 was the smallest molecular weight molecule in the system.

Pulse time (low energy, p_1) = 500 μs
Dummy Scans (ds) = 0
Number of Scans (ns) = 96
Relaxation Delay (d_1) = 2 seconds

After scans were taken, an additional 10-30 μL aliquot of (*R*)-product stock solution (91.0 mg in 500 μL toluene) was added gravimetrically to the tube. Tube was inverted until solution appeared well mixed, and was inserted into the NMR to cool to 0°C. Sample was analyzed by ^{1}H and ^{2}H NMR, using the conditions above.

Titration: in-situ monitoring of reaction by ^{1}H and ^{2}H NMR. A screw-top NMR tube was flamed dried under vacuum and backflushed with Argon. An (*S*) initiator stock solution (0.12 M in Toluene) and an aldehyde stock solution (0.80M in Toluene) were prepared gravimetrically. The initiator solution (250 μL, 0.030 mmol), diisopropylzinc solution (500 μL, 0.425 mmol), and toluene-*d*8 (150 μL, for locking) were weighed into the NMR tube. Sample was inserted into the machine (Bruker DRX-500), cooled to 273K, locked and shimmed. After initial ^{2}H and ^{1}H spectra were taken, 200 μL of aldehyde stock solution (0.16 mmol) was added and reaction was inserted into the spectrometer. Alternative ^{1}H and ^{2}H spectra were taken under the conditions given below.

Initial Conditions:

[(*S*) initiator] = 27 mM
[diisopropylzinc] = 386 mM
[aldehyde] = 145 mM

Qualitative ^{1}H spectra were taken under the given conditions:

Dummy Scans (ds) = 4
Number of Scans (ns) = 16
Relaxation Delay (d_1) = 2 seconds
Temperature = 273K (0 °C)

A qualitative ^{2}H NMR spectra was taken under the following conditions, to optimize throughput (128 spectra every 8.5 minutes).

Pulse time (low energy, p_1) = 100 μs
Dummy Scans (ds) = 4
Number of Scans (ns) = 128
Acquisition Time = 3.7 seconds
Relaxation Delay (d_1) = 0.2 seconds
Temperature = 273K (0 °C)

Titration: DOSY analysis of initiator-product-zinc complexes. A screw-top NMR tube was flamed dried under vacuum and backflushed with Argon. An (*S*) initiator stock solution (0.1 M in toluene-*d8*) and an (*R*) product stock solution (0.2 M in toluene-*d8*) were prepared gravimetrically. The initiator solution (100 μL, 0.020 mmol) and the diisopropylzinc solution (110 μL, 0.10 mmol) were weighed into the NMR tube. Sample was inserted into the machine at room temperature (Bruker AV-600), locked and shimmed. A DOSY spectrum was acquired using the parameters below (the T_1 relaxation time and 90-degree flip angle for the initiator molecule were determined in a prior experiment). After the initial DOSY spectrum was collected, product solution was added (50 μL, 0.22 mmol, 1.1 eq) and an additional DOSY was run. After completion, another 50 uL aliquot (100 μL total, 0.5 mmol, 2.5 eq) was added and a final DOSY was collected. Analysis of the raw DOSY file was done in MestreNova, after phase correction and baseline correction. Diffusivities for each peak were extracted using the "Peak Heights" algorithm, with overlapping peak deconvolution applied.

Pulse Time (p_1, for 90° flip angle) = 8.5μsec
Relaxation Delay (d_1) = 75 seconds ($T_{1,\text{initiator}}$ = 11.5 sec)
Gradient Strength = 53.5 gauss/cm
Gradient Time (Δ) = 50 ms
Gradient Range = 5% to 95%
Number of scans per point (ns) = 4
Number of gradient points = 36

E. Purity Determination

Diisopropylzinc Titration. Adapted from reference 1. *Preparing 0.5M LiCl in THF:* Anhydrous LiCl (2.1 g, 50 mmol) was added to a Schlenk flask. Flask was placed under high vacuum and heated at 160°C for 6 hours. Flask was flushed with argon and cooled to room temperature. 100 mL of THF was added, and solution was stirred for ~2 hours until all solids were dissolved. *Titration Procedure:* Iodine (1079.9mg) was placed in a 20.0 mL septa-topped vial and flushed with argon. 20.0 mL of 0.5M LiCl in THF was added to the vial, and mixed until all I_2 was dissolved. Three 5.0 mL crimp top vials were flamed dried and backflushed with argon. A weighed amount of the iodine stock solution was added to the vial. Balance was tared on the vial. The diisopropylzinc solution was added dropwise, until solution gave a clear endpoint (the titration solution went from black, to orange, to yellow, to clear). Vial was weighed after the endpoint was reached, and the concentration of [diisopropylzinc] was determined using the formula below. Titration was repeated in triplicate. Over-titrated samples were ignored.

a = amount of I_2 added to stock (mg)
b = amount of LiCl in THF added to stock (mg)
c = amount of stock added to vial (mg)
d = amount of zinc added to vial (mg)

$$[\text{diisopropyl zinc}](\text{M}) = 1.708\,\frac{\text{c}}{\text{d}}\left(\frac{\text{a}}{\text{a}+\text{b}}\right)$$

F. Safety Assessment

No unexpected or unusally high safety hazards were encountered. Diisopropylzinc was purchased and utilized as a 1M solution in toluene. At this concentration, solution could be handled using standard laboratory techniques for air-sensitive materials, without the use of a glovebox.

3. Experimental Results

A. Sampling Analysis at Varied [Initiator]

Three vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Aliquots were varied time points and analyzed by LC-UV.

Table S1. Reaction concentrations for sampling analysis of reactions with varied [initiator]

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	Initiator *S*-3 (mM)	Biphenyl (mM)
220-B1	113.6	260.1	15.42	7.29
220-B2	114.5	259.0	11.09	5.24
220-B3	114.6	252.6	7.89	3.73

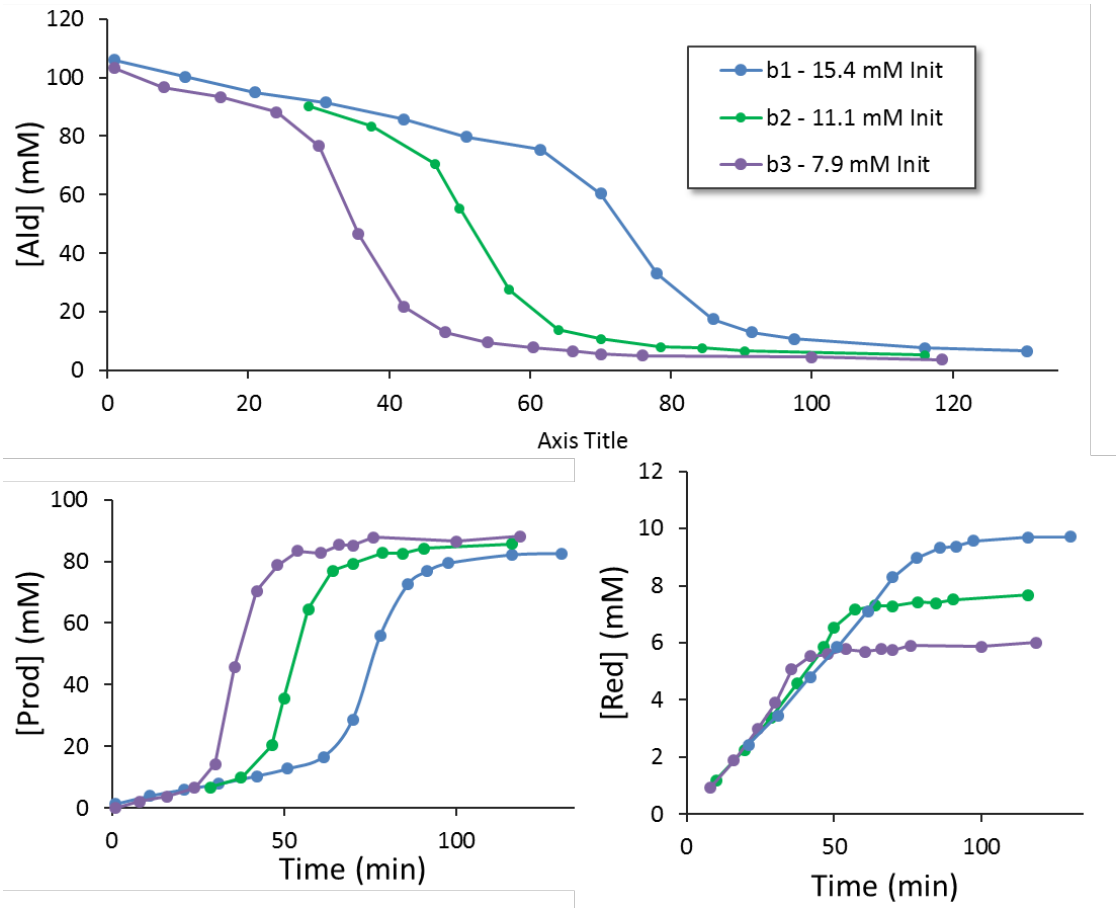


Figure S3. Time course data for reaction at -12°C. [ald] = 115 mM, [Zn(*i*Pr)$_2$] = 260 mM, [(*S*) initiator] = 15 mM (blue), 11 mM (green) and 8 mM (purple) in toluene. Time course data shown for starting aldehyde (top), secondary alcohol product (bottom left) and primary alcohol reduction product (bottom right). Test ID: SOA220.

B. Sampling Analysis with no Initiator – 16% ee Product Added

Two vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Aliquots were taken at varied time points and analyzed by LC-UV. Data was used for validation of the COPASI model. 16% ee catalyst added.

Table S2. Reaction conditions for sampling experiment using 5 mol% of 16% ee (*R*) catalyst in toluene.

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	Product 2 (mM)	Biphenyl (mM)
189-B1	61.0	113.2	2.8	13.0
189-B4	58.3	112.0	2.9	13.1

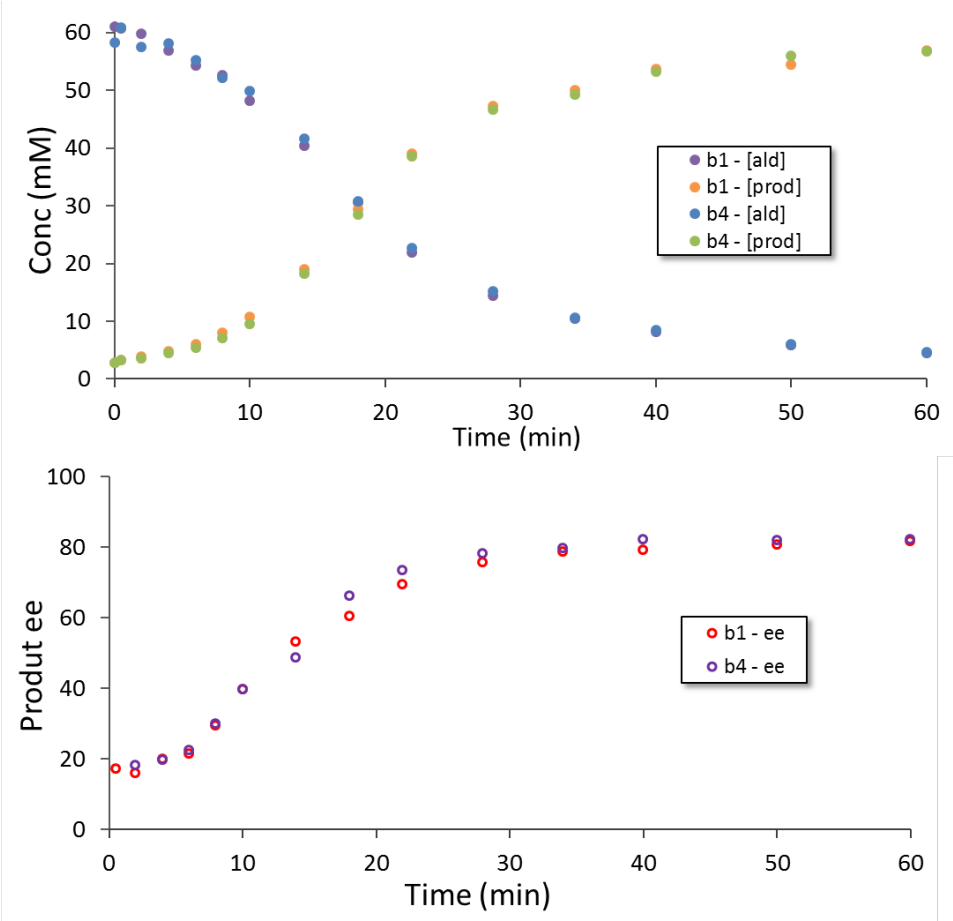


Figure S4. Time course data for reaction at -12°C. $[ald]_0$ = 60 mM, $[Zn(iPr)_2]_0$ = 113 mM, $[prod]_0$ = 3 mM in toluene. $ee_{0,prod}$ = 16%. Time course [ald] and [product] (top, reverse phase) and ee (bottom, normal phase). Test ID: SOA189. Duplicate trials (b1 and b4).

C. Sampling Analysis with no Initiator – 16% ee Product Added (2)

Two vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Aliquots were taken at varied time points and analyzed by LC-UV. Data was used for validation of the COPASI model. 16% ee catalyst added. Varied $[ald]_0$.

Table S3. Reaction conditions for sampling experiment using 16% ee (*R*) catalyst, replicate.

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	Product 2 (mM)	Biphenyl (mM)
190-B1	61.2	159.6	3.1	13.7
190-B4	76.5	164.6	3.1	13.5

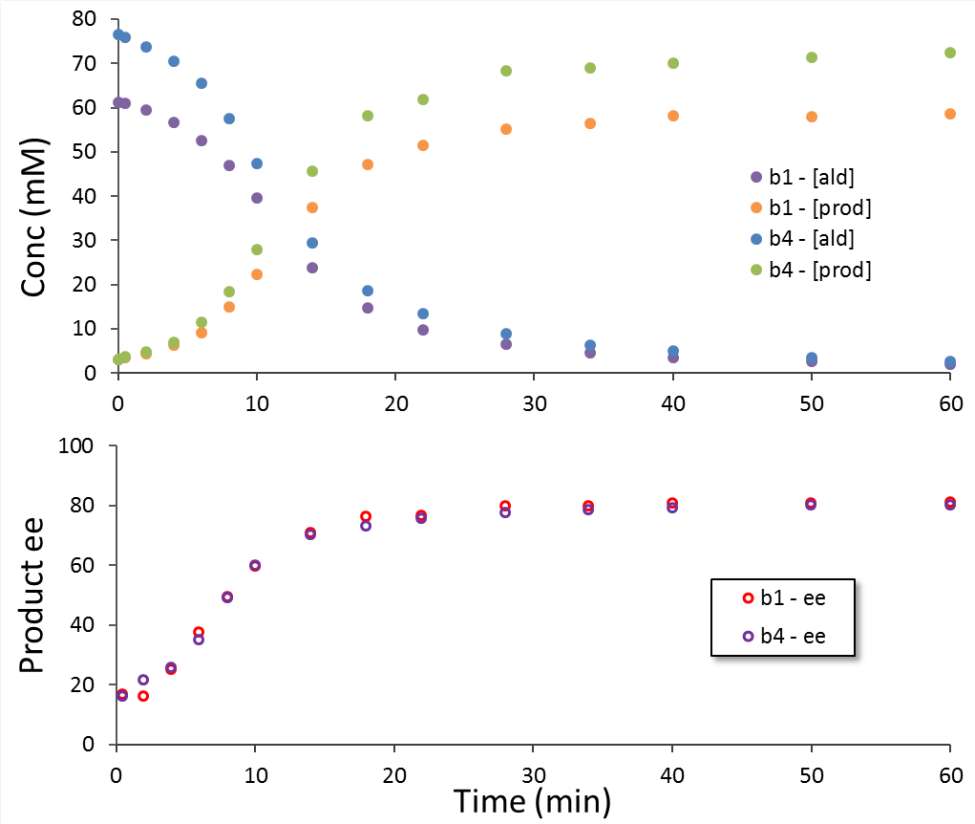


Figure S5. Time course data for reaction at -12°C. $[ald]_0$ = varied, $[Zn(iPr)_2]_0$ = 160 mM, $[prod]_0$ = 3 mM in toluene. $ee_{0,prod}$ = 16%. Time course [ald] and [product] (top, reverse phase) and ee (bottom, normal phase). Test ID: SOA190.

D. Sampling Analysis with no Initiator – 80% ee Product Added

Two vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Aliquots were taken at varied time points and analyzed by LC-UV. Concentration data was determined using reversed phase LC and ee data attained using normal phase LC. Data was used for validation of the COPASI model. 79.7% ee catalyst added.

Table S4. Reaction conditions for sampling experiment using 80% ee (*R*) catalyst.

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	Product 2 (mM)	Biphenyl (mM)
191-B1	49.7	90.1	2.2	9.1
191-B4	51.5	91.4	2.2	9.1

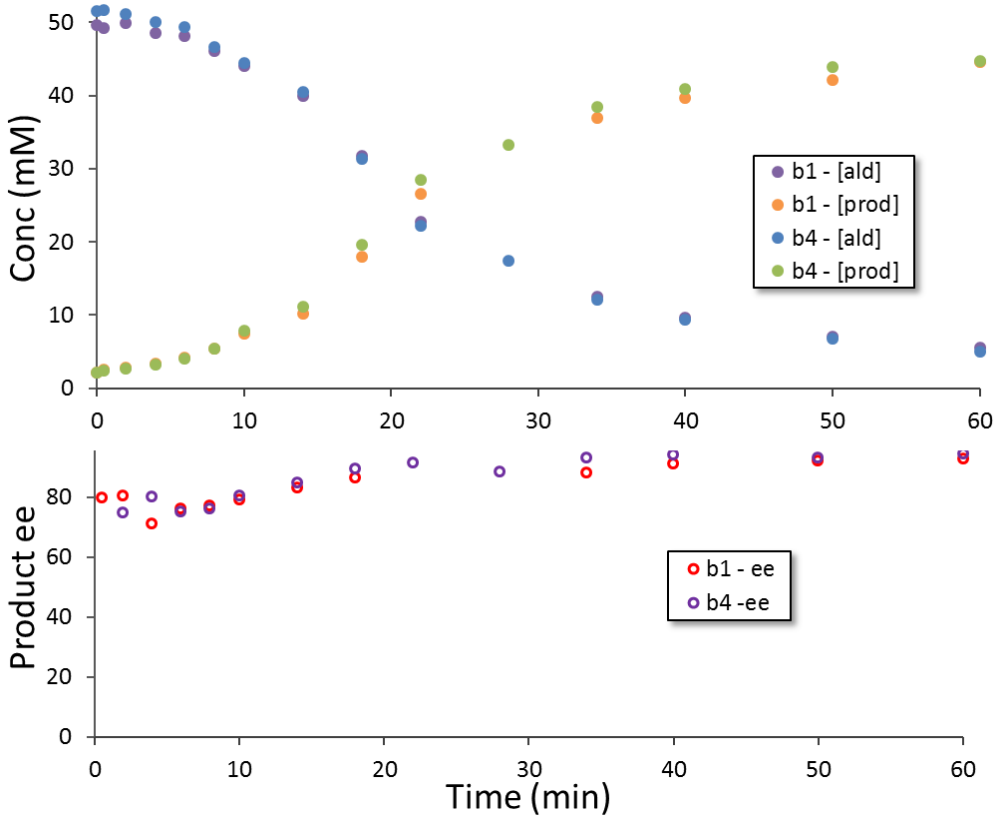


Figure S6. Time course data for reaction at -12°C. [ald]$_o$ = 50mM, [Zn(*i*Pr)$_2$]$_o$ = 90 mM, [prod]$_o$ = 2 mM in toluene. ee$_{o,prod}$ = 79.7%. Time course [ald] and [product] (top, reverse phase) and ee (bottom, normal phase). Test ID: SOA191.

E. Sampling Analysis with Initiator – Varied [Zn(iPr)$_2$]

Four vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Aliquots were taken at varied time points and analyzed by LC-UV. 20 mM initiator used in all trials, at varied [Zn(iPr)$_2$]. At concentrations greater than 2.0 eq, [Zn(iPr)$_2$] had little influence on the induction period.

Table S5. Reactions conditions for measurement of [Zn(*i*Pr)$_2$] influence on induction period.

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	Product 2 (mM)	Biphenyl (mM)
209-B1	111.6	289.8	19.4	16.0
209-B2	110.6	223.2	20.0	16.5
209-B3	115.2	176.8	18.9	15.6
209-B4	108.8	134.6	20.3	16.7

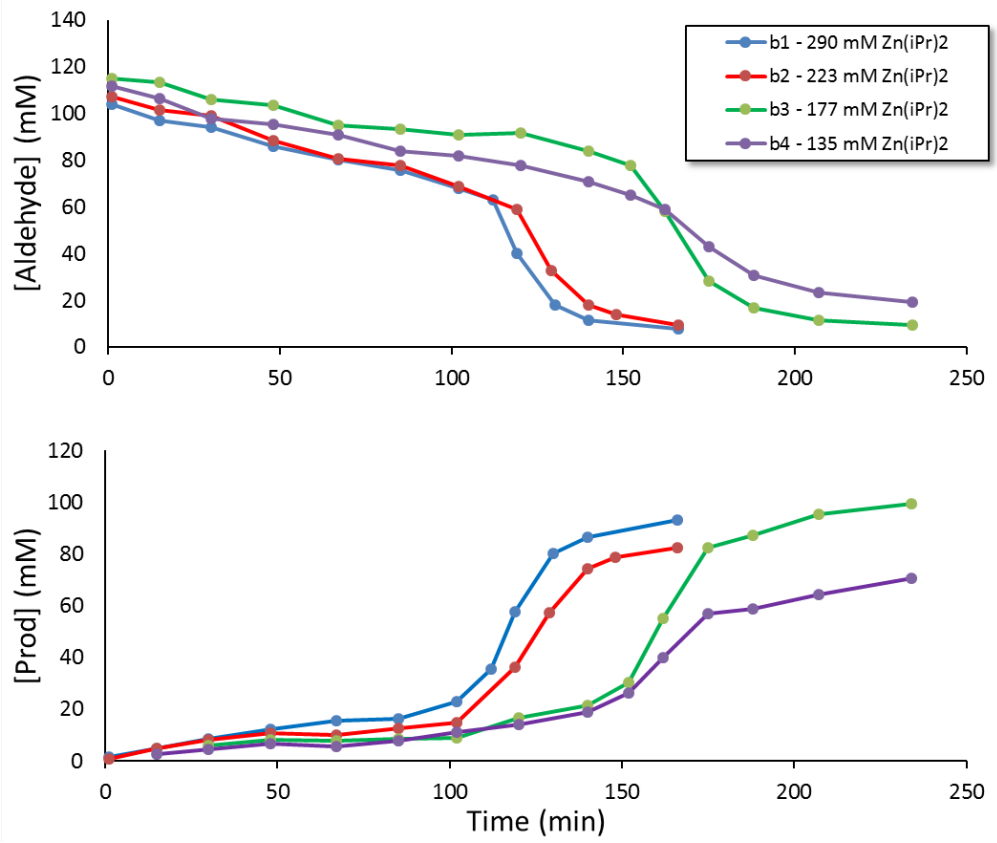


Figure S7. Time course data at -12°C. [ald]$_0$ = 50mM, [Zn(*i*Pr)$_2$]$_0$ = 290 mM (blue), 223 mM (red), 177 mM (green), 135 mM (purple), [(*S*) initiator]$_0$ = 20 mM in toluene. Time course data for [aldehyde] (top) and [product] (bottom). Test ID: SOA209.

F. Reaction Calorimetry – Varied [Initiator]

Vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Reaction commenced by injection of aldehyde. Reaction was performed in duplicate over two different days. Given data shown after tau correction. Final ee of the reaction was racemic in all three cases.

Table S6. Reaction conditions for reaction calorimetry studies at varied [initiator].

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	*S*-3 Initiator (mM)	Biphenyl (mM)
216-B1	112.2	278.4	17.4	7.9
216-B2	110.5	275.7	12.9	5.9
216-B3	109.7	279.4	8.9	4.1
216-B4	111.3	276.3	None	9.5
218-B1	110.4	262.9	17.5	8.0
218-B2	110.1	258.9	12.9	5.9
218-B3	108.7	260.7	8.9	4.1

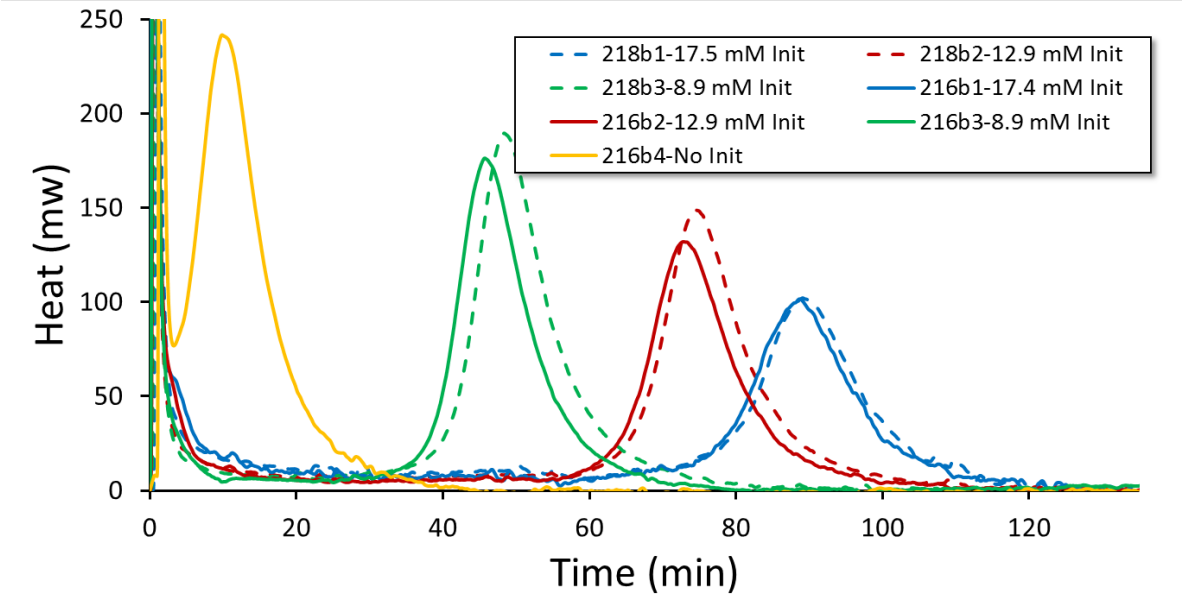


Figure S8. Raw heat flow data from reaction calorimetry experiments (post tau correction). [aldehyde]$_0$ = 110 mM, [Zn(*i*Pr)$_2$] = 260 to 280 mM, [(*S*) initiator] = 0 mM (yellow), 9 mM (green), 13mM (green), or 17 mM (blue). Duplicate experiments shown in dashed lines (SOA218).

Processed data provided below. While the shape of the processed data during the first ~5 minutes of reaction is dependent on data processing treatment, the method of data processing was validated by comparison to LC data (see page 58).

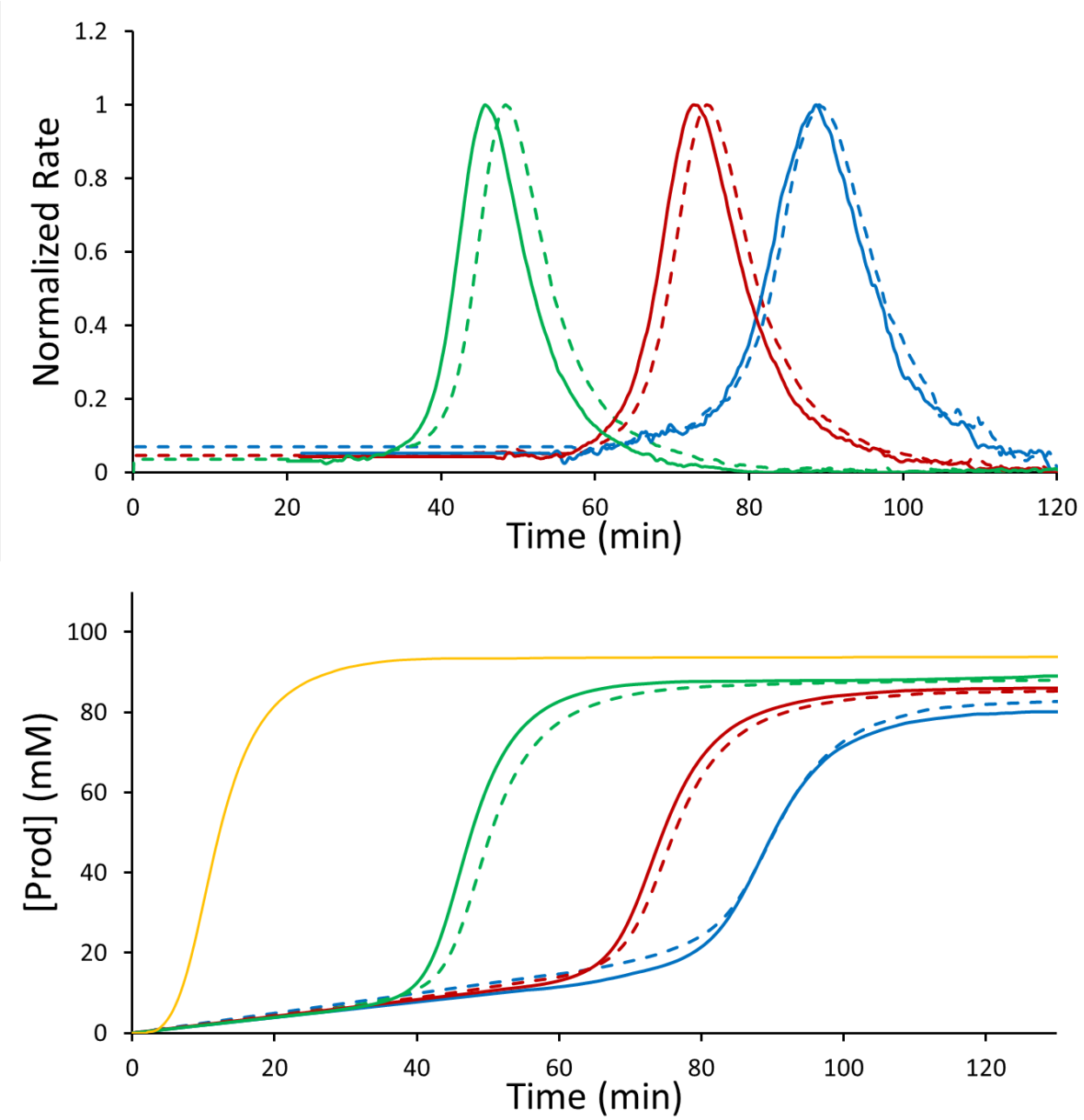


Figure S9. Processed data, showing normalized rate vs. time (top) and [prod] vs. time (bottom). Heat of mixing removed by extending the zero-order regime back to t = 0. Validation given on page 58. $[aldehyde]_0$ = 110 mM, $[Zn(iPr)_2]$ = 260 to 280 mM, [(*S*) initiator] = 0 mM (yellow), 9 mM (green), 13mM (green), or 17 mM (blue). Duplicate experiments shown in dashed lines (SOA218).

G. Amplification of Enantiomeric Excess in Calorimetry Data

Product mixtures from reactions at different initiator concentrations were subjected to further reaction by addition of 4.0 mL of diisopropyl zinc solution (0.86M stock, 3.45 mmol) and aldehyde (2.4 mmol, 80 mM) to a solution containing 0.3 mL of the filtered reaction mixture estimated to contain ca. 0.003 mmol product. The resulting ee after amplification was > 90% for SOA218 B1 through B3. From this we may estimate that the product ee after the calorimetry reaction was between 0.5% and 1% ee, values too low to measure accurately by chiral HPLC.

H. Reaction Calorimetry – Amine Initiator

There remained a question as to whether the inhibitory effect of the chiral trigger was unique to 2° alcohols, or if this was a more general feature of chiral induction by small molecules. This was tested by comparing the induction time resulting from the addition of TMEDA, a common amine ligand in organozinc catalysis and another structural motif used in isotopically driven chiral induction. These results show that addition of TMEDA to the reaction mixture does indeed suppress the reaction rate, suggesting an inhibitory effect. The level of suppression appears to smaller when compared to oxygen based ligands, likely due the weaker Zn-N bonding.

Table S7. Reaction conditions for TMEDA triggered reaction calorimetry studies at -12°C.

Sample	Aldehyde (mM)	Zinc (mM)	TMEDA (mM)
227-B1	112.0	317	0
227-B2	109.8	319	12.4
227-B4	112.4	320	60.6

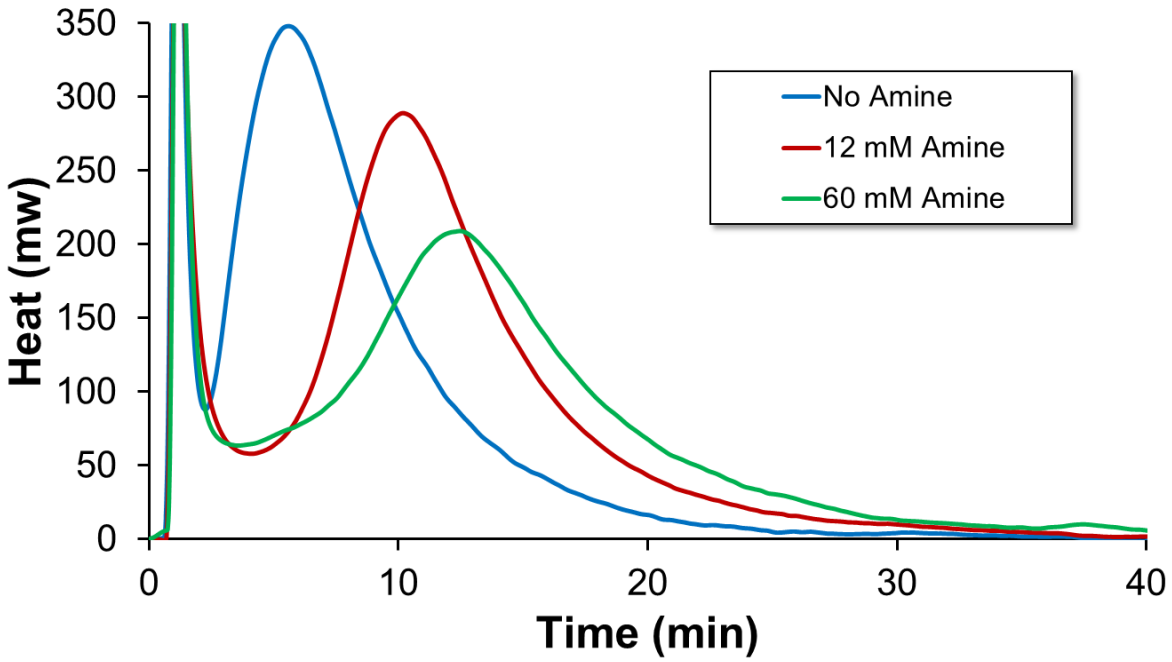


Figure S10. Raw heat flow data from SOA227 using added TMEDA at -12°C. Data shown post Tau Correction.

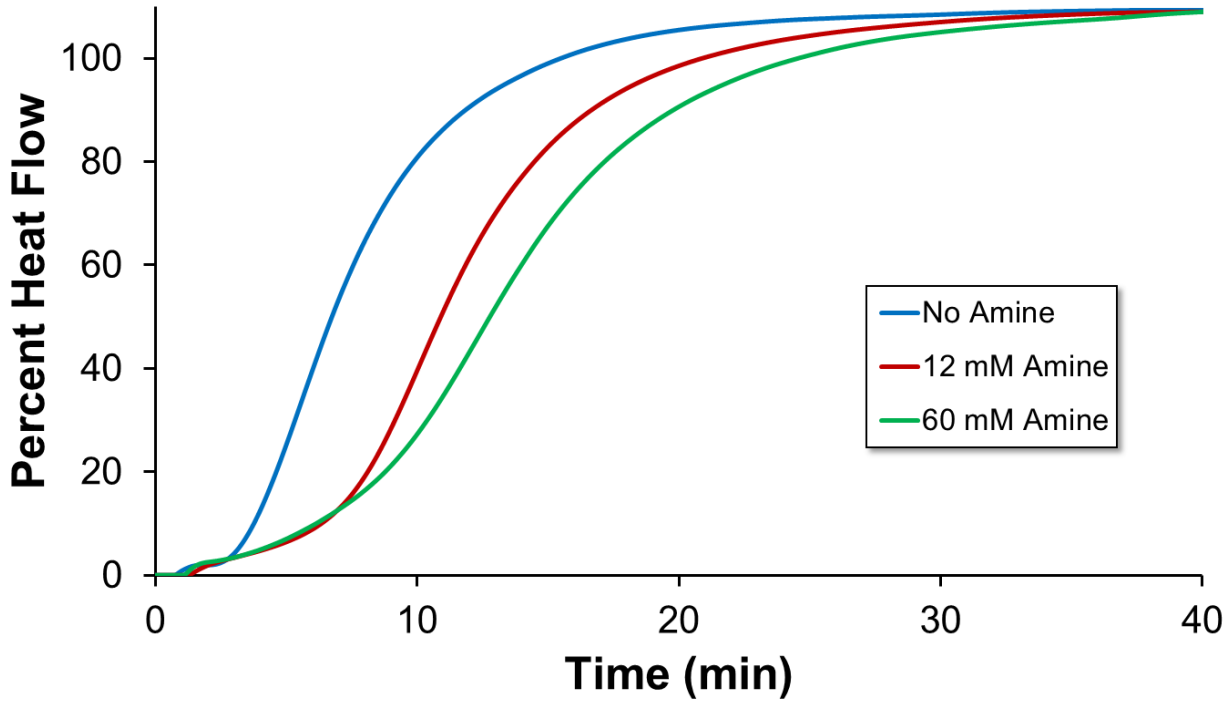


Figure S11. Percent heat flow vs. time plot from SOA227. Heat of mixing removed via subtraction of a standard curve. If the reaction shows mass balance fraction heat flow = fraction conversion.

I. Reaction Calorimetry – Varied [Product]

Vials were prepared gravimetrically and placed in the calorimeter (see sections 2B, 2C for procedure) at -12°C. Reaction commenced by injection of aldehyde. Given data shown after tau correction. Data used for validation of COPASI model.

Table S8. Reaction conditions for product catalyzed reaction calorimetry studies at -12°C.

Sample	Aldehyde 1 (mM)	Zn(*i*Pr)$_2$ (mM)	Product 2 (mM)	Product ee	Biphenyl (mM)
189-B2	56.6	113.2	2.8	16.5	13.0
189-B3	56.4	111.8	2.9	16.5	13.1
190-B2	65.8	163.9	3.1	16.5	13.6
190-B3	58.9	162.5	3.1	16.5	13.6
191-B2	49.6	90.1	2.2	79.7	9.1
191-B3	51.5	91.4	2.2	79.7	9.1

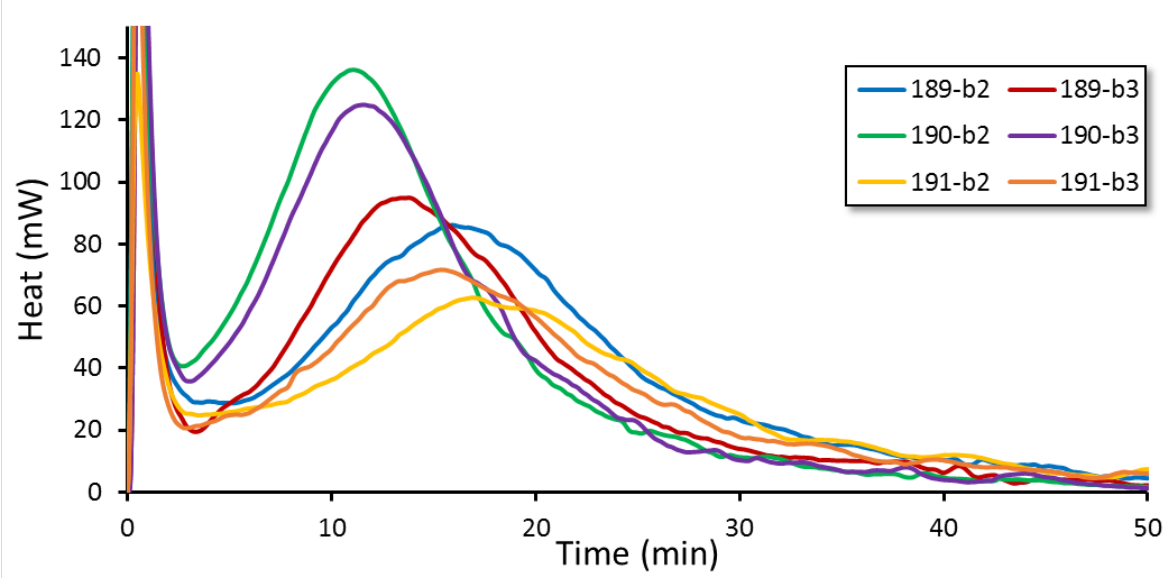


Figure S12. Raw heat flow data from time course reaction calorimetry experiments. Reagent concentrations varied (see Table **S8**). Data shown post tau correction. Test IDs: SOA189-191.

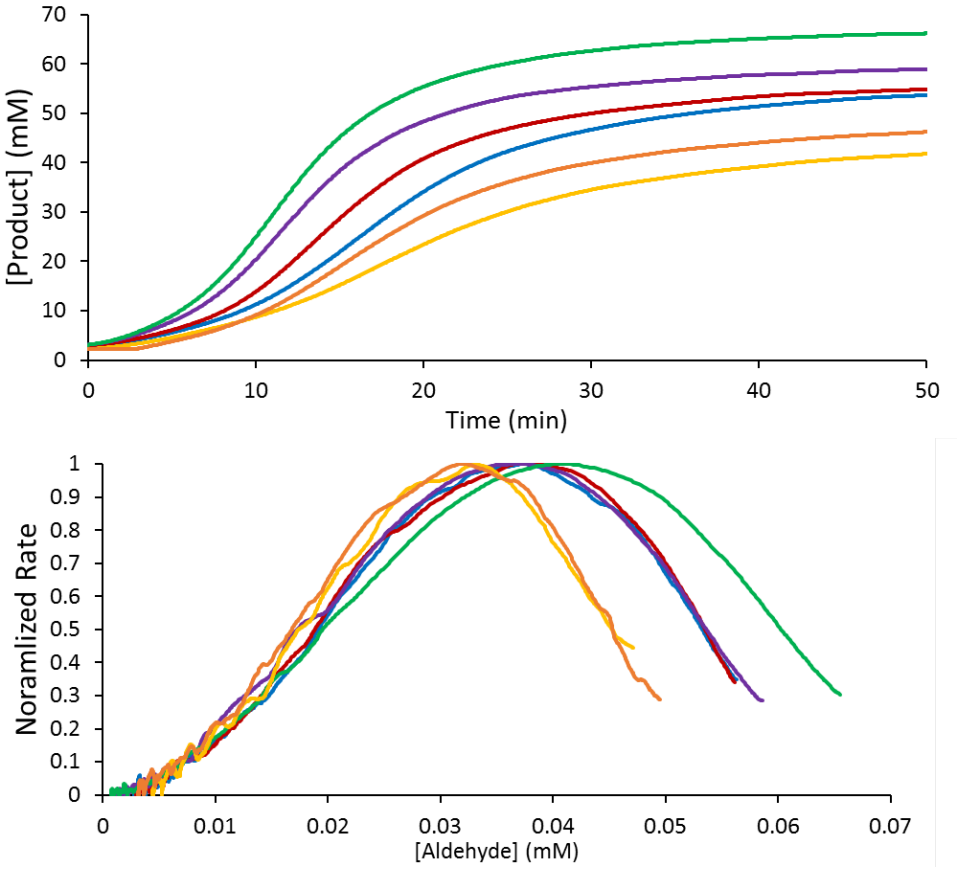


Figure S13. Processed reaction calorimetry data for varied initiator trials. Colors correlated with legend in Fig. S12. Normalization to maximum rate vs. [aldehyde]. Test IDs: SOA189-191.

J. NMR Titration Results (Set 1) – ^{2}H

A solution containing *(R)* product (1.5M in Toluene) was titrated into a screw top NMR containing 0.06 mmol (60 mM) of *(R)* or *(S)* initiator and 0.60 mmol (0.6M) diisopropyl zinc. Initiators were enantiopure, and product was 90% ee. After each titration step, ^{1}H and ^{2}H NMR was acquired. Exact conditions and procedure on page 10.

Table S9. Conditions for ^{1}H and ^{2}H NMR titration of (*R*) and (*S*) initiator with (*R*) product.

	Titration with (*R*) Initiator (matched)			**Titration with (*S*) Initiator (mismatched)**		
Titration Point	***R-3* (mM)**	**[Product] (mM)**	**Equiv**	***S-3* (mM)**	**[Product] (mM)**	**Equiv**
0	55.7	-	0.0	56.4	-	0.00
10	55.2	7.2	0.1	55.8	8.4	0.15
20	54.7	14.9	0.3	55.2	16.3	0.3
40	53.6	30.2	0.6	54.1	31.7	0.6
60	52.5	45.0	0.9	53.0	47.0	0.9
80	51.5	58.6	1.1	51.9	61.0	1.2
110	50.1	80.6	1.6	50.5	83.9	1.7

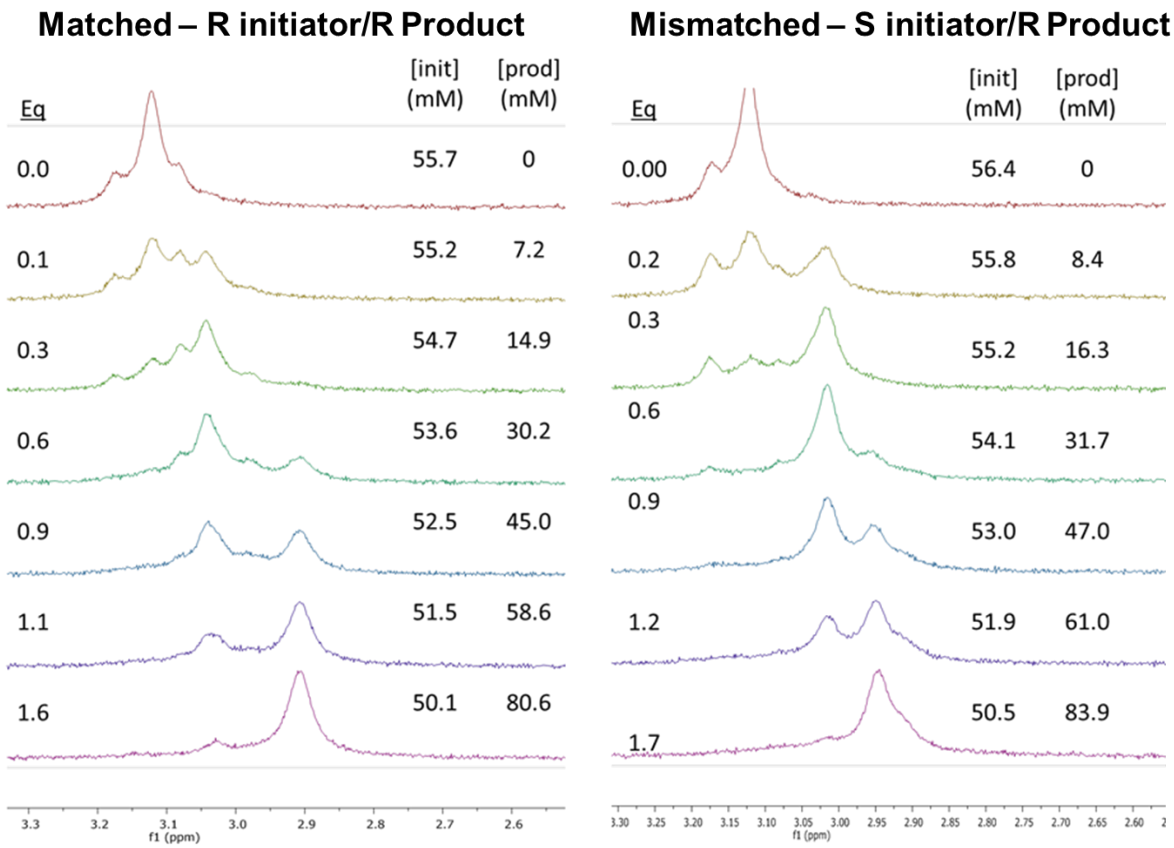


Figure S14. ^{2}H NMR of mismatched and matched titration of (*R*) product with (*R*) and *(S)* initiator, respectively. Product was titrated into a solution containing 0.06M of initiator 0.6M diisopropyl zinc (15:85 toluene-*d8*:toluene). Peaks are assigned to D atoms in the OCD_3 group on the initiator. Spectra referenced to CD_3 in to toluene-*d*8. Test ID: SOA215.

^{2}H NMR revealed two initial initiator-zinc-complexes, though monitoring of the ROC*D*$_3$ peak of the initiator. Two (mismatched) or three (matched) peaks appeared as the titration proceeded, converging on a final species at > 1.7 equiv.

K. NMR Titration Results (Set 1) - ^{1}H

A ^{1}H spectra was acquired at each titration point for both the matched case (*R* product, *R* initiator) and mismatched case (*R* product, *S* initiator). Spectra are provided, segmented into four regions. Tentative NMR assignments are provided, based on COSY, ^{13}C, HMBC and HSQC data from additional experiments (see page 64). All spectra referenced to 2.09 for the toluene CH_3. Conditions taken under qualitative conditions (see page 10 for NMR parameters).

The aromatic region shows the emergence and disappearance of two transient peaks, and converges to a final peak at ~ 1.7 eq of product. All peaks are associated with the aromatic CH on the pyrimidine ring.

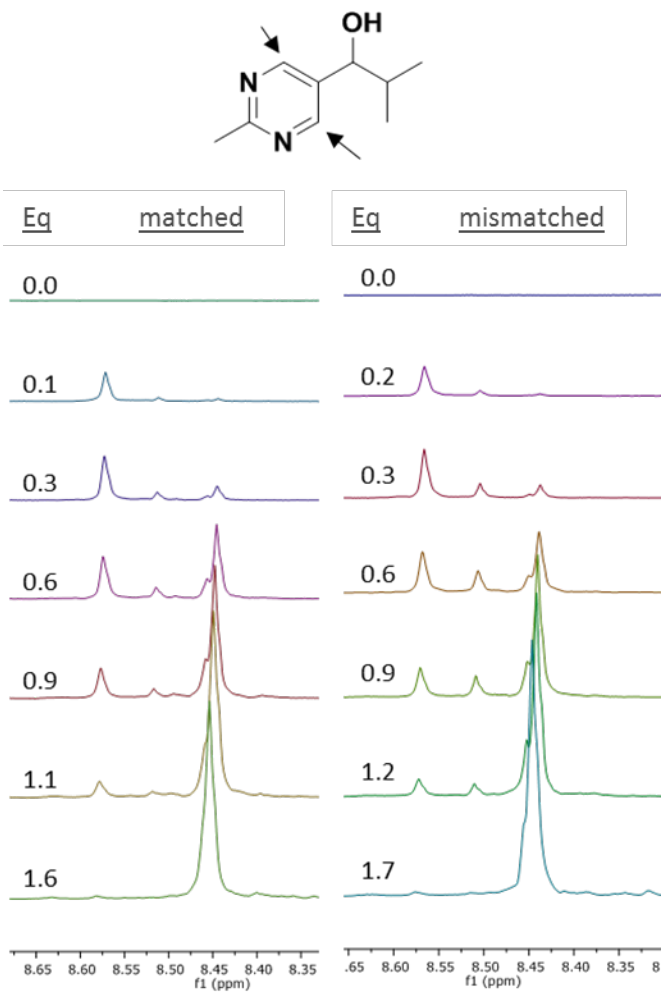


Figure S15. ^{1}H spectra in the aromatic region of matched and mismatched titration of with (*R*) product. Peaks correlate to the aromatic CH signals on the pyrimidine ring. Spectra referenced to toluene CH_3. Test ID: SOA215.

The region from 4.5 to 3.3 ppm shows transitions in the benzylic CH of the product, and the CH_2 and CH protons from the initiator. Assignments only provided for matched case, but peak assignments are analogous for the mismatched titration.

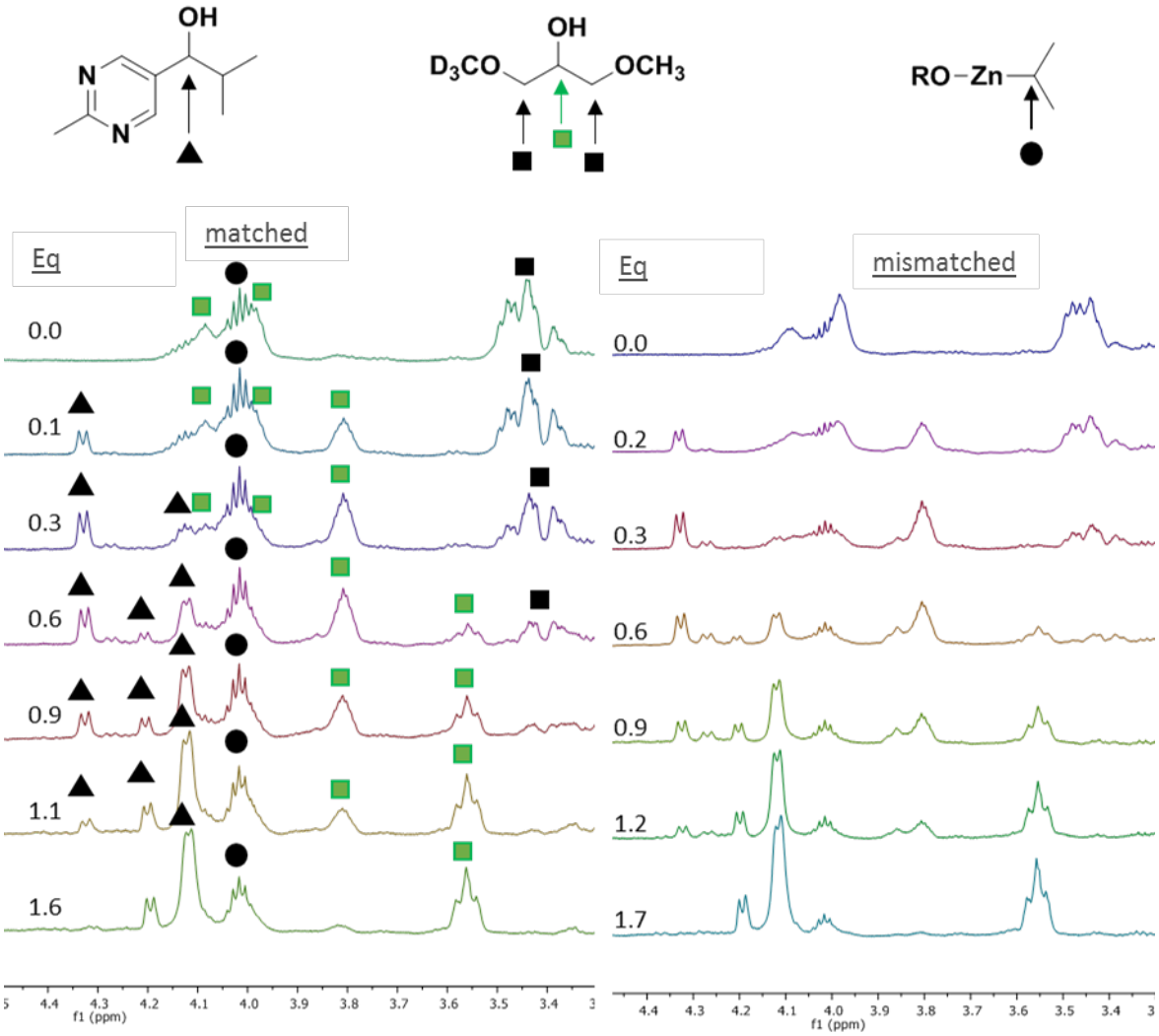


Figure S16. ^{1}H spectra from 3.3 to 4.5 ppm of matched (left) and mismatched (right) titration of 60 mM initiator solution with (*R)* product. Peak assignments based on 2D NMR (page 64). Spectra referenced to toluene CH_3. Test ID: SOA215.

The region from 3.3 to 2.3 ppm shows transitions in the benzylic CH_3 of the product as well as the CH_3 and CH_2 protons from the initiator. Large shifts are seen in the CH_3 of the initiator, and the chemical shifts are not identical between the matched and mismatched complexes. The quartet at 3.2 ppm is a consistent impurity resulting from the exposure of the $Zn(iPr)_2$ to air (likely the cubic zinc isopropoxide).

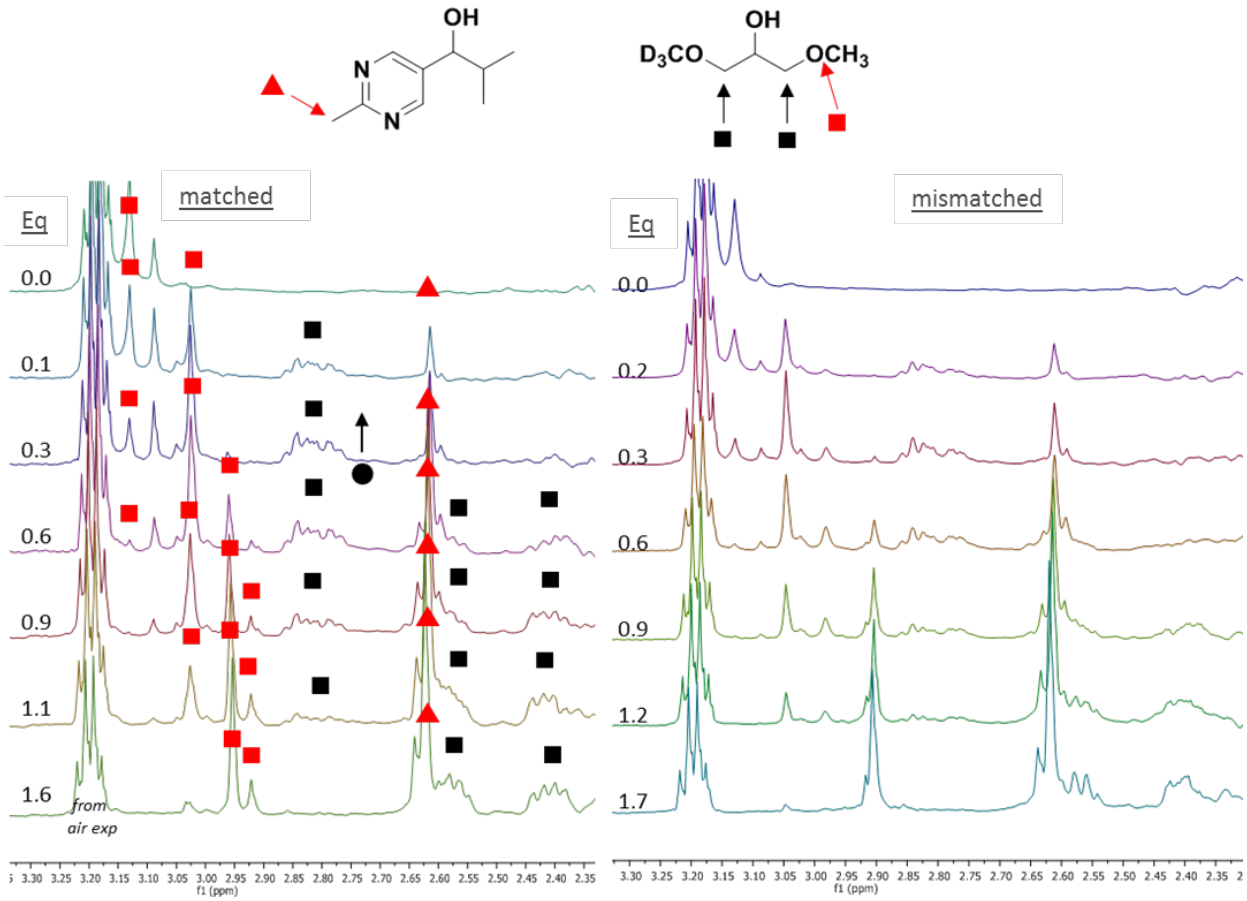


Figure S17. ^1H spectra from 3.3 to 2.3 ppm of matched (left) and mismatched (right) of 60 mM initiator solution with *(R)* product. Peak assignments based on 2D NMR (page 64). Spectra referenced to toluene CH_3. Note differences in initiator-OCH_3 peaks between mismatched and matched complexes. Test ID: SOA215.

The region from 2.3 to 0.4 ppm shows transitions in the benzylic alkyl chains associated with the product and zinc isopropyl groups. However, many of these peaks are obscured or cannot be assigned due to overlap with toluene, Zn(*i*Pr)$_2$ and the Zn(*i*Pr)$_2$ byproducts from exposure to air.

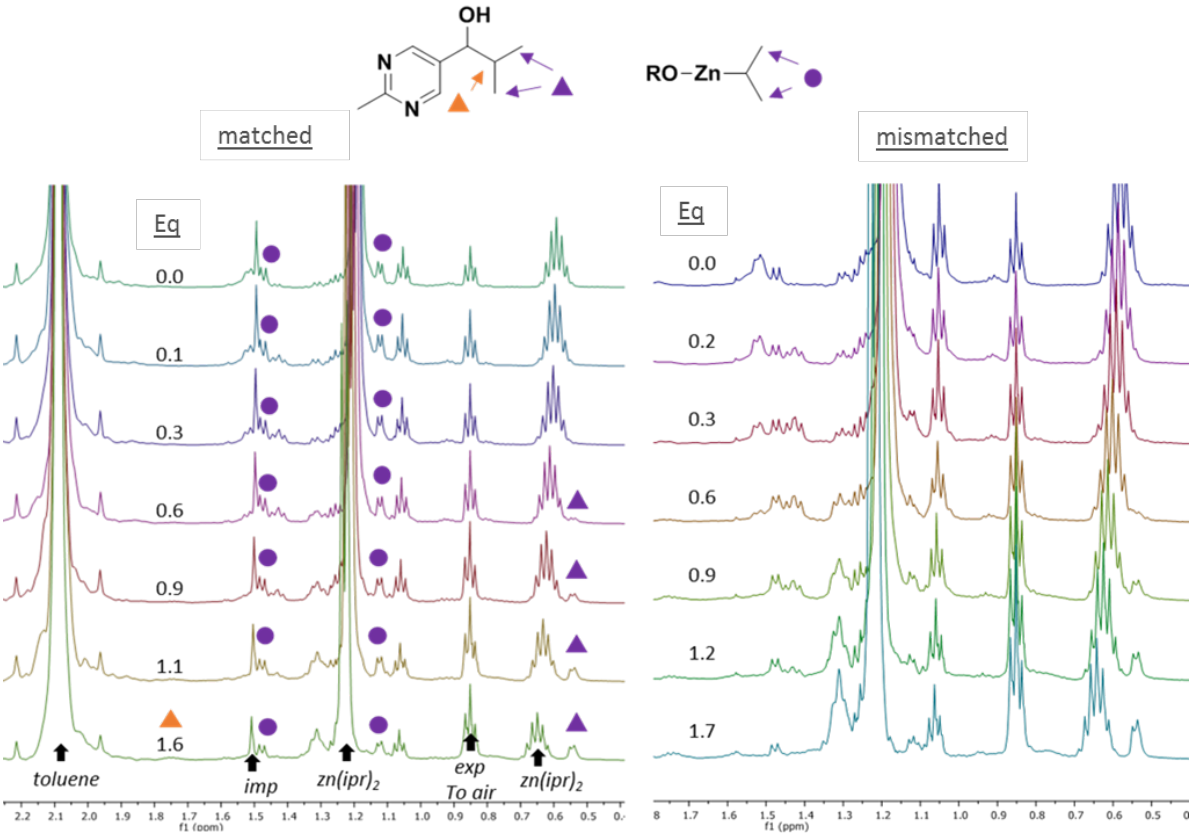


Figure 18. ^{1}H spectra from 2.3 to 0.4 ppm of matched (left) and mismatched (right) titration of 60 mM initiator solution with (*R)* product. Peak assignments based on 2D NMR (page 64). Spectra referenced to toluene CH$_3$. Some peaks not assigned due to overlap in 2D spectra. Residual peaks from Zn(*i*Pr)$_2$, dialkyzinc degradation products, and toluene are given. Test ID: SOA215.

L. NMR Titration Results (Set 2) – ^{2}H

As a validation of the previous results, a second titration was performed. In this experiment, (*R*) and (*S*) product were titrated into an NMR tube containing (*S)* initiator (0.06mmol) and diisopropyl zinc (0.60mmol). Both products were ~90% ee. These results agree with results from the previous titration. Procedure and NMR protocols given on page 10. Quantitative ^{2}H spectra given below.

Table S10. Conditions for ^{1}H and ^{2}H NMR titration of (S) initiator with (*R*) and (*S*) product.

	Titration with (*R*) product (mismatched)			**Titration with (*S*) product (matched)**		
Titration Point	**[Initiator] (mM)**	**[Product] (mM)**	**Equivalents**	**[Initiator] (mM)**	**[Product] (mM)**	**Equivalents**
0	50.9	-	0.00	51.0	-	0.00
10	50.4	9.2	0.18	50.5	9.0	0.18
20	50.0	17.0	0.34	50.0	18.6	0.37
40	49.0	34.1	0.70	49.0	35.5	0.72
60	48.0	51.0	1.06	48.1	52.0	1.08
80	47.1	66.9	1.42	47.1	68.5	1.45
110	45.7	90.8	1.99	45.8	91.1	1.99

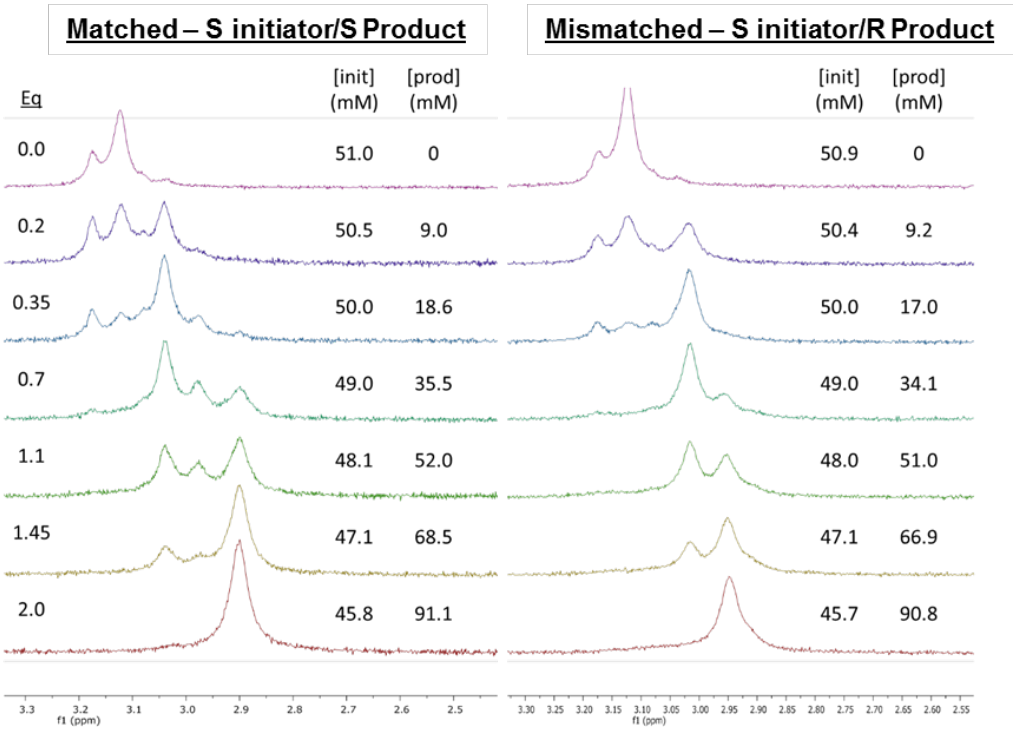


Figure S19. ^{2}H NMR of matched and mismatched titration of (*R*) with (*R*) and (*S*) product respectively. Product was titrated into a solution containing 0.06M of initiator 0.6M diisopropyl zinc (15:85 toluene-*d8*:toluene). Peaks are assigned to D atoms in the OCD_3 group on the initiator. Spectra referenced to CD_3 in to toluene-*d*8. Test ID: SOA221.

M.NMR Titration Results (Set 2) – ^{1}H

Below are the ^{1}H results of the validation study. ^{1}H spectra taken are qualitative, see page 10 for NMR protocols and experimental procedure. Assignments are tentative and based on 2D NMR performed in an additional experiment (page 64).

In the aromatic region, the titration again reveals three peaks relating the pyrimidine CH protons. The observed trend matches the results seen in the first experimental set, validating these results. The remainder of the spectra are given on subsequent pages, and agree with the trends seen in the first titration.

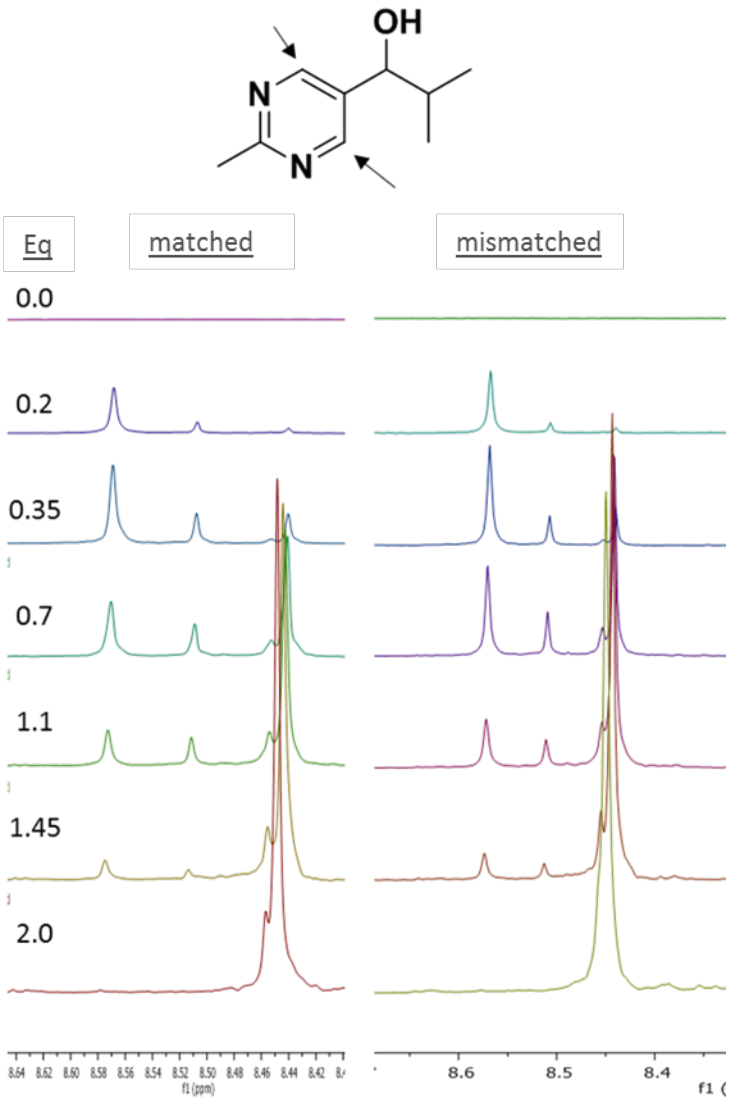


Figure S20. ^{1}H spectra in the aromatic region of matched and mismatched titration of (*S*) initiator with (*R*) and (*R*) product. Peaks correlate to the aromatic CH signals on the pyrimidine ring. Spectra referenced to toluene CH_3 at 2.09 ppm. Test ID: SOA221.

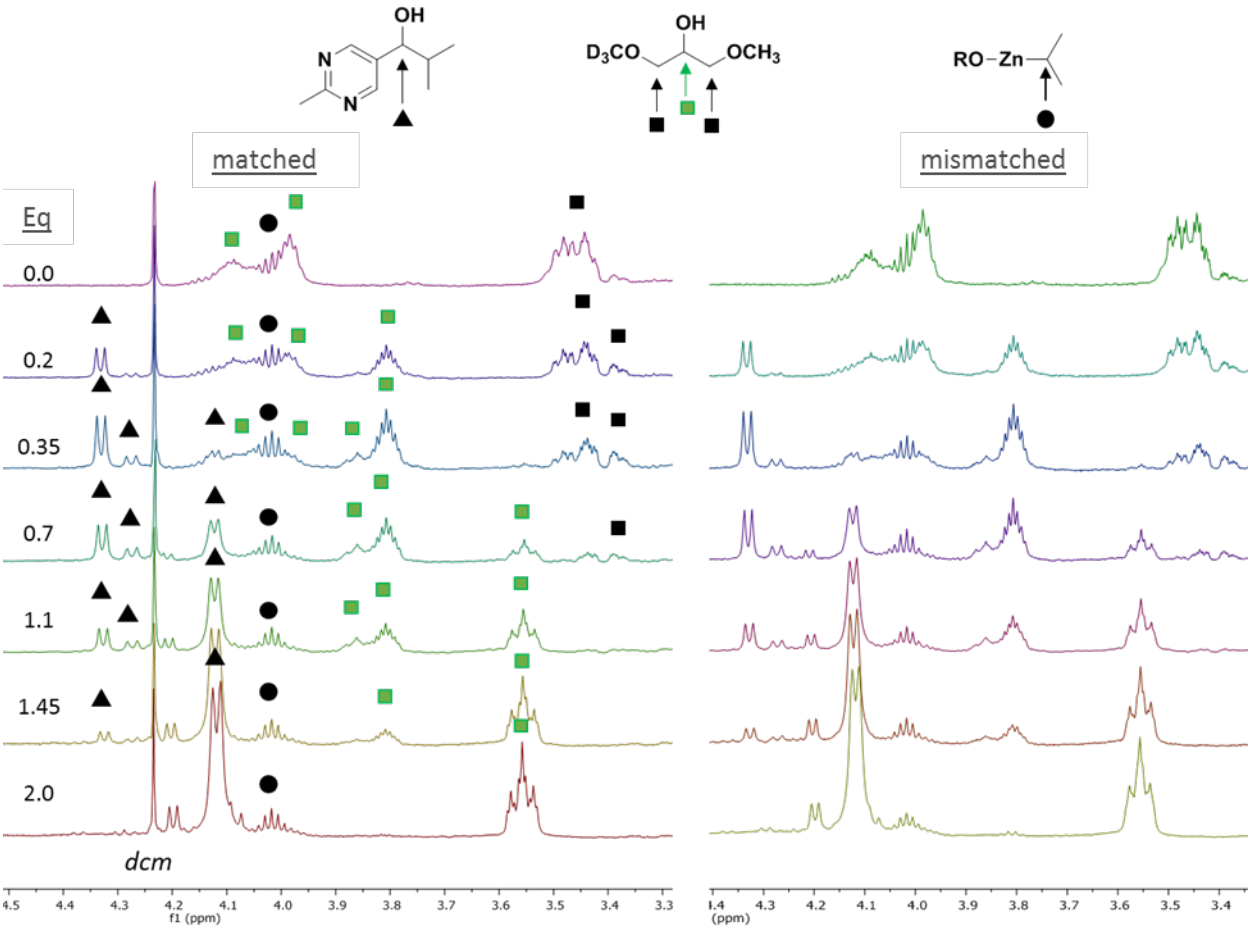


Figure S21. ^{1}H spectra from 3.3 to 4.5 ppm of matched (left) and mismatched (right) titration of 60 mM initiator solution with *(S)* and *(R)* product, respectively. Peak assignments based on 2D NMR (page 64). Spectra referenced to toluene CH_3. Minor amount of residual dichloromethane present from cleaning of NMR tube. Test ID: SOA221.

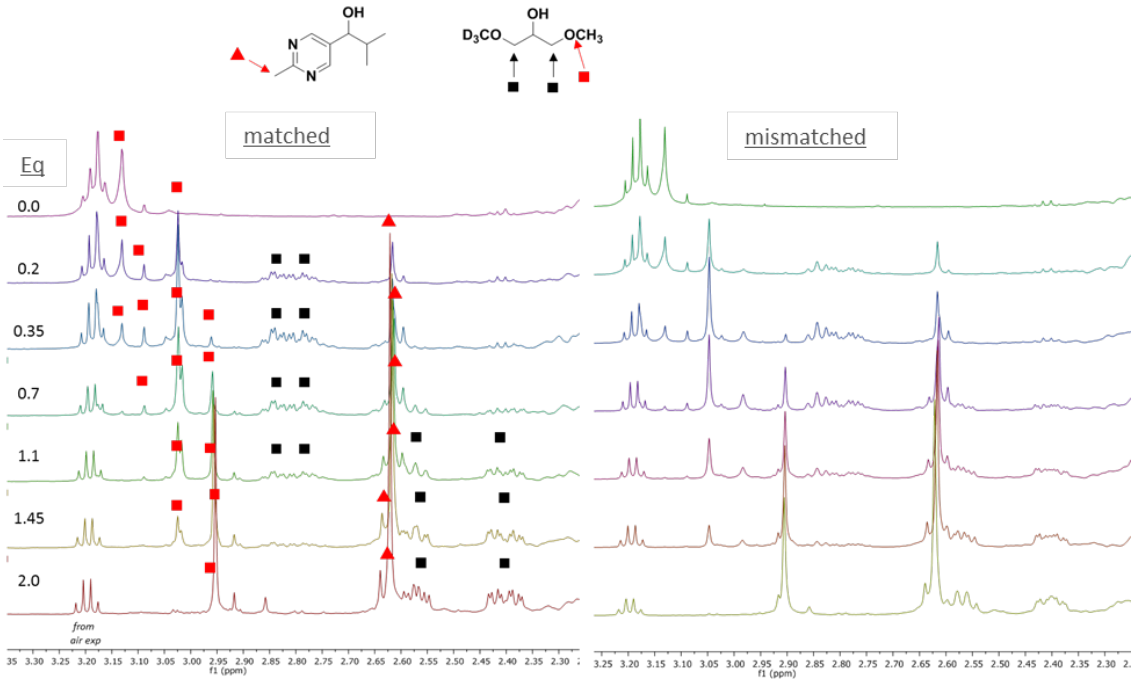


Figure 22. ^{1}H spectra from 3.3 to 2.3 ppm of matched (left) and mismatched (right) of 60 mM initiator solution with (S)and (*R*) product, respectively. Peak assignments based on 2D NMR (page 64). Spectra referenced to toluene CH_3. Test ID: SOA221.

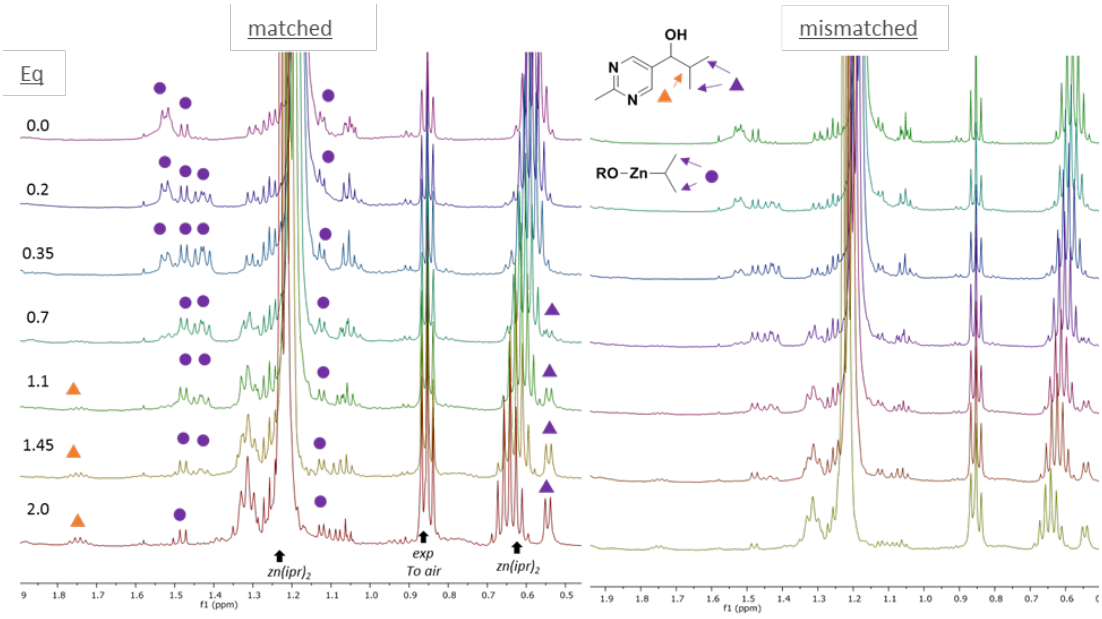


Figure 23. ^{1}H spectra from 2.3 to 0.4 ppm of matched (left) and mismatched (right) titration of 60 mM (*S*) initiator solution with (*R)* and *(S)* product. Peak assignments based on 2D NMR (page 64). Spectra referenced to toluene CH_3. Some peaks not assigned due to overlap in 2D spectra. Residual peaks from $zn(ipr)_2$, dialkyzinc degradation products, and toluene are given. Test ID: SOA221.

N. NMR Titration Results - Comparison between Matched and Mismatched

While most peaks appear with identical chemical shifts in the matched and mismatched complexes, the OCD_3 (in ^2H NMR) and the OCH_3 peak (in ^1H NMR) display different chemical shifts depending on the diastereomer. The ^2H signal correlated with OCD_3 on the initiator splits into three unique peaks in the matched complex, while the mismatched complex forms shows only two forms (or more likely three overlapping forms). The increased peak separation in the matched complex may suggest that OCD_3 is more rigidly bound in the matched diastereomer, whereas the deuteron may experience more free rotation in the mismatched dimer. This suggests a "CD_3 inside" of the matched complex, and a "CD_3 outside" of the mismatched complex.

We see the opposite trend in the ^1H spectra, with the matched diastereomers displaying less peak separation than the mismatched complexes. By analogy to the argument above, this may suggest a "CH_3 outside" for the matched complex and a "CH_3 inside" of the mismatched complex.

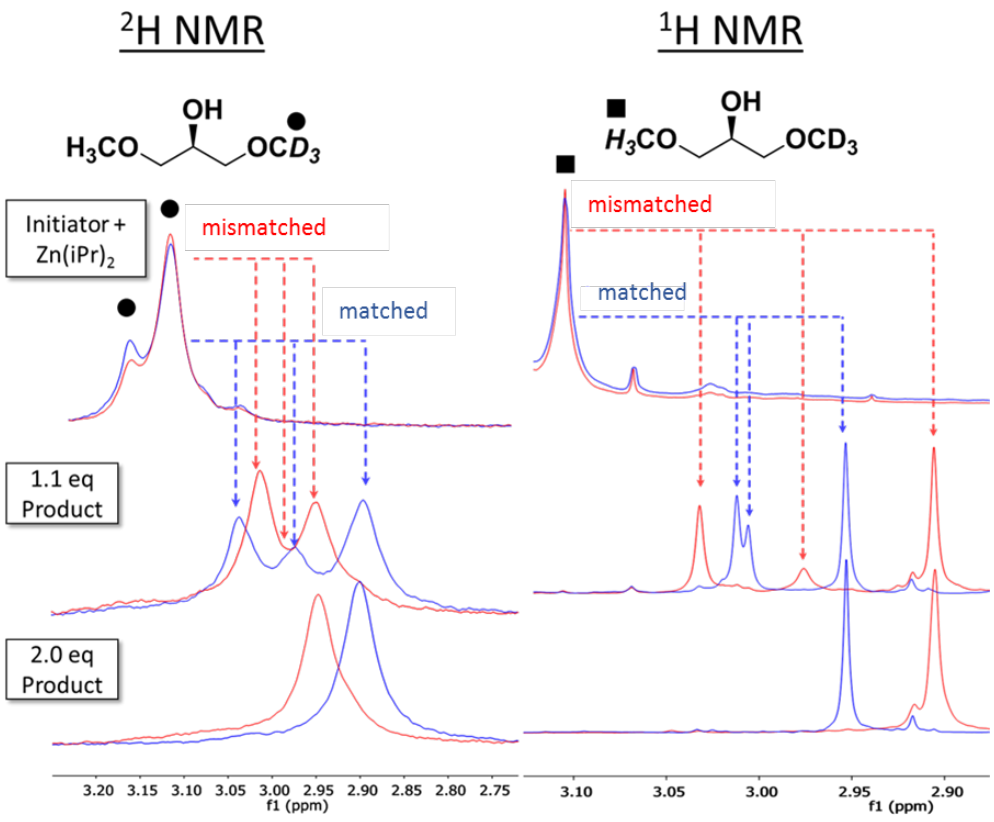


Figure 24. Comparison of OCD_3 (^2H NMR) and OCH_3 (^1H NMR) signals in the matched (blue) and mismatched (red) complex at three titration points. [$Zn(iPr)_2$] = 0.6M, [initiator] = 0.06M, [product] = 0 mM (top), 33 mM (middle), 60 mM (bottom). Test ID: SOA221.

O. In-situ NMR monitoring Results ^{2}H

To probe whether the species observed in the titration experiments were relevant to the running reaction, a reaction was monitored *in-situ* using ^{1}H and ^{2}H NMR. After initiating the reaction by addition of aldehyde, the screw top NMR tube was placed in the spectrometer at 273K. ^{1}H and ^{2}H spectra were taken in alternation as the reaction proceeded. Procedure and NMR parameters given on page 10. The ^{2}H spectrum is given below.

Table S11. Conditions for *in-situ* NMR monitoring of initiator reaction

Sample	Aldehyde 1 (mM)	Zn(iPr)$_2$ (mM)	*S*-3 Initiator (mM)
212	126.0	403.2	28.7

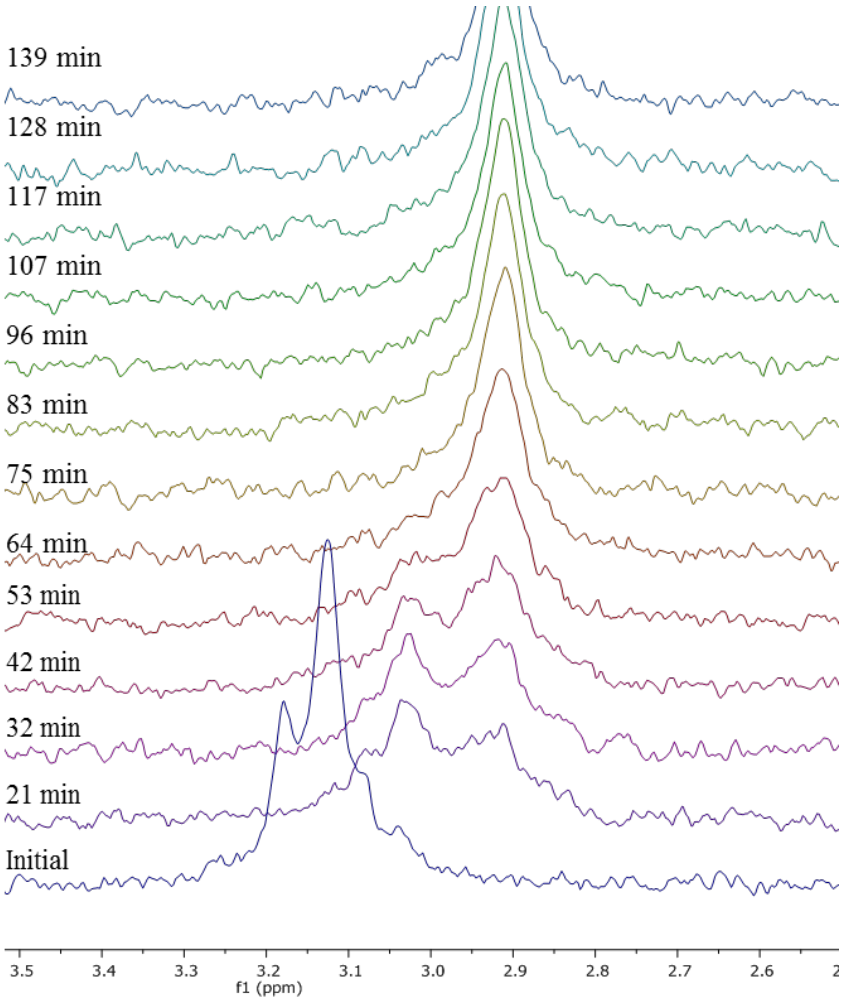


Figure S25. ^{2}H NMR time course from *in-situ* monitoring experiment at 273K. [ald]$_0$ = 126 mM, [initiator]$_0$ = 30 mM, [Zn(*i*Pr)$_2$] = 403 mM. Gaussian apodization applied for smoothing (0.3 Hz). Spectra referenced to CD$_3$ in tol-*d8*. Test ID: SOA212

P. In-situ NMR monitoring Results ^{1}H

^{1}H NMR was used to determine reaction progress. The normalized integrals of the aldehyde protons show that induction period ends after around 60 minutes, giving way to autocatalysis. This correlates with saturation in the complex at 2.88 pm in the ^{2}H NMR, suggesting that this complex is suppressing autocatalysis. Due to the complexity of the spectra, no additional peak assignments were made.

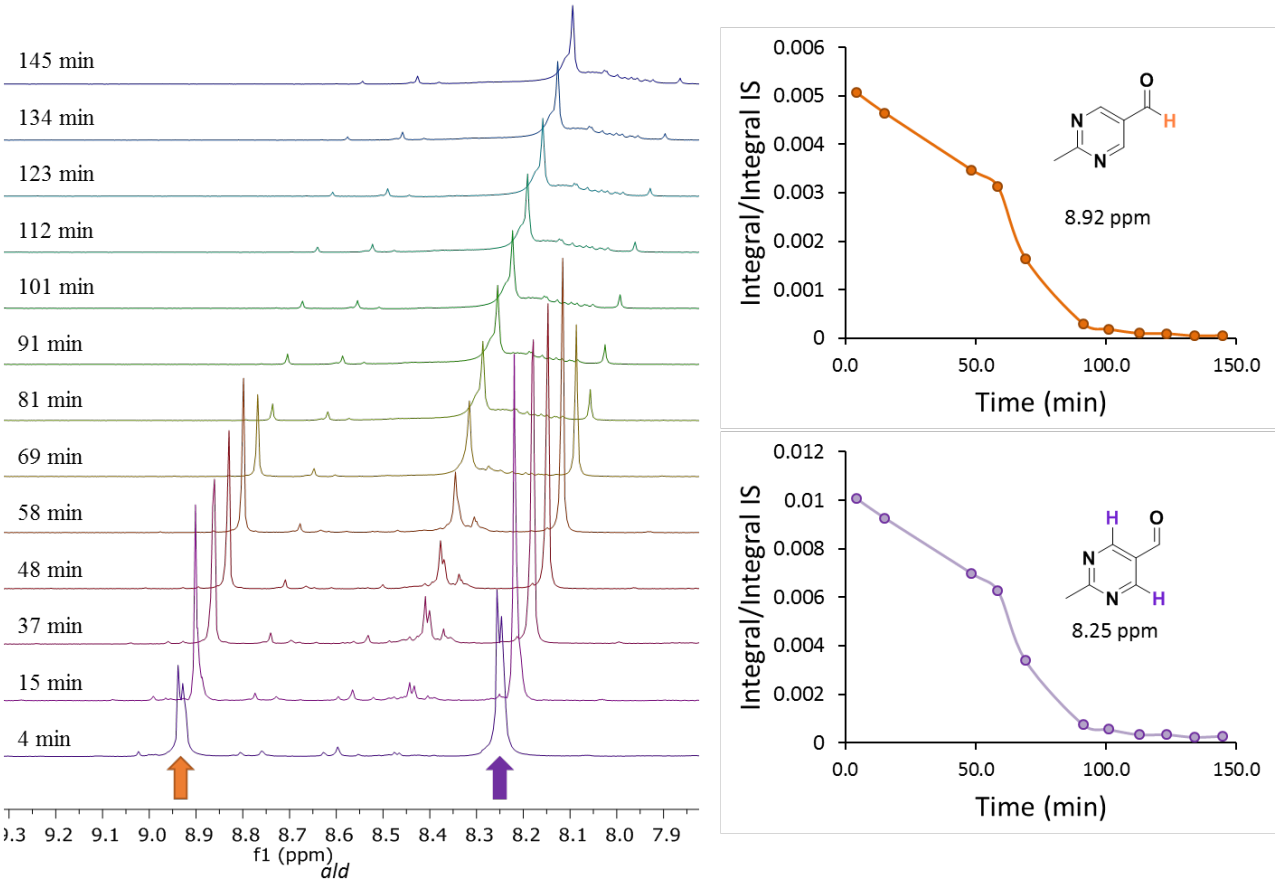


Figure S26. ^{1}H NMR of running reaction at 273K, from 7.8 to 9.3 ppm. Aldehyde signals at 8.92 ppm and 8.25 ppm were integrated over the time course (and normalized by the integral of the CH_3 proton on tol-*d8*). Reaction conditions give in Table S11 and NMR protocols give on page 10. All spectra referenced to the CH_3 proton on toluene. Solvent was 15:85 toluene-*d8*:toluene. Test ID: SOA212.

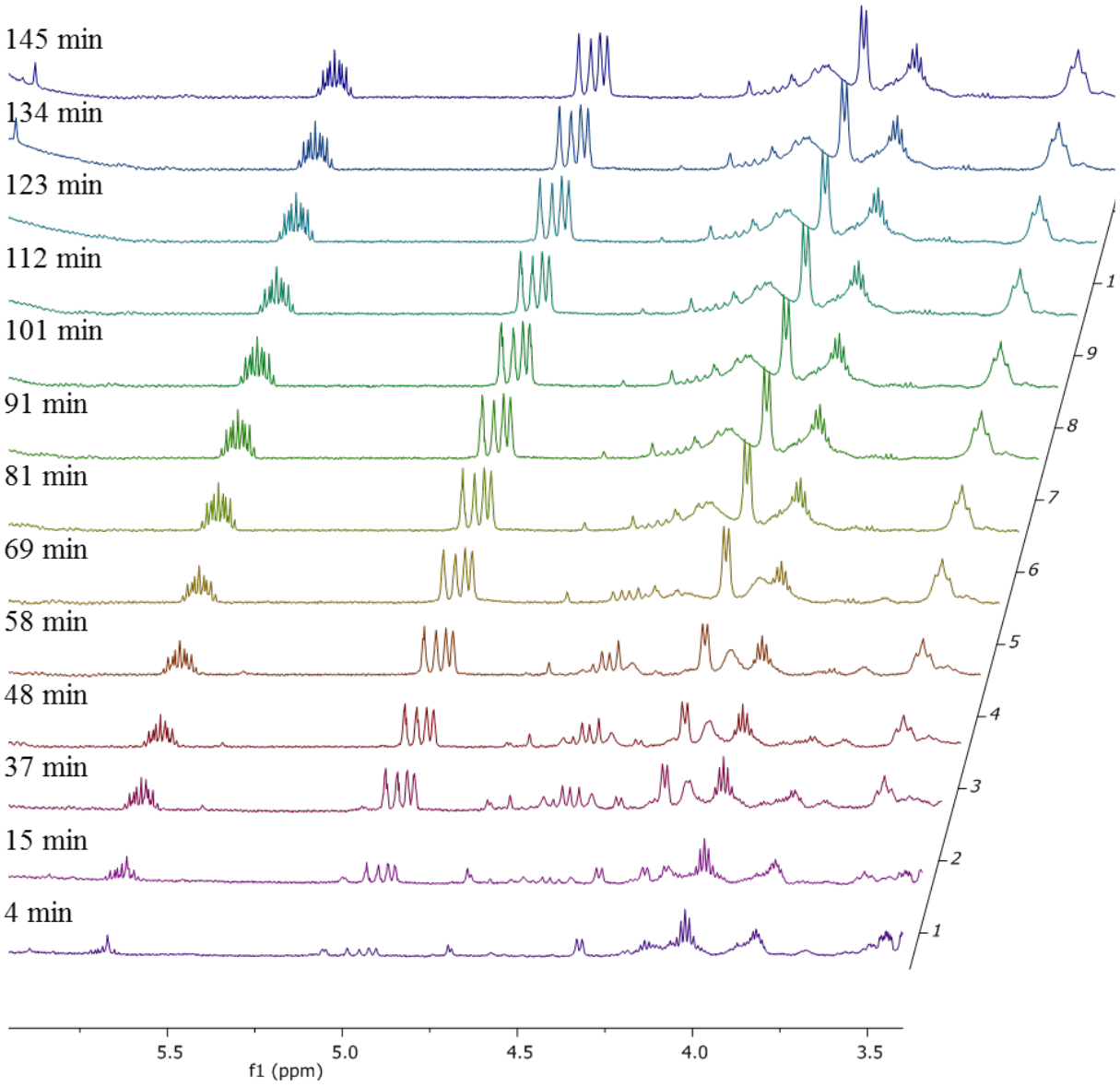


Figure 27. ^{1}H NMR of running reaction at 273K, from 3.4 to 6.0 ppm. Reaction conditions give in Table S11 and NMR protocols given on page 10. All spectra referenced to the CH_3 proton on toluene. Solvent was 15:85 toluene-*d8*:toluene. Test ID: SOA212.

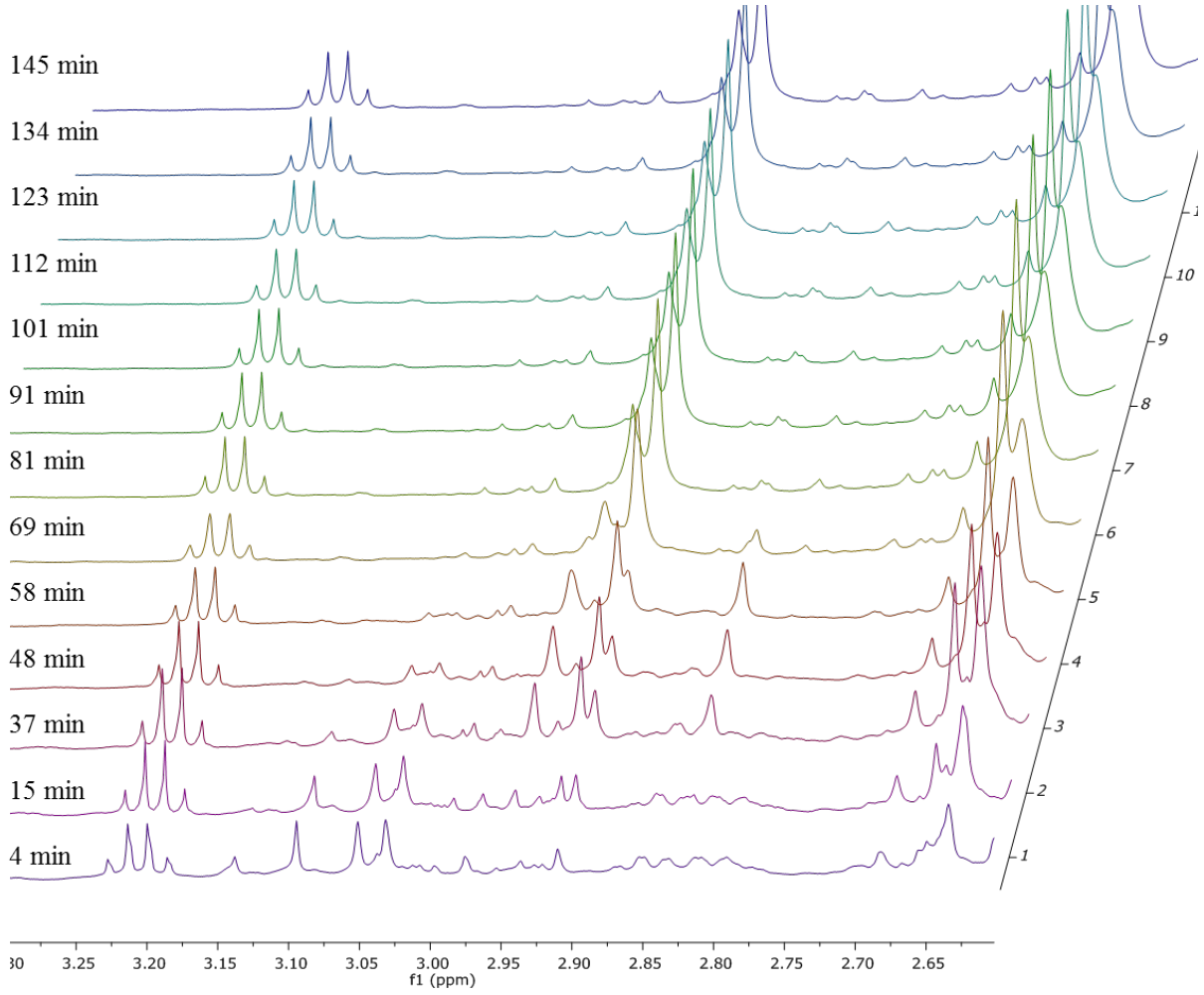


Figure S28. ^{1}H NMR of running reaction at 273K, from 2.6 to 3.3 ppm. Reaction conditions give in Table S11 and NMR protocols given on page 10. All spectra referenced to the CH_3 proton on toluene. Solvent was 15:85 toluene-*d8*:toluene. Test ID: SOA212.

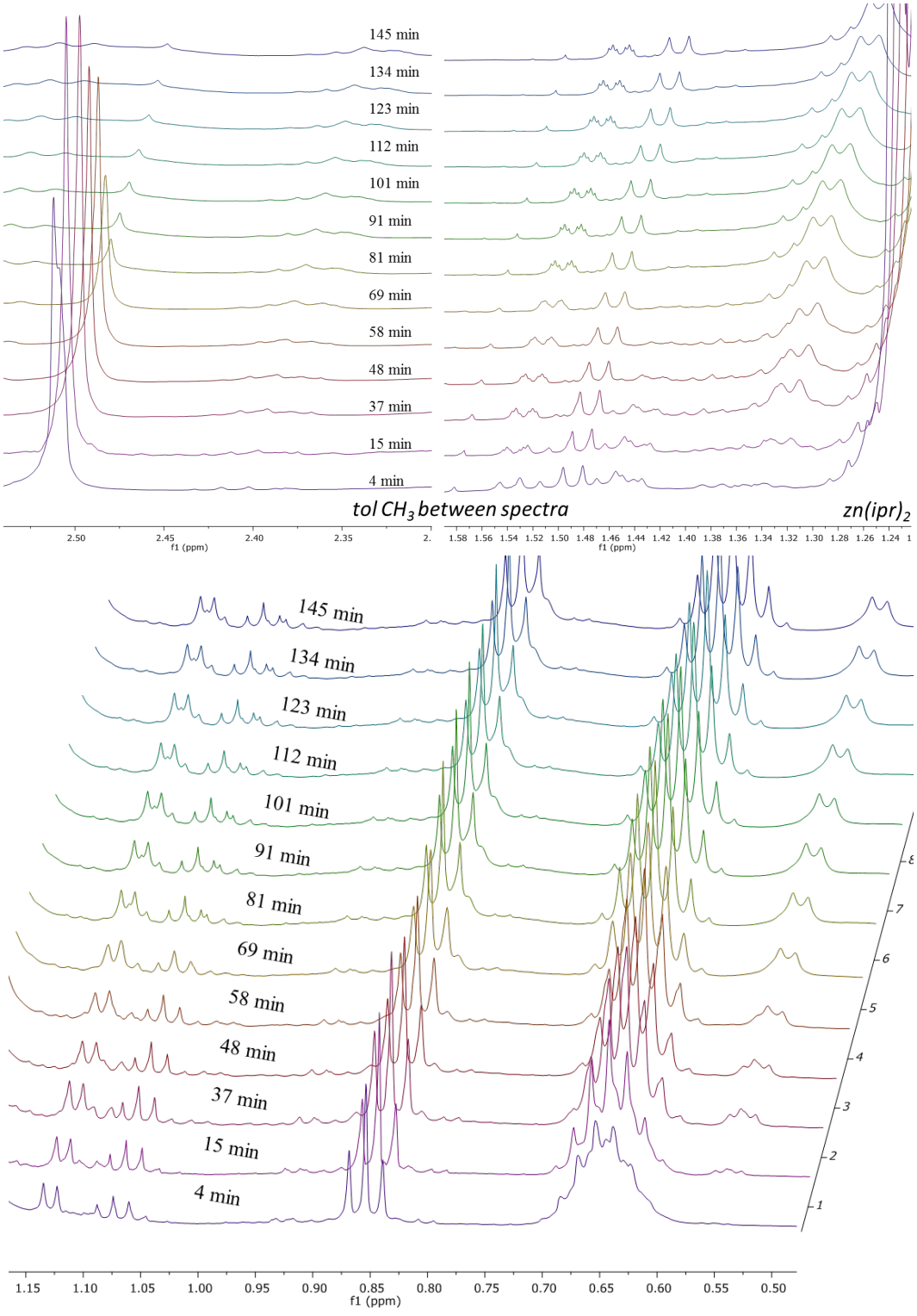


Figure 29. ^{1}H NMR of running reaction at 273K, from 2.3 to 2.6ppm (top left) 1.2 to 1.6 ppm (top right) and 0.5 to 1.2 ppm (bottom). Reaction conditions give in Table S11 and NMR protocols given on page 10. All spectra referenced to the CH_3 proton on toluene. Solvent was 15:85 toluene-*d8*:toluene. Test ID: SOA212.

Q. NMR Titration: Racemic Interaction at High Product Ratios

The *in-situ* monitoring results suggested the formation of a 2:1 product-initiator complex during the initial regime, which acted to suppress autocatalysis. The time-course spectra showed that once the initiator was saturated in this 2:1 complex, no changes in initiator bound complex occurred. This was verified using an *ex-situ* titration experiment using racemic product and racemic initiator. No changes were seen in the ^{2}H spectra at ratios higher than 2:1.

Table S12. Conditions for racemic titration at high [prod].

Titration Point	[product] (mM)	[initiator] (mM)	product-initiator ratio
1 to 1	43.7	45.7	1.0
2 to 1	42.9	24.2	1.8
3 to 1	37.4	12.9	2.9
4 to 1	41.8	9.5	4.4

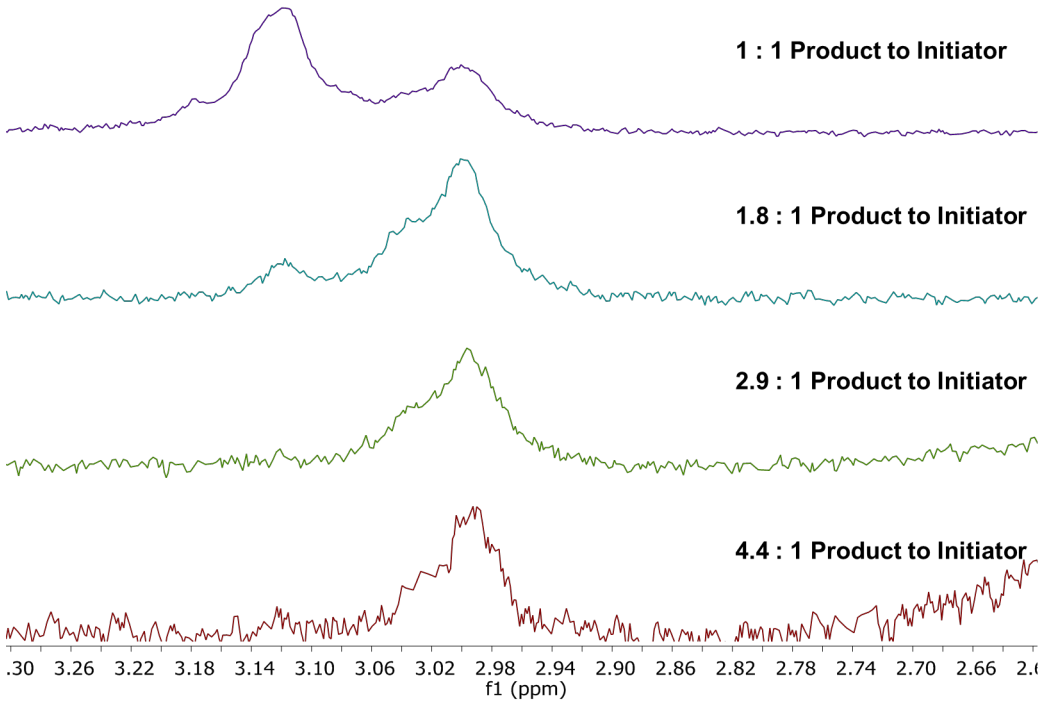


Figure S30. ^{2}H NMR of racemic product-initiator complex at various ratios (273K). Titration conditions given in Table 11, [zn(ipr)$_2$] = ~ 400 mM. Spectra were baseline corrected (Whittaker Smoother) and a 0.2 Hz exponential apodization was applied. Test ID: SOA228.

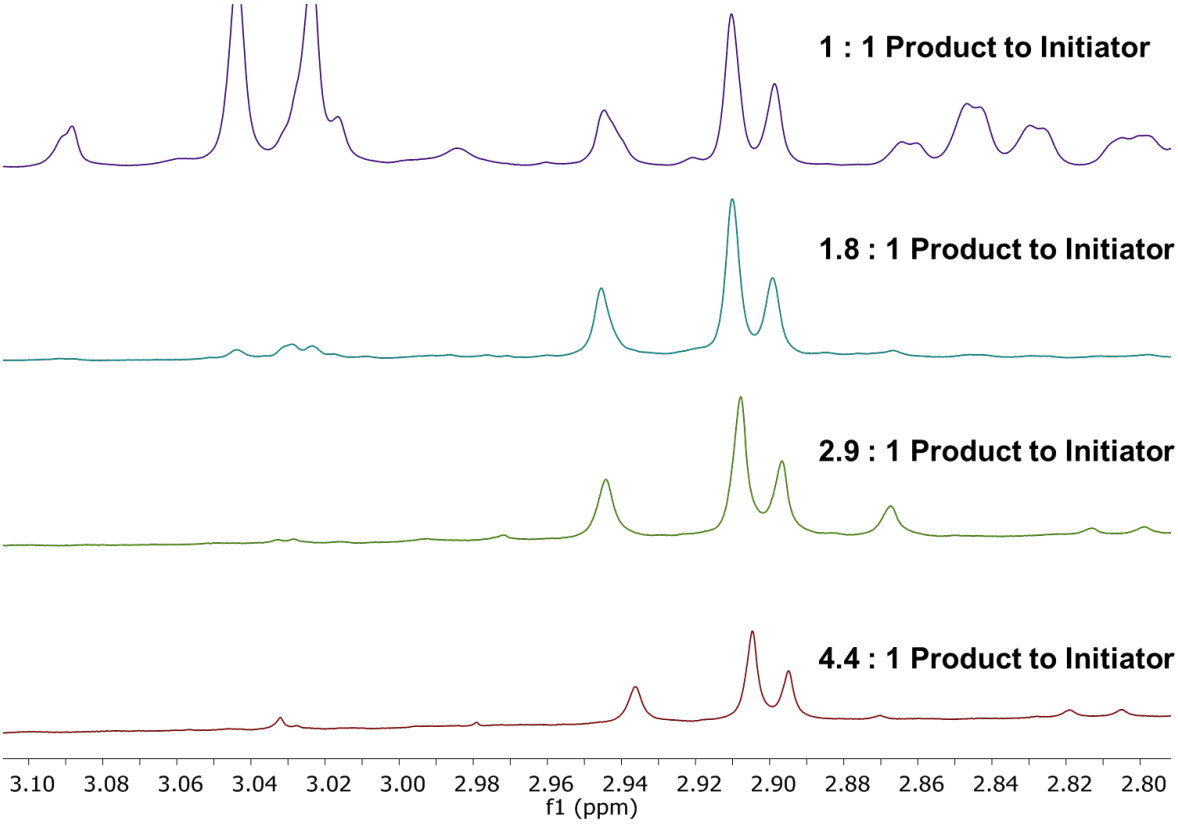


Figure S31. ^{1}H NMR (OCH_3 region) of racemic product-initiator complex at various ratios (273K). Titration conditions given in Table 11, [$zn(ipr)_2$] = ~ 400 mM. Spectra were baseline corrected (Whittaker Smoother) Test ID: SOA228.

R. DOSY- NMR Titration

Diffusion ordered spectroscopy (DOSY) was used to determine the diffusivities of the given initiator-zinc and initiator-zinc-product complexes. A DOSY spectra was acquired at three different titration points at 298K; 0:1, 1.1:1 and 2.5:1 product: initiator. After processing, diffusivities of each distinct peak were determined. These diffusivities were used to roughly estimate the molecular weight based on a diffusion ladder previously published.[3]

Table S13. Conditions for DOSY determination of diffusivities.

Titration Point	[initiator] (mM)	[zn(ipr)$_2$] (mM)	[product] (mM)	equivalents
0	9.9	104.6	0	0.0
1	9.3	98.3	11.1	1.2
2	8.7	92.4	21.4	2.5

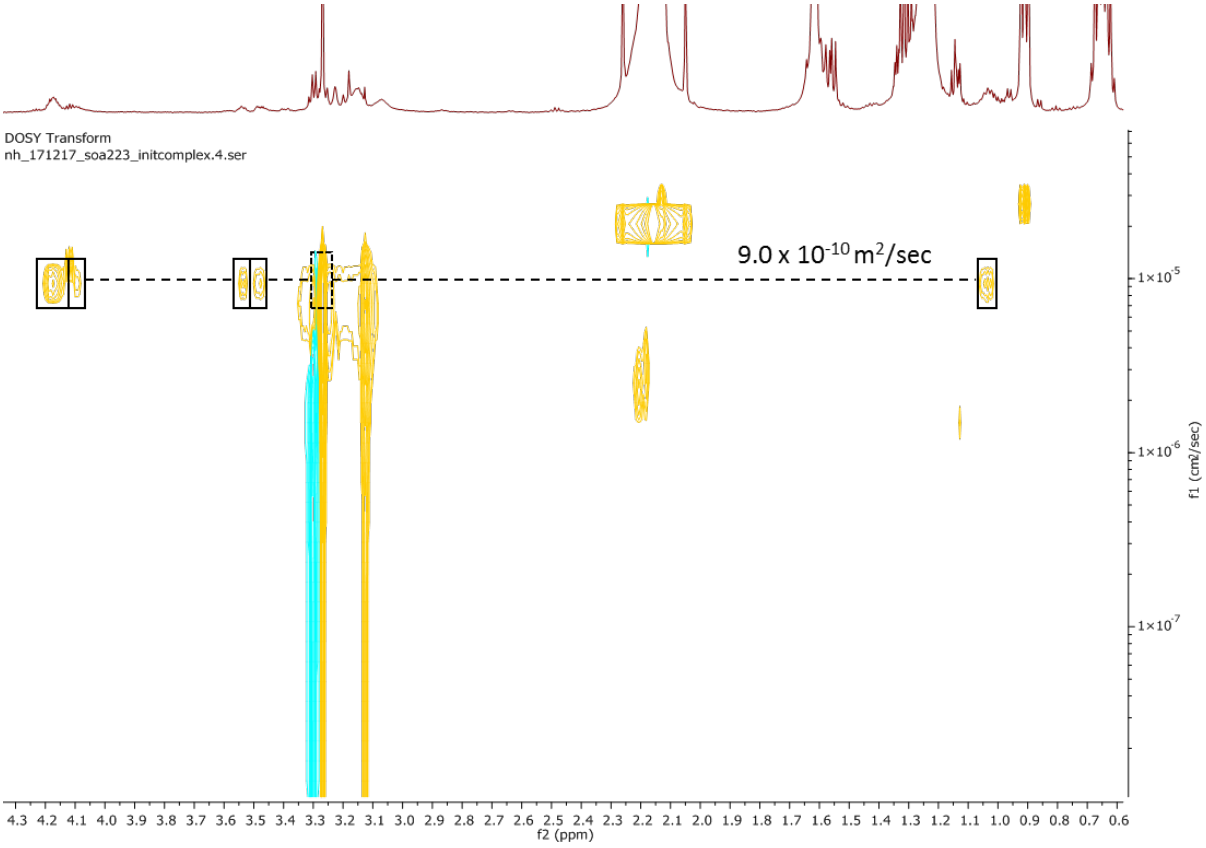


Figure S32. DOSY of zinc-initiator complex at 298K. [(*S*) initiator] = 9.9 mM, [Zn(*i*Pr)$_2$] = 105 mM. One initiator complex seen (black boxes), diffusivity = 9.01 x 10^{-10} m^2/sec Smearing due to phasing errors. Solution is 10% toluene in toluene-*d8*. Test ID: SOA223.

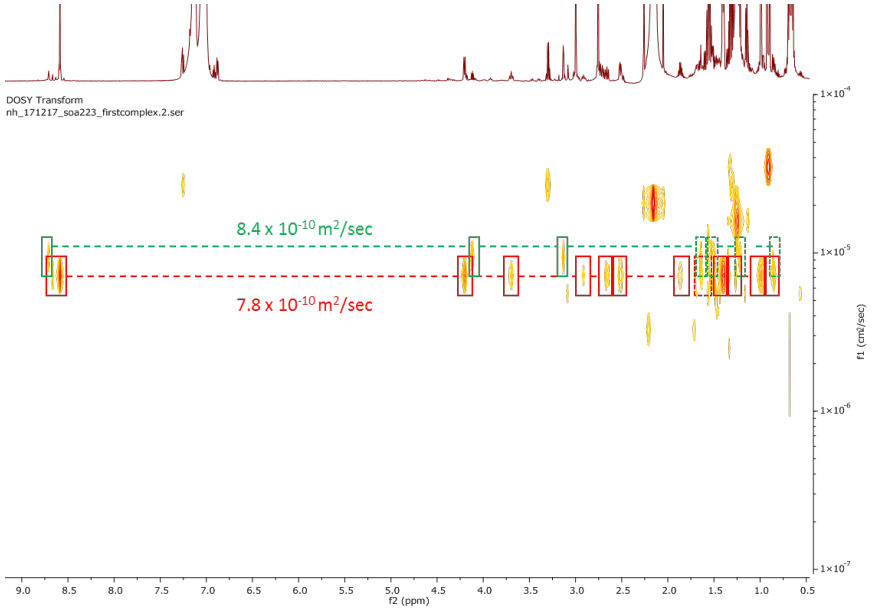


Figure S33. DOSY of zinc-initiator-product complex at 298K. [(*S*) initiator] = 9.3 mM, [Zn(*i*Pr)$_2$] = 98 mM. [prod] = 11.1 mM. Two initiator-product-zinc complexes seen, diffusivity = 8.46 x 10^{-10} m^2/sec (green) and 7.80 x 10^{-10} m^2/sec (red) Solution is 10% toluene in toluene-*d8*. Test ID: SOA223.

Figure S34. DOSY of zinc-initiator-product complex at 298K. [(*S*) initiator] =8.7 mM, [Zn(*i*Pr)$_2$] = 92 mM. [prod] = 21.4 mM. initiator-product-zinc complexes, diffusivity = 7.80 x 10^{-10} m^2/sec (red) and product tetramer complex: 5.54 x 10^{-9} m^2/sec (blue) Solution is 10% toluene in toluene-*d8*. Test ID: SOA223.

The intensity decay as a result of gradient strength can be used to determine the diffusivity (**D**, diffusion coefficient), via the Stejskal Tanner equation:[4]

$$I = I_0 e^{-D\,\gamma^2 g^2 \delta^2 \left(\Delta - \frac{\delta}{3}\right)}$$

where I = observed signal, I_0 = signal intensity in absence of gradient, D = diffusivity, γ = gyromagnetic ratio, g = gradient strength, δ = gradient duration, Δ = gradient delay before rephasing. Processing was performed within the MestreNova software, where *I* was determined via peak heights (with deconvolution).

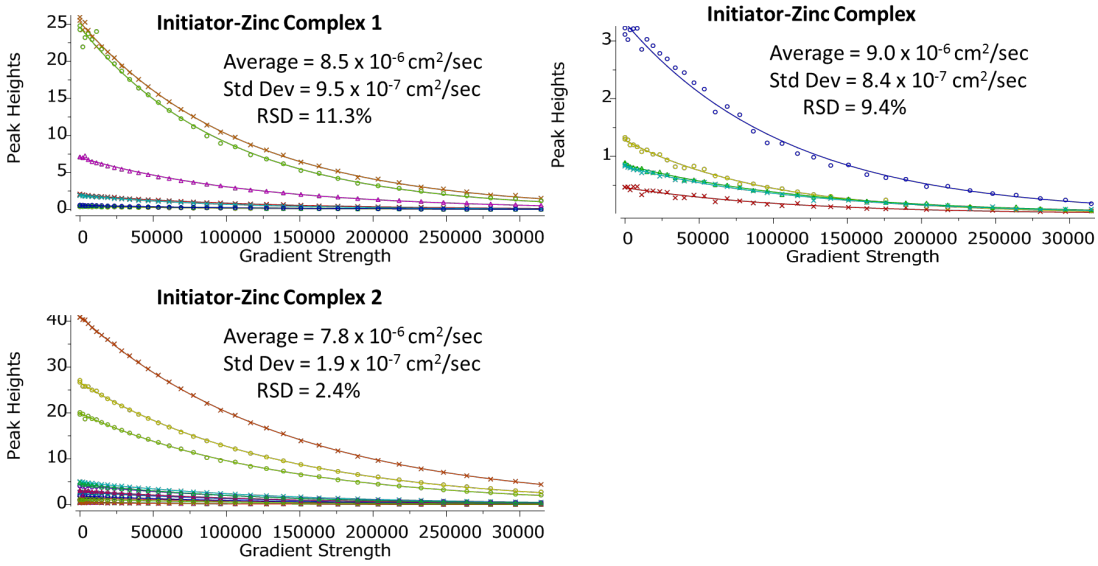


Figure S35. Diffusion curves from DOSY experiments. Each line represents the gradient dependent decay curve fit to the experimental data for a given peak. The average of all curve fits, as well as the standard deviation are given for each set complex with a similar diffusivity. (RSD = standard deviation/average).

The diffusivity can be used to roughly approximate the molecular weight. Broadly, the relationship between a D and the MW can be approximated by the equation:

$$D = c\,M^{-\alpha}$$

where D is the diffusivity (m^2/sec), M is the molecular weight (g/mol), and α represents the shape of the molecule (α = 1 for spherical, α = 1/3 for rod like molecules) and *c* is prefactor (like Stoke-Einstein, *c* depends on the viscosity and temperature of the system). A DOSY ladder[3] has been utilized previously to estimate the molecular weight of zinc complexes in the Soai reaction. We applied the same ladder ($c = 10^{-7.56}$, α = -0.56) from reference 3 to estimate the molecular weight of the unknown complexes from their diffusivities. The estimated molecular weights for toluene, $zn(ipr)_2$ and the product tetramer complex acted as an internal check for the validity of the approximation.

Table S14. Diffusion coefficients acquired from DOSY experiments and estimated molecular weights.

Complex	Diffusivity (cm^2/sec)	Diffusivity (m^2/sec)	Estimated MW	Actual MW
Toluene	2.07E-05	2.07E-09	104.71	92.14
Diisopropyl Zinc	1.59E-05	1.59E-09	167.72	151.57
Initiator Zinc Complex	9.00E-06	9.00E-10	463.36	-
Prod-Init-Zinc Complex 1	8.46E-06	8.46E-10	517.50	-
Prod-Init-Zinc Complex 2	7.80E-06	7.80E-10	598.27	-
Prod-Prod Tetramer	5.54E-06	5.54E-10	1102.12	1094.11

A reasonable molecular weight is predicted for the control compounds using the given DOSY ladder. From DFT calculations and NMR evidence, we anticipate a structure containing one initiator molecule coordinated to two products. A DOSY ladder of molecular weight vs. diffusivity was previously reported under identical conditions[3] and was used to determine the viability of this structure. The molecular weight of the proposed structure plotted against the experimental diffusivity fits nicely on the DOSY curve.

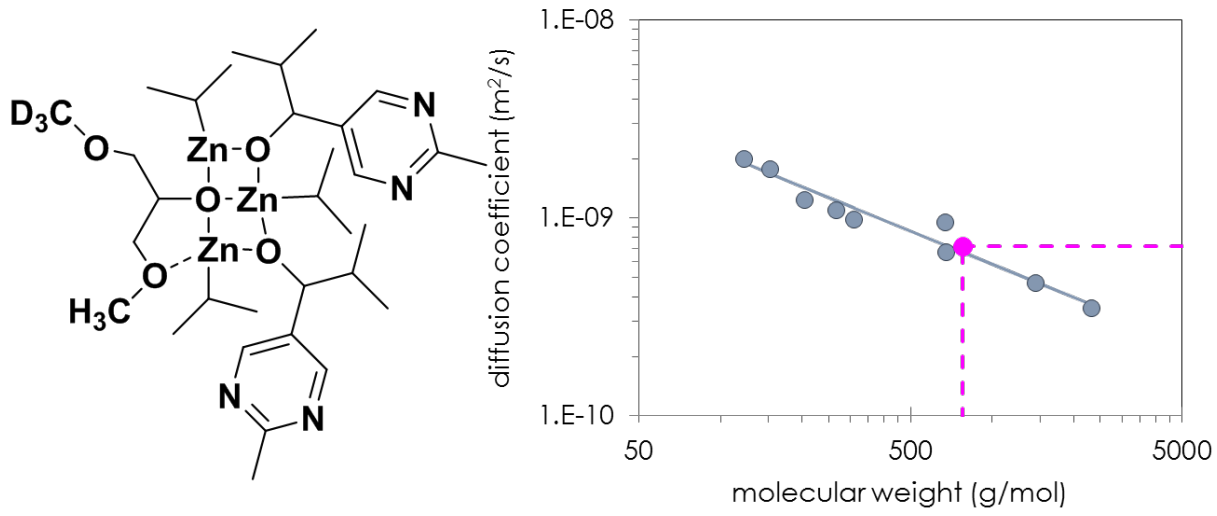


Figure S36. Proposed structure from DFT calculations (left), molecular weight estimation for prod-init-zinc complex 2 on DOSY previously reported DOSY ladder.

4. Kinetic Modeling using COPASI

A. General Methodology

Kinetic modeling was employed to determine the most viable mechanism for the reaction and estimate kinetic parameters for the reaction. This was done using the software COPASI.[5] Time course data from the LC analysis was fit to a variety of kinetic models. The COPASI software would attempt to determine the values of the kinetic constants needed to fit the time course data. This was done by starting at random values of the kinetic constants (typically between 1×10^{-6} and 1×10^{6} for each constant) and performing a particle swarm optimization to find a general fit by minimization of the variance between the model fit and the experimental data. Fit was refined using sequential Hookes and Jeeves optimizations until a minimum was reached.

The model was validated by using determined kinetic constants to predict plots of ee vs. conversion and normalized rate vs. [A] for a variety of initial conditions. These predicted plots were compared with the reaction calorimetry data (rate vs. [A]) or ee data (ee vs. conversion) that were performed under those initial conditions (Initial conditions being the starting concentrations $[A]_0$, $[X_L]_0$ and $[X_D]_0$).

B. Kinetic Model

In kinetic modeling, it is important to find a model which (a) accurately represents the observed experimental data and (b) accurately represents the possible chemistry occurring in the system and (c) contains no superfluous or kinetically irrelevant steps. While inclusion of many kinetic steps may assist in giving a seemingly good fit to the experimental data, it results in an underdetermined system in which the kinetic constants are nearly meaningless. Typically, in an underdetermined system, repeated fits from different initial conditions (i.e. different starting values of the kinetic constants) will lead to wildly different values for all the kinetic constants. A model must converge on similar values for some of the relevant kinetic constants (those involved in the rate determining or enantiodetermining processes). Moreover, the more experimental data used in the fit, the better the model will reflect the true kinetics of the system.

The model below was determined to be the most accurate representation of the system, considering the experimental data, literature precedent of Soai reaction kinetics,[6] and the spectroscopic data on hand. This model contains several key steps.

(1) A background reaction which both the L and D product monomers, X_L and X_D are formed at equal rates (k_1)
(2) Homochiral dimerization to form homochiral dimers Y_{LL} and Y_{DD} (K_2)
(3) Heterochiral dimerization to form an inactive dimer, Y_{LD} (K_3)
(4) Autocatalytic formation of the homochiral dimer from two aldehyde molecules, catalyzed by the homochiral dimer itself (k_4)
(5) Sequestration of two monomer species by the initiator to give an inactive 2:1 product: initiator complex (Z_{LL} and Z_{DL}), (K_5)

(6) First order reduction of the aldehyde by a zinc-hydride species to give the primary alcohol byproduct (k_6)

Previous studies[6] showed that the distribution of homochiral and heterochiral dimers is stochastic, so the system was constrained such that $2K_2 = K_3$. As in previous work, our data show zero order in diisopropyl zinc concentration. Since this reactant makes no impact on the observed reaction kinetics, diisopropyl zinc was not included in the model. Similarly, we observed ca. second order kinetics in aldehyde, which was simplified to one ternary elementary step ($2A + Y_{LL} \rightarrow 2Y_{LL}$) rather than two ($Y_{LL} + A \rightarrow D_{LL}$ $D_{LL} \rightarrow 2Y_{LL}$) to avoid superfluous inclusion of steps not kinetically relevant. Similarly, the spectroscopic evidence suggests a 2:1 product: initiator complex, which was represented in the step ($N_L + 2X_L \rightarrow Z_{LL}$). Thus, the final kinetic model is given below.

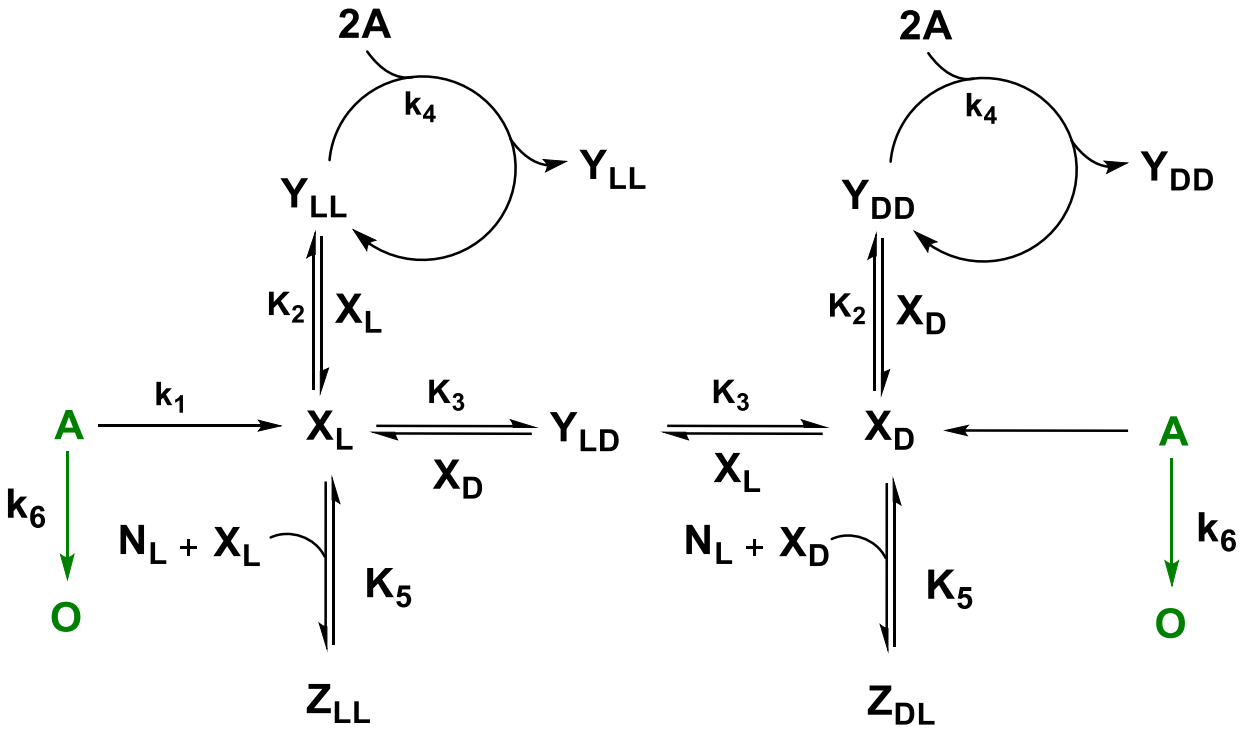


Figure S37. Minimal kinetic model giving accurate fits to experimental data. A = aldehyde, X_L and X_D = L and D product monomers, Y_{LL} and Y_{DD} = homochiral product dimers, Y_{LD} = heterochiral dimer, N_L = L initiator, O = reduction product, and Z_{LL} and Z_{DL} = initiator complexes. Constraint: $K_3 = 2K_2$.

C. Parameter Estimation Results

COPASI was used to fit a set of experimental data containing three levels of initiator. The data set contained a slight decrease in mass balance over the course of the reaction, likely due to formation of a second byproduct in addition to **4**, which was observed but was not identified or quantified. The primary alcohol byproduct only accounts for 48% of the missing mass balance. This results in an overestimation of the side products as a single species O, as the model attempts to account for the incomplete mass balance. The unaccounted for side product could possibly be an acetal species previously identified during Soai reaction induction periods.

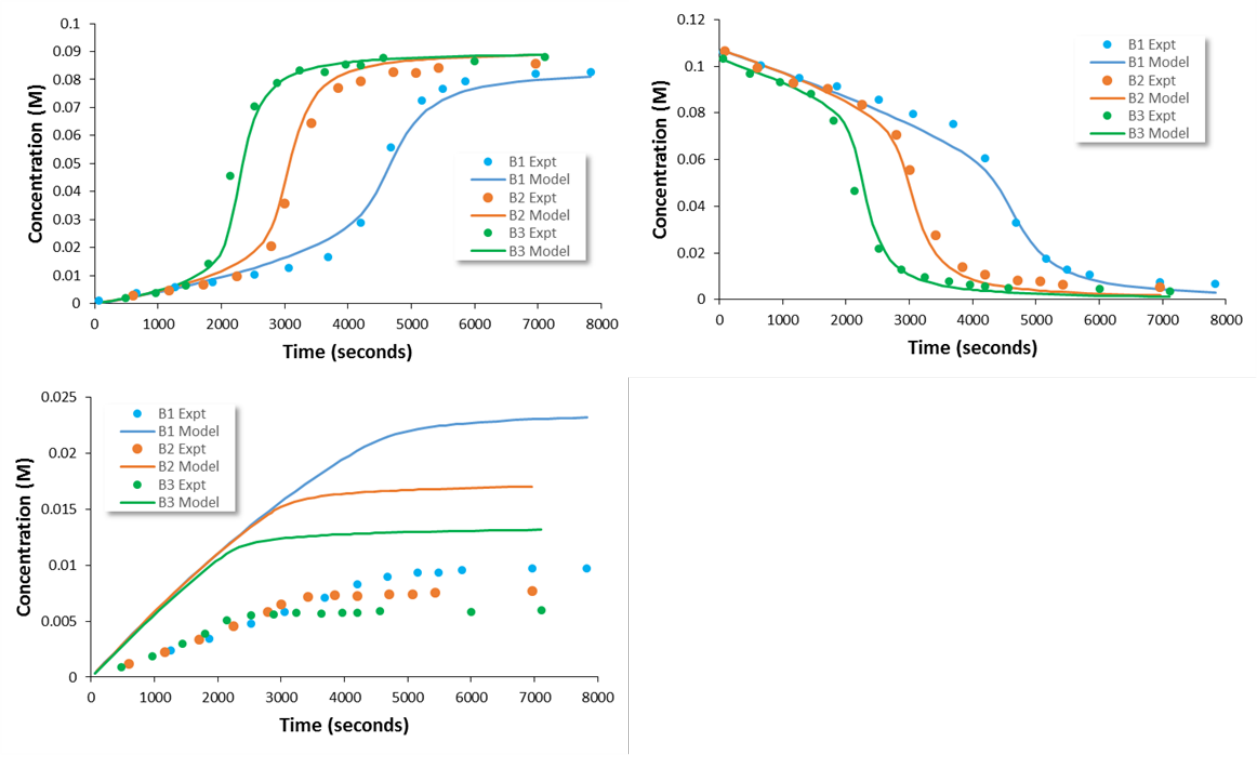


Figure S38. COPASI model fits (lines) compared to experimental data (lines). Data from page 14. [ald] = 115 mM, [Zn(*i*Pr)2] = 260 mM, [(*S*) initiator] = 15 mM (blue), 11 mM (orange) and 8 mM (green).

Table S15. Kinetic constants from COPASI parameter estimation fit

Entry	RMS Fit	k_1	K_{homo} (K_2)	k_{auto} (k_4)	K'_{homo} (K_5)	k_6
1	0.00366	1.68E-05	2.18E+07	3.81	5.48E+28	5.68E-05
2	0.00369	1.69E-05	2.72E+07	3.79	6.84E+28	5.63E-05
3	0.00326	1.17E-05	3.25E+07	3.12	8.21E+28	5.03E-05
4	0.00362	1.73E-05	4.25E+07	3.75	1.09E+29	5.62E-05
5	0.00362	1.54E-05	4.11E+07	3.73	1.09E+29	5.65E-05
AVERAGE		1.56E-05	3.30E+07	3.64E+00	8.48E+28	5.52E-05
STDEV		2.06E-06	7.96E+06	2.62E-01	2.19E+28	2.47E-06
RSD		13%	24%	7%	26%	4%

All values for the kinetic constants came close to converging, within an order of magnitude. The values of K_5 were much larger than K_2 throughout, suggesting that initiator binding is stronger than dimerization.

D. Validation of the Kinetic Model

These kinetic constants were then used to predict the results of another experimental data set, and the prediction was then compared the observed experimental results. Data was compared as rate vs. [A] (reaction calorimetry) and ee vs conversion (LC). Processing the data in this manner corrects for small, random changes in induction period during the reaction. The initial conditions used for the model prediction and the experiments are given below:

Table S16. Initial conditions for model validation

Condition	Description	Compare to	[A] (mM)	[B] (mM)	[cat] (mM)	ee_{cat}
1	17% ee - Low Zinc	189b2,189b3,190b3	57	112	2.8	16.5
2	17% ee - High Zinc	189b2,189b3,190b3	57	162	3.1	16.5
3	17% ee - High Ald	190b2	66	164	3.1	16.5
4	80% ee	191b2,b3	48	91	2.1	79.7
5	17% ee - Low Zinc	189b1,b4,190b1	61	114	2.8	16.5
6	17% ee - High Zinc	189b1,b4,190b1	61	165	3.1	16.5
7	17% ee - High Ald	190b4	77	164	3.1	16.5
8	80% ee	191b1,b4	50	90	2.2	79.7

The model predicted each of the data sets quite well, indicating that the model can provide an accurate representation of the reaction system, within this range of initial conditions. Interesting, no initiator was included in these validation sets, suggesting that the autocatalytic driving force operates identically in the presence and absence of the initiator. Thus, the initiator's role is simply to sequester monomer until a sufficient amount of autocatalyst forms. This suggests the autocatalytic process is governed by the same kinetic driving forces in the presence and absence of the initiator.

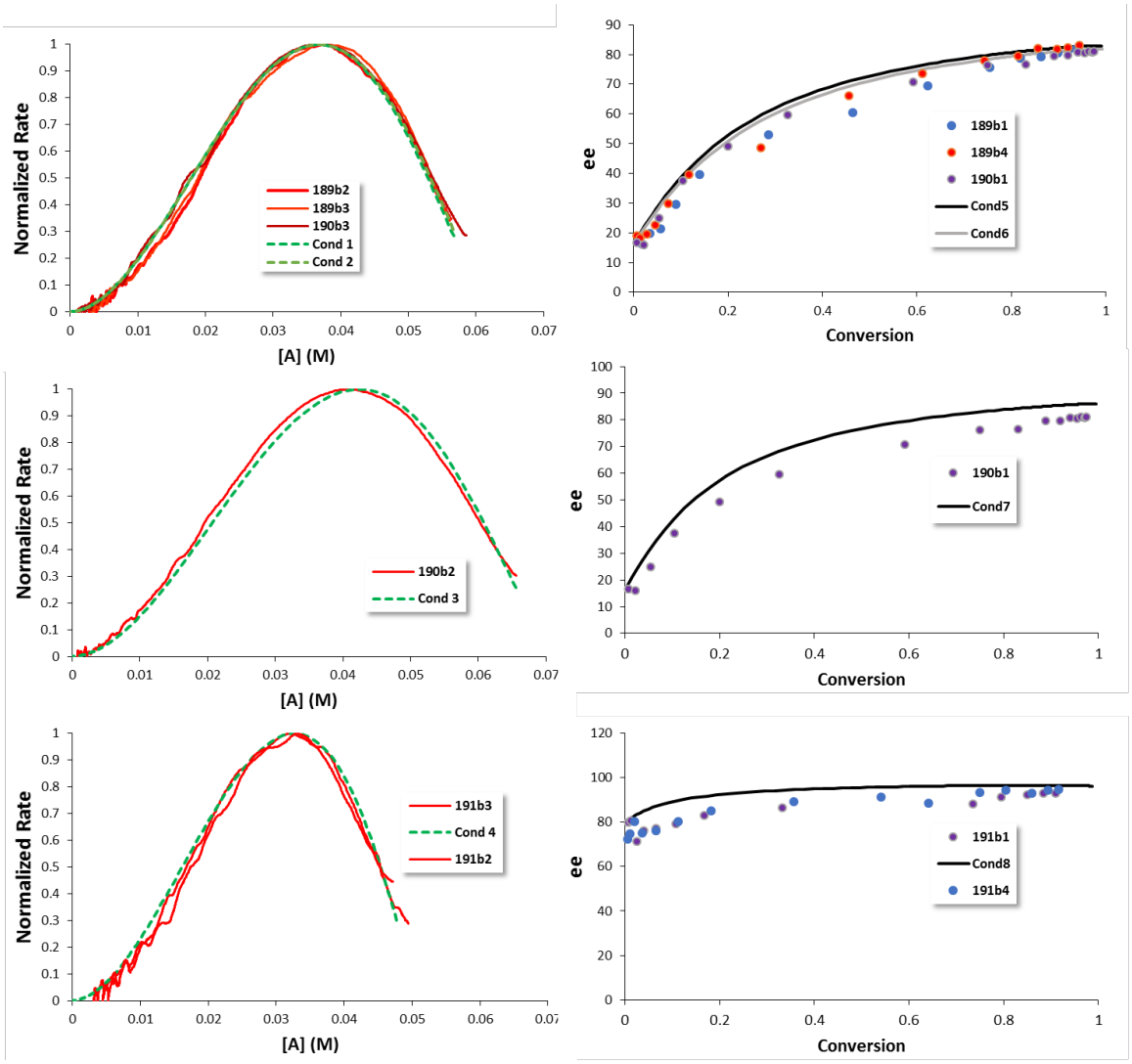
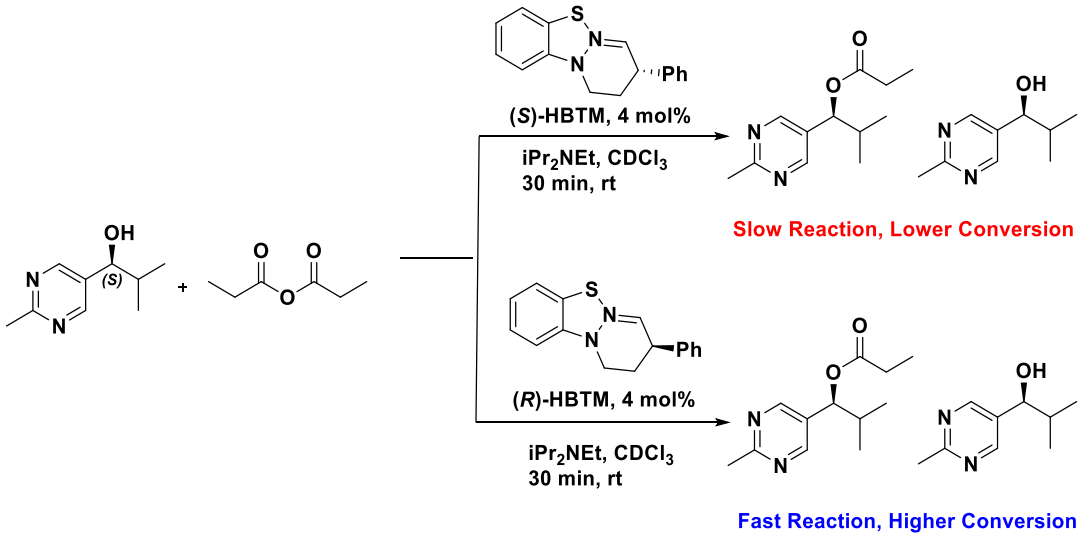


Figure 39. Experimental calorimetry data (left, solid red lines) compared to model prediction (green dashes). Experimental ee data (right, dots) vs. model prediction (solid lines). Kinetic constants from Table S15, fit 1 used for model estimation.

5. Calibration, Quantitation and Configuration

A. CEC Method for Absolute Configuration of Product



The competing enantioselective conversion (CEC method)[7] was used to determine the absolute configuration of the product. In this enantioselective reaction, the mismatched acylation of benzylic alcohols proceeds faster than the matched case. This allows for the relative conversions to be used to determine absolute conversion (given identical catalyst loadings and reaction times).

Competing reactions were setup between both hands of the product (unknown stereochemistry) and (*R*) and (*S*)-HBTM. A solution of alcohol (7.4 μmol), HBTM catalyst (0.3 μmol), diisopropylethylamine (22.3 μmol) was prepared in a 1.0 mL vial in $CDCl_3$ (100 μL total volume). Reaction was initiated by addition of three equivalents of propionic anhydride (22.2 μmol). After thirty minutes, the reaction was quenched with 50 μL of methanol-*d4*. $CDCl_3$ was added (0.5 mL) and crude mixture was analyzed by ^1H and ^{13}C NMR.

The relative rates of the reactions could be ascertained by integration of the benzylic CH proton (Alcohol: 4.3 ppm, Ester: 5.4 ppm).

Table S17. Results from CEC determination of absolute configuration.

Product Sample	HBTM Chirality	SM Integration	Product Integration	Conv	Rate	Assignment
A	R	5.35	1	15.7%	Slow	R
A	S	1.04	1	49.0%	Fast	R
B	R	1.06	1	48.5%	Fast	S
B	S	6.60	1	13.2%	Slow	S

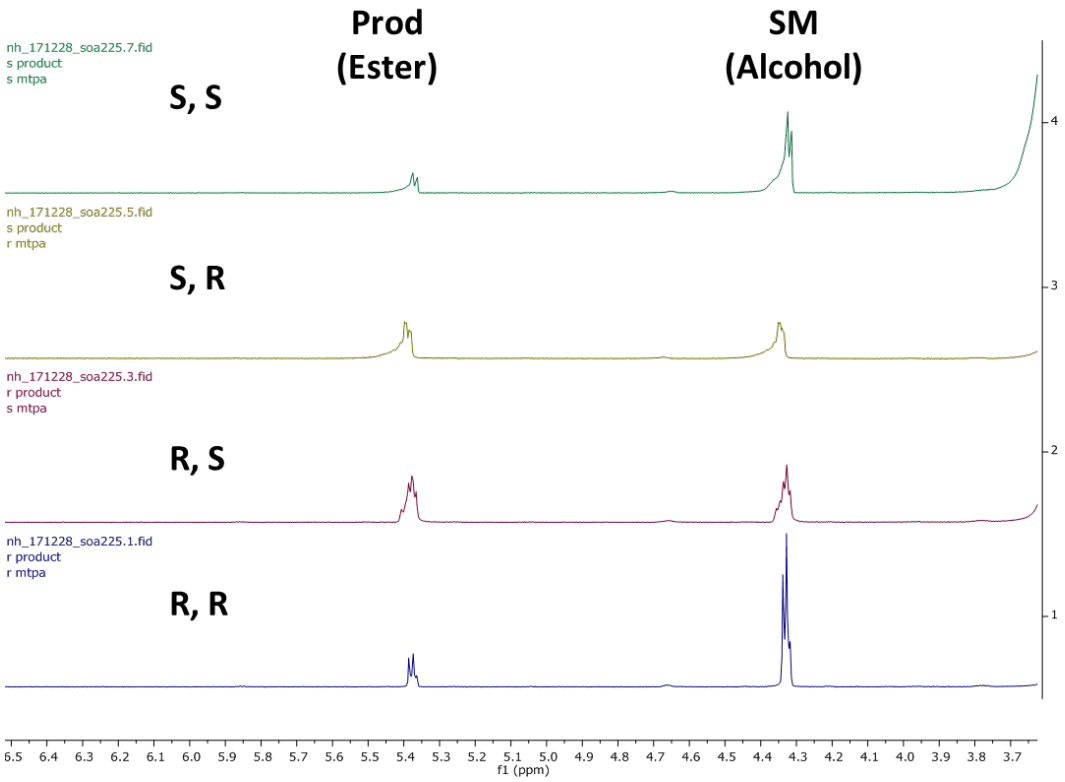
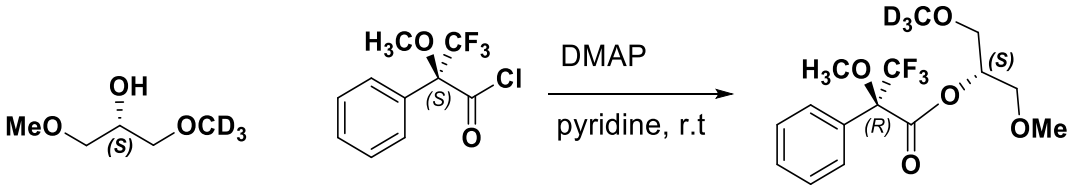


Figure S40. ^{1}H NMR of the benzylic proton in the CEC determination of absolute configuration. Conversion determined by relative integrations. Poor shimming resulted from an overly concentrated sample, but does not largely influence quantitation Test ID: SOA225.

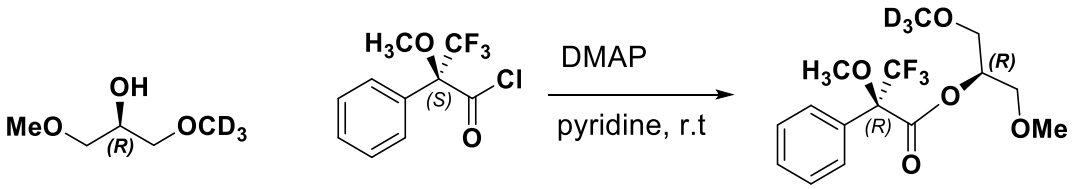
B. Mosher's Assay for Determination of Initiator ee

(*S*)-1-methoxy-3-(methoxy-*d3*)propan-2-yl (*R*)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate



Enantiomeric excess of the (*S*) hand of the initiator was determined using the Mosher's assay. (*S*) initiator (0.11 mmol, 55mM) was added to an argon flushed vial containing *N,N*-dimethylaminopyridine (DMAP, 0.02 mmol, 10 mM) in 2.0 mL of pyridine (dried over KOH and distilled). (*S*)-MTPA-Cl (0.27mmol, 0.14M) was added to the reaction mixture and the solution was stirred overnight at room temperature for 12 hours. Reaction mixture was checked by TLC to ensure consumption of starting material (via I_2 stain). Pyridine was removed in-*vacuo* and the crude mixture was dissolved in $CDCl_3$ for analysis by NMR.
Enantiomeric excess was determined by relative integration of the OCH_3 proton at 3.30 ppm ((*S*) initiator adduct) and 3.39 ppm ((*R*) initiator adduct). Final enantiomeric excess was 97.8% ee.

(*R*)-1-methoxy-3-(methoxy-*d3*)propan-2-yl (*R*)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate



Enantiomeric excess of the (*R*) hand of the initiator was determined using the Mosher's assay. (*R*) initiator (0.13 mmol, 63mM) was added to an argon flushed vial containing *N,N*-dimethylaminopyridine (DMAP, 0.02 mmol, 10 mM) in 2.0 mL of pyridine (dried over KOH and distilled). (*S*)-MTPA-Cl (0.33mmol, 0.16M) was added to the reaction mixture and the solution was stirred overnight at room temperature for 12 hours. Reaction mixture was checked by TLC to ensure consumption of starting material (via I_2 stain). Pyridine was removed in-*vacuo* and the crude mixture was dissolved in $CDCl_3$ for analysis by NMR.

Enantiomeric excess was determined by relative integration of the OCH_3 proton at 3.30 ppm ((*S*) initiator adduct) and 3.39 ppm ((*R*) initiator adduct). Final enantiomeric excess was 98.0% ee.

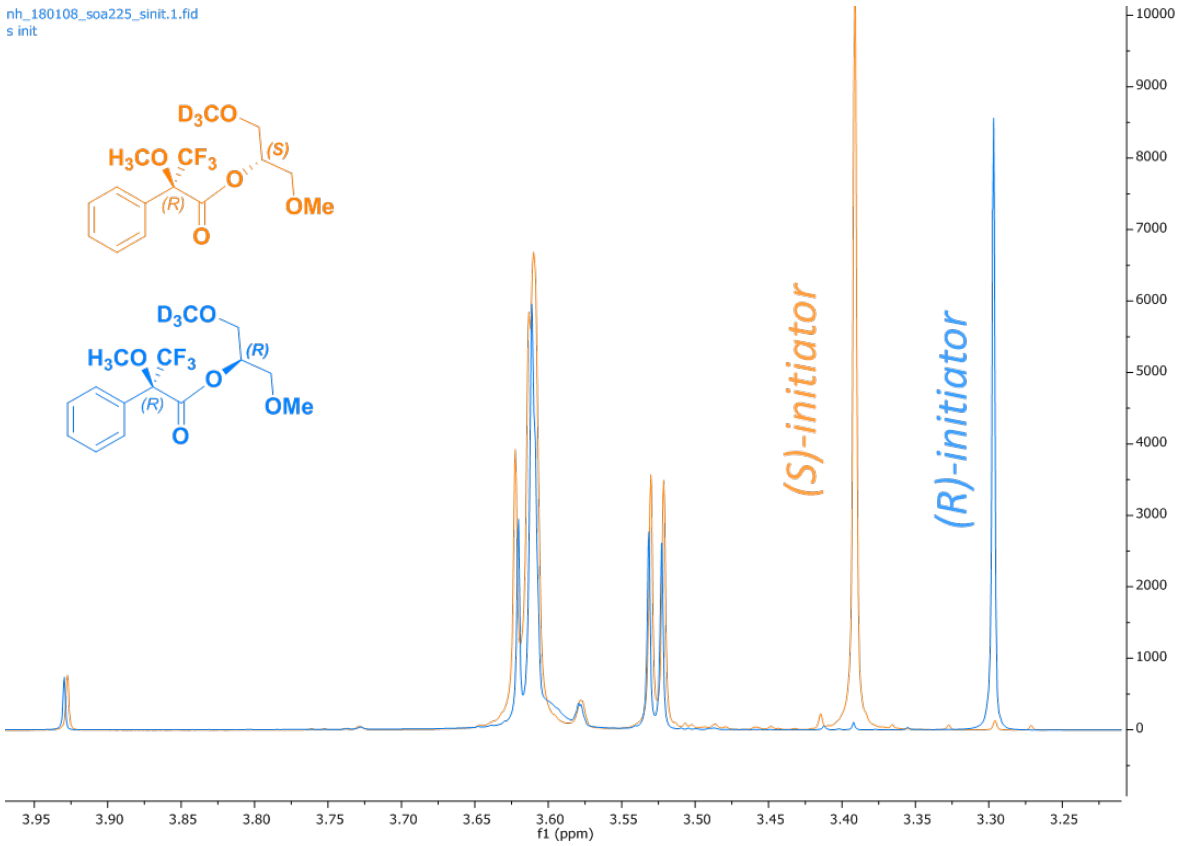


Figure S41. Mosher assay for determination of enantiomeric excess. ^{1}H NMR from crude reaction mixture for the (*S*)-MTPA-(*R*) initiator adduct (blue) and (*S*)-MTPA-(*S*) initiator adduct (orange).

C. LC Calibration for Quantitative Analysis

A calibration curve was established to quantify the [aldehyde], [product] and [reduction byproduct] in the quenched aliquot mixtures. Standard injection was performed at 5 µL and area was determined by integration at 254 nm. If the area was greater than the range of the calibration curve, sample was rerun and quantified using a 2 µL injection. Calibrations curves are given below.

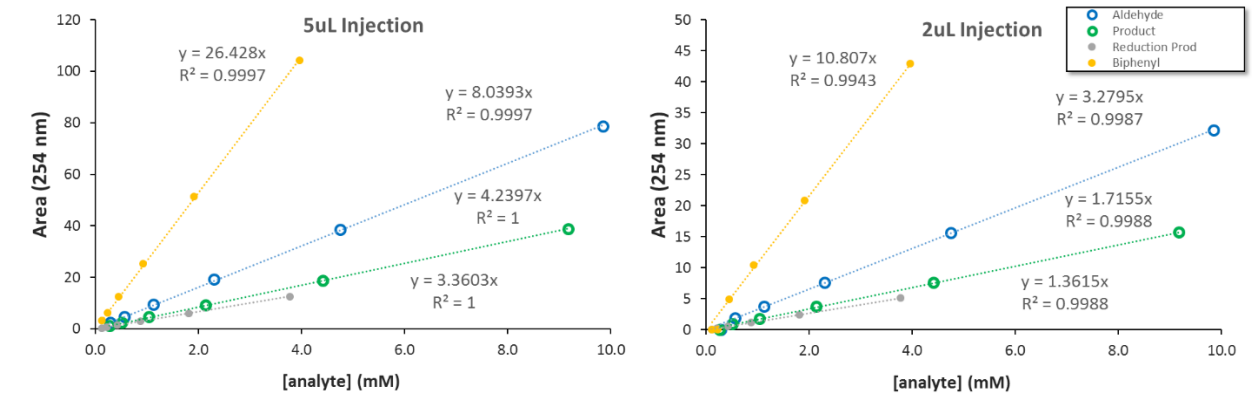


Figure S42. LC calibration curves for biphenyl (yellow), aldehyde (blue), product (green) and reduction product (grey) at 5 µL (left) and 2 µL (right). Areas taken at 254 nm.

Area was converted to concentration via the calibration curve. The concentration of the internal standard (biphenyl) was used to determine a dilution factor via the following equation:

$$DF = \frac{[IS]_{reaction}}{[IS]_{aliquot}}$$

where $[IS]_{reaction}$ is the gravimetrically determined concentration of biphenyl in the reaction mixture and $[IS]_{aliquot}$ is the [biphenyl] in the aliquot (determined via LC). The concentration of analyte was determined using this dilution factor and the aliquot concentration.

$$[Product]_{reaction} = DF * [Product]_{aliquot}$$

where DF is the dilution factor and $[Product]_{aliquot}$ is the aliquot concentration determined by LC.

D. Reaction Calorimetry Data Analysis

Data Processing. All data obtained from reaction calorimetry was Tau corrected within the Insight software by Omnical. Data was baseline corrected linearly. Following baseline correction, three operations were performed: heat of mixing removal, determination of rate, and determination of conversion profiles.

Heat of mixing (HOM) removal can be performed in three different ways, via removal of a standard curve, extension of a zero-order regime, or addition of a standard slope. The most common method is via subtraction of a heat of mixing curve, collected under experimentally identical conditions. This typically works well for systems close to room temperature which use small injection volumes. Systems which have variation in their heat of mixing due to differences in syringe temperature at time of injection may need to be scaled to fit each experimental set. This typically occurs for very high or low temperature reactions.

For systems where this is difficult or not possible, the initial slope following the heat of mixing may be mimicked and traced back to the origin. Alternatively, systems which contain a zero-order induction period can be treated by adding a horizontal line back to the origin. The best method for HOM can be determined by comparison of the post-processed data to the secondary data collected using aliquots couple with NMR analysis, LC, or GC analysis. The impact of heat of mixing is minimal in systems with an induction period or low injection volumes. Examples of heat of mixing removal methods and their influence on the final processed data are provided in Fig. S43.

After heat of mixing correction, the conversion data can be acquired by integration of the spectra (units of mW*min). This area is determined by the trapezoid law: $0.5(q_2 - q_1)(t_2 - t_1)$ where q_1 is the heat at time point 1 (t_1) and q_2 is the heat at the later time point 2 (t_2). Summing the area of these trapezoids over the course of the run will give the cumulative area. The fraction conversion (at a given time t) is determined by dividing the cumulative area at time t over the maximum area. This should be normalized if the final conversion is not 100%. Multiplying fraction conversion by $[Product]_0$ or (1- fraction conversion) by $[SM]_0$ will give the concentration vs. time plots for the product and starting material respectively (assuming mass balance is maintained). The total heat output of the reaction can be determined by using the maximum area (cumulative area at t_{final} in mW*min). Enthalpy can then be calculated from the equation below.

$$Heat\ Output\ (Q, kJ) = \frac{60 * A_{max}}{(1 * 10^6)}$$

$$\Delta H\ (kCal/mol) = \frac{Q}{4{,}184 * m * c}$$

where Q is total heat (kJ), A_{max} is the maximum cumulative area (mW*min), m is the mmol of substrate converted (for 100% conversion) and c is the fraction conversion attained (0 to 1). Heat versus time data can be converted into rate versus time by the following equation:

$$rate\ (mM/min) = \frac{60 * q}{V\ (\Delta H)}$$

where q = heat from calorimeter (mW), V is the vial volume (L) and ΔH is the reaction enthalpy (mJ/mol).

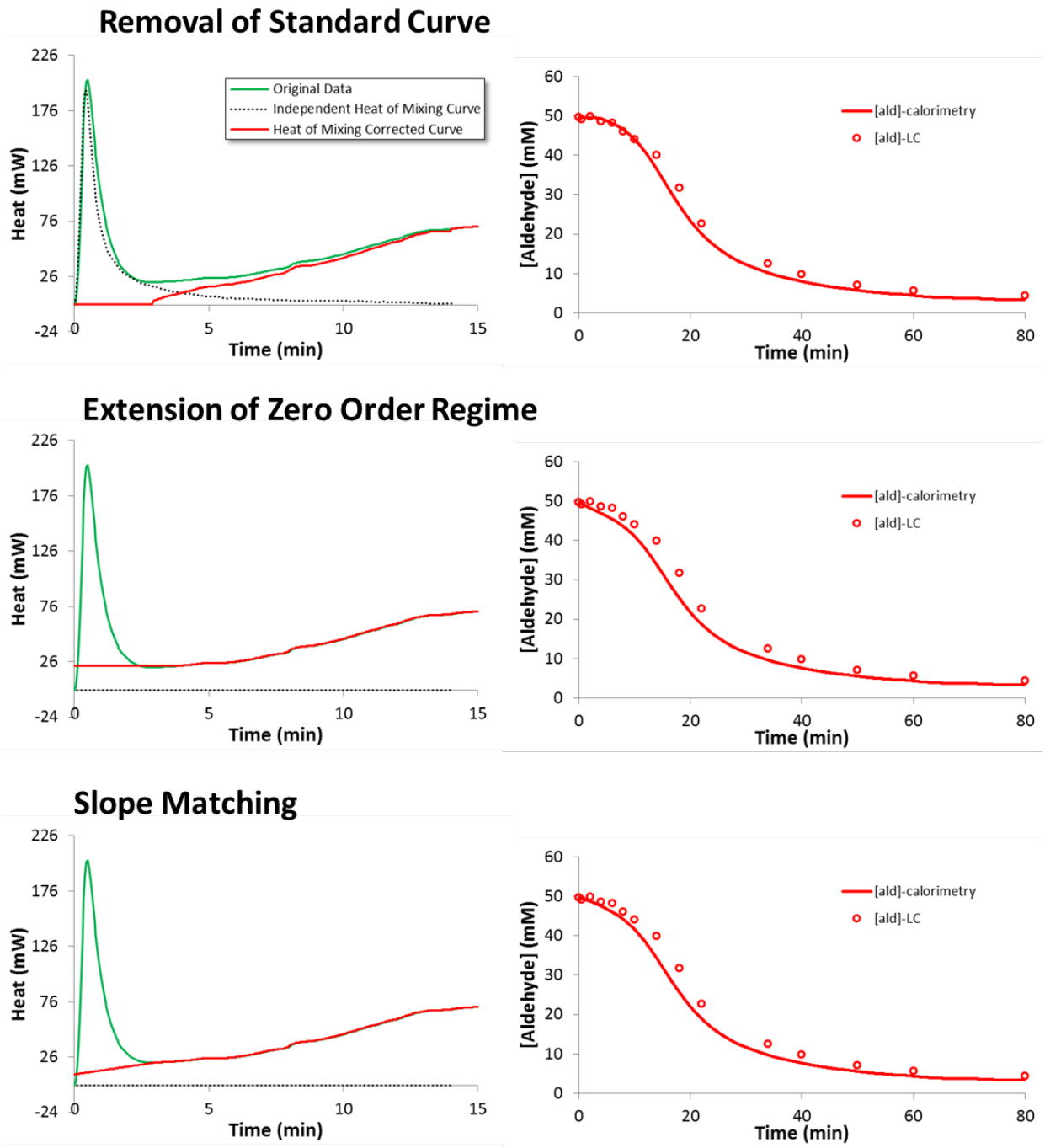


Figure S43. (left) Types of heat of mixing removal. Initial data set is given in green and post processed heat of mixing data given in red. (right) Comparison of post processed data for each HOM correction. Reaction calorimetry data shown in red lines, LC validation data shown as red circles.

Data Validation. To ensure that the heat produced by the reaction properly reflects the productive reaction taking place, validation runs must be performed to ensure that predicted conversion from the reaction calorimetry data matches the true conversion seen. In this case, the calorimetry data was compared to aliquot data under identical conditions, both in the presence and absence of the initiator. Validation data given below:

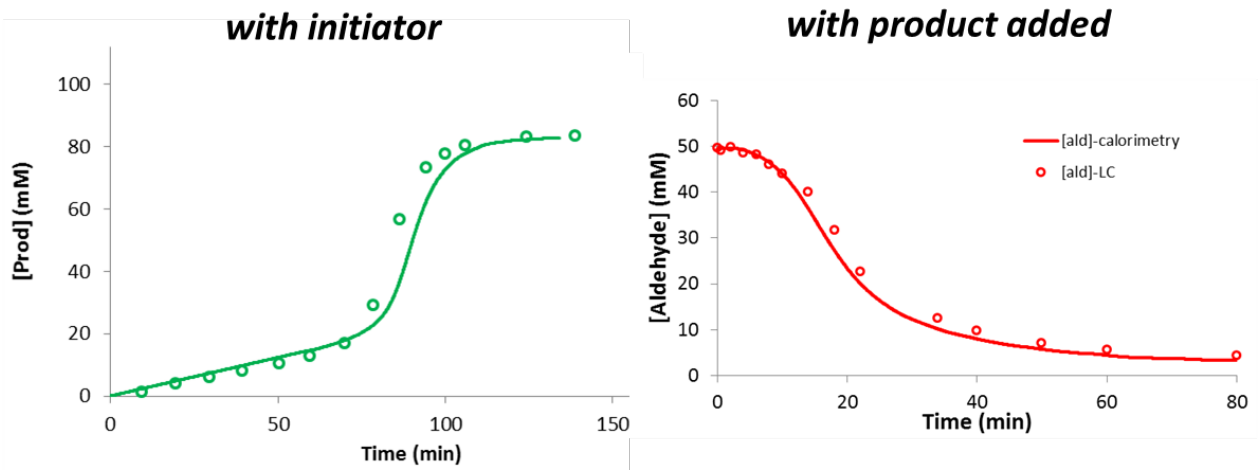
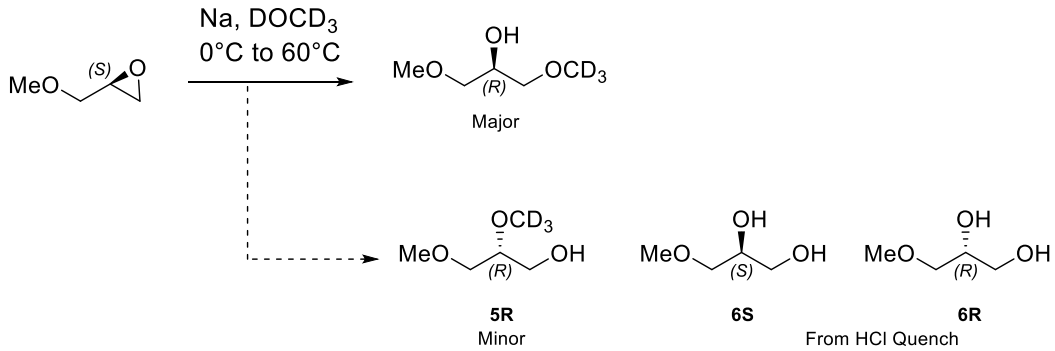


Figure S44. Reaction calorimetry data vs. LC for a reaction containing $[Ald]_0$ = 110 mM, $[zn(ipr)_2]$ = 260 mM, [initiator] = 17 mM (left) and $[Ald]_0$ = 50 mM, $[zn(ipr)_2]$ = 90 mM, [product] = 2.1 mM ee_{prod} = 79.7%. One calorimeter vial was left untouched, which aliquots were taken from a second vial and analyzed by LC.

E. Purity Assessment of Initiator

Particularly in symmetry breaking experiments, it is necessary to ensure that chiral induction is occurring using the desired isotopomers, not through the action of a minor byproduct. The synthesis of the isotopic chiral trigger in this study has the potential for formation of two chiral byproducts. Epoxide opening from the disfavored position will yield the undesired primary alcohol, **5.** Moreover, premature quenching of the reaction with HCl will yield the enantiomeric diols **6R** and **6S**.



While careful control of the synthesis and rigorous purification (total of 3 distillations and 1 chromatography column) were employed to minimize contamination with any of these byproducts, it is important to verify the absolute purity of the synthesized material analytically. Qualitatively, the NMR spectra of the initiator looks very clean.

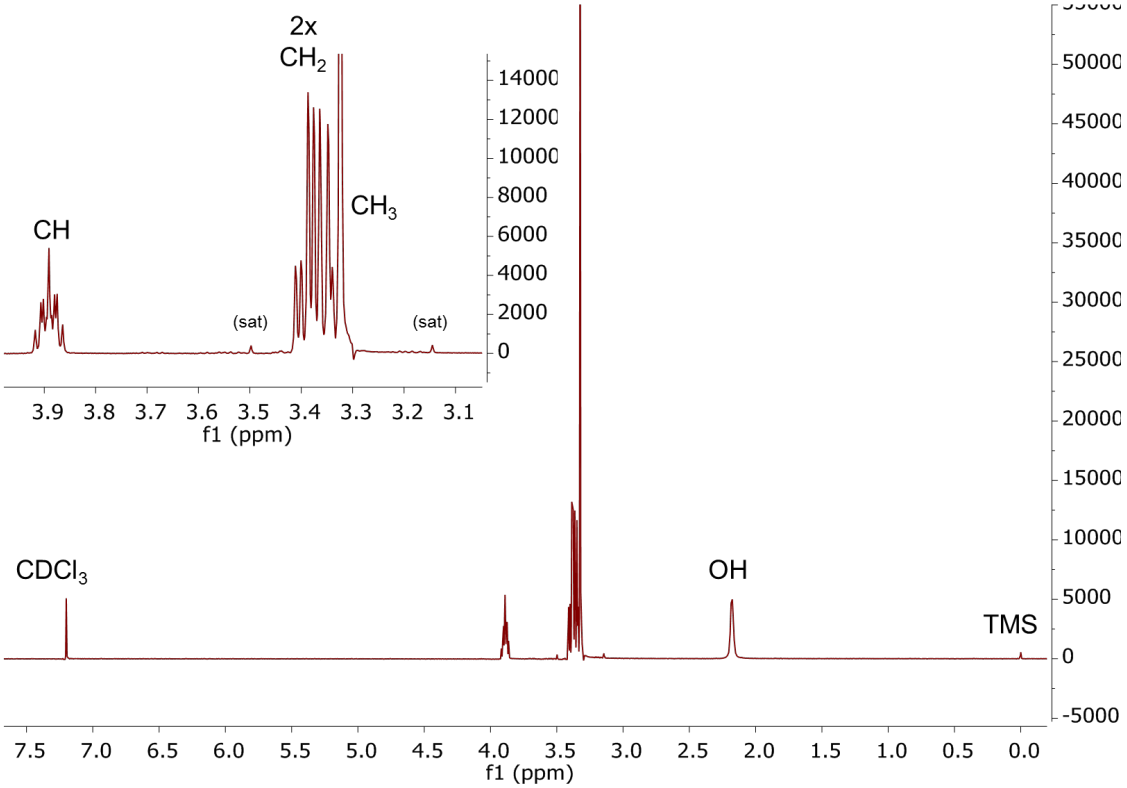


Figure S45. NMR spectra of the racemic initiator after purification. In $CDCl_3$ with TMS added.

Attempts at quantitative NMR vs. an internal standard (trimethoxybenzene) confirmed ~100% purity, but replicates of the Q-NMR studies revealed a variation of ± 5% due to weighing errors, baseline correction, integral selection, shimming, ect.

As QNMR was not ideal for the detection of minor impurities, GC-FID was employed. Commercial registries reported boiling points of 168°C, 180°C, and 220°C for the CH_3 analogs of major, minor, and diol products respectively. This suggests facile separation and detection of product purity by gas chromatography. GC-FID showed some small impurities at 1% or less in the reaction mixture. These impurities are insignificant, and likely do not influence the reaction kinetics or NMR studies. The GC chromatograms are provided below.

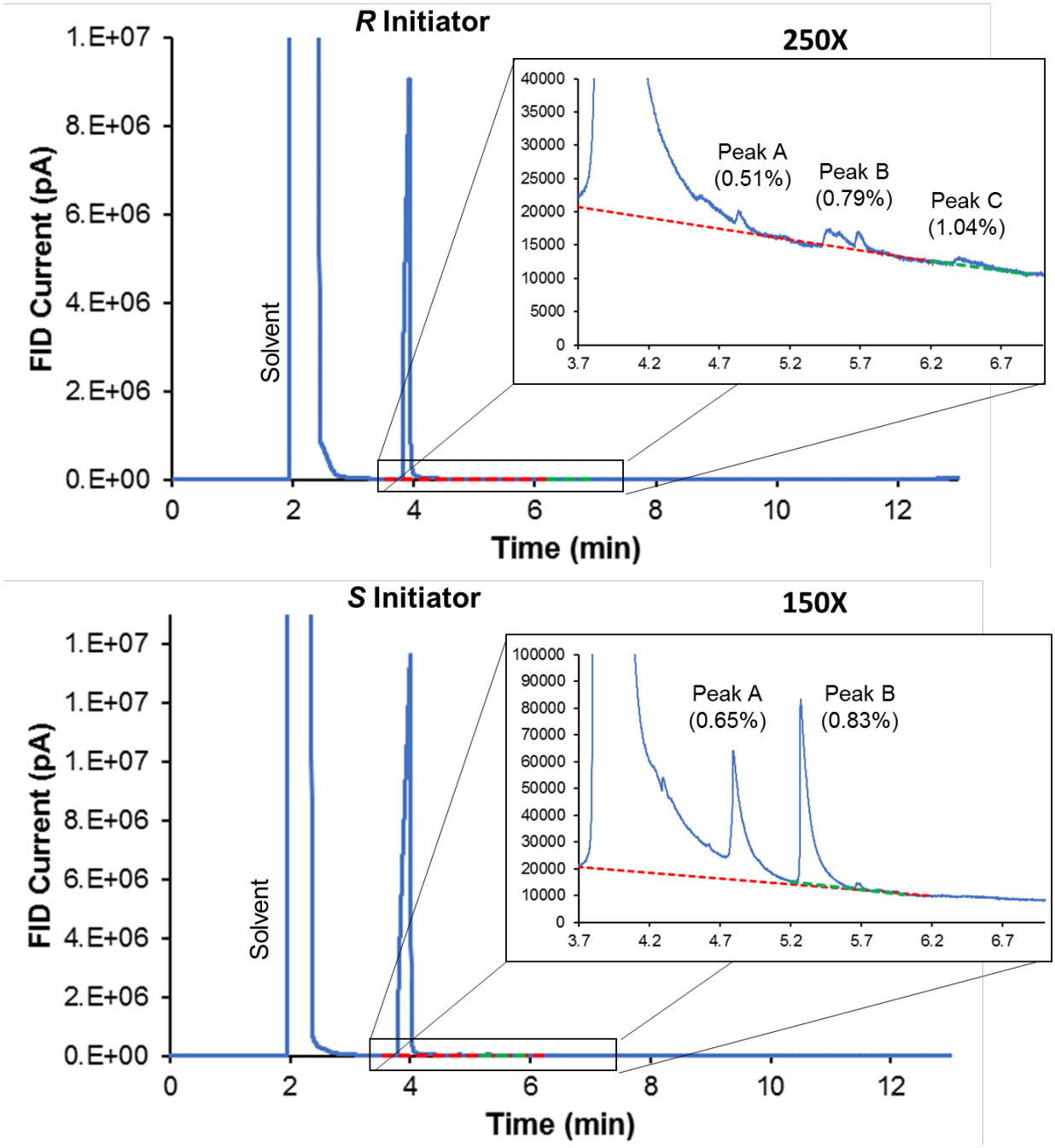


Figure S46. GC-FID chromatograms of the initiator (3.9 min) and associated impurities. (top) R initiator (bottom) S initiator.

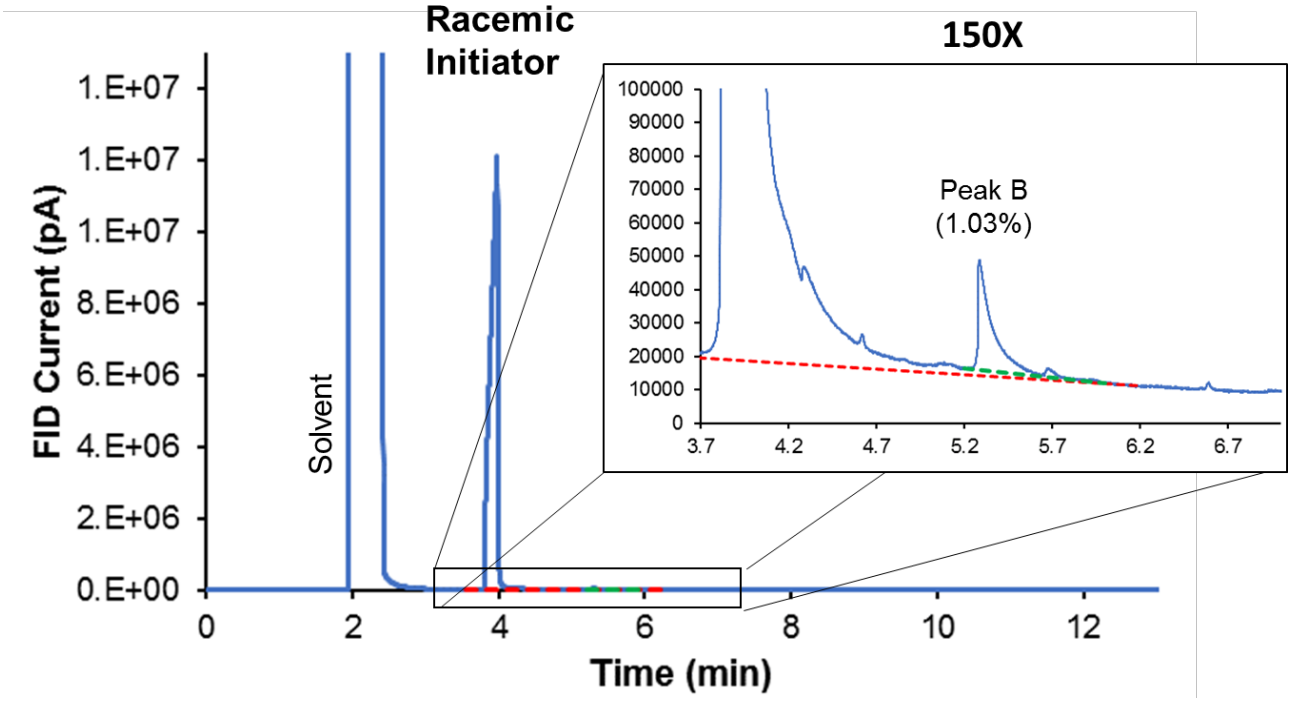


Figure S47. GC-FID chromatograms of the racemic initiator (3.9 min) and associated impurities.

6. Spectra

A. 2D NMR Assignments of Zinc-Initiator Complexes

General Methodology. 2D NMR spectroscopy was used to assign peaks for the zinc-initiator complex and zinc-initiator-product complexes. These studies were also aimed towards discerning the structure of the zinc-initiator bound complexes, and to corroborate results from DOSY spectroscopy by demonstrating that initiator and product peaks exhibited identical diffusion coefficients. This provides evidence that the change in chemical shift resulting from product addition is indeed due to formation of a zinc-initiator complex. Product was titrated in at 0°C until one structure predominated in the ^{2}H NMR spectrum. Following this, ^{1}H, ^{2}H, ^{13}C, COSY, HSQC and HMBC spectra were acquired of the resulting complex at 0°C.

Peak assignments are indicated on each spectrum using the following legend: triangles represent peaks associated with the product, squares represent peaks associated with the initiator, and circles represent peaks associated with the isopropyl group associated with a zinc alkoxide. The color scheme represents these location on molecule

For Product:

Red = Benzylic CH_3 and associated carbon
Blue = Aromatic CH and associated carbon
Unfilled Blue Triangle = Aromatic quaternary carbons
Black = Benzylic CH and associated carbon
Orange = Isopropyl CH and associated carbon
Purple = Isopropyl CH_3 and associated carbon

For initiator

Black = CH_2 and associated carbon
Red = CH_3 and associated carbon
Green = CH and associated carbon

For zinc alkoxide

Purple = Isopropyl CH_3 and associated carbon
Black = Isopropyl CH and associated carbon

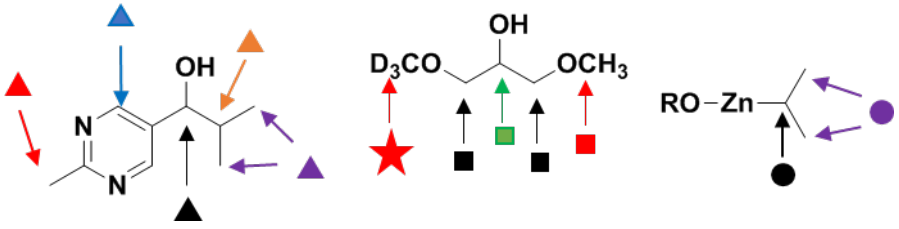


Figure S48. Legend for Peak Assignments in 2D NMR experiments.

2D Spectra of Zinc Initiator Complex. A zinc-initiator complex was formed via addition of (*S*) initiator solution (70 mM final concentration) into a solution containing diisopropylzinc (0.7M) in a toluene/toluene-*d8* (9:2) mixture. ^{1}H, ^{2}H, ^{13}C, COSY, HSQC and HMBC spectra were taken of the resulting mixture and are provided below. Three different chemical species are seen in the ^{1}H, ^{2}H and ^{13}C NMR.

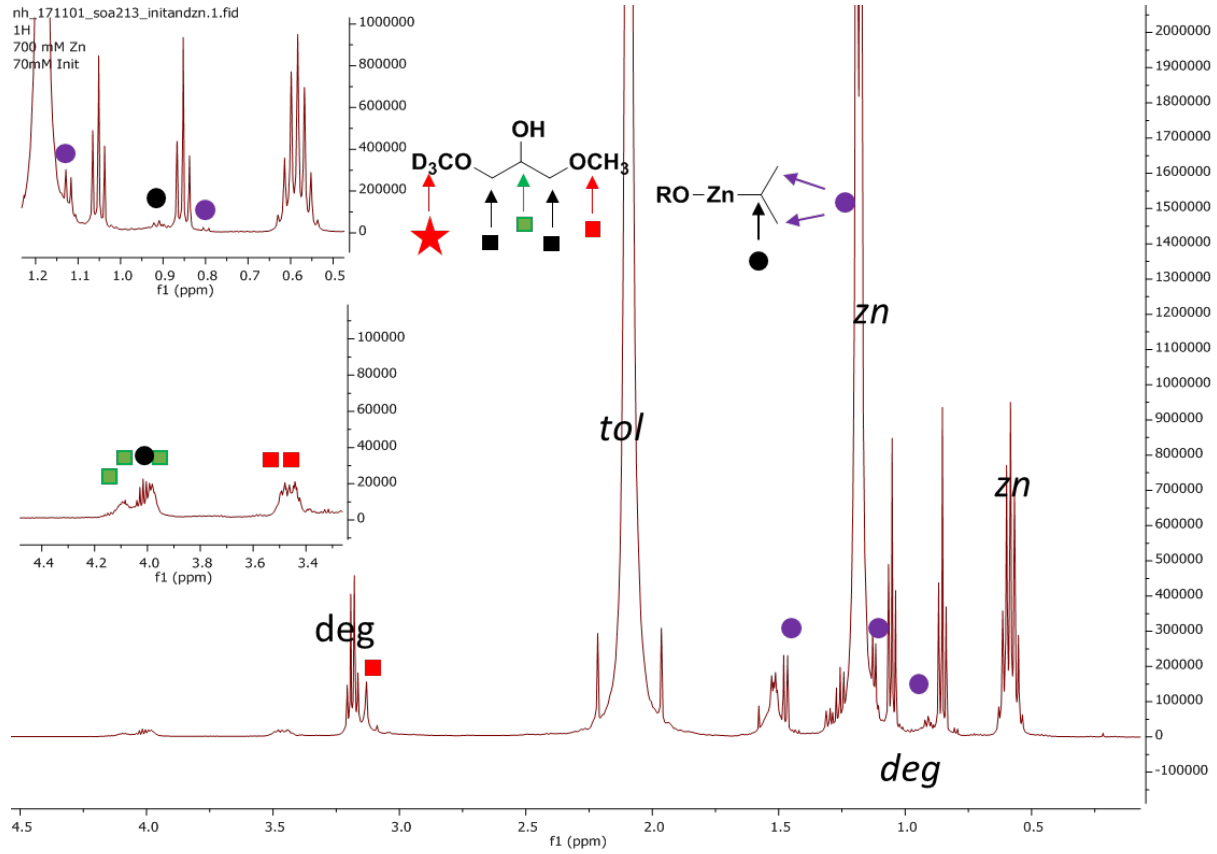


Figure S49. ^{1}H NMR of 70mM (*S*) initiator in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). "deg" denotes formation of the zinc-alkoxide species when zn(ipr)$_2$ is exposed to air. "zn "denotes zn(ipr)$_2$.

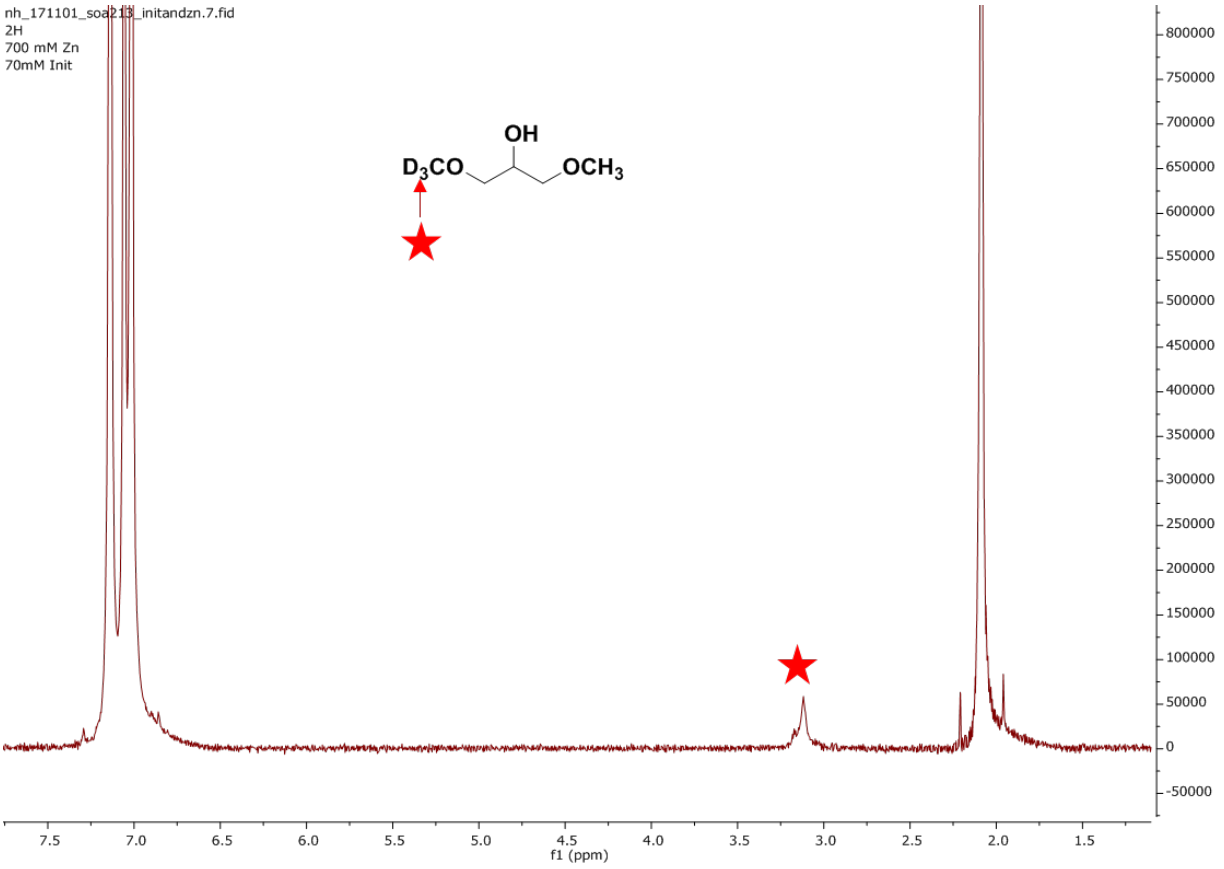


Figure S50. ^{2}H NMR of 70mM (*S*) initiator in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2).

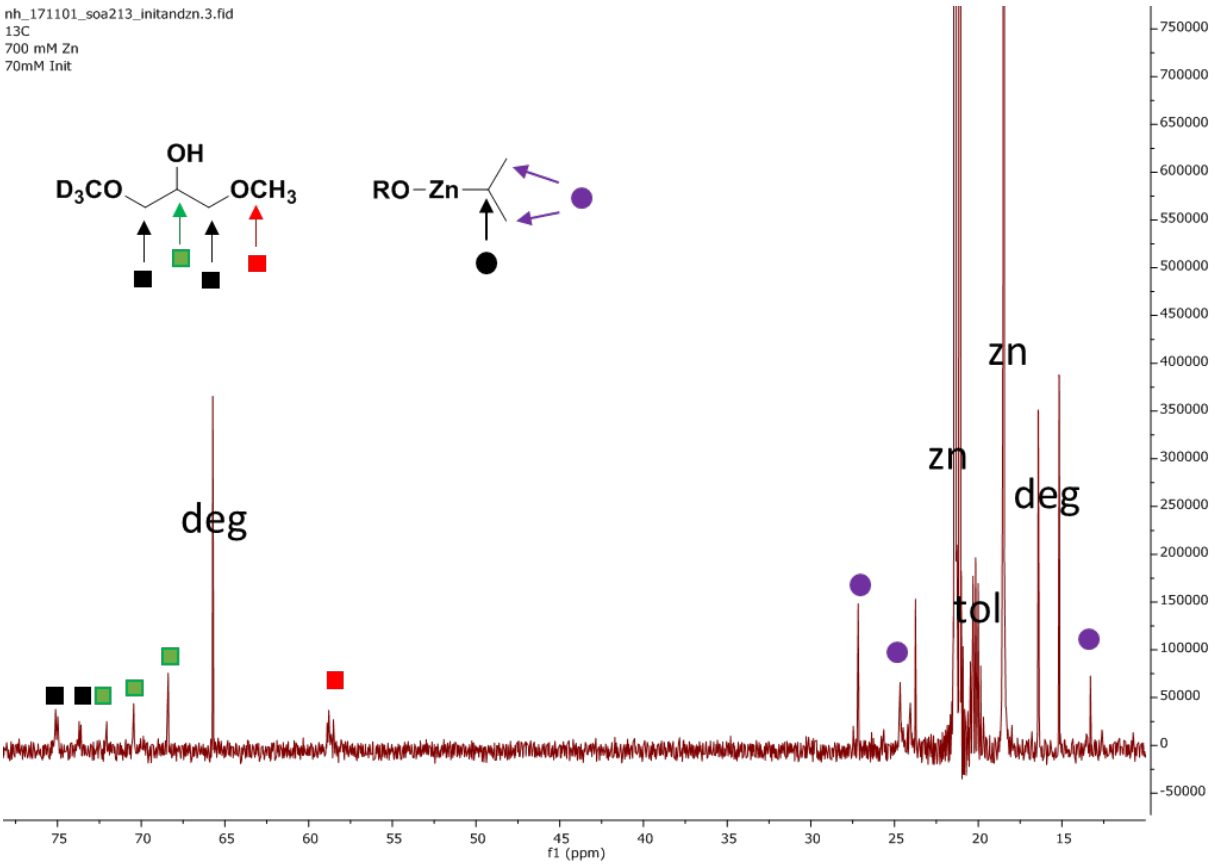


Figure S51. ^{13}C NMR of 70mM (*S*) initiator in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). "deg" denotes formation of the zinc-alkoxide species when zn(ipr)$_2$ is exposed to air. "zn "denotes zn(ipr)$_2$

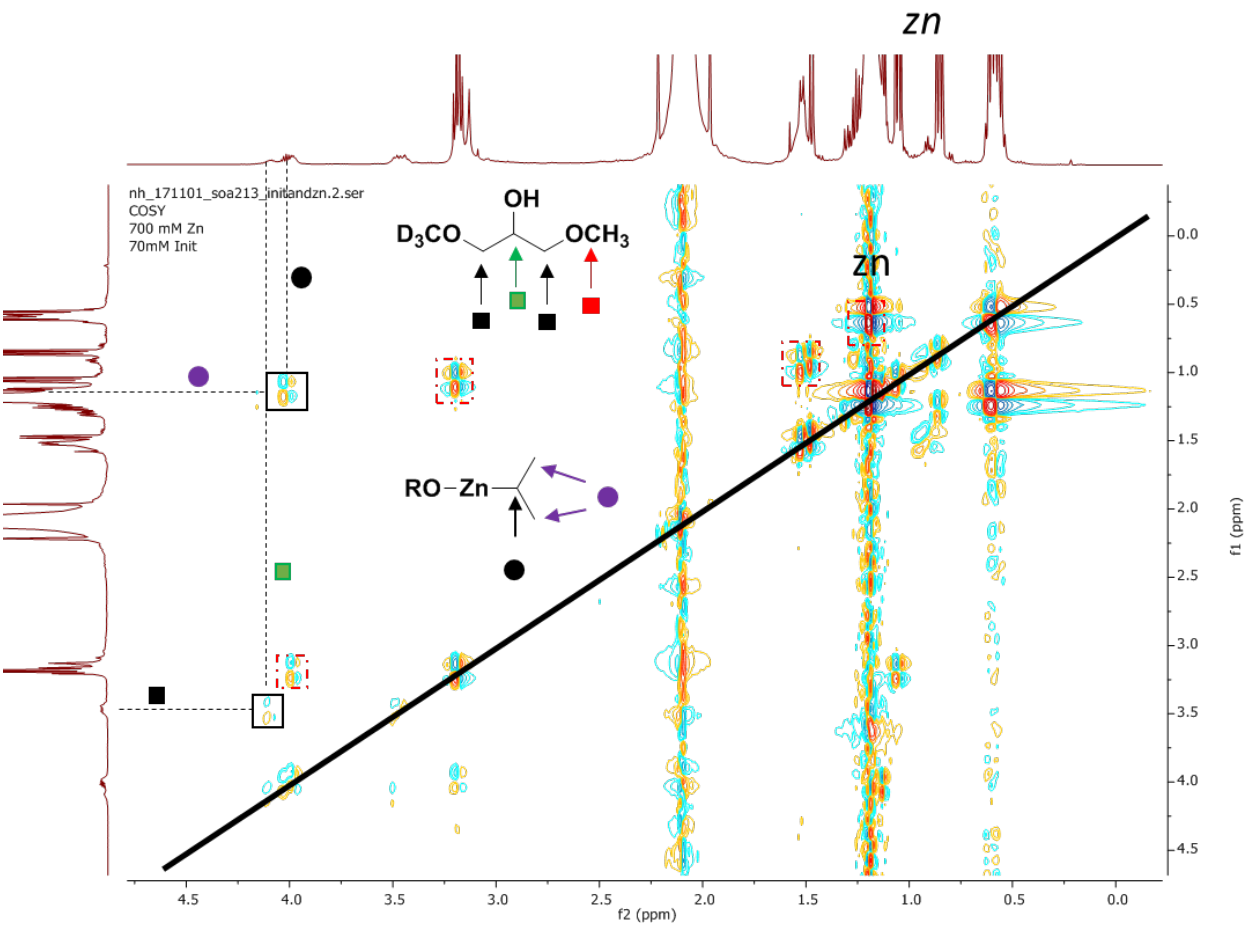


Figure S52. COSY Spectra of 70mM (*S*) initiator in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air.

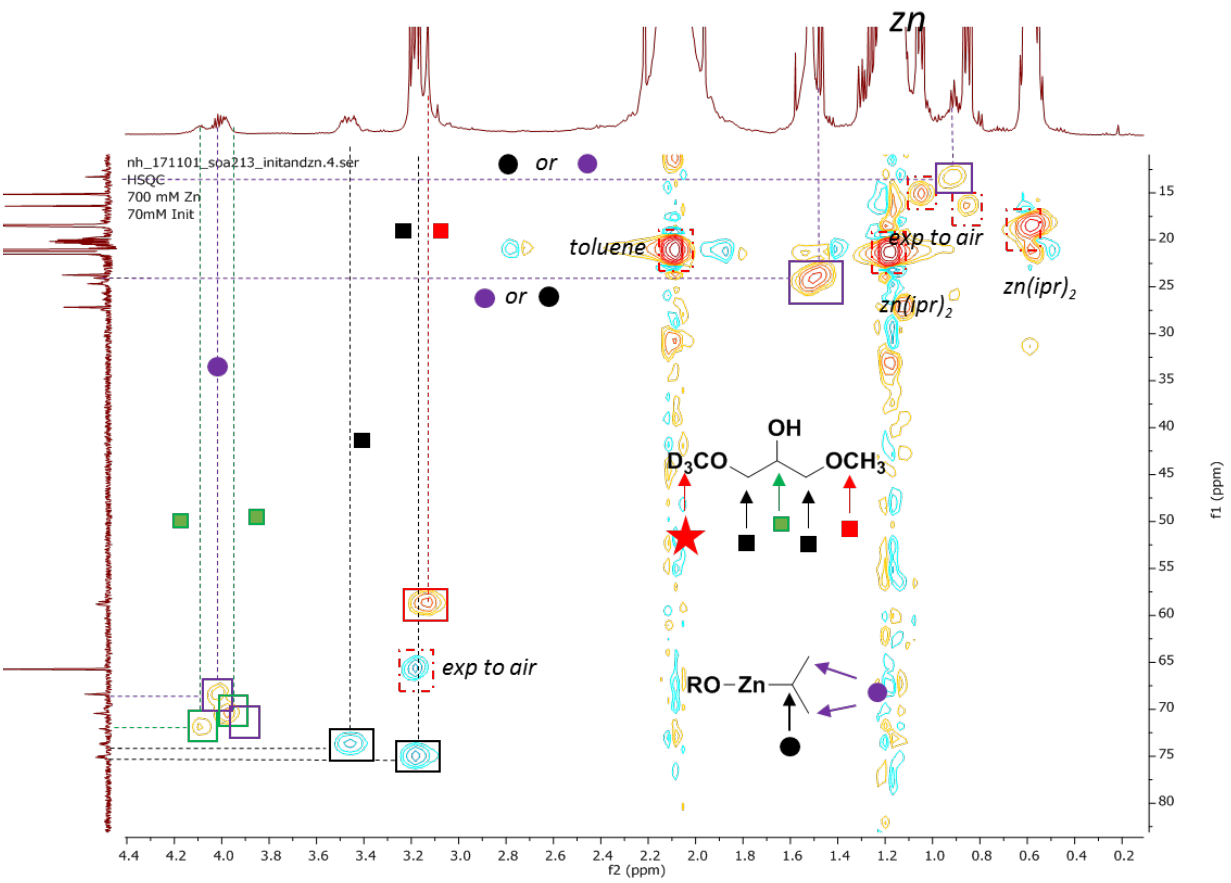


Figure S53. HSQC Spectra of 70mM (*S*) initiator in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air.

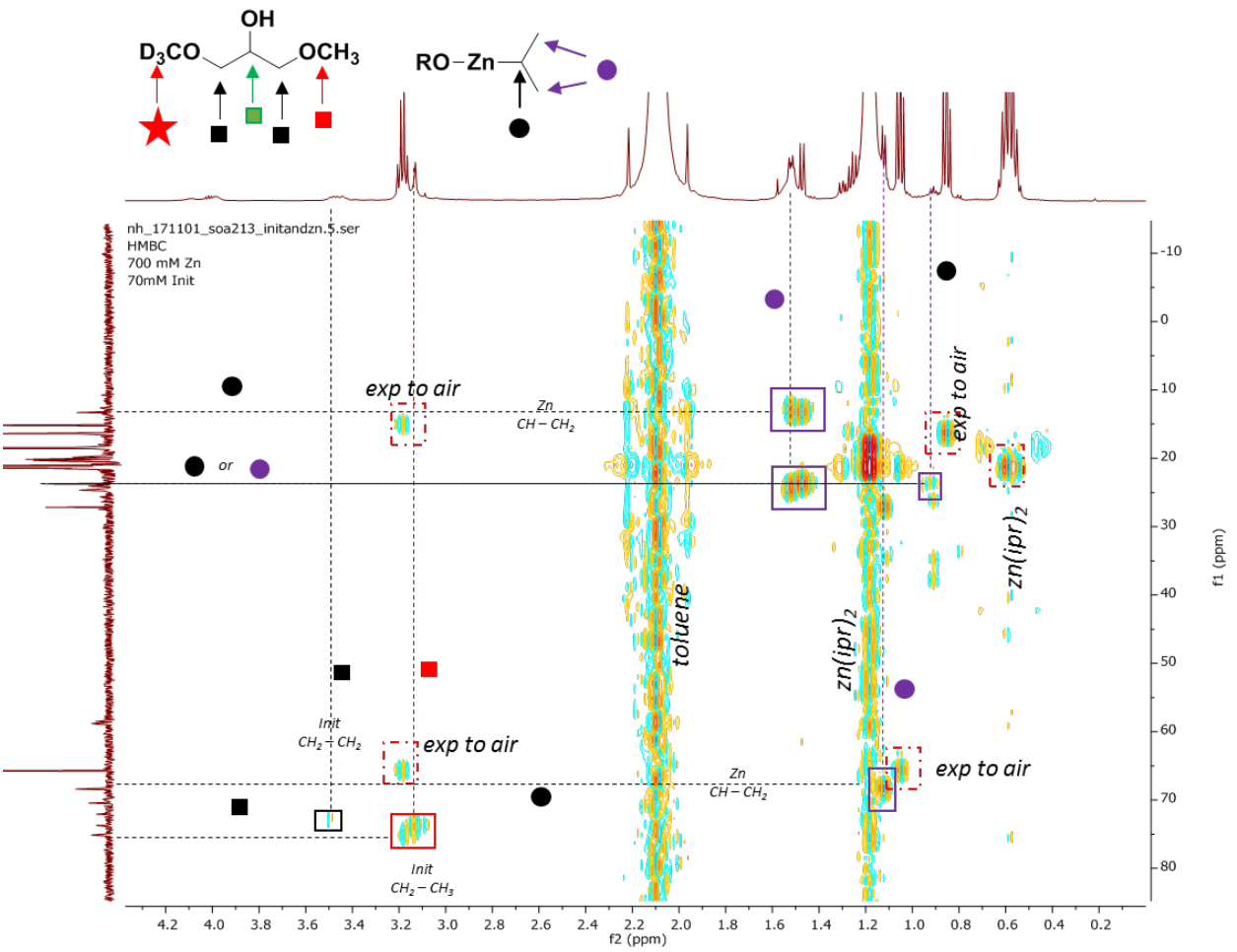


Figure S54. HMBC Spectra (~2,3 bonds) of 70mM (*S*) initiator in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares represent areas containing either zn(ipr)$_2$, toluene, or byproduct resulting from zn(ipr)$_2$ exposure to air.

2D Spectra of Zinc-Initiator-Product Complex (~20:2:1). A solution of product was added to the reaction mixture until one major species appeared in the ^{2}H NMR spectra. ^{1}H, ^{2}H, ^{13}C, COSY, HSQC and HMBC spectra were taken of the resulting complex and are provided below. Two to four initiator-zinc-product complexes were observed.

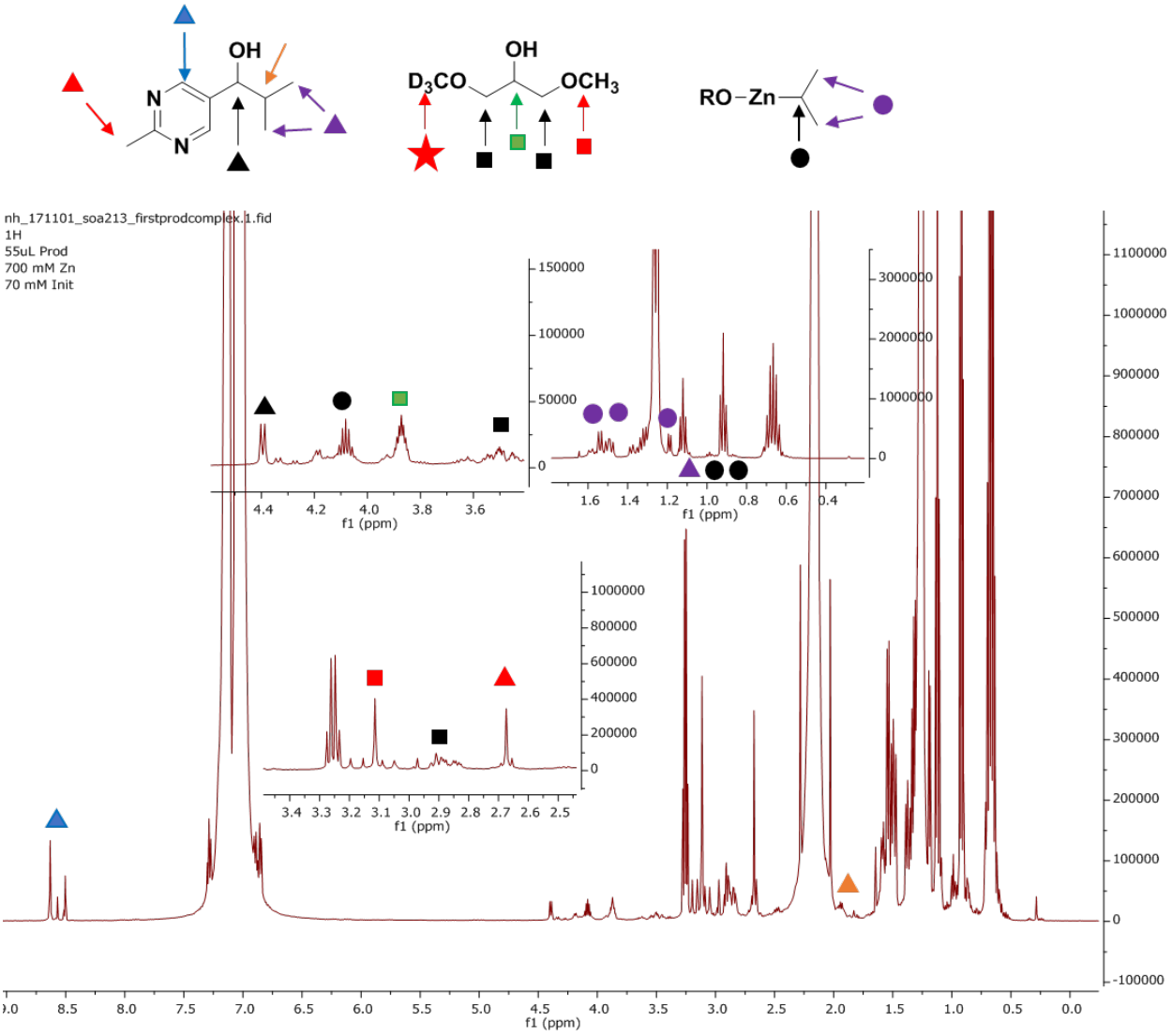


Figure S55. ^{1}H NMR of 70mM (*S*) initiator, 35mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Peaks that are labeled neither in the inset or the main spectra either could not be assigned or are related to toluene, diisopropylzinc, or the degradation production of diisopropylzinc.

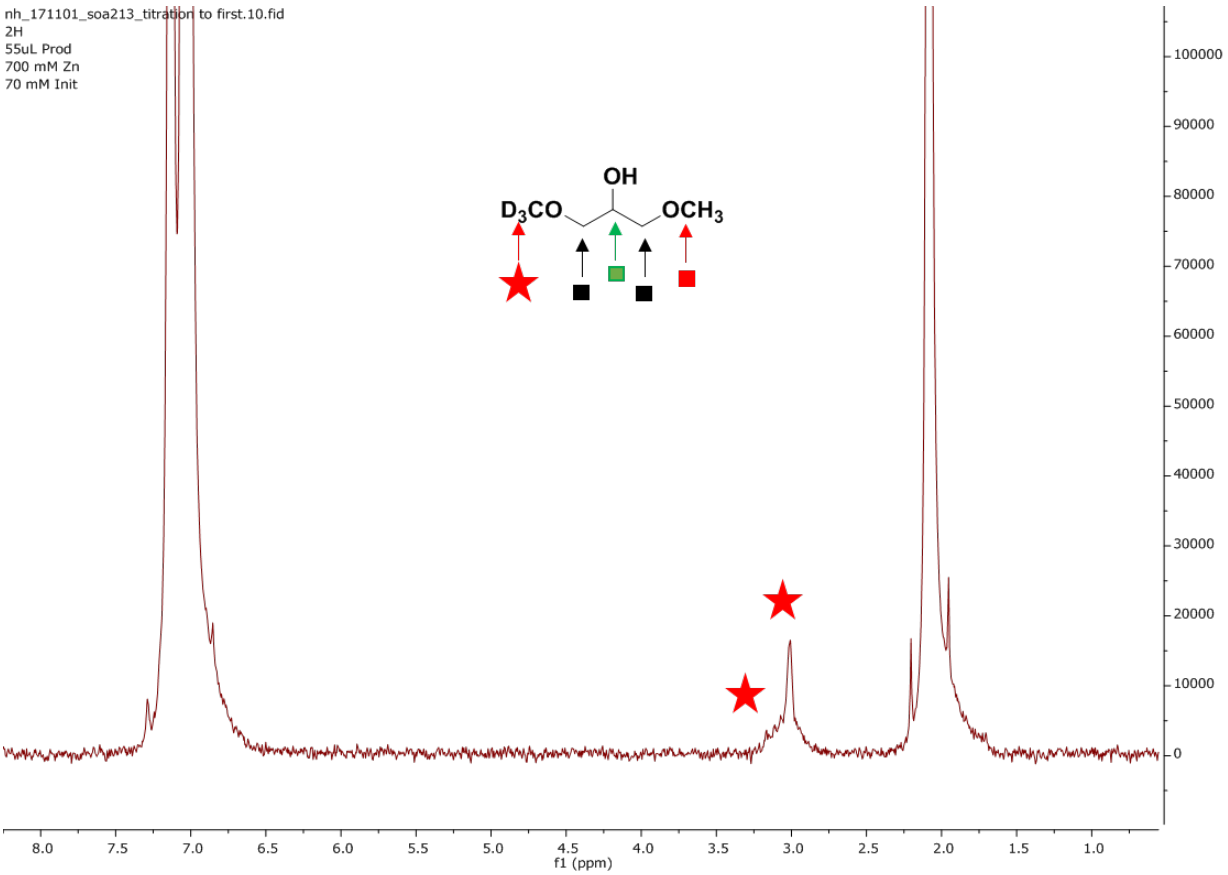


Figure S56. ^{2}H NMR of 70mM (*S*) initiator, 35mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Unlabeled peaks are toluene-*d8*.

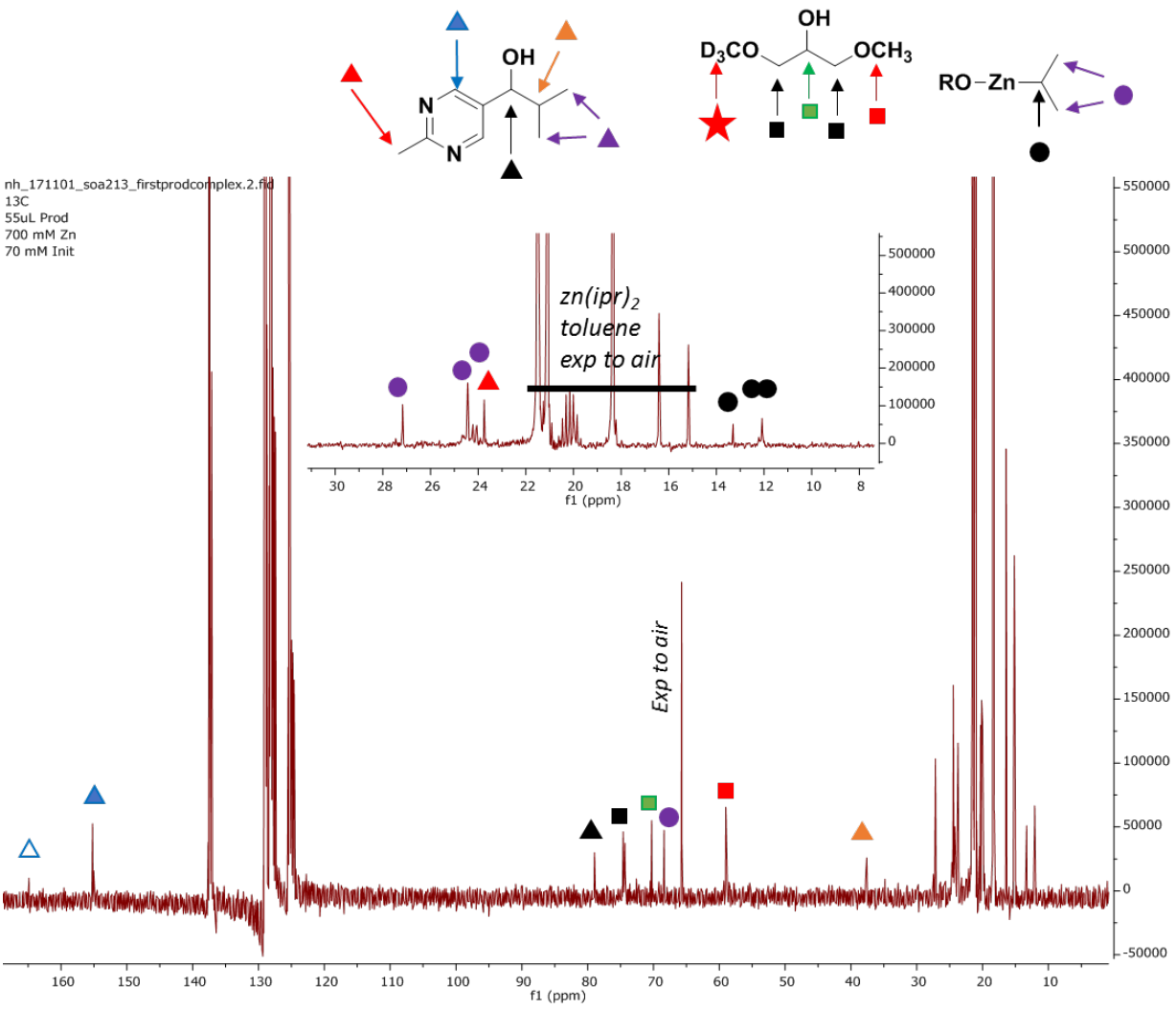


Figure S57. ^{13}C NMR of 70mM (*S*) initiator, 35mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Peaks that are labeled neither in the inset or the main spectra either could not be assigned or are related to toluene, diisopropylzinc, or the degradation production of diisopropylzinc. Open blue triangle represents quaternary aromatic carbons.

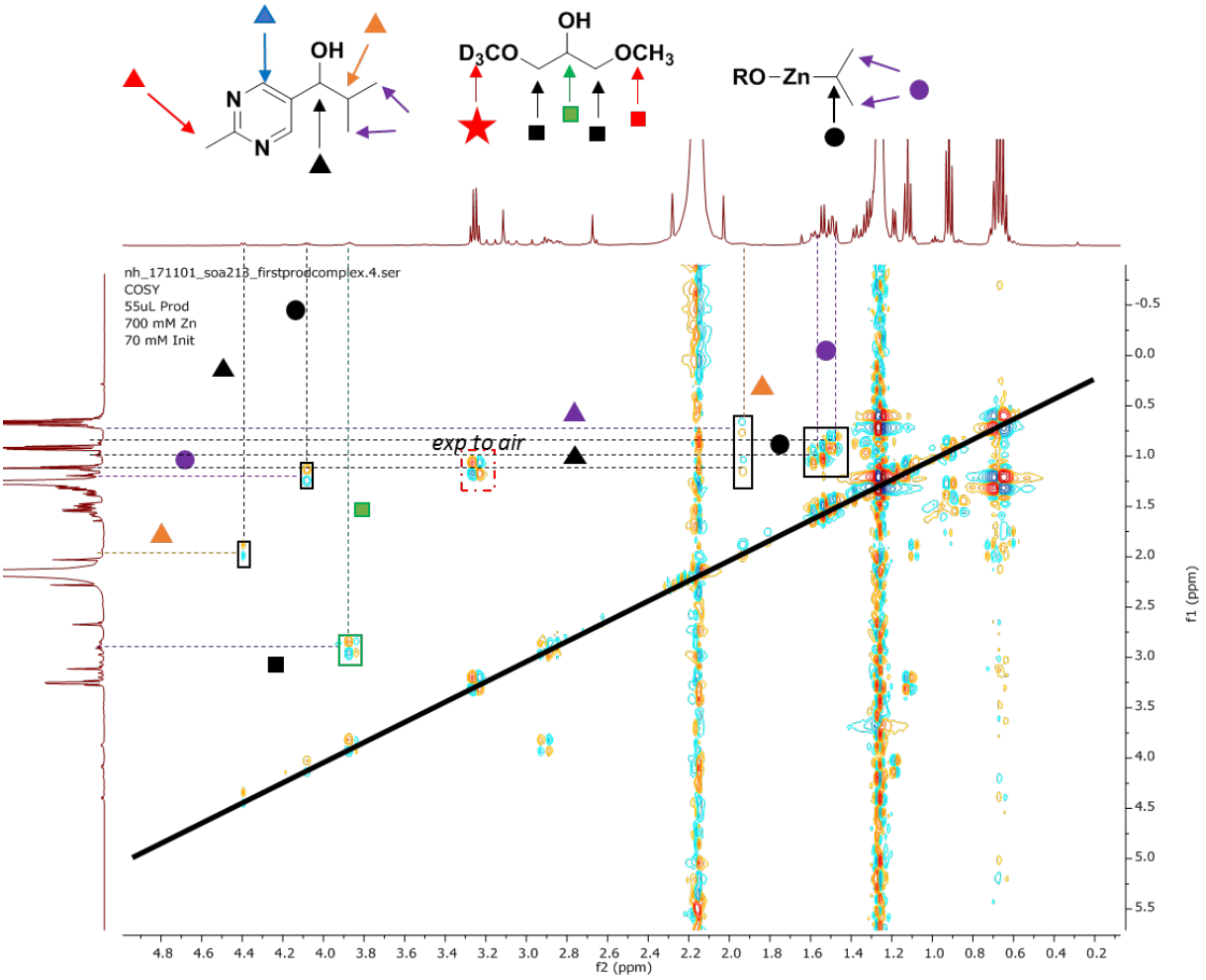


Figure S58. COSY Spectra of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either zn(ipr)$_2$, toluene, or byproduct resulting from zn(ipr)$_2$ exposure to air.

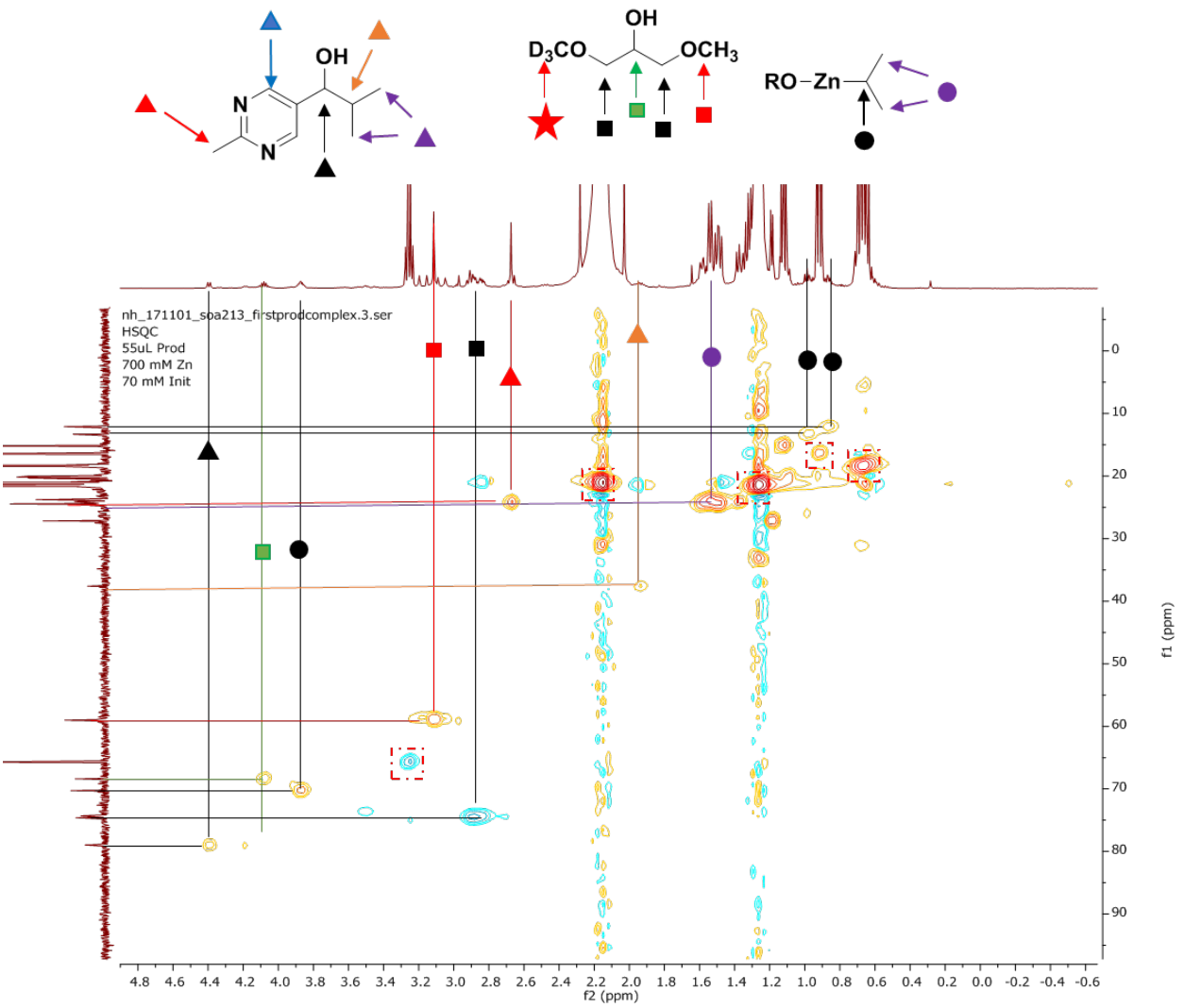


Figure S59. HSQC spectra of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either zn(ipr)$_2$, toluene, or byproduct resulting from zn(ipr)$_2$ exposure to air. Phasing: blue = CH$_2$, orange/red = CH/CH$_3$.

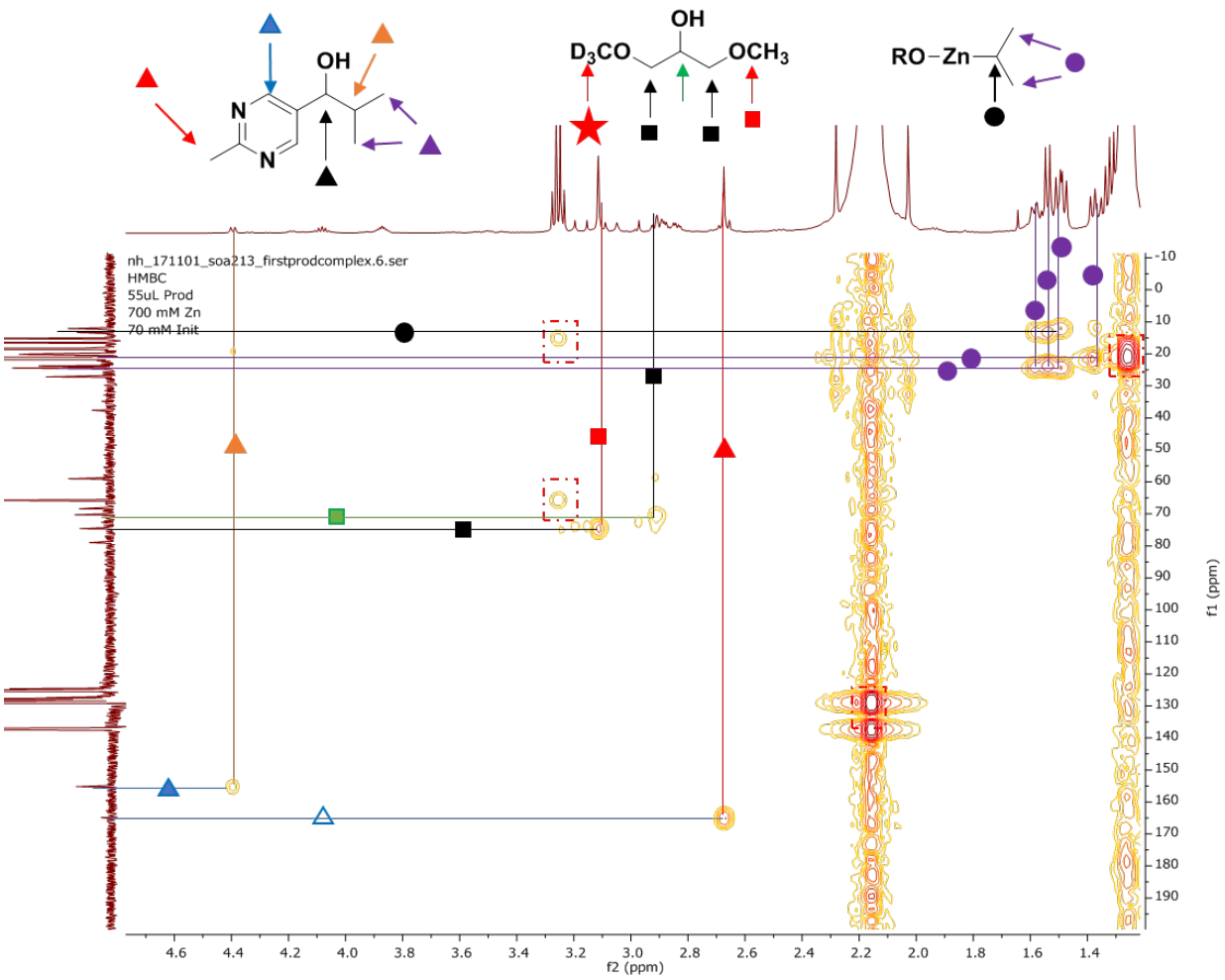


Figure S60. HMBC spectra (2-3 bonds) of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 1.2 to 4.8 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air. Light blue triangle = aromatic quaternary carbon.

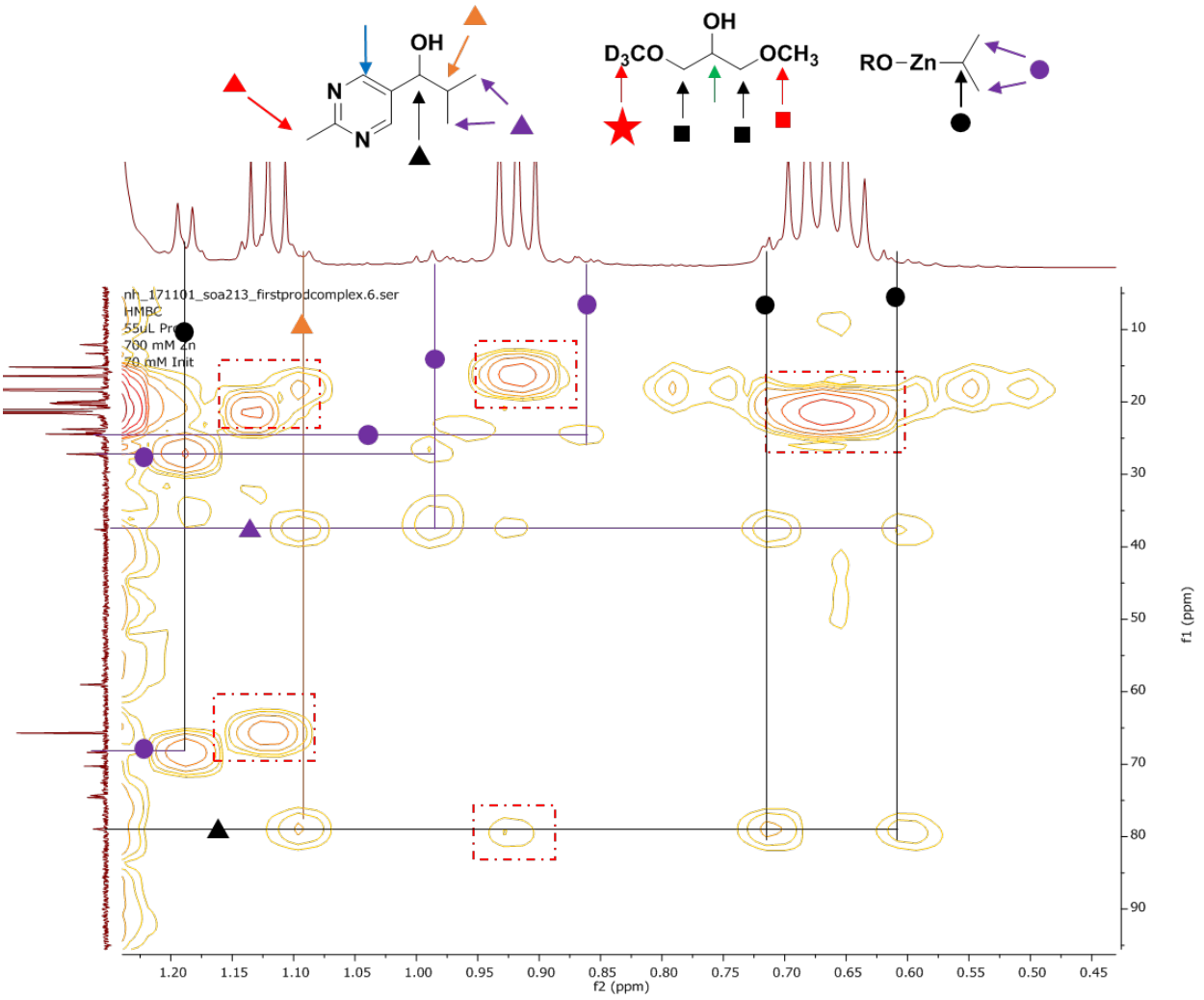


Figure S61. HMBC spectra (2-3 bonds) of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 0.4 to 1.2 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either zn(ipr)$_2$, toluene, or byproduct resulting from zn(ipr)$_2$ exposure to air.

2D Spectra of Zinc-Initiator-Product Complex (~10:1:2). A solution of product was added to the reaction mixture until a final single species appeared in the ^{2}H NMR spectra. ^{1}H, ^{2}H, ^{13}C, COSY, HSQC and HMBC spectra were taken of the resulting complex and are provided below. This data shows only one complex present.

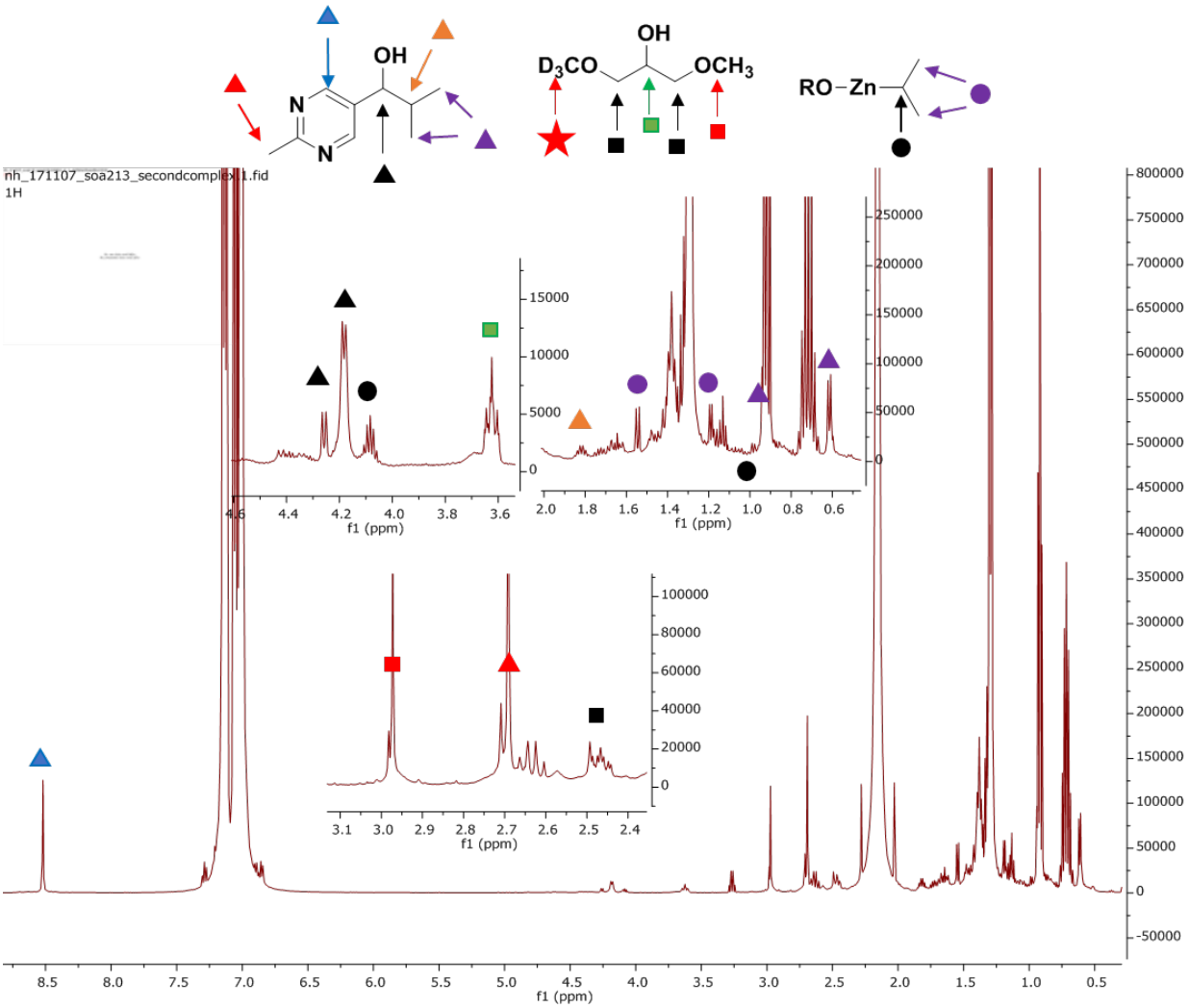


Figure S62. ^{1}H NMR of 70mM (*S*) initiator, ~140mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Peaks that are labeled neither in the inset or the main spectra either could not be assigned or are related to toluene, diisopropylzinc, or the degradation production of diisopropylzinc.

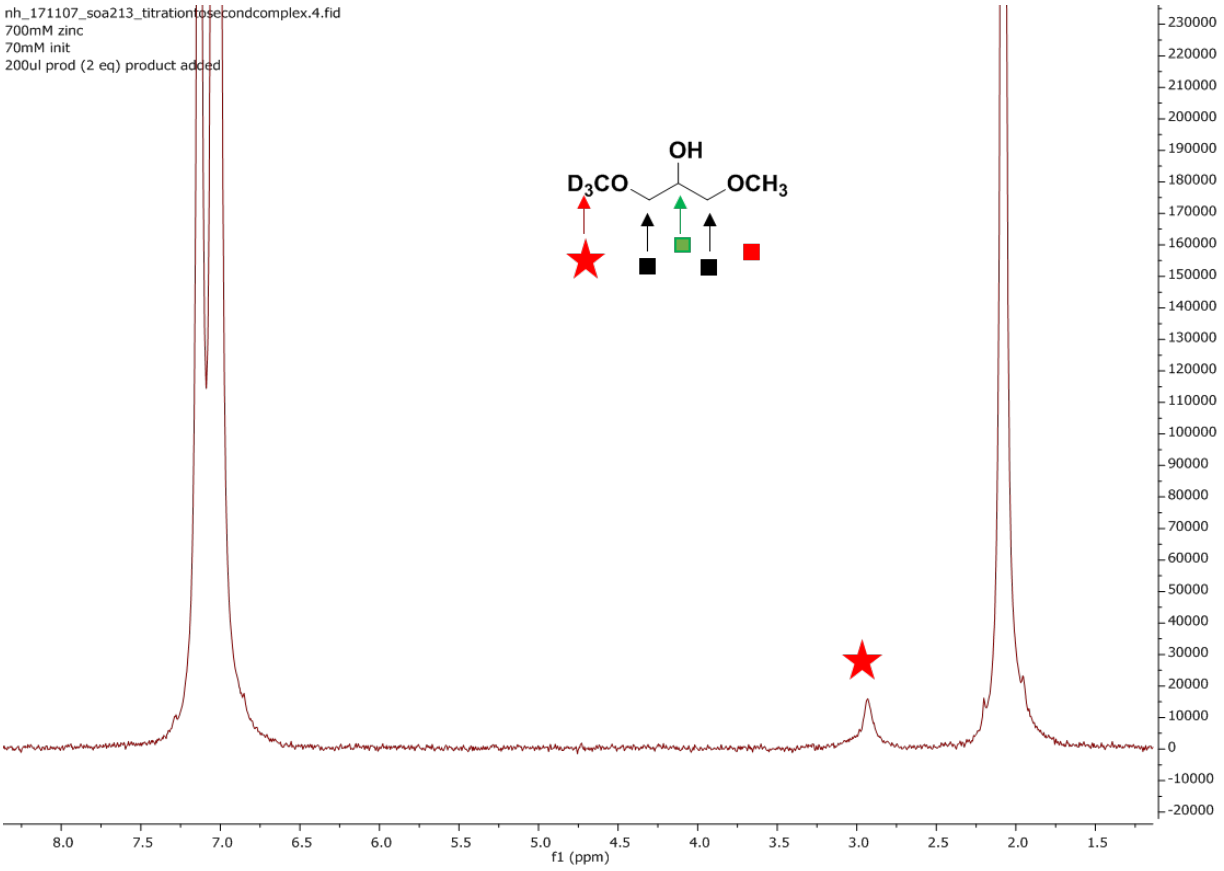


Figure S63. ^{1}H NMR of 70mM (*S*) initiator, ~140mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Peaks that are not labeled are toluene-*d8*.

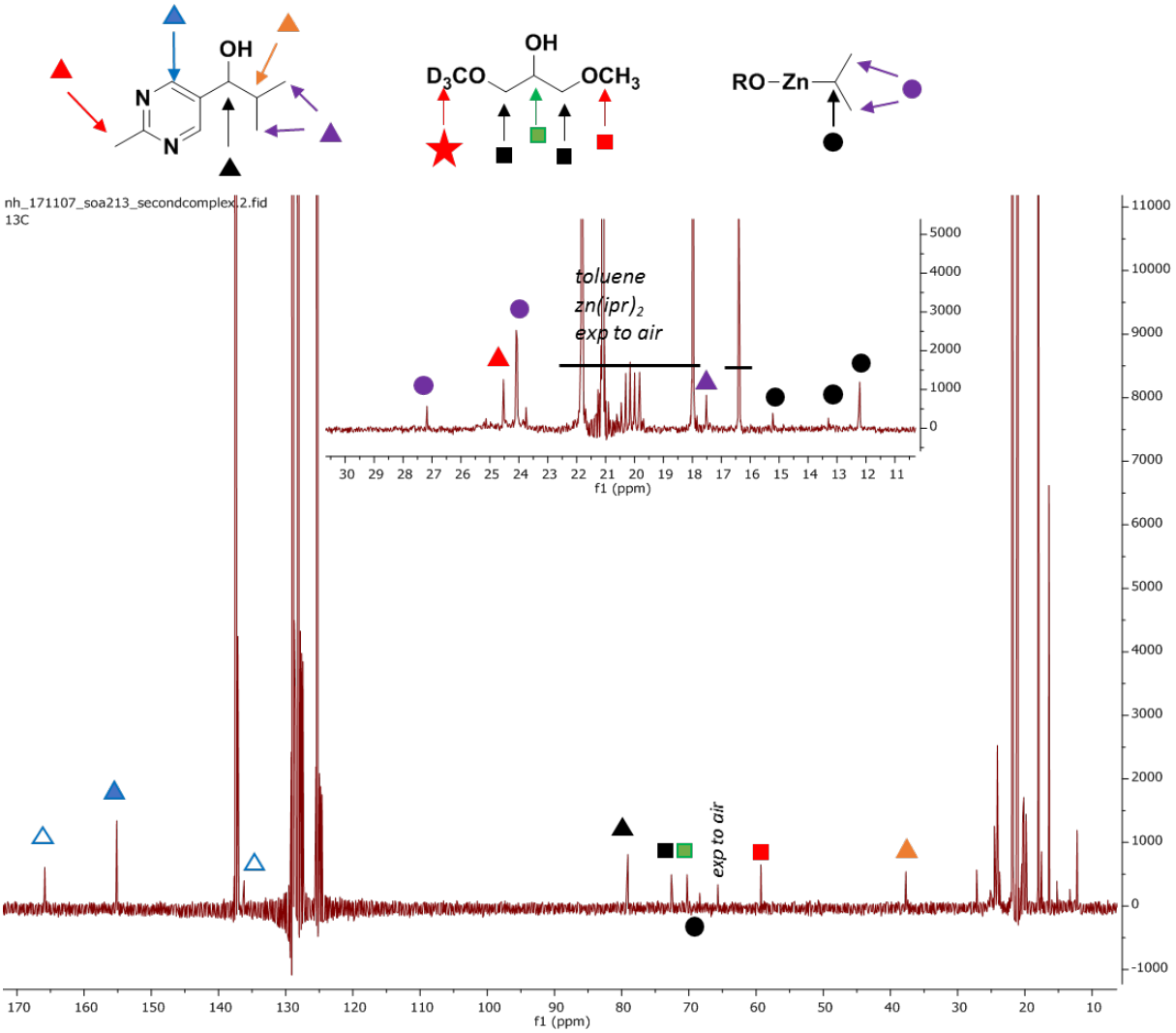


Figure S64. ^{13}C NMR of 70mM (*S*) initiator, 35mM product in 0.7M diisopropylzinc at 273K. Solvent = toluene/toluene-*d8* (9:2). Peaks that are labeled neither in the inset or the main spectra either could not be assigned or are related to toluene, diisopropylzinc, or the degradation production of diisopropylzinc. Open blue triangles represent quaternary aromatic carbons.

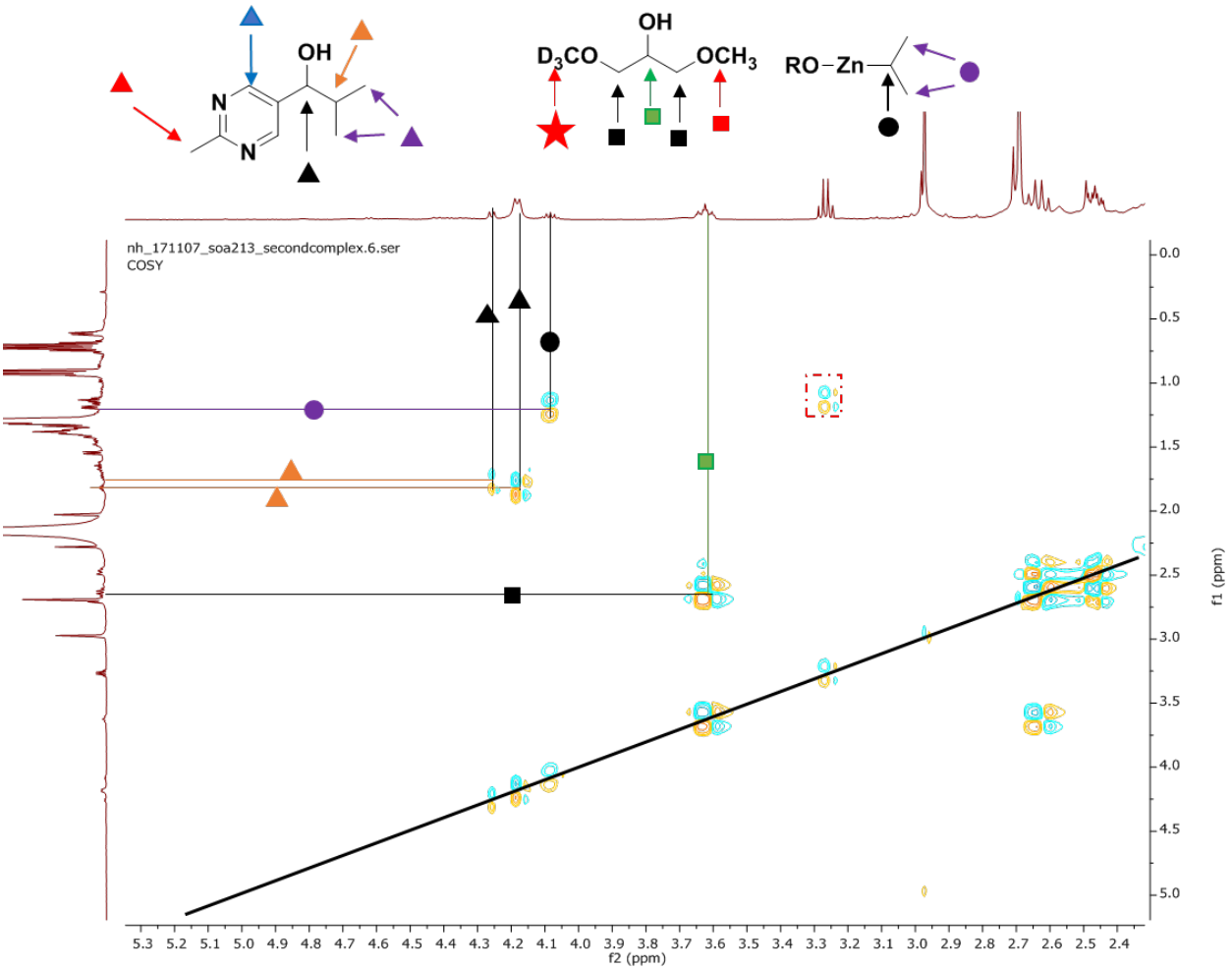


Figure S65. COSY Spectra of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 5.3 to 2.4ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air.

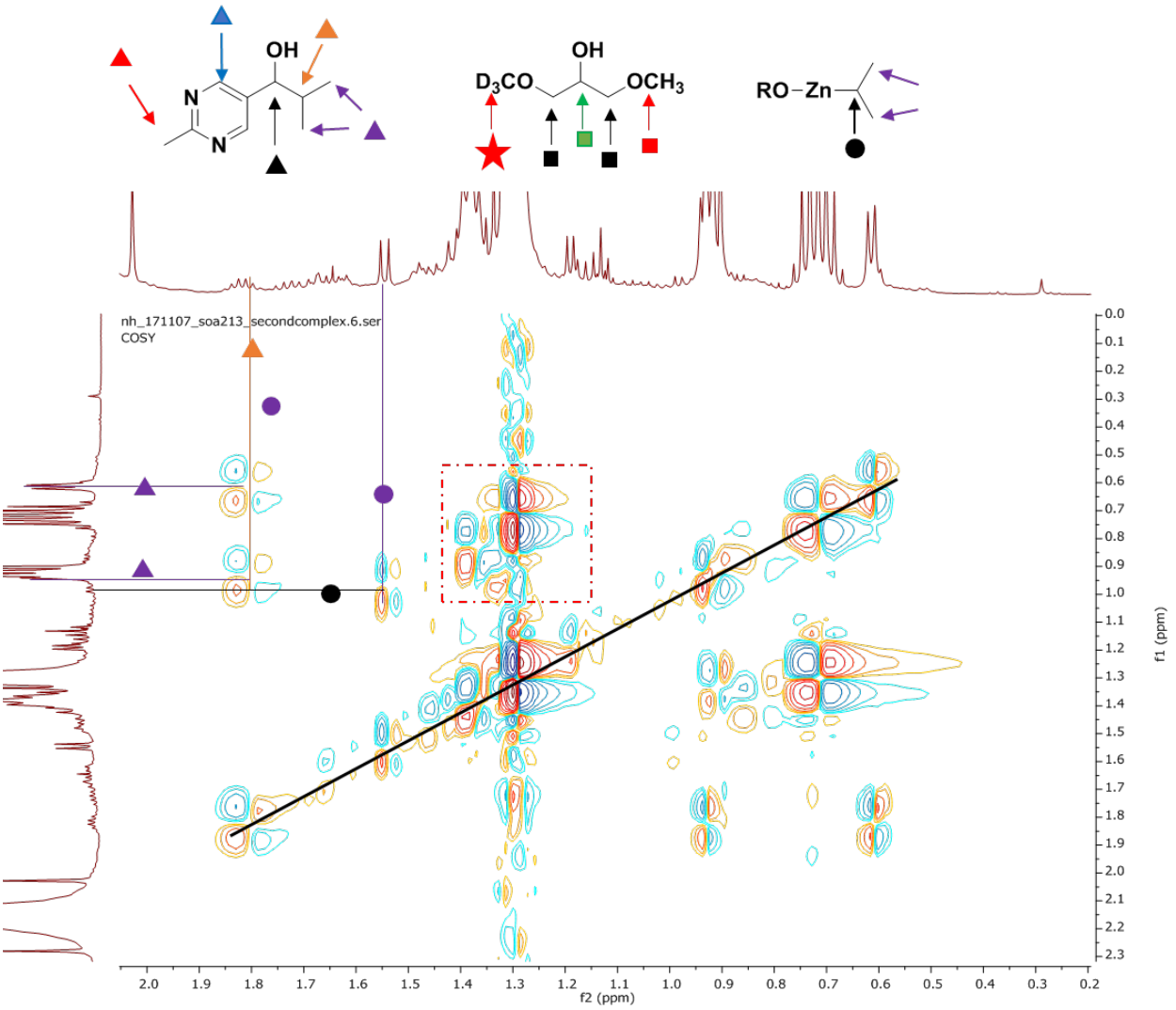


Figure S66. COSY Spectra of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 0.2 to 2.1 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air.

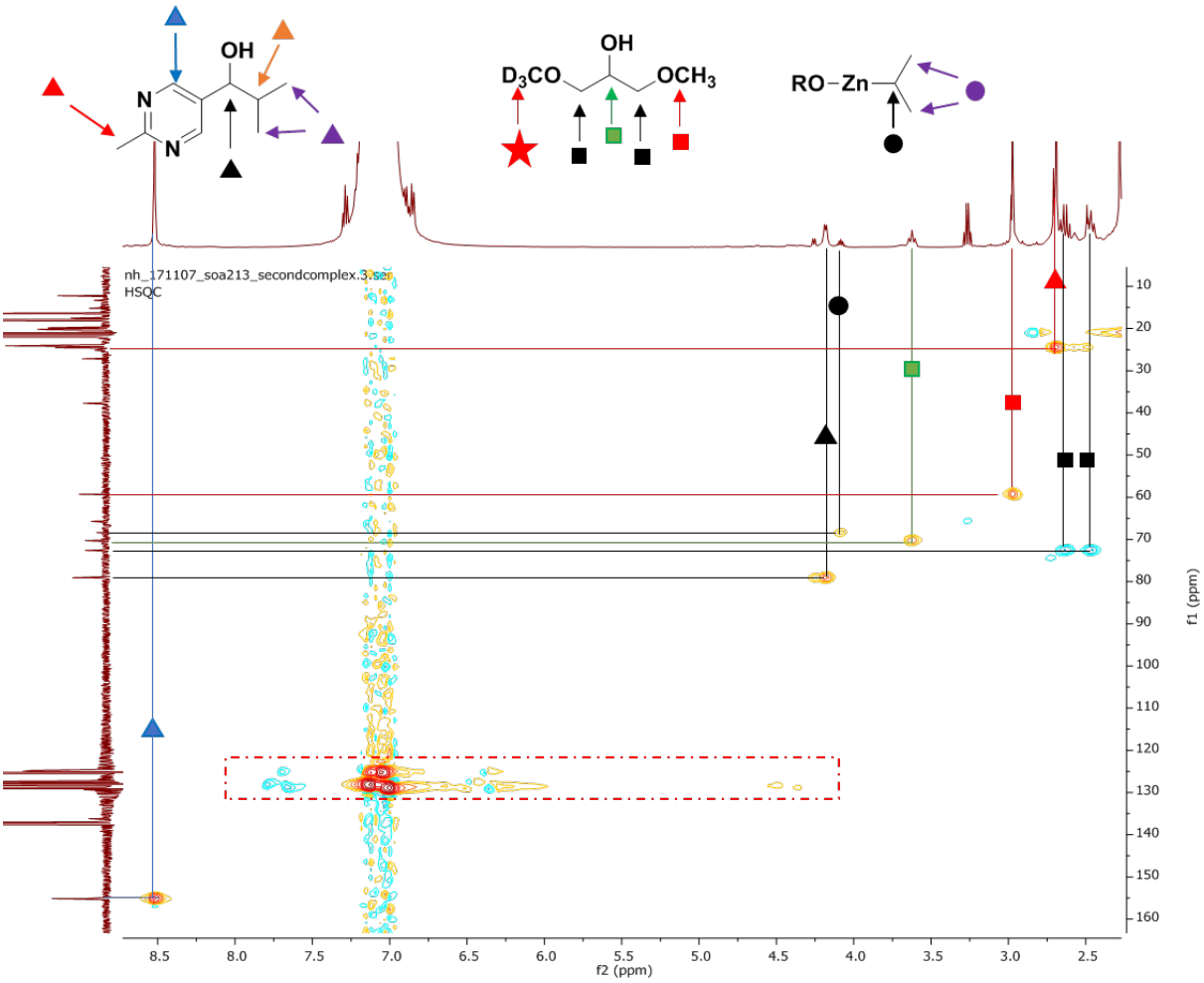


Figure S67. HSQC spectra of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 2.4 to 8.5 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air. Phasing: blue = CH_2, red/orange = CH/CH_3.

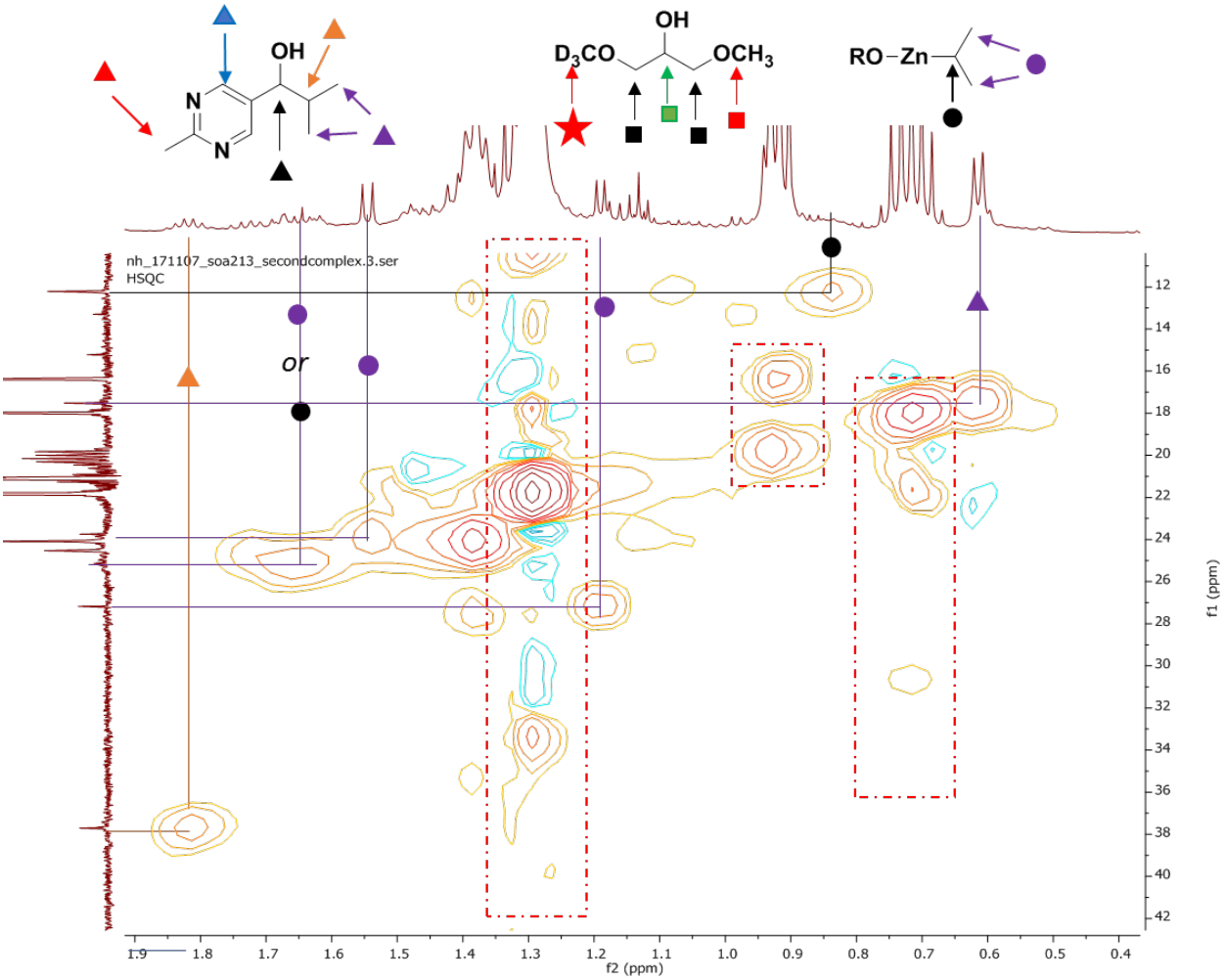


Figure S68. HSQC spectra of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 0.4 to 1.9 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air. Phasing: blue = CH_2, red/orange = CH/CH_3.

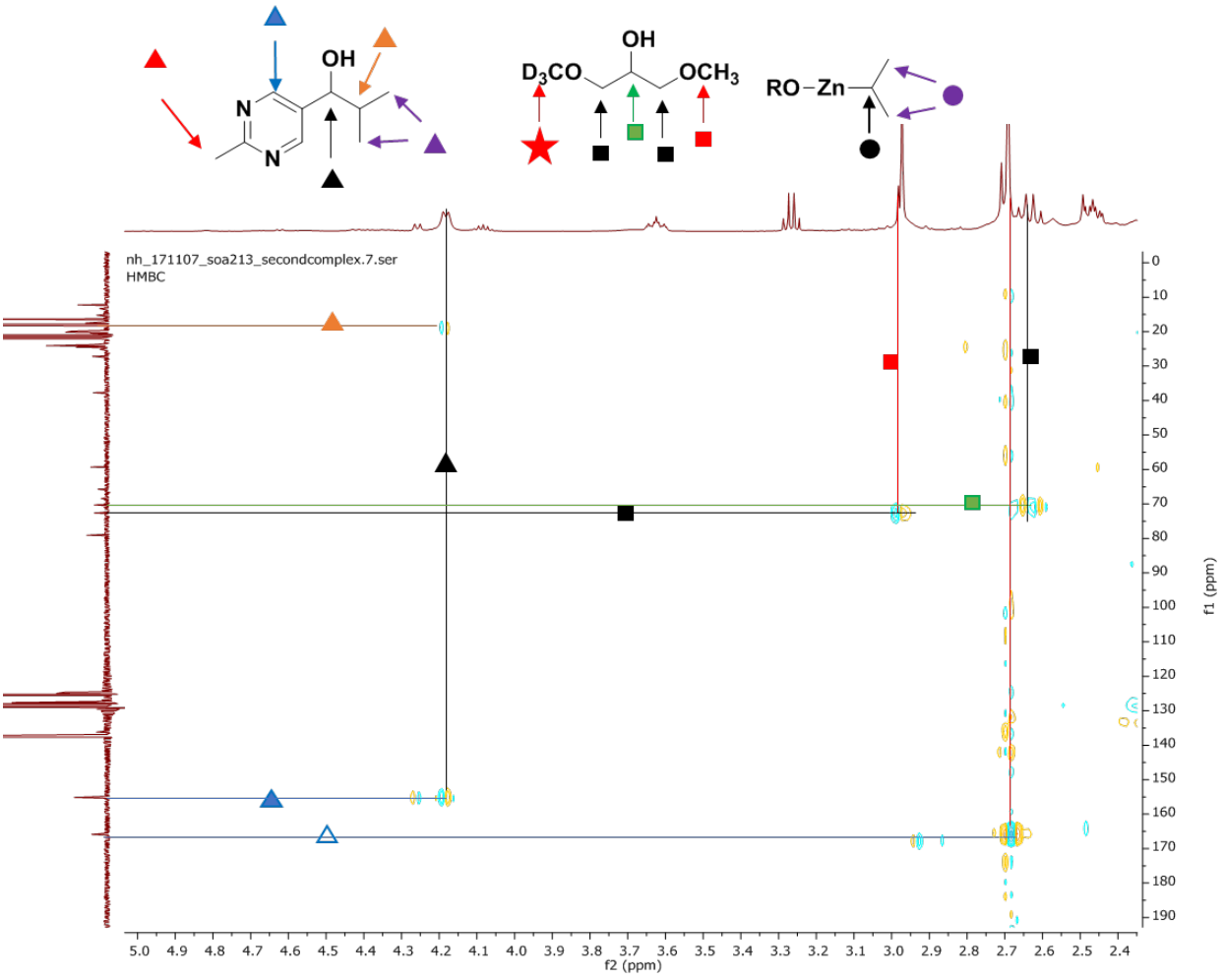


Figure S69. HMBC spectra (~2 to 3 bonds) of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 2.4 to 5.0 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either $zn(ipr)_2$, toluene, or byproduct resulting from $zn(ipr)_2$ exposure to air. Open blue triangle = quaternary aromatic carbon.

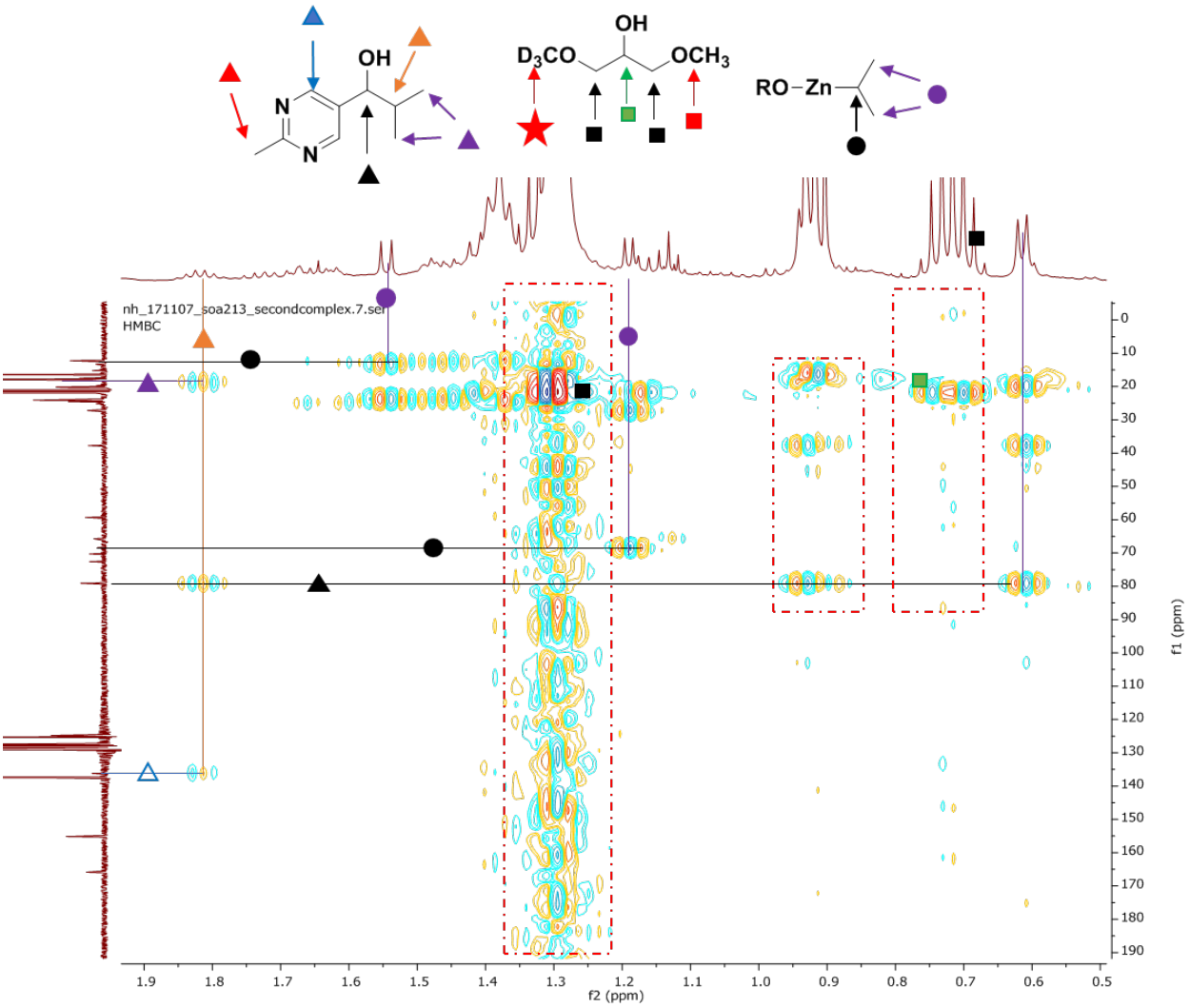


Figure S70. HMBC spectra (~2 to 3 bonds) of 70mM (*S*) initiator, ~35mM product in 0.7M diisopropylzinc at 273K from 0.5 to 1.9 ppm. Solvent = toluene/toluene-*d8* (9:2). Lines represent correlations, dashed squares or unlabeled peaks represent areas containing either zn(ipr)$_2$, toluene, or byproduct resulting from zn(ipr)$_2$ exposure to air. Open blue triangle = quaternary aromatic carbon.

B. Supplemental NMR Structures

(*R*) Initiator

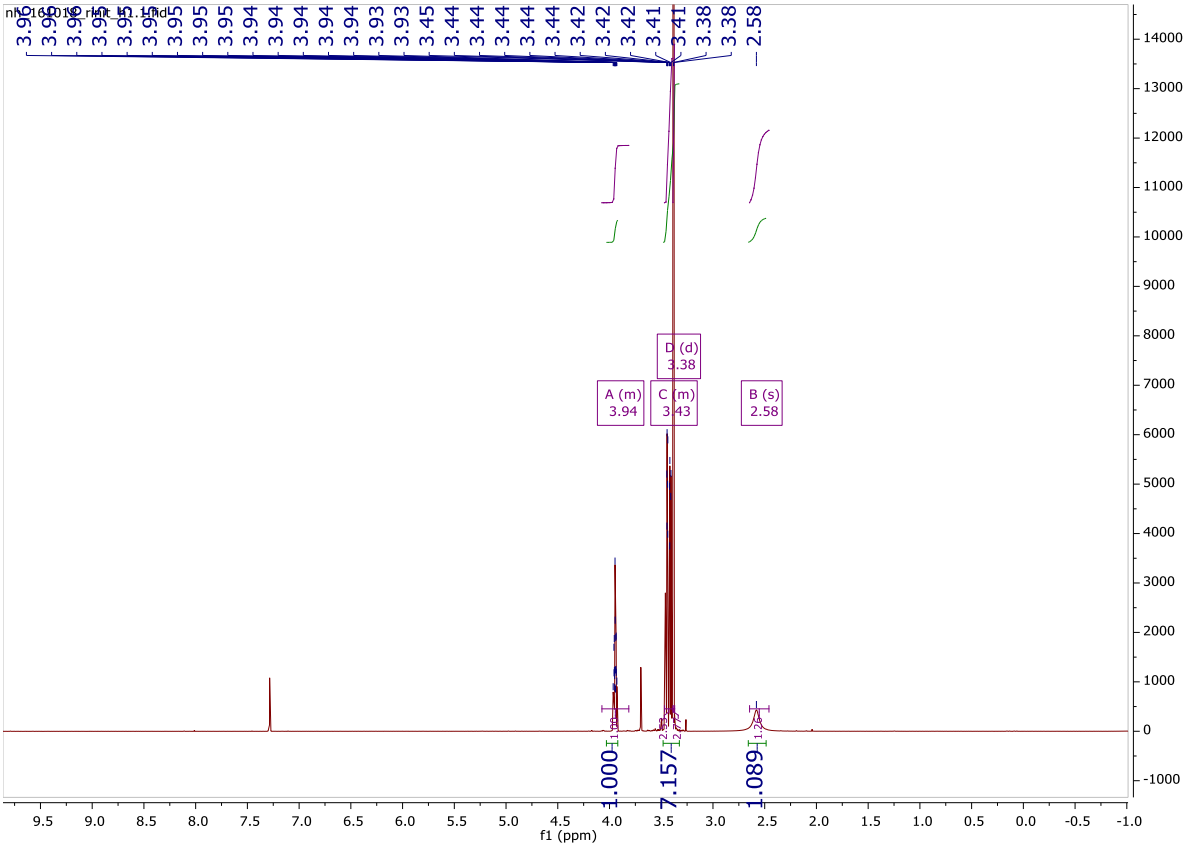


Figure S71. ^{1}H NMR of (*R*) initiator in $CDCl_3$.

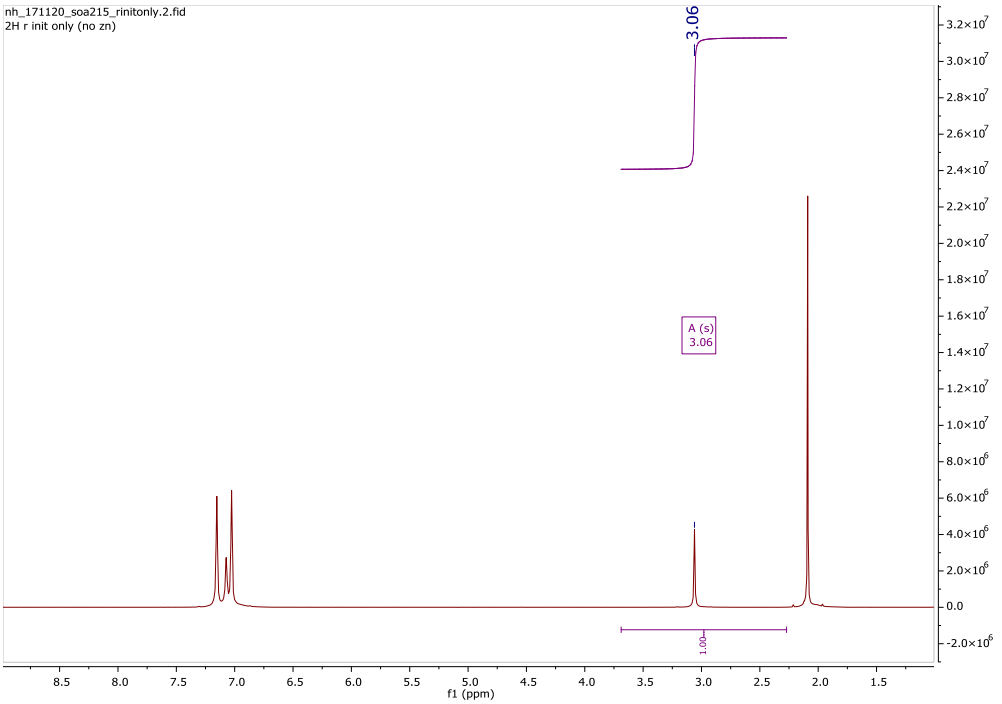


Figure S72. ^{2}H NMR of (*R*) initiator in toluene-*d8*.

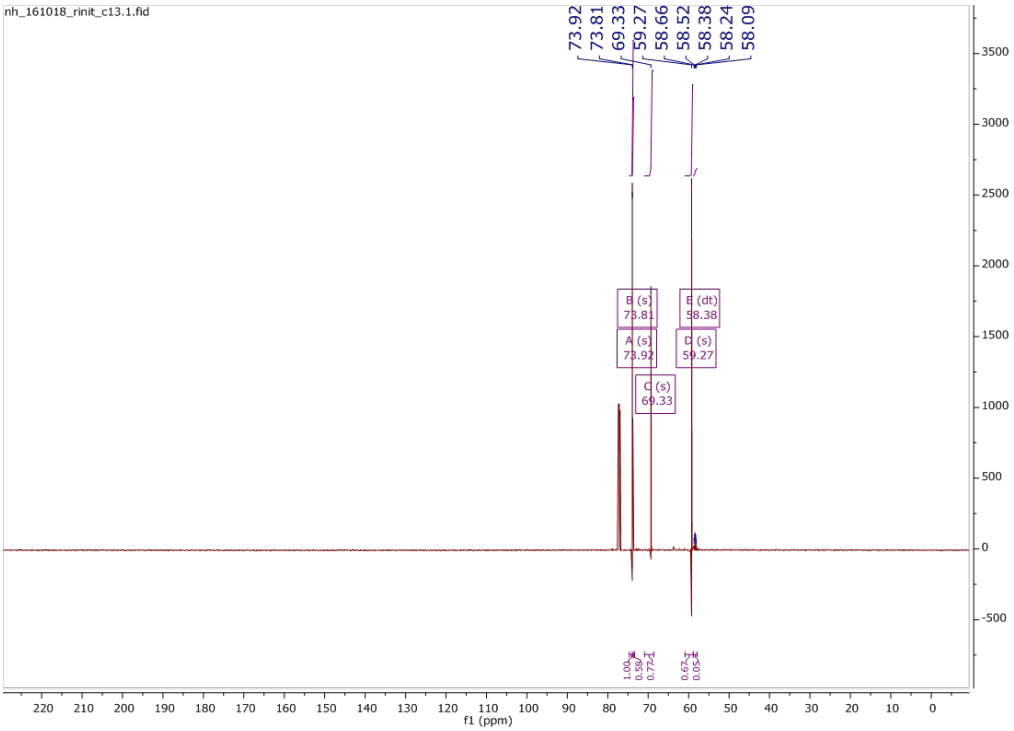


Figure S73. ^{13}C NMR of (*R*) initiator in $CDCl_3$.

(*S*) Initiator

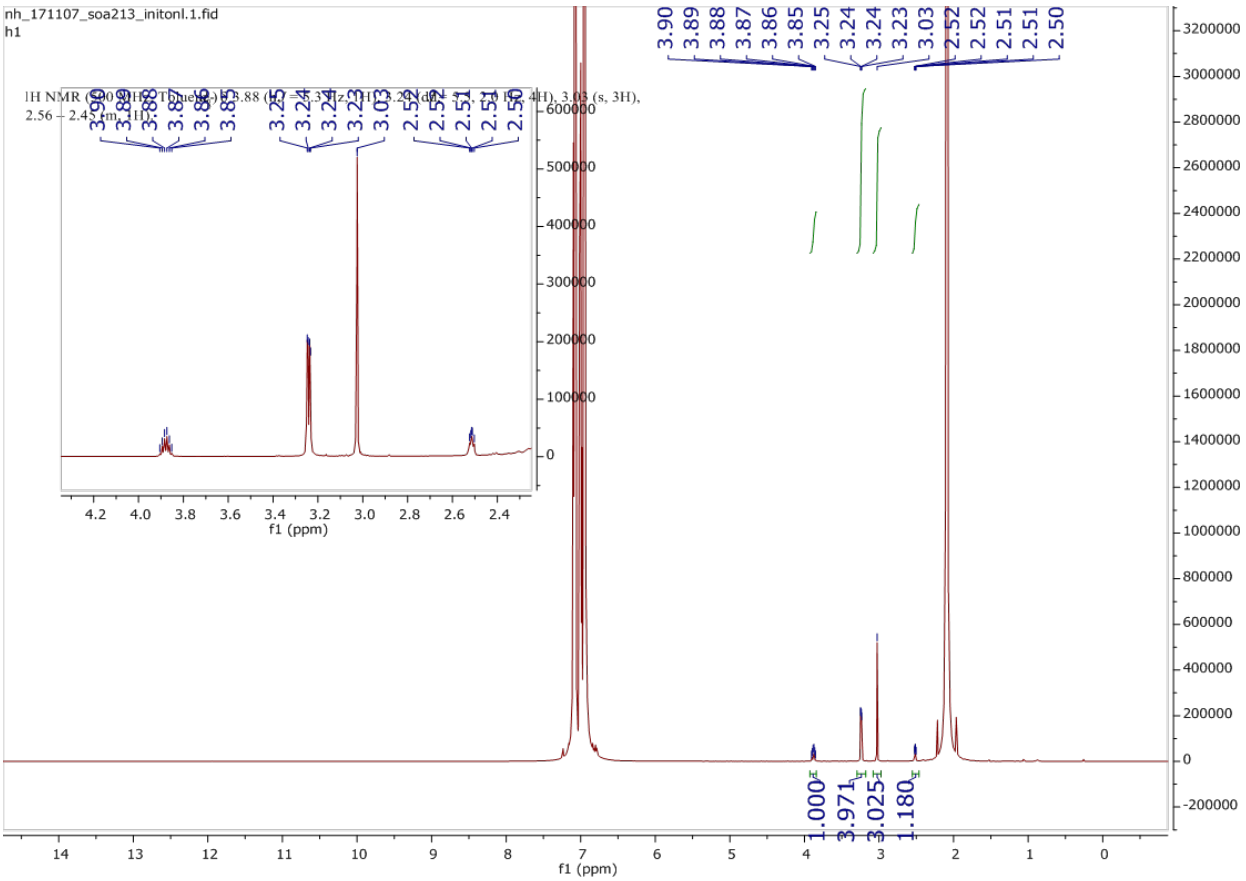


Figure S74. ^{1}H NMR of (*S*) initiator in toluene-*d8*.

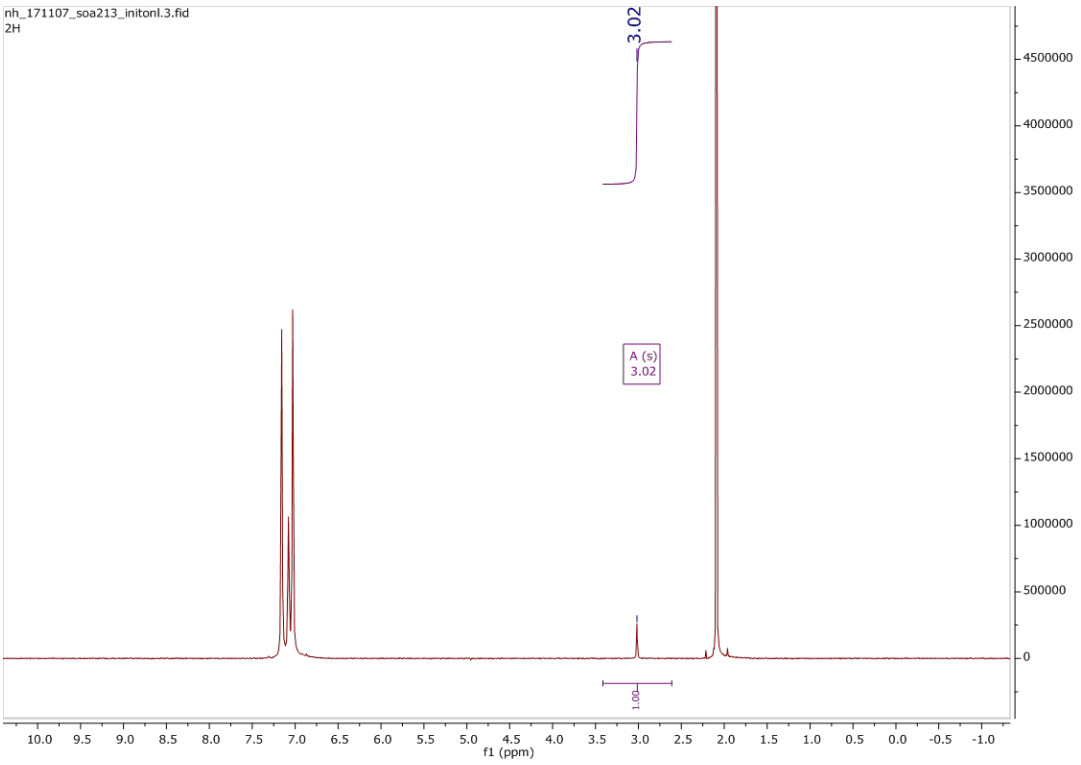


Figure S75. ^{2}H NMR of (*S*) initiator in toluene-*d8*.

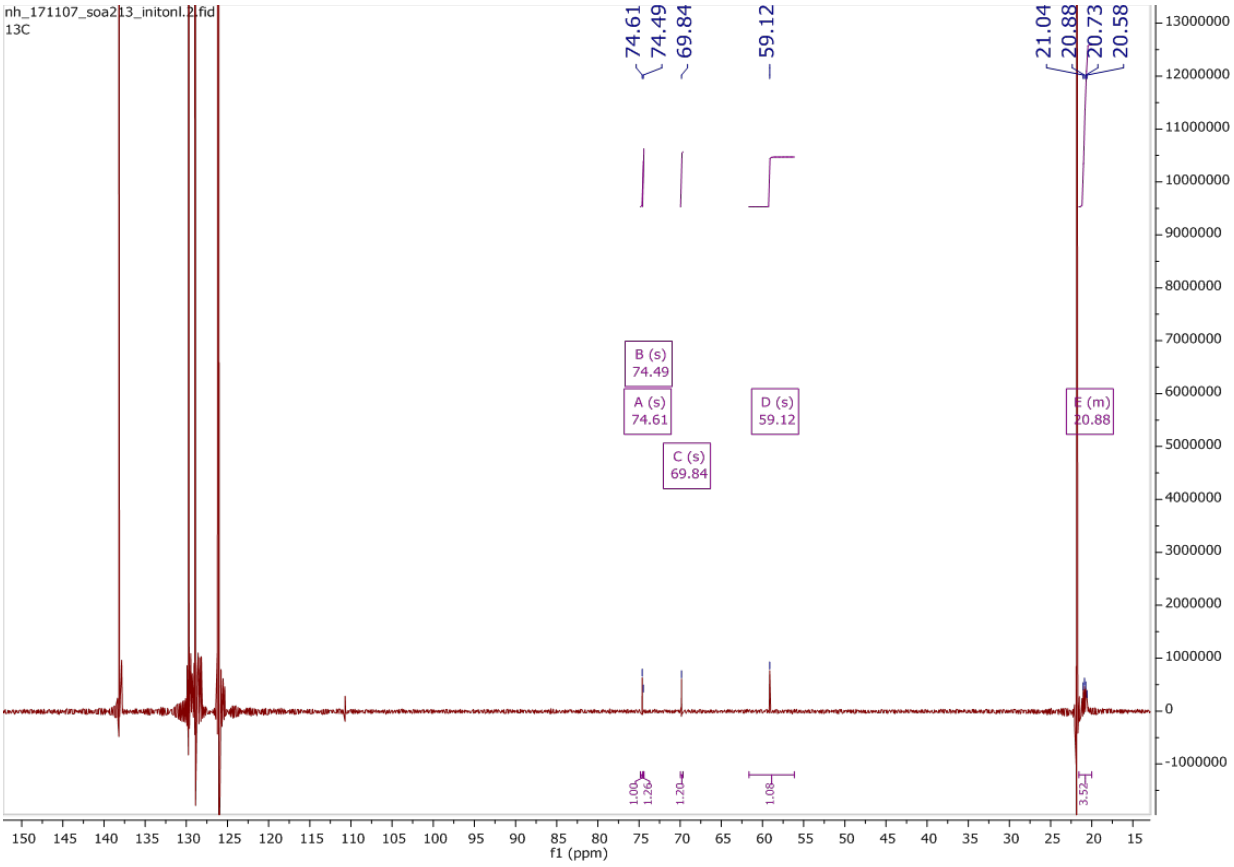


Figure S76. ^{13}C NMR of (*S*) initiator in toluene-*d8*.

7. DFT Calculations of Zinc-Product-Initiator Complex

A. General Methodology

All calculations were performed in Gaussian 09.[8] Initial conformers were generated in Avogadro, and geometry minimized within Gaussian using the 6-36G(d,p) basis set for all nitrogen, carbon, hydrogen and oxygen and SDD basis set for zinc. B3LYP functional used and solvent effects were estimated using a continuum model (PCM, toluene). Generally, several conformers of the same structure were input to ensure the minimized structure was found.

B. Minimized Achiral Structures

To approximate the structure of the initiator-product-zinc complex, seventeen possible structures (all $Zn_3C_{32}N_4H_{58}O_5$) were submitted for geometry optimization and frequency calculations. The starting structures were varying diastereomers of varied connectivity, all incorporating (*R*,*R*) products. These structures converged on four general structure. The highest energy structure consisted of a square product dimer with a bridging initiator molecule along the top face. The lowest energy structure was a contained two fused square dimer systems, with the initiator contributing the central oxygen. All calculated structures are provided in Appendix A, with relative electronic energies (ZPE corrected) provided in **bold** and relative free energies provided in italics (kcals/mol).

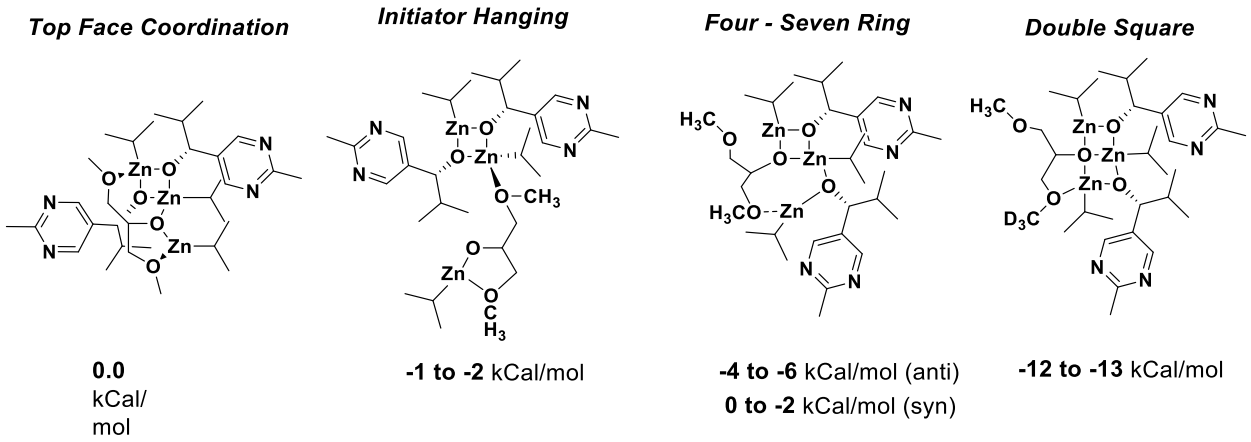


Figure S77. Minimized structures found in DFT study. All energy values relative to the highest energy structure (left).

C. Minimized Chiral Structures

All possible diastereomers of the double square dimer structure were calculated, with both (*R*,*R*), (*S*,*S*) and (*R*,*S*) product configurations considered. The lowest energy structure was the (*R*,*R*) product structure h_3 with all bonds -syn to each other. The highest energy diastereomers result in cleavage of the central-zinc oxygen bond, giving a six-membered ring rather than the double square dimer orientation.

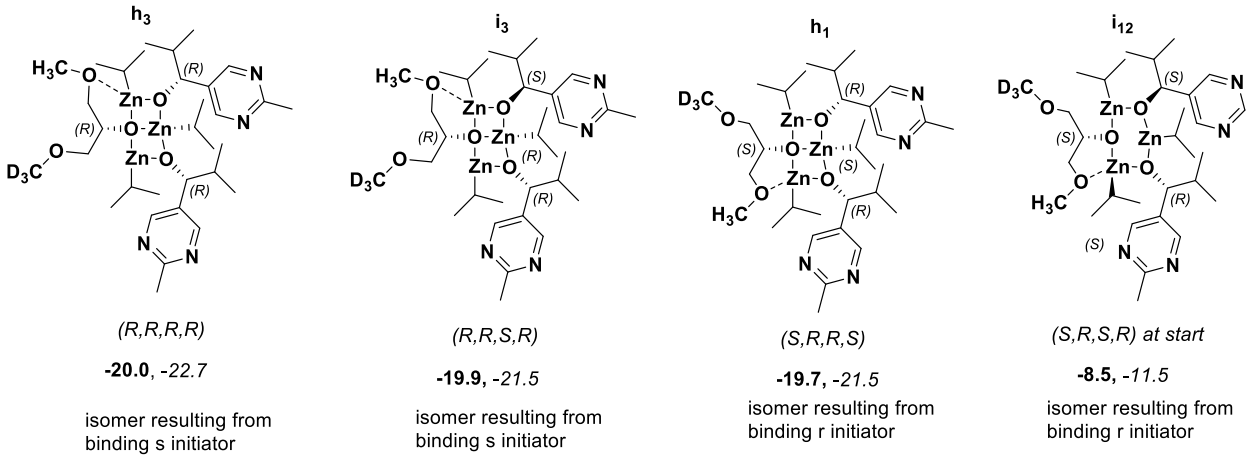


Figure S78. Calculated energies of the double square dimer orientation, including the three lowest energy orientations and the highest energy orientation (right). Binding of methoxy group to Zn elevates the priority in the CIP naming rules, meaning that *S*-**3** becomes designated as *R* when OCH_3 is bound, and *R*-**3** becomes *S* when OCH_3 is bound.

Each of the diastereomers gave nearly identical energy when calculating the binding between the (*R*) and (*S*) enantiomer of the initiator. In the case of the lowest energy diastereomers, binding of the (*S*) initiator (mismatched initiator-product interaction) gives a "CD_3 out" conformation, while binding the (*R*) initiator (matched interaction) gives the "CH_3 out". This is consistent with the trends observed in ^{1}H and ^{2}H NMR.

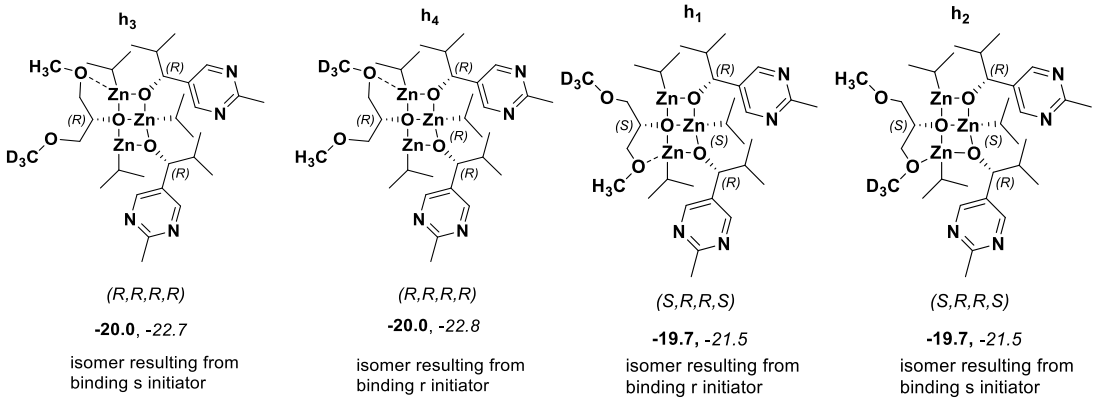
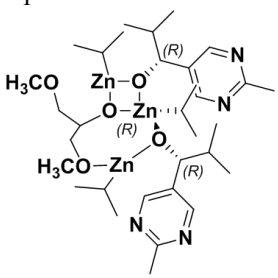


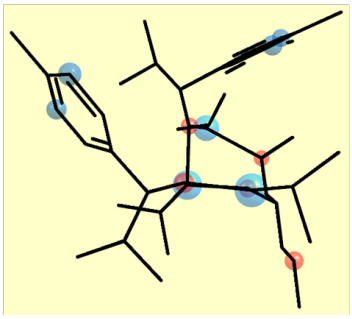
Figure S79. Isomeric differences between (*R*) and (*S*) initiator binding.

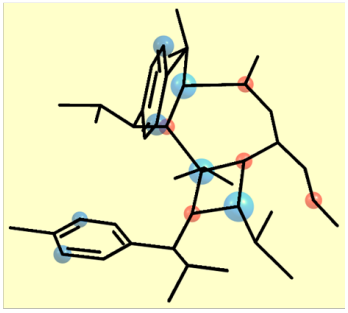
8. DFT Structures

a_1



-4.7, *-6.1*





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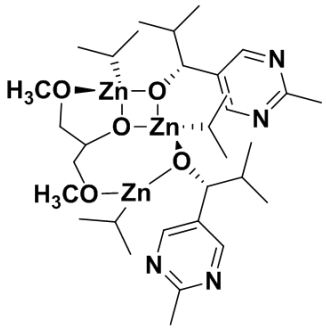
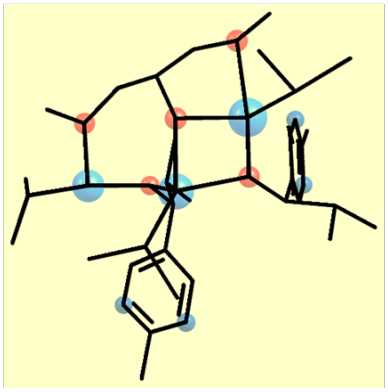
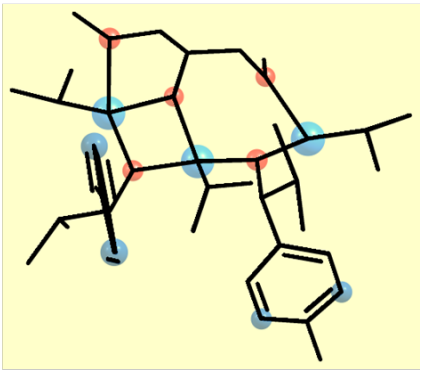
a_2



-0.6, *-2.8*





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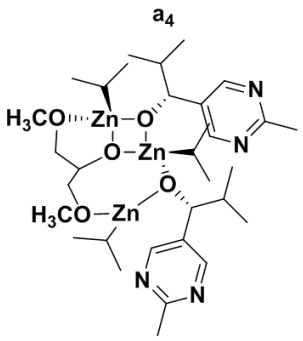
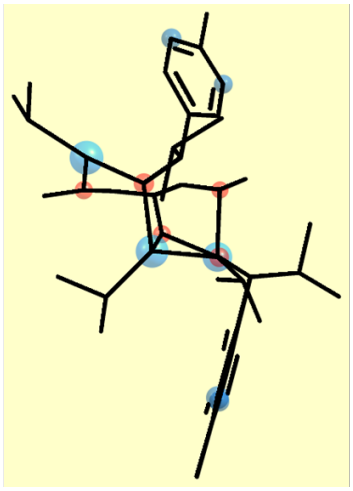
30	2.819790000	-1.493976000	-0.816013000
6	4.543228000	-2.437534000	-1.048633000
6	5.520542000	-2.221827000	0.117155000
6	5.198617000	-2.091721000	-2.397085000
1	4.265856000	-3.500477000	-1.071128000
1	5.480430000	-1.032955000	-2.454591000
1	4.542250000	-2.304217000	-3.248986000
1	6.122092000	-2.671974000	-2.544724000
1	5.815336000	-1.170734000	0.218350000
1	6.445092000	-2.799014000	-0.036885000
1	5.096264000	-2.534516000	1.077059000
6	0.786597000	-1.452819000	2.633782000
1	0.050473000	-2.222019000	2.916812000
6	0.801755000	-0.404696000	3.758034000
6	2.152379000	-2.149512000	2.548245000

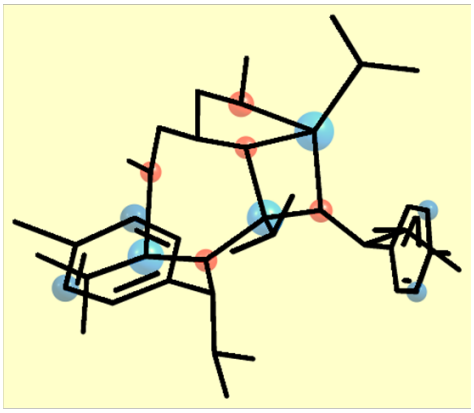
1	2.165489000	-2.955987000	1.803795000
1	2.449716000	-2.599585000	3.510529000
1	2.951127000	-1.442440000	2.284385000
1	-0.180330000	0.056353000	3.908417000
1	1.513233000	0.405481000	3.553145000
1	1.102834000	-0.847758000	4.722750000

a_4



-5.2, *-5.7*





Zero-point correction= 0.868496 (Hartree/Particle)
Thermal correction to Energy= 0.926816
Thermal correction to Enthalpy= 0.927760
Thermal correction to Gibbs Free Energy= 0.769697
Sum of electronic and zero-point Energies= -2530.174249
Sum of electronic and thermal Energies= -2530.115929
Sum of electronic and thermal Enthalpies= -2530.114985
Sum of electronic and thermal Free Energies= -2530.273048

6	-1.047156000	2.906226000	-1.775172000
6	-1.061458000	1.377362000	-1.731847000
1	-0.582398000	3.276640000	-2.702473000
8	-0.294498000	3.345930000	-0.646696000
1	-2.072044000	3.300649000	-1.714781000
8	0.240451000	0.851846000	-1.677875000
6	-1.823107000	0.823570000	-2.931453000
1	-1.623054000	1.095952000	-0.829931000
1	-1.185160000	0.881344000	-3.822675000
1	-2.748255000	1.390106000	-3.119629000
8	-2.165454000	-0.553135000	-2.692630000
6	-2.586356000	-1.212541000	-3.888442000
6	-0.278345000	4.761436000	-0.496383000
1	0.345271000	4.985804000	0.370493000
1	-1.292556000	5.142396000	-0.320243000
1	0.144749000	5.252360000	-1.382639000
1	-3.473185000	-0.725803000	-4.315031000
1	-2.831495000	-2.242297000	-3.627889000
1	-1.779343000	-1.207280000	-4.630498000
30	1.731307000	1.920355000	-0.815286000
30	0.579561000	-0.886277000	-0.614508000
8	1.623217000	0.454566000	0.565200000
6	2.471956000	0.123874000	1.650219000
6	3.576118000	-0.831924000	1.220096000
1	1.873468000	-0.413210000	2.408372000
6	3.019820000	1.392977000	2.357771000

1	3.596268000	1.955082000	1.608932000
6	3.957377000	1.044476000	3.524463000
6	1.870671000	2.282712000	2.853231000
1	1.193619000	2.563040000	2.042963000
1	2.259442000	3.200728000	3.306901000
1	1.280924000	1.760668000	3.617704000
1	4.838638000	0.487213000	3.195810000
1	3.438624000	0.437704000	4.277332000
1	4.304094000	1.956540000	4.021137000
6	4.469256000	-0.551396000	0.179271000
6	3.764457000	-2.074318000	1.824672000
7	5.431117000	-1.392566000	-0.208872000
6	5.516233000	-2.563335000	0.449730000
7	4.717272000	-2.942009000	1.457854000
6	6.588033000	-3.521704000	0.004244000
1	4.406714000	0.388842000	-0.363939000
1	6.661659000	-4.360260000	0.697883000
1	7.553197000	-3.011305000	-0.064541000
1	6.357194000	-3.908496000	-0.994774000
1	3.116697000	-2.389924000	2.643183000
8	-1.337862000	-0.960323000	0.379281000
6	-1.497703000	-0.543524000	1.743736000
6	-1.684467000	-1.741480000	2.705501000
6	-2.606652000	0.497396000	1.837636000
1	-0.560312000	-0.038255000	2.015352000
6	-3.967279000	0.194933000	1.944963000
6	-2.322368000	1.865445000	1.749371000
1	-2.632127000	-2.237529000	2.446767000
6	-1.766178000	-1.278089000	4.169325000
6	-0.559339000	-2.771100000	2.534870000
1	-0.480952000	-3.117532000	1.502434000
1	-0.732713000	-3.639688000	3.178661000
1	0.407781000	-2.338383000	2.818514000
1	-2.602822000	-0.596904000	4.347585000
1	-0.845339000	-0.759831000	4.463572000
1	-1.886998000	-2.137546000	4.836372000
7	-3.261937000	2.816069000	1.751680000
7	-4.931556000	1.124133000	1.945408000
6	-4.538355000	2.404475000	1.846793000
6	-5.606358000	3.464148000	1.869172000
1	-4.308465000	-0.835396000	2.038314000
1	-1.291798000	2.203398000	1.657750000
1	-6.568824000	3.044225000	1.572617000
1	-5.336697000	4.294428000	1.212521000
1	-5.710861000	3.869599000	2.882883000
30	-2.764014000	-1.655290000	-0.642907000
6	-4.398291000	-2.674889000	-1.089420000
6	-5.574772000	-1.750207000	-1.440921000
6	-4.778756000	-3.661794000	0.026489000
1	-4.145944000	-3.261377000	-1.983226000
1	-5.022575000	-3.146418000	0.963917000
1	-3.976388000	-4.375417000	0.243541000
1	-5.669077000	-4.245883000	-0.251681000
1	-5.866079000	-1.119366000	-0.592482000
1	-6.463193000	-2.335422000	-1.722547000
1	-5.345062000	-1.084818000	-2.280440000
6	1.207348000	-2.653865000	-1.349158000
6	2.156090000	-2.464919000	-2.545549000
6	0.070862000	-3.619258000	-1.721192000
1	1.786452000	-3.126513000	-0.542324000
1	-0.552721000	-3.217586000	-2.531620000
1	-0.589986000	-3.830944000	-0.870014000
1	0.451929000	-4.591354000	-2.076782000
1	1.657338000	-1.959269000	-3.382900000
1	2.526159000	-3.429823000	-2.932102000

1	3.036636000	-1.866560000	-2.285020000
6	3.010840000	3.331893000	-1.442455000
6	2.723751000	3.727690000	-2.901522000
6	4.504451000	3.019471000	-1.265840000
1	2.782485000	4.205038000	-0.812106000
1	2.918729000	2.896645000	-3.591155000
1	3.359575000	4.567088000	-3.227490000
1	1.682313000	4.033660000	-3.054509000
1	4.814394000	2.152149000	-1.862989000
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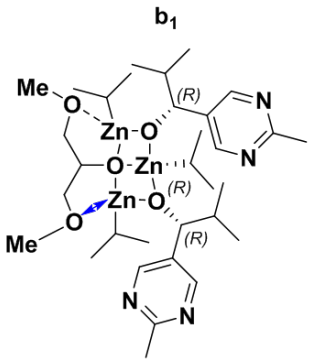
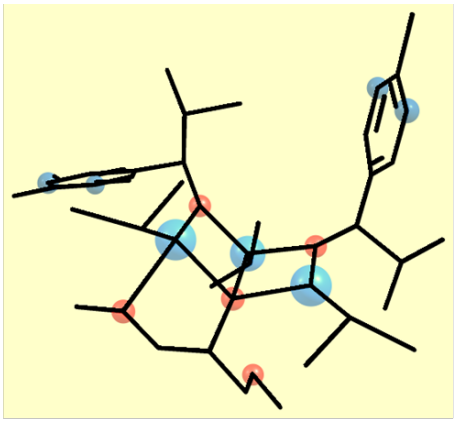
1	5.134055000	3.862986000	-1.592741000

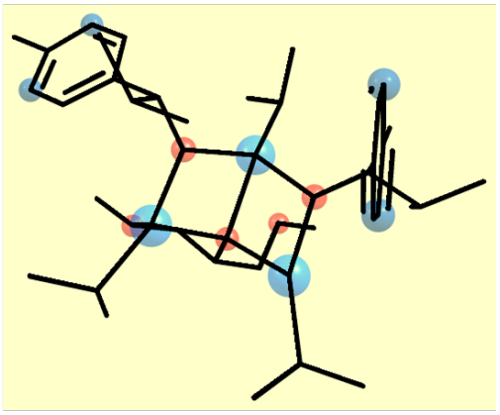
b1



-13.8, *-16.3*

3.3 angstroms





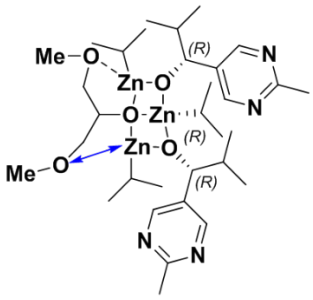
Zero-point correction= 0.868373 (Hartree/Particle)
Thermal correction to Energy= 0.926883
Thermal correction to Enthalpy= 0.927827
Thermal correction to Gibbs Free Energy= 0.766603
Sum of electronic and zero-point Energies= -2530.188029
Sum of electronic and thermal Energies= -2530.129519
Sum of electronic and thermal Enthalpies= -2530.128574
Sum of electronic and thermal Free Energies= -2530.289798

6	-1.944979000	-3.064610000	0.254844000
6	-0.470634000	-3.005760000	0.646703000
1	-2.071233000	-2.793259000	-0.800730000
8	-2.658721000	-2.147734000	1.084490000
1	-2.336947000	-4.080844000	0.406765000
8	0.009956000	-1.670464000	0.510278000
6	0.342763000	-4.025543000	-0.150604000
1	-0.391409000	-3.306074000	1.703199000
1	-0.022960000	-5.038816000	0.090192000
1	1.399852000	-3.984879000	0.161901000
8	0.220462000	-3.769359000	-1.534379000
6	0.899847000	-4.719670000	-2.336559000
6	-4.061052000	-2.140388000	0.821450000
1	-4.515509000	-1.403367000	1.483269000
1	-4.264919000	-1.865077000	-0.220665000
1	-4.492172000	-3.129191000	1.024488000
1	0.745562000	-4.431148000	-3.377869000
1	0.503476000	-5.734144000	-2.180094000
1	1.978994000	-4.730371000	-2.123664000
30	2.016179000	-1.222935000	0.916034000
30	-0.084485000	-0.459216000	-1.344863000
8	-1.183040000	0.700483000	-0.042058000
6	-1.836513000	1.924162000	-0.366261000

6	-3.325291000	1.682297000	-0.569509000
1	-1.433822000	2.273520000	-1.330518000
6	-1.546083000	3.039235000	0.671248000
1	-1.925175000	2.691032000	1.643863000
6	-2.267039000	4.349485000	0.313940000
6	-0.039054000	3.287236000	0.808603000
1	0.503233000	2.369672000	1.044538000
1	0.160051000	4.016866000	1.600575000
1	0.374575000	3.690564000	-0.123145000
1	-3.354651000	4.238034000	0.296568000
1	-1.951268000	4.711103000	-0.672459000
1	-2.022667000	5.129382000	1.042274000
6	-4.207432000	1.400367000	0.479781000
6	-3.916503000	1.693945000	-1.833239000
7	-5.507173000	1.150245000	0.302337000
6	-5.963390000	1.183517000	-0.963908000
7	-5.216365000	1.448120000	-2.045537000
6	-7.429820000	0.914009000	-1.170500000
1	-3.853916000	1.373714000	1.510080000
1	-7.658601000	0.850935000	-2.234909000
1	-8.028489000	1.716474000	-0.725244000
1	-7.722705000	-0.015962000	-0.673953000
1	-3.316967000	1.911731000	-2.716924000
8	1.889439000	-0.197360000	-0.711302000
6	2.907220000	0.453342000	-1.461789000
6	4.133970000	-0.466179000	-1.696488000
6	3.277010000	1.781876000	-0.821334000
1	2.489607000	0.682559000	-2.455462000
6	3.837636000	1.894311000	0.456877000
6	3.064938000	2.998996000	-1.467969000
1	4.532357000	-0.732118000	-0.705226000
6	5.244709000	0.247872000	-2.483257000
6	3.719918000	-1.755803000	-2.419558000
1	2.914389000	-2.278660000	-1.898826000
1	4.572421000	-2.437124000	-2.512429000
1	3.363407000	-1.529235000	-3.432088000
1	5.631895000	1.122529000	-1.953910000
1	4.877214000	0.582610000	-3.461155000
1	6.082767000	-0.433188000	-2.662888000
7	3.357732000	4.188556000	-0.925560000
7	4.140358000	3.063067000	1.025673000
6	3.883585000	4.172796000	0.307822000
6	4.211844000	5.493496000	0.950390000
1	4.055708000	1.006900000	1.050261000
1	2.637679000	3.018920000	-2.471025000
1	5.255321000	5.508893000	1.279955000
1	3.592771000	5.645641000	1.841214000
1	4.036573000	6.311085000	0.250313000
6	-0.424336000	-0.693046000	-3.310238000
6	-0.392237000	0.631901000	-4.091165000
6	-1.705522000	-1.477667000	-3.630209000
1	0.426995000	-1.298096000	-3.654844000
1	-2.605035000	-0.958155000	-3.274462000
1	-1.695116000	-2.472507000	-3.171627000
1	-1.835799000	-1.619143000	-4.716579000
1	-1.203393000	1.306610000	-3.788423000
1	-0.512372000	0.468801000	-5.175287000
1	0.547727000	1.179654000	-3.950968000
6	3.082700000	-1.841563000	2.479114000
6	4.439236000	-2.444751000	2.079210000
6	2.298990000	-2.805729000	3.384873000
1	3.283014000	-0.929583000	3.059957000
1	4.320439000	-3.353588000	1.475645000
1	5.024120000	-2.729435000	2.967531000
1	5.052631000	-1.746147000	1.498992000

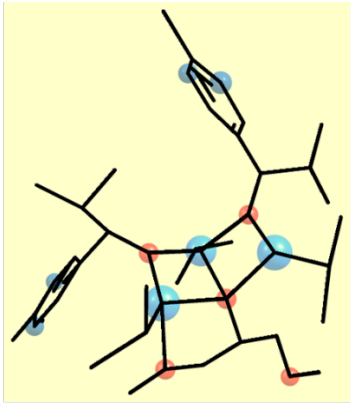
1	2.048746000	-3.740750000	2.867054000
1	1.360740000	-2.369218000	3.744736000
1	2.889272000	-3.085655000	4.271186000
30	-1.234617000	-0.316252000	1.626714000
6	-1.336880000	-0.224066000	3.616011000
6	-0.303104000	0.724837000	4.244631000
1	-1.094139000	-1.246247000	3.942618000
6	-2.749454000	0.097989000	4.130142000
1	-3.067886000	1.109420000	3.844443000
1	-2.795534000	0.057535000	5.230301000
1	-3.502191000	-0.602065000	3.750234000
1	0.726069000	0.460619000	3.973692000
1	-0.359935000	0.709926000	5.344832000
1	-0.462022000	1.765615000	3.935208000

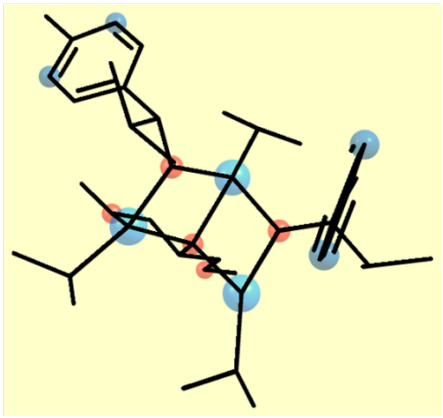
b3



-13.2, *-15.0*

4.7 angstroms





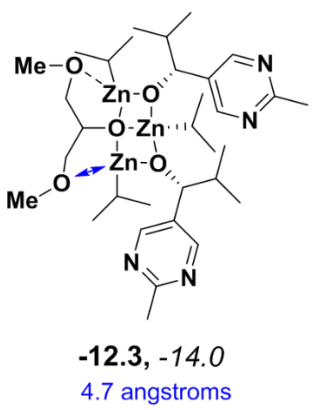
Zero-point correction= 0.868511 (Hartree/Particle)
Thermal correction to Energy= 0.926902
Thermal correction to Enthalpy= 0.927846
Thermal correction to Gibbs Free Energy= 0.767689
Sum of electronic and zero-point Energies= -2530.187026
Sum of electronic and thermal Energies= -2530.128635
Sum of electronic and thermal Enthalpies= -2530.127691
Sum of electronic and thermal Free Energies= -2530.287847

6	-2.036908000	-2.951902000	0.085614000
6	-0.548052000	-2.970771000	0.413888000
1	-2.195512000	-2.615833000	-0.950004000
8	-2.680671000	-2.051766000	0.987928000
1	-2.454604000	-3.959706000	0.195529000
8	-0.024786000	-1.644286000	0.395975000
6	0.205178000	-3.858407000	-0.581378000
1	-0.424377000	-3.397316000	1.419478000
6	-4.099117000	-2.027063000	0.831036000
1	-4.495889000	-1.311519000	1.551014000
1	-4.521038000	-3.020101000	1.030749000
1	-4.378419000	-1.711893000	-0.181633000
30	-0.061660000	-0.350792000	-1.380321000
30	2.012323000	-1.320441000	0.821089000
8	1.938849000	-0.295130000	-0.813815000
6	2.985017000	0.366890000	-1.514606000
6	3.203912000	1.765802000	-0.960831000
1	2.663170000	0.483726000	-2.562188000
6	4.288996000	-0.474446000	-1.539772000
1	4.602679000	-0.618526000	-0.493830000

6	5.422677000	0.251437000	-2.282219000
6	4.048023000	-1.853970000	-2.170346000
1	3.249504000	-2.405687000	-1.667906000
1	4.959044000	-2.460109000	-2.127785000
1	3.765120000	-1.751566000	-3.224972000
1	5.686828000	1.201475000	-1.810512000
1	5.138470000	0.459413000	-3.321119000
1	6.322493000	-0.371539000	-2.306376000
6	3.601986000	2.015731000	0.358116000
6	3.020882000	2.909565000	-1.736865000
7	3.803192000	3.241947000	0.844096000
6	3.598489000	4.271029000	0.000154000
7	3.208868000	4.154444000	-1.277839000
6	3.815058000	5.656389000	0.546283000
1	3.768224000	1.194335000	1.054084000
1	3.752800000	6.395032000	-0.253649000
1	4.789391000	5.724993000	1.038975000
1	3.056367000	5.887039000	1.302458000
1	2.709248000	2.822210000	-2.778216000
8	-1.028984000	0.827271000	-0.005375000
6	-1.639586000	2.083655000	-0.281281000
6	-1.385583000	3.111808000	0.850515000
6	-3.117979000	1.897136000	-0.586188000
1	-1.175026000	2.492507000	-1.193427000
6	-4.059648000	1.520189000	0.378390000
6	-3.640952000	2.068920000	-1.867881000
1	-1.818864000	2.696077000	1.772635000
6	-2.064438000	4.460379000	0.560484000
6	0.116951000	3.313600000	1.077696000
1	0.624678000	2.369275000	1.280779000
1	0.292995000	3.985603000	1.924143000
1	0.583652000	3.762958000	0.193017000
1	-3.151638000	4.374086000	0.482209000
1	-1.693677000	4.888758000	-0.378951000
1	-1.842942000	5.177243000	1.357658000
7	-4.932880000	1.884176000	-2.172321000
7	-5.352501000	1.325459000	0.107634000
6	-5.740563000	1.515769000	-1.167635000
6	-7.197058000	1.298046000	-1.478471000
1	-3.762819000	1.370806000	1.416305000
1	-2.990717000	2.370161000	-2.689336000
1	-7.820271000	1.950059000	-0.857905000
1	-7.486605000	0.267066000	-1.249016000
1	-7.395062000	1.501659000	-2.531230000
6	3.050750000	-2.085624000	2.331287000
6	2.154884000	-2.735833000	3.398391000
6	4.025745000	-1.082252000	2.970870000
1	3.652703000	-2.882324000	1.869394000
1	3.501079000	-0.232733000	3.425245000
1	4.742505000	-0.676974000	2.247244000
1	4.611565000	-1.557326000	3.772880000
1	1.497249000	-2.003632000	3.881735000
1	2.760707000	-3.194402000	4.195315000
1	1.516393000	-3.523886000	2.983905000
1	0.089635000	-3.453168000	-1.601175000
8	-0.310844000	-5.171194000	-0.496734000
1	1.282677000	-3.847866000	-0.342021000
6	0.316417000	-6.068809000	-1.395163000
1	-0.151180000	-7.045952000	-1.256542000
1	1.394437000	-6.156279000	-1.191961000
1	0.184557000	-5.753094000	-2.440954000
30	-1.211009000	-0.310256000	1.592388000
6	-1.328780000	-0.235569000	3.585053000
6	-2.751644000	0.035543000	4.100743000
6	-0.331321000	0.749083000	4.217466000

1	-1.049775000	-1.248750000	3.909099000
1	-0.527203000	1.783843000	3.909473000
1	0.707687000	0.524421000	3.947897000
1	-0.389566000	0.729517000	5.317511000
1	-3.112513000	1.030139000	3.806630000
1	-2.790806000	0.004409000	5.201488000
1	-3.477052000	-0.698944000	3.733333000
6	-0.595824000	-0.528522000	-3.312390000
6	0.426470000	-1.291761000	-4.170178000
1	-0.615606000	0.510763000	-3.677188000
6	-2.004194000	-1.105957000	-3.526994000
1	1.428878000	-0.853041000	-4.115730000
1	0.134650000	-1.305369000	-5.233253000
1	0.518603000	-2.340636000	-3.858165000
1	-2.065938000	-2.155057000	-3.207841000
1	-2.290640000	-1.089278000	-4.591314000
1	-2.773848000	-0.552251000	-2.978213000

b_4



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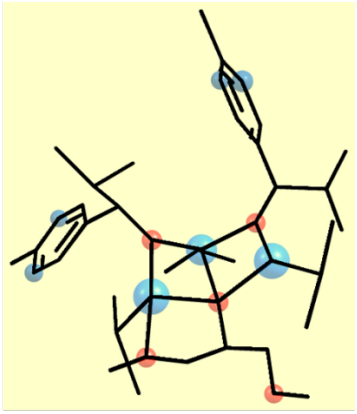
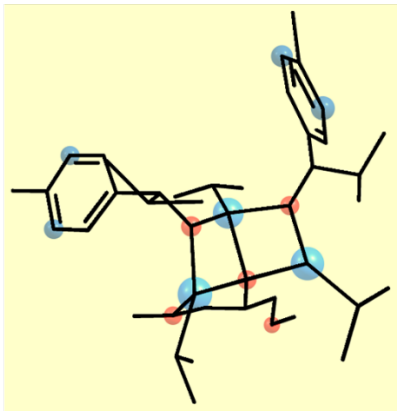
4.7 angstroms





Zero-point correction= 0.868529 (Hartree/Particle)
Thermal correction to Energy= 0.927012
Thermal correction to Enthalpy= 0.927957
Thermal correction to Gibbs Free Energy= 0.767892
Sum of electronic and zero-point Energies= -2530.185656
Sum of electronic and thermal Energies= -2530.127173
Sum of electronic and thermal Enthalpies= -2530.126229
Sum of electronic and thermal Free Energies= -2530.286293

6	-1.523243000	-3.249496000	-0.710163000
6	-0.089257000	-3.125011000	-0.199294000
1	-1.625127000	-2.739788000	-1.680028000
8	-2.390045000	-2.643840000	0.246845000
1	-1.782444000	-4.306887000	-0.842223000
8	0.195852000	-1.762383000	0.115083000
6	0.892754000	-3.666006000	-1.243071000
1	0.007668000	-3.735598000	0.709667000
6	-3.769262000	-2.727740000	-0.104906000
1	-4.338810000	-2.263138000	0.701014000
1	-4.076345000	-3.776330000	-0.207579000
1	-3.971030000	-2.197867000	-1.044081000
30	-0.114553000	-0.075238000	-1.316022000
30	2.134277000	-1.133431000	0.630112000
8	1.885310000	0.123770000	-0.819488000

6	2.789892000	1.017346000	-1.454863000
6	2.747081000	2.382258000	-0.786240000
1	2.446345000	1.159077000	-2.492980000
6	4.225315000	0.434863000	-1.538283000
1	4.563829000	0.251903000	-0.506899000
6	5.202949000	1.424182000	-2.193746000
6	4.243349000	-0.898653000	-2.300480000
1	3.583934000	-1.646877000	-1.853240000
1	5.256577000	-1.313593000	-2.321794000
1	3.921843000	-0.753245000	-3.339140000
1	5.292242000	2.355573000	-1.628580000
1	4.879205000	1.678326000	-3.210564000
1	6.201011000	0.980777000	-2.267739000
6	3.089567000	2.588841000	0.555452000
6	2.346239000	3.532048000	-1.465810000
7	3.055575000	3.785645000	1.144793000
6	2.661413000	4.826262000	0.385788000
7	2.296636000	4.746845000	-0.901914000
6	2.621477000	6.177452000	1.047315000
1	3.403727000	1.755791000	1.182403000
1	3.580983000	6.396199000	1.525666000
1	1.860757000	6.191977000	1.835615000
1	2.390344000	6.952588000	0.315828000
1	2.052447000	3.475597000	-2.514423000
8	-1.072349000	0.584048000	0.364671000
6	-1.692854000	1.857309000	0.504011000
6	-1.678886000	2.353172000	1.974418000
6	-3.095007000	1.832665000	-0.085571000
1	-1.107610000	2.587123000	-0.079536000
6	-4.105596000	0.984889000	0.383932000
6	-3.473481000	2.647814000	-1.151771000
1	-2.248581000	1.623488000	2.569719000
6	-2.361196000	3.723528000	2.117242000
6	-0.248891000	2.417359000	2.526057000
1	0.258771000	1.452506000	2.457429000
1	-0.255555000	2.719546000	3.578512000
1	0.350844000	3.149742000	1.974440000
1	-3.411662000	3.699006000	1.815065000
1	-1.853195000	4.479074000	1.505364000
1	-2.320110000	4.061741000	3.157555000
7	-4.697412000	2.632608000	-1.697828000
7	-5.332432000	0.942744000	-0.139378000
6	-5.581496000	1.775150000	-1.168639000
6	-6.961479000	1.728385000	-1.767352000
1	-3.920824000	0.310746000	1.219881000
1	-2.759713000	3.346563000	-1.588690000
1	-7.719649000	1.869191000	-0.990762000
1	-7.145899000	0.748456000	-2.221155000
1	-7.070418000	2.499920000	-2.530252000
6	3.349719000	-1.844175000	2.037731000
6	2.664446000	-2.856051000	2.969395000
6	4.050629000	-0.737912000	2.843537000
1	4.124955000	-2.382526000	1.472362000
1	3.338199000	-0.128307000	3.412846000
1	4.625877000	-0.058848000	2.203754000
1	4.754637000	-1.165823000	3.573913000
1	1.864761000	-2.390814000	3.557802000
1	3.380981000	-3.281777000	3.688990000
1	2.219356000	-3.693873000	2.421012000
1	0.814296000	-3.079016000	-2.173337000
8	0.589200000	-5.026790000	-1.477272000
1	1.926730000	-3.559432000	-0.871747000
6	1.428907000	-5.619280000	-2.451859000
1	1.117157000	-6.660491000	-2.558627000
1	2.485477000	-5.592237000	-2.145180000

1	1.337006000	-5.115669000	-3.425870000
30	-1.221001000	-1.005871000	1.522933000
6	-1.722845000	-1.581943000	3.369555000
6	-1.038515000	-0.794896000	4.498487000
6	-1.541165000	-3.095407000	3.571300000
1	-2.801622000	-1.369545000	3.429195000
1	-0.484178000	-3.385965000	3.524641000
1	-2.073044000	-3.678216000	2.812579000
1	-1.913061000	-3.415581000	4.557682000
1	0.048980000	-0.942705000	4.499576000
1	-1.399732000	-1.120208000	5.487133000
1	-1.218092000	0.282980000	4.426801000
6	-0.672381000	0.079796000	-3.241528000
6	0.251394000	-0.681863000	-4.206131000
1	-0.550388000	1.153340000	-3.457115000
6	-2.142850000	-0.268419000	-3.521207000
1	1.305740000	-0.411433000	-4.078413000
1	-0.010487000	-0.486687000	-5.258975000
1	0.178932000	-1.768448000	-4.064458000
1	-2.354179000	-1.329766000	-3.333763000
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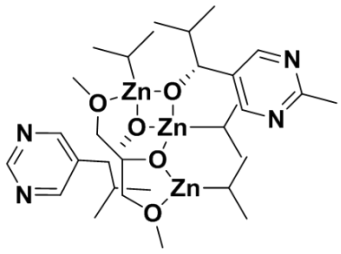
1	-2.834577000	0.314214000	-2.904080000

b_5



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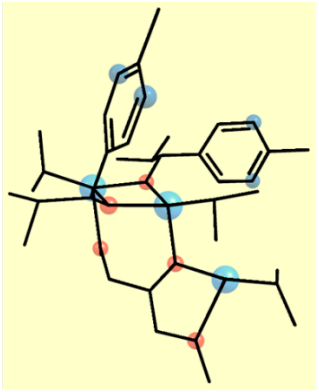

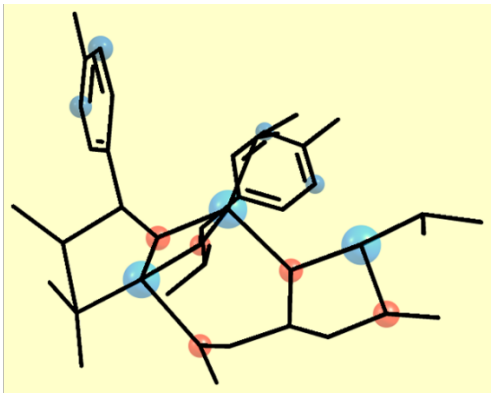

Zero-point correction= 0.868611 (Hartree/Particle)
Thermal correction to Energy= 0.926038
Thermal correction to Enthalpy= 0.926982
Thermal correction to Gibbs Free Energy= 0.770758
Sum of electronic and zero-point Energies= -2530.166047
Sum of electronic and thermal Energies= -2530.108621
Sum of electronic and thermal Enthalpies= -2530.107677
Sum of electronic and thermal Free Energies= -2530.263901

6	-2.138120000	-3.768763000	-0.540699000
6	-1.545739000	-2.798245000	0.485234000
1	-1.541215000	-3.759681000	-1.465014000
8	-3.467713000	-3.331539000	-0.823492000
1	-2.165014000	-4.794324000	-0.146167000
8	-1.653752000	-1.463536000	0.018513000
6	-0.097197000	-3.211085000	0.753944000
1	-2.130142000	-2.917321000	1.413217000

6	-4.120544000	-4.117644000	-1.819899000
1	-5.115236000	-3.696378000	-1.962527000
1	-4.208812000	-5.160162000	-1.489343000
1	-3.567919000	-4.086998000	-2.767691000
30	-0.086139000	0.085130000	-0.517216000
30	2.117152000	-0.754171000	1.407252000
8	1.678153000	-1.002168000	-0.544880000
6	2.505492000	-1.112237000	-1.687392000
6	2.931677000	0.256901000	-2.206926000
1	1.923242000	-1.588608000	-2.497023000
6	3.737345000	-2.032137000	-1.445594000
1	4.357485000	-1.550109000	-0.677051000
6	4.589218000	-2.187998000	-2.715989000
6	3.313171000	-3.412466000	-0.927439000
1	2.782442000	-3.344704000	0.023520000
1	4.190424000	-4.051821000	-0.780043000
1	2.657034000	-3.913865000	-1.650869000
1	4.988195000	-1.233723000	-3.069715000
1	4.002779000	-2.629260000	-3.531846000
1	5.437868000	-2.853251000	-2.525819000
6	3.493575000	1.243480000	-1.390628000
6	2.793370000	0.627702000	-3.545817000
7	3.869374000	2.445485000	-1.838753000
6	3.685351000	2.688581000	-3.148492000
7	3.161483000	1.820941000	-4.028040000
6	4.077112000	4.049096000	-3.659975000
1	3.647164000	1.062364000	-0.328454000
1	4.287138000	4.009221000	-4.730274000
1	4.946814000	4.426994000	-3.117869000
1	3.256471000	4.759959000	-3.503685000
1	2.362042000	-0.068845000	-4.264905000
8	0.530703000	0.517957000	1.401625000
6	0.440786000	1.777945000	2.055880000
6	0.249598000	1.644840000	3.599858000
6	-0.700681000	2.599007000	1.480986000
1	1.368835000	2.356102000	1.896258000
6	-2.032222000	2.171688000	1.542379000
6	-0.521386000	3.862841000	0.920079000
1	-0.654863000	1.038583000	3.752064000
6	0.039506000	3.015590000	4.269570000
6	1.423105000	0.935995000	4.282237000
1	1.600196000	-0.061414000	3.879192000
1	1.233581000	0.831882000	5.356288000
1	2.347932000	1.513687000	4.166373000
1	-0.869394000	3.517819000	3.930236000
1	0.886392000	3.683134000	4.066645000
1	-0.030861000	2.898937000	5.355994000
7	-1.533043000	4.626377000	0.482573000
7	-3.060042000	2.908745000	1.116371000
6	-2.768274000	4.119632000	0.603498000
6	-3.921667000	4.954285000	0.116734000
1	0.478903000	4.284857000	0.823895000
1	-4.733653000	4.950564000	0.849124000
1	-4.322848000	4.535448000	-0.813382000
1	-3.596520000	5.977759000	-0.074156000
6	3.846293000	-1.222667000	2.321874000
6	3.706357000	-2.074157000	3.593359000
6	4.773048000	-0.022085000	2.575313000
1	4.338573000	-1.857195000	1.570772000
1	4.348178000	0.678299000	3.304357000
1	4.978844000	0.548439000	1.661760000
1	5.746862000	-0.343115000	2.979981000
1	3.215430000	-1.524851000	4.406790000
1	4.691593000	-2.383560000	3.978860000
1	3.127069000	-2.987433000	3.416958000

1	-0.061428000	-4.292519000	0.960377000
8	0.537660000	-2.515985000	1.825735000
1	0.508745000	-2.985334000	-0.124056000
6	0.029565000	-2.815105000	3.122263000
1	0.715433000	-2.369991000	3.843343000
1	-0.004915000	-3.901201000	3.283555000
1	-0.970959000	-2.395241000	3.275912000
30	-3.422992000	-0.984632000	-0.465871000
6	-5.172783000	-0.110787000	-0.742620000
6	-5.745214000	0.439924000	0.575145000
6	-6.183137000	-1.025945000	-1.451070000
1	-4.965695000	0.741349000	-1.402044000
1	-6.418886000	-1.915392000	-0.853628000
1	-5.826670000	-1.365780000	-2.429955000
1	-7.133447000	-0.496647000	-1.617882000
1	-5.908428000	-0.353003000	1.316255000
1	-6.723608000	0.913593000	0.399898000
1	-5.091171000	1.197488000	1.017994000
6	-0.695746000	0.897644000	-2.265793000
6	-0.985950000	-0.201665000	-3.301695000
1	0.203028000	1.429181000	-2.608263000
6	-1.835785000	1.924612000	-2.250941000
1	-0.148895000	-0.899937000	-3.419635000
1	-1.199990000	0.221029000	-4.297270000
1	-1.860916000	-0.805624000	-3.024545000
1	-2.782191000	1.495898000	-1.895776000
1	-2.035230000	2.317164000	-3.262379000
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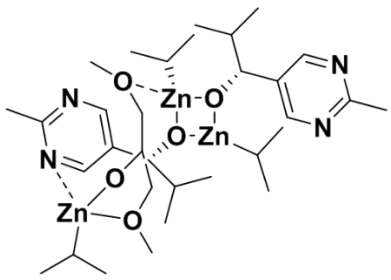
1	-2.275620000	1.195710000	1.959267000

c_2



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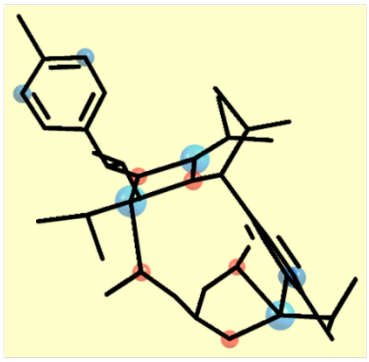

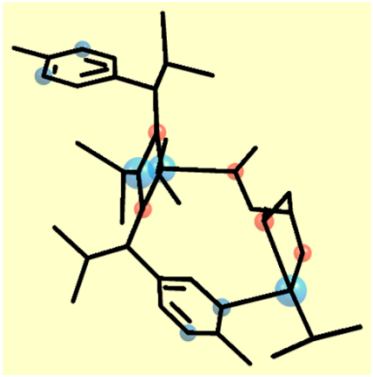

Zero-point correction= 0.868556 (Hartree/Particle)
Thermal correction to Energy= 0.926950
Thermal correction to Enthalpy= 0.927894
Thermal correction to Gibbs Free Energy= 0.768733
Sum of electronic and zero-point Energies= -2530.172118
Sum of electronic and thermal Energies= -2530.113724
Sum of electronic and thermal Enthalpies= -2530.112780
Sum of electronic and thermal Free Energies= -2530.271941

6	-1.557249000	0.193597000	-2.452052000
6	-2.582720000	-0.952119000	-2.600260000
1	-1.832730000	0.994086000	-3.152010000

8	-0.179409000	-0.168419000	-2.637228000
1	-1.610916000	0.591490000	-1.441307000
8	-3.852215000	-0.444756000	-2.326653000
6	-2.242383000	-2.179965000	-1.745841000
1	-2.540736000	-1.314655000	-3.644514000
6	0.181822000	-0.412528000	-3.993216000
1	-0.064373000	0.448578000	-4.629278000
1	-0.318628000	-1.302060000	-4.393982000
1	1.261124000	-0.576194000	-4.016766000
30	1.538742000	1.037769000	-1.115306000
30	1.055415000	-0.715152000	1.357700000
8	2.085304000	-0.722963000	-0.358937000
6	3.192317000	-1.492035000	-0.809382000
6	4.495820000	-0.839713000	-0.372827000
1	3.187755000	-1.495637000	-1.912567000
6	3.076915000	-2.971676000	-0.362900000
1	3.032406000	-2.976375000	0.736166000
6	4.295804000	-3.800117000	-0.798550000
6	1.786369000	-3.602511000	-0.903748000
1	0.904809000	-3.024814000	-0.617358000
1	1.667014000	-4.624114000	-0.527834000
1	1.811898000	-3.651722000	-1.999522000
1	5.226439000	-3.435092000	-0.355861000
1	4.412883000	-3.782161000	-1.889143000
1	4.171291000	-4.845780000	-0.499496000
6	4.799201000	-0.561057000	0.965791000
6	5.476341000	-0.445903000	-1.282886000
7	5.932112000	0.026686000	1.354102000
6	6.806469000	0.360516000	0.385371000
7	6.623011000	0.148058000	-0.925507000
6	8.083249000	1.028894000	0.818255000
1	4.100280000	-0.823290000	1.759501000
1	8.727507000	1.210866000	-0.042529000
1	8.612142000	0.405232000	1.545974000
1	7.864569000	1.981353000	1.312742000
1	5.333704000	-0.614727000	-2.350562000
8	0.525244000	1.069940000	0.668935000
6	-0.040306000	2.213754000	1.284677000
6	0.275312000	2.258825000	2.807028000
6	-1.527836000	2.309369000	0.965995000
1	0.425408000	3.112839000	0.846211000
6	-2.338984000	1.188476000	0.794715000
6	-2.169433000	3.530713000	0.743695000
1	-0.051756000	1.295106000	3.222361000
6	-0.475015000	3.374563000	3.551204000
6	1.787497000	2.414747000	3.035757000
1	2.374213000	1.666522000	2.496892000
1	2.029449000	2.330343000	4.100159000
1	2.125167000	3.402056000	2.696993000
1	-1.559737000	3.243599000	3.518527000
1	-0.239586000	4.360330000	3.131609000
1	-0.174608000	3.390197000	4.603670000
7	-3.463599000	3.640754000	0.425268000
7	-3.629270000	1.272559000	0.435904000
6	-4.155564000	2.503737000	0.278337000
6	-5.602035000	2.609056000	-0.115352000
1	-1.614748000	4.465702000	0.817670000
1	-6.219151000	1.931828000	0.480800000
1	-5.728738000	2.331474000	-1.168398000
1	-5.947525000	3.635300000	0.013035000
6	0.762928000	-2.001297000	2.850198000
6	-0.442005000	-1.660477000	3.740851000
6	2.024193000	-2.205584000	3.707881000
1	0.547764000	-2.954218000	2.345404000
1	2.322522000	-1.283677000	4.222583000

1	2.883849000	-2.542764000	3.117592000
1	1.854401000	-2.962390000	4.489658000
1	-0.290755000	-0.721981000	4.288470000
1	-0.611728000	-2.441785000	4.498064000
1	-1.371368000	-1.554413000	3.169873000
1	-2.862804000	-3.027469000	-2.070761000
8	-2.536655000	-1.894065000	-0.368395000
1	-1.183927000	-2.454381000	-1.845382000
6	-2.484358000	-3.055139000	0.457182000
1	-1.478080000	-3.493039000	0.453059000
1	-3.203950000	-3.811748000	0.117987000
1	-2.738580000	-2.745660000	1.472372000
30	-4.606712000	-0.648396000	-0.606413000
6	-6.116683000	-1.259570000	0.540012000
6	-5.795323000	-1.174407000	2.039901000
6	-6.626852000	-2.661194000	0.165279000
1	-6.932897000	-0.549329000	0.337762000
1	-5.858264000	-3.429477000	0.321943000
1	-6.934016000	-2.721974000	-0.885020000
1	-7.494455000	-2.956915000	0.777452000
6	2.053758000	2.602304000	-2.240313000
6	3.047532000	2.274690000	-3.366078000
1	2.563032000	3.282961000	-1.541509000
6	0.823312000	3.340464000	-2.791171000
1	3.970315000	1.821166000	-2.986959000
1	3.337112000	3.181246000	-3.921524000
1	2.619300000	1.581873000	-4.101212000
1	0.244814000	2.709022000	-3.476116000
1	1.113165000	4.241052000	-3.355886000
1	0.140070000	3.662264000	-1.996631000
1	-1.937348000	0.185290000	0.892522000
1	-4.993168000	-1.868901000	2.323509000
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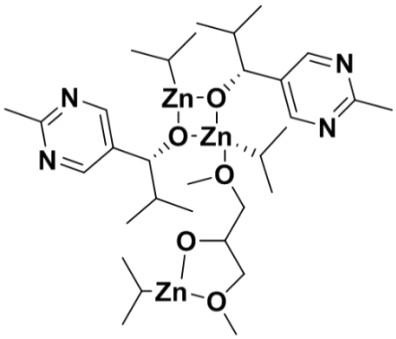
1	-5.471529000	-0.170575000	2.337114000

C_3



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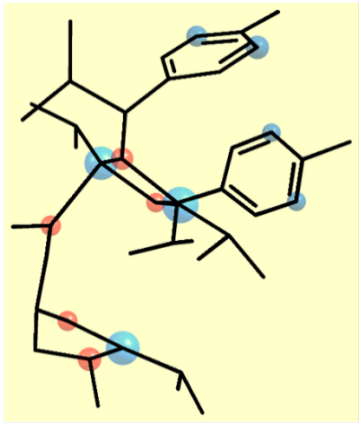

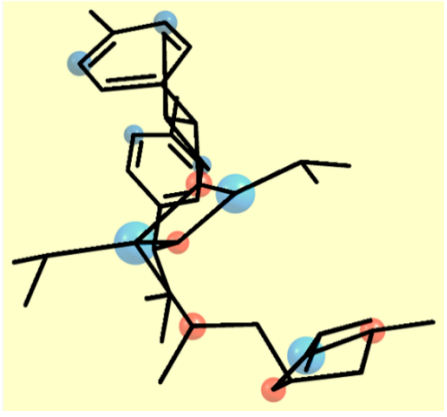

Zero-point correction= 0.869212 (Hartree/Particle)
Thermal correction to Energy= 0.927441
Thermal correction to Enthalpy= 0.928385
Thermal correction to Gibbs Free Energy= 0.769056
Sum of electronic and zero-point Energies= -2530.165082
Sum of electronic and thermal Energies= -2530.106853
Sum of electronic and thermal Enthalpies= -2530.105909
Sum of electronic and thermal Free Energies= -2530.265238

6	-4.466025000	-2.149856000	-1.286456000
6	-3.749540000	-2.226640000	0.070925000
1	-4.134936000	-2.948065000	-1.966915000
8	-4.188600000	-0.872534000	-1.868768000
1	-5.550409000	-2.250957000	-1.134764000
8	-4.003759000	-1.107488000	0.864287000
6	-2.242306000	-2.470441000	-0.146479000
1	-4.165543000	-3.120772000	0.566509000
6	-4.865848000	-0.662391000	-3.104976000
1	-5.954115000	-0.734668000	-2.975747000
1	-4.545574000	-1.399183000	-3.852481000
1	-4.606435000	0.338792000	-3.450553000
30	0.319038000	0.403272000	-0.979170000
30	0.774140000	-1.627657000	1.242756000
8	0.959520000	-1.522939000	-0.761148000
6	1.999862000	-2.015118000	-1.599257000
6	3.263411000	-1.192330000	-1.379736000
1	1.692186000	-1.857217000	-2.647713000
6	2.220991000	-3.536588000	-1.429805000
1	2.565827000	-3.711909000	-0.400594000
6	3.301569000	-4.052281000	-2.393494000
6	0.909657000	-4.307648000	-1.627669000
1	0.147049000	-3.982535000	-0.917960000
1	1.070674000	-5.382912000	-1.494720000
1	0.517965000	-4.152208000	-2.640980000
1	4.265113000	-3.558979000	-2.236989000
1	3.005821000	-3.885613000	-3.436763000
1	3.451226000	-5.128739000	-2.261738000
6	4.020967000	-1.248799000	-0.203135000
6	3.710595000	-0.252054000	-2.309353000
7	5.058978000	-0.446004000	0.041836000
6	5.370496000	0.453289000	-0.910922000
7	4.746880000	0.568705000	-2.093664000
6	6.476934000	1.422704000	-0.602319000
1	3.781433000	-1.969258000	0.577016000
1	6.886042000	1.845874000	-1.521382000
1	7.266671000	0.936163000	-0.025145000
1	6.069436000	2.238668000	0.007349000
1	3.207472000	-0.151299000	-3.271534000
8	0.211491000	0.332416000	0.986761000
6	0.455240000	1.355492000	1.954484000
6	-0.860666000	1.895793000	2.562214000
6	1.354655000	2.425825000	1.352159000
1	1.022824000	0.902203000	2.784001000
6	0.895916000	3.504078000	0.590707000
6	2.747435000	2.352953000	1.473662000
1	-1.446752000	2.343905000	1.746186000
6	-0.589928000	2.974827000	3.623764000
6	-1.689930000	0.752895000	3.165319000
1	-1.926201000	-0.016416000	2.427633000
1	-2.631091000	1.138598000	3.573405000
1	-1.147162000	0.278389000	3.992820000
1	-0.065012000	3.843678000	3.217069000
1	0.019519000	2.569939000	4.441310000
1	-1.530671000	3.326335000	4.059760000
7	3.584775000	3.218949000	0.896778000
7	1.710634000	4.387873000	0.000198000
6	3.029613000	4.204106000	0.168428000
6	3.964818000	5.164333000	-0.514477000
1	3.205601000	1.558264000	2.062600000
1	3.410452000	6.008075000	-0.926946000
1	4.492754000	4.656482000	-1.329707000
1	4.723432000	5.524075000	0.186455000
6	1.710465000	-2.482580000	2.799750000
6	1.834055000	-4.012756000	2.709321000
6	1.169662000	-2.063855000	4.177717000
1	2.731043000	-2.075820000	2.727734000
1	0.136320000	-2.395061000	4.340108000
1	1.179940000	-0.976864000	4.315079000
1	1.770203000	-2.499425000	4.992537000

1	0.858244000	-4.511436000	2.759775000
1	2.435807000	-4.416313000	3.539386000
1	2.311026000	-4.338594000	1.777934000
1	-2.106060000	-3.433757000	-0.663544000
8	-1.464798000	-2.468566000	1.055642000
1	-1.812630000	-1.686259000	-0.772616000
6	-1.925074000	-3.385778000	2.048863000
1	-2.040283000	-4.394883000	1.629686000
1	-2.875726000	-3.051947000	2.475949000
1	-1.167447000	-3.410389000	2.830902000
30	-4.183211000	0.559850000	0.096651000
6	-4.407033000	2.501399000	-0.168684000
6	-5.239020000	3.129027000	0.964470000
6	-4.981012000	2.872071000	-1.544937000
1	-3.391165000	2.916742000	-0.106762000
1	-5.982628000	2.451818000	-1.699029000
1	-4.346594000	2.523760000	-2.367224000
1	-5.074708000	3.963731000	-1.649432000
6	-0.055505000	1.272674000	-2.730026000
6	-0.810642000	0.297706000	-3.652124000
1	0.937679000	1.444287000	-3.169963000
6	-0.770538000	2.629610000	-2.659945000
1	-0.266817000	-0.643047000	-3.796952000
1	-0.971938000	0.737366000	-4.649453000
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1	-1.755772000	2.552384000	-2.182499000
1	-0.940709000	3.040114000	-3.668262000
1	-0.192513000	3.374010000	-2.103499000
1	-0.169468000	3.671866000	0.445050000
1	-6.266169000	2.744135000	0.977222000
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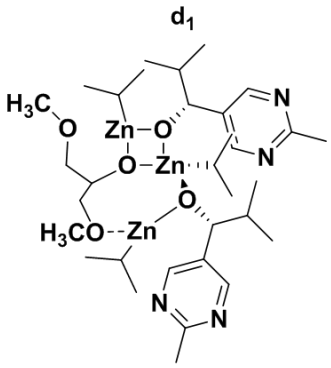
1	-4.806939000	2.938437000	1.953008000

d_1



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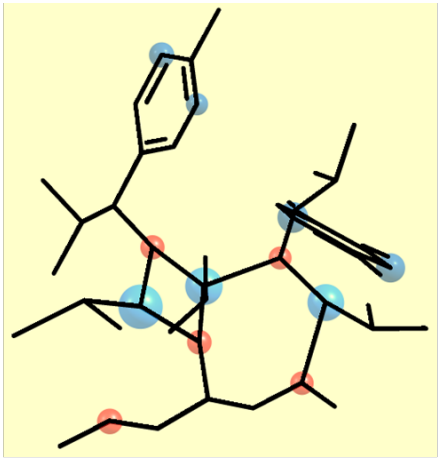

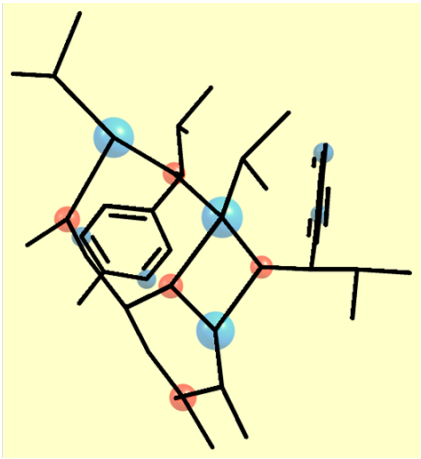

Zero-point correction= 0.869251 (Hartree/Particle)
Thermal correction to Energy= 0.927524
Thermal correction to Enthalpy= 0.928469
Thermal correction to Gibbs Free Energy= 0.769241
Sum of electronic and zero-point Energies= -2530.173502
Sum of electronic and thermal Energies= -2530.115229
Sum of electronic and thermal Enthalpies= -2530.114285
Sum of electronic and thermal Free Energies= -2530.273512

6	-1.437912000	-3.889888000	-1.241916000
6	-0.344026000	-3.208089000	-0.411959000
1	-1.478208000	-3.443637000	-2.248789000
8	-2.678148000	-3.707256000	-0.580036000
1	-1.222758000	-4.965685000	-1.354403000
8	-0.611399000	-1.847509000	-0.210678000
6	1.007218000	-3.410343000	-1.110212000
1	-0.318571000	-3.723940000	0.562593000
1	0.987112000	-2.937908000	-2.096669000
1	1.207897000	-4.484109000	-1.244111000
8	2.112791000	-2.812515000	-0.428348000
6	2.464504000	-3.449226000	0.800622000
6	-3.767861000	-4.271043000	-1.291592000
1	-4.670927000	-4.070243000	-0.712624000
1	-3.649489000	-5.358386000	-1.408600000
1	-3.871919000	-3.821421000	-2.289868000
1	1.708530000	-3.285275000	1.575454000
1	3.408034000	-3.009223000	1.128940000
1	2.606634000	-4.526960000	0.648183000
30	-2.179679000	-1.200143000	0.778080000
6	-3.488768000	-1.391725000	2.265065000
6	-4.799363000	-2.066052000	1.829491000
1	-3.729281000	-0.360522000	2.564244000
6	-2.891262000	-2.102204000	3.491154000
1	-5.281882000	-1.544131000	0.994412000
1	-5.526572000	-2.098446000	2.657071000
1	-4.630543000	-3.102072000	1.513251000
1	-2.587064000	-3.130092000	3.254698000
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1	-2.013864000	-1.577479000	3.884722000
30	-0.229545000	-0.190578000	-1.398529000
8	-1.777289000	0.490000000	-0.288162000
6	0.273700000	-0.166308000	-3.356923000
6	0.378838000	1.253736000	-3.938720000
6	-0.638198000	-1.028984000	-4.245369000
1	-0.596710000	1.758482000	-3.944618000
1	0.727046000	1.244382000	-4.984927000
1	1.069668000	1.890016000	-3.374067000
1	-1.674767000	-0.668124000	-4.232270000
1	-0.661332000	-2.079199000	-3.930427000
1	-0.314028000	-1.017860000	-5.299447000
1	1.284455000	-0.607200000	-3.410749000
6	-2.729480000	1.526462000	-0.460344000
6	-2.097236000	2.877330000	-0.159641000
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6	-3.423513000	1.481663000	-1.847717000
1	-2.646028000	1.625291000	-2.612080000
6	-4.465115000	2.602613000	-1.995937000
6	-4.079277000	0.114964000	-2.087764000
1	-3.351948000	-0.698669000	-2.039303000
1	-4.556306000	0.083119000	-3.073314000
1	-4.857698000	-0.078838000	-1.338264000
1	-4.020590000	3.597748000	-1.906984000
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1	-4.957192000	2.542857000	-2.972184000
6	-1.143353000	3.487443000	-0.983093000
6	-2.409142000	3.595820000	0.995019000
7	-0.571611000	4.660711000	-0.697375000
6	-0.953727000	5.263140000	0.444494000
7	-1.854322000	4.774409000	1.309298000
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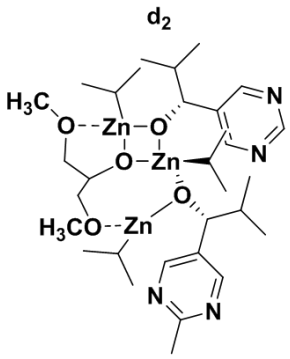
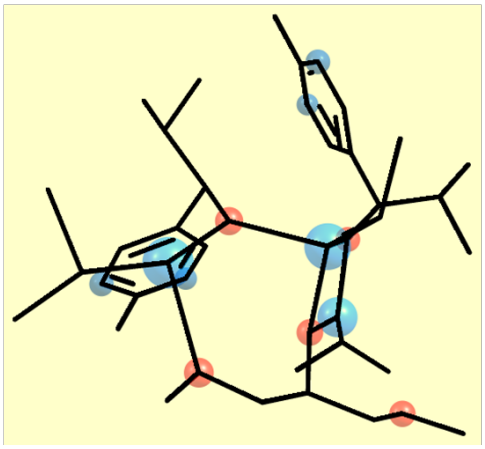
1	-0.822983000	3.014818000	-1.909701000
1	-0.546409000	7.318935000	-0.020545000
1	0.771799000	6.492634000	0.801496000

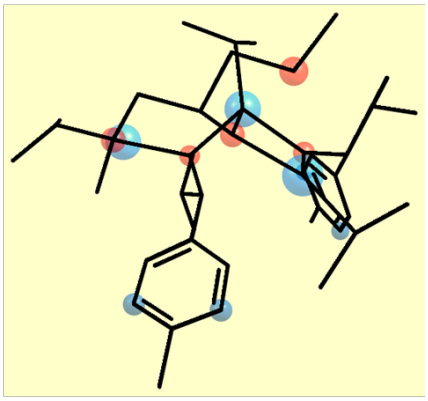
1	-0.682335000	6.964871000	1.720797000
1	-3.142253000	3.204744000	1.701216000
8	1.568333000	0.419694000	-0.322705000
6	1.633485000	1.383266000	0.732964000
6	2.846516000	2.339041000	0.590127000
6	1.579021000	0.679688000	2.081722000
1	0.726065000	1.997214000	0.655268000
6	2.623451000	-0.086210000	2.604864000
6	0.436333000	0.723546000	2.885635000
1	3.762680000	1.728920000	0.657185000
6	2.883545000	3.373145000	1.727520000
6	2.846198000	3.049136000	-0.771868000
1	2.834152000	2.339863000	-1.603621000
1	3.739688000	3.674281000	-0.874849000
1	1.969543000	3.699219000	-0.870966000
1	2.974158000	2.907121000	2.712544000
1	1.971398000	3.981709000	1.727273000
1	3.732778000	4.051817000	1.598908000
7	0.328149000	0.076633000	4.050474000
7	2.546790000	-0.747192000	3.765694000
6	1.391385000	-0.644071000	4.444078000
6	1.269485000	-1.398385000	5.740482000
1	3.573245000	-0.174869000	2.076121000
1	-0.428807000	1.305605000	2.570429000
1	2.240117000	-1.790358000	6.046886000
1	0.571230000	-2.235436000	5.625460000
1	0.865937000	-0.750078000	6.523164000
30	3.045639000	-0.604289000	-0.874715000
6	4.789605000	-1.175484000	-1.608029000
6	5.870388000	-1.294788000	-0.520234000
6	5.268243000	-0.282185000	-2.764016000
1	4.595023000	-2.179968000	-2.005727000
1	5.449547000	0.748863000	-2.437066000
1	4.546308000	-0.242461000	-3.587096000
1	6.216684000	-0.655367000	-3.179779000
1	6.091379000	-0.326801000	-0.053764000
1	6.815541000	-1.662819000	-0.947544000
1	5.587176000	-1.988652000	0.279389000

d_2



-3.9, *-5.3*





Zero-point correction= 0.869184 (Hartree/Particle)
Thermal correction to Energy= 0.927416
Thermal correction to Enthalpy= 0.928360
Thermal correction to Gibbs Free Energy= 0.769140
Sum of electronic and zero-point Energies= -2530.172312
Sum of electronic and thermal Energies= -2530.114080
Sum of electronic and thermal Enthalpies= -2530.113136
Sum of electronic and thermal Free Energies= -2530.272356

6	-0.858080000	-4.023875000	-1.317683000
6	0.082547000	-3.245380000	-0.392778000
1	-0.916146000	-3.520878000	-2.297032000
8	-2.135221000	-4.055248000	-0.704295000
1	-0.487703000	-5.050232000	-1.480647000
8	-0.352729000	-1.929038000	-0.199043000
6	1.507774000	-3.280026000	-0.959200000
1	0.077851000	-3.776571000	0.573432000
1	1.518868000	-2.869837000	-1.972917000
1	1.875775000	-4.315821000	-0.999661000
8	2.444741000	-2.482774000	-0.224456000
6	2.662298000	-2.910031000	1.122676000
6	-3.116017000	-4.706389000	-1.493108000
1	-4.053430000	-4.670376000	-0.934779000
1	-2.848833000	-5.757174000	-1.680054000
1	-3.254090000	-4.203490000	-2.461518000
1	1.783767000	-2.724250000	1.747579000
1	3.504275000	-2.334131000	1.509380000
1	2.915324000	-3.977404000	1.146705000
30	-1.937553000	-1.521671000	0.886489000
6	-3.051872000	-2.034493000	2.453778000
6	-4.172383000	-3.023466000	2.094358000
1	-3.526189000	-1.101437000	2.792345000
6	-2.200483000	-2.570548000	3.618013000
1	-4.846590000	-2.627945000	1.325281000
1	-4.790186000	-3.264076000	2.974908000
1	-3.768698000	-3.970126000	1.716545000
1	-1.676845000	-3.495268000	3.342380000
1	-2.825877000	-2.811338000	4.493212000
1	-1.444890000	-1.847975000	3.946028000
30	-0.349161000	-0.269600000	-1.452829000
8	-1.882898000	0.201806000	-0.169608000
6	-3.020750000	1.050078000	-0.211143000
6	-2.609030000	2.497786000	0.009243000
1	-3.674594000	0.781937000	0.637479000
6	-3.881785000	0.866920000	-1.490518000
1	-3.275039000	1.179527000	-2.351493000

6	-5.141835000	1.746842000	-1.442889000
6	-4.270653000	-0.603383000	-1.695011000
1	-3.394377000	-1.244398000	-1.816193000
1	-4.893842000	-0.714374000	-2.589075000
1	-4.851422000	-0.975644000	-0.840960000
1	-4.902520000	2.811303000	-1.368180000
1	-5.769117000	1.484105000	-0.581855000
1	-5.744688000	1.602750000	-2.345288000
6	-1.893269000	3.248954000	-0.930531000
6	-2.901569000	3.178174000	1.191811000
7	-1.518919000	4.515019000	-0.725901000
6	-1.865841000	5.070220000	0.450638000
7	-2.543157000	4.447833000	1.426291000
6	-1.464853000	6.503669000	0.675239000
1	-1.606273000	2.815033000	-1.886281000
1	-1.966958000	7.155155000	-0.048313000
1	-0.388263000	6.629126000	0.523830000
1	-1.731668000	6.819191000	1.684460000
1	-3.453162000	2.678281000	1.988656000
8	1.431379000	0.581578000	-0.557871000
6	1.394151000	1.659779000	0.385927000
6	2.365878000	2.805839000	0.008063000
6	1.606856000	1.105623000	1.787543000
1	0.377446000	2.072606000	0.355776000
6	2.852381000	0.761961000	2.315810000
6	0.524643000	0.835198000	2.632144000
1	3.388512000	2.395984000	0.008368000
6	2.310328000	3.954187000	1.029226000
6	2.073715000	3.336908000	-1.403281000
1	2.084128000	2.536507000	-2.146999000
1	2.822818000	4.081525000	-1.693078000
1	1.091958000	3.822898000	-1.437483000
1	2.597811000	3.635527000	2.034988000
1	1.298086000	4.371212000	1.086478000
1	2.983556000	4.763511000	0.728969000
7	0.652358000	0.272522000	3.836924000
7	3.014029000	0.194993000	3.518967000
6	1.900428000	-0.033954000	4.233312000
6	2.052344000	-0.674860000	5.586327000
1	3.770183000	0.951806000	1.759011000
1	-0.486849000	1.080229000	2.311143000
1	3.100775000	-0.897529000	5.787557000
1	1.465737000	-1.597683000	5.638615000
1	1.668717000	-0.008871000	6.366269000
30	3.058177000	-0.336434000	-0.884399000
6	4.913685000	-0.588126000	-1.524759000
6	5.851221000	-1.140716000	-0.439457000
6	5.489889000	0.687431000	-2.160914000
1	4.822559000	-1.350709000	-2.311178000
1	5.578107000	1.502688000	-1.432135000
1	4.874263000	1.055437000	-2.989033000
1	6.499977000	0.507570000	-2.559688000
1	5.967359000	-0.442058000	0.398630000
1	6.859141000	-1.316381000	-0.845386000
1	5.497025000	-2.092607000	-0.030148000
6	-0.246386000	-0.218691000	-3.473299000
6	1.104521000	-0.690339000	-4.036265000
6	-0.597036000	1.154329000	-4.070782000
1	-1.008950000	-0.930489000	-3.825254000
1	0.097397000	1.935838000	-3.736320000
1	-1.608558000	1.479926000	-3.802532000
1	-0.549575000	1.143764000	-5.172657000
1	1.934819000	-0.057820000	-3.692698000
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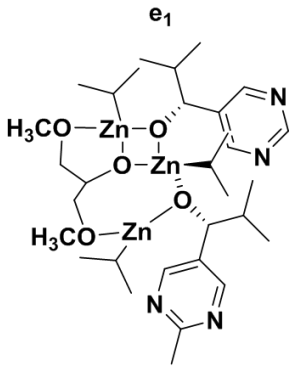
1	1.342231000	-1.723671000	-3.755571000

e_1



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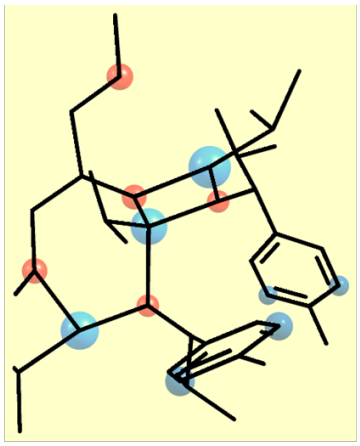
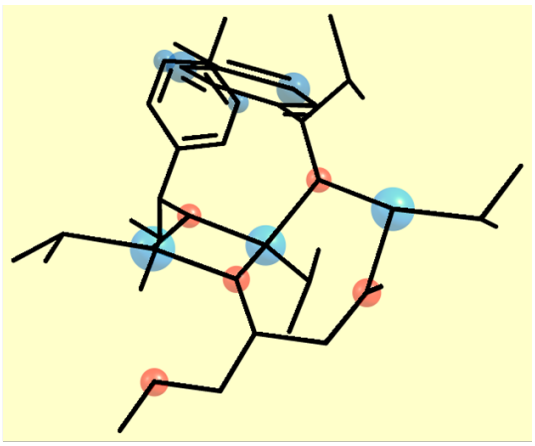


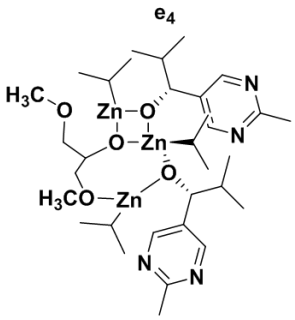


Zero-point correction= 0.868140 (Hartree/Particle)
Thermal correction to Energy= 0.925880
Thermal correction to Enthalpy= 0.926824
Thermal correction to Gibbs Free Energy= 0.769282
Sum of electronic and zero-point Energies= -2530.174456
Sum of electronic and thermal Energies= -2530.116716
Sum of electronic and thermal Enthalpies= -2530.115772
Sum of electronic and thermal Free Energies= -2530.273315

6	-1.571968000	-3.760066000	-1.401164000
6	-0.446142000	-3.137474000	-0.565553000
1	-1.606030000	-3.289331000	-2.397524000
8	-2.797295000	-3.547658000	-0.720477000
1	-1.397890000	-4.840076000	-1.540082000
8	-0.668755000	-1.775905000	-0.327445000
6	0.888879000	-3.362010000	-1.286251000
1	-0.426554000	-3.681820000	0.393717000
1	0.890397000	-2.814846000	-2.233238000
1	1.031263000	-4.431595000	-1.501424000
8	2.033515000	-2.882819000	-0.570488000
6	2.384766000	-3.655688000	0.577887000
6	-3.915571000	-4.064171000	-1.422631000
1	-4.802003000	-3.847577000	-0.823246000
1	-3.833378000	-5.152270000	-1.561585000
1	-4.024193000	-3.592903000	-2.410432000
1	1.685604000	-3.498418000	1.405575000
1	3.380878000	-3.331792000	0.886611000
1	2.421312000	-4.722738000	0.324525000
30	-2.232322000	-1.078846000	0.640207000
6	-3.561051000	-1.343803000	2.095745000
6	-5.012033000	-1.177196000	1.614407000
1	-3.357521000	-0.545712000	2.823863000
6	-3.376323000	-2.690538000	2.812938000
1	-5.194149000	-0.191054000	1.171447000
1	-5.726930000	-1.297633000	2.444645000
1	-5.279139000	-1.926428000	0.858266000
1	-3.511877000	-3.534842000	2.126650000
1	-4.106328000	-2.815208000	3.629517000
1	-2.377788000	-2.787010000	3.255285000
30	-0.142172000	-0.096482000	-1.417198000
8	-1.718454000	0.611000000	-0.373085000
6	0.492646000	-0.080593000	-3.334460000
6	0.832711000	1.322280000	-3.865496000
6	-0.455852000	-0.796237000	-4.310567000
1	-0.063945000	1.952468000	-3.941941000
1	1.268431000	1.284860000	-4.877757000

1	1.546475000	1.853414000	-3.225342000
1	-1.428052000	-0.290387000	-4.371002000
1	-0.654877000	-1.834913000	-4.019434000
1	-0.049661000	-0.822005000	-5.335557000
1	1.436133000	-0.654433000	-3.325424000
6	-2.584979000	1.715029000	-0.572163000
6	-1.875110000	3.009643000	-0.203910000
1	-3.432995000	1.613967000	0.127054000
6	-3.196285000	1.750929000	-1.998439000
1	-2.368487000	1.877202000	-2.711356000
6	-4.165965000	2.932510000	-2.163506000
6	-3.908159000	0.430969000	-2.325918000
1	-3.222961000	-0.419001000	-2.290542000
1	-4.346333000	0.468705000	-3.329182000
1	-4.723846000	0.242647000	-1.616068000
1	-3.676065000	3.897469000	-2.005742000
1	-4.995584000	2.857754000	-1.449375000
1	-4.597715000	2.938064000	-3.169626000
6	-0.816066000	3.545280000	-0.942600000
6	-2.217507000	3.743554000	0.934892000
7	-0.175542000	4.669401000	-0.598765000
6	-0.595452000	5.291441000	0.516466000
7	-1.597892000	4.869715000	1.304399000
6	0.119540000	6.551447000	0.925991000
1	-0.462654000	3.054045000	-1.847338000
1	-0.599427000	7.320706000	1.220283000
1	0.744406000	6.917351000	0.110234000
1	0.759013000	6.358782000	1.795441000
1	-3.032384000	3.407000000	1.576915000
8	1.611167000	0.355019000	-0.216099000
6	1.635538000	1.224733000	0.917331000
6	2.946613000	2.049244000	1.001675000
6	1.345907000	0.446078000	2.191789000
1	0.813657000	1.941823000	0.786724000
6	2.158911000	-0.582631000	2.672804000
6	0.216345000	0.702424000	2.973204000
1	3.778946000	1.337058000	1.126318000
6	2.946368000	2.988616000	2.218640000
6	3.184655000	2.850167000	-0.287267000
1	3.204362000	2.205592000	-1.169995000
1	4.140136000	3.382965000	-0.234984000
1	2.392544000	3.593110000	-0.435526000
1	2.865021000	2.444915000	3.163813000
1	2.109209000	3.694860000	2.164076000
1	3.870252000	3.574937000	2.247260000
7	-0.085613000	0.018688000	4.082292000
7	1.883986000	-1.289137000	3.774328000
6	0.760543000	-0.961674000	4.437092000
6	0.413220000	-1.763086000	5.662550000
1	3.080267000	-0.856823000	2.157017000
1	-0.475118000	1.494796000	2.689025000
1	1.279476000	-2.329663000	6.007109000
1	-0.394678000	-2.468249000	5.433564000
1	0.052346000	-1.107310000	6.458868000
30	3.070268000	-0.720970000	-0.728977000
6	4.892141000	-1.290874000	-1.250297000
6	5.903283000	-1.095287000	-0.107080000
6	5.377907000	-0.610252000	-2.539962000
1	4.796528000	-2.367019000	-1.443745000
1	5.465226000	0.476509000	-2.421295000
1	4.706813000	-0.794586000	-3.386114000
1	6.374421000	-0.979752000	-2.826636000
1	6.015471000	-0.038175000	0.163446000
1	6.901368000	-1.454786000	-0.400950000
1	5.620326000	-1.638075000	0.802361000

e_4



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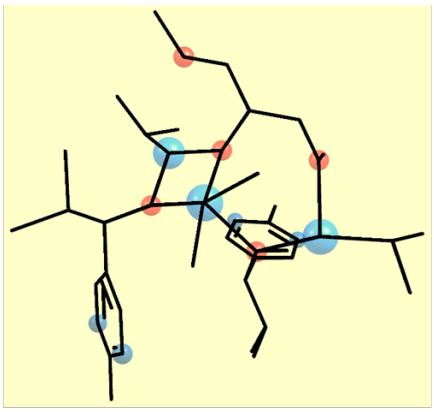
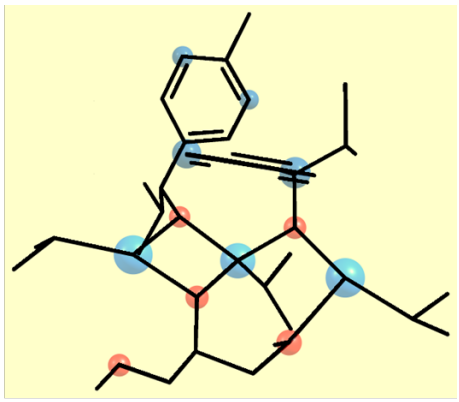


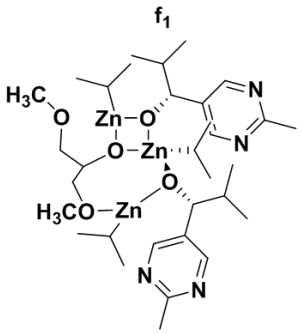


Zero-point correction= 0.868246 (Hartree/Particle)
Thermal correction to Energy= 0.926825
Thermal correction to Enthalpy= 0.927769
Thermal correction to Gibbs Free Energy= 0.767446
Sum of electronic and zero-point Energies= -2530.173031
Sum of electronic and thermal Energies= -2530.114452
Sum of electronic and thermal Enthalpies= -2530.113507
Sum of electronic and thermal Free Energies= -2530.273831

6	-0.239966000	-4.099324000	-1.179326000
6	0.521044000	-3.151337000	-0.246203000
1	-0.292291000	-3.665575000	-2.191725000
8	-1.544280000	-4.279145000	-0.655451000
1	0.278292000	-5.070521000	-1.251548000
8	-0.104274000	-1.901292000	-0.145068000
6	1.970221000	-3.017796000	-0.735384000
1	0.531329000	-3.631806000	0.746097000
1	1.985842000	-2.648553000	-1.764998000
1	2.466713000	-3.999603000	-0.713412000
8	2.754117000	-2.081261000	0.009929000
6	2.997657000	-2.458429000	1.365768000
6	-2.352112000	-5.123219000	-1.457732000
1	-3.326043000	-5.196542000	-0.969917000
1	-1.917509000	-6.130182000	-1.544856000
1	-2.485743000	-4.712300000	-2.469296000
1	2.084275000	-2.411862000	1.967127000
1	3.724424000	-1.752992000	1.770289000
1	3.415654000	-3.472492000	1.409895000
30	-1.811920000	-1.679696000	0.807758000
6	-2.963017000	-2.316519000	2.301168000
6	-4.001536000	-3.358171000	1.854898000
1	-3.509540000	-1.426157000	2.645892000
6	-2.136073000	-2.842025000	3.487190000
1	-4.655237000	-2.982483000	1.058671000
1	-4.650297000	-3.660004000	2.693248000
1	-3.519723000	-4.268385000	1.479033000
1	-1.543533000	-3.722387000	3.206081000
1	-2.786920000	-3.153226000	4.320789000
1	-1.444105000	-2.087055000	3.876287000
30	-0.220377000	-0.280926000	-1.433626000
8	-1.883100000	0.022821000	-0.282485000
6	-3.100392000	0.723058000	-0.491495000
6	-2.917817000	2.196660000	-0.161222000
1	-3.845900000	0.336102000	0.225297000
6	-3.695855000	0.493002000	-1.905997000
1	-2.970469000	0.876063000	-2.637912000

6	-5.020647000	1.251333000	-2.090686000
6	-3.901509000	-1.003176000	-2.179860000
1	-2.965109000	-1.561255000	-2.111777000
1	-4.313209000	-1.158257000	-3.182991000
1	-4.610739000	-1.435690000	-1.462051000
1	-4.900959000	2.332439000	-1.977946000
1	-5.766087000	0.919428000	-1.357056000
1	-5.434070000	1.063644000	-3.086959000
6	-2.148380000	3.072185000	-0.931445000
6	-3.492651000	2.776295000	0.973333000
7	-1.970128000	4.362297000	-0.621167000
6	-2.576646000	4.808489000	0.492075000
7	-3.335369000	4.060419000	1.309899000
6	-2.405676000	6.260873000	0.849013000
1	-1.648867000	2.726940000	-1.834810000
1	-3.358597000	6.791228000	0.741794000
1	-1.666696000	6.728887000	0.197663000
1	-2.097872000	6.364665000	1.893601000
1	-4.109417000	2.173582000	1.640982000
8	1.370347000	0.847401000	-0.457015000
6	1.169907000	1.829252000	0.568356000
6	2.019955000	3.105608000	0.342044000
6	1.374161000	1.196113000	1.938431000
1	0.114782000	2.127546000	0.509209000
6	2.616271000	1.011506000	2.547547000
6	0.290213000	0.702264000	2.672956000
1	3.083008000	2.820478000	0.403004000
6	1.747302000	4.161916000	1.426060000
6	1.771142000	3.703397000	-1.050200000
1	1.932577000	2.967973000	-1.841474000
1	2.444507000	4.548972000	-1.226870000
1	0.743377000	4.074074000	-1.133303000
1	1.984679000	3.803855000	2.431530000
1	0.692845000	4.460962000	1.415174000
1	2.345396000	5.059891000	1.240746000
7	0.417166000	0.086276000	3.851182000
7	2.777582000	0.396793000	3.727230000
6	1.665507000	-0.047402000	4.333964000
6	1.817145000	-0.739674000	5.661414000
1	3.530431000	1.375828000	2.078436000
1	-0.720645000	0.807594000	2.281500000
1	2.871183000	-0.829779000	5.926292000
1	1.360632000	-1.733941000	5.627684000
1	1.296896000	-0.176598000	6.443513000
30	3.067794000	0.126758000	-0.857605000
6	4.875452000	-0.075841000	-1.626631000
6	5.928579000	-0.418779000	-0.560693000
6	5.307088000	1.133091000	-2.471229000
1	4.778288000	-0.943113000	-2.294506000
1	5.397577000	2.043413000	-1.866029000
1	4.602479000	1.347697000	-3.282049000
1	6.291580000	0.958935000	-2.931539000
1	6.070291000	0.400985000	0.154823000
1	6.908931000	-0.604445000	-1.025143000
1	5.664080000	-1.315216000	0.009795000
6	-0.034330000	-0.225609000	-3.448270000
6	1.130880000	-1.052942000	-4.016404000
6	0.020512000	1.203509000	-4.012542000
1	-0.962592000	-0.685567000	-3.819938000
1	0.903555000	1.750788000	-3.659764000
1	-0.856763000	1.798343000	-3.732090000
1	0.067246000	1.205095000	-5.114333000
1	2.108070000	-0.695893000	-3.658872000
1	1.171408000	-1.001329000	-5.117197000
1	1.057899000	-2.114829000	-3.752552000

f_1



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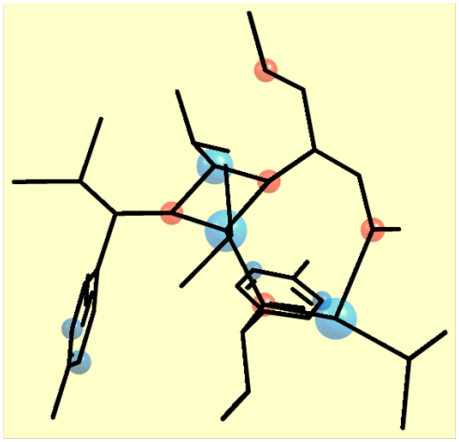

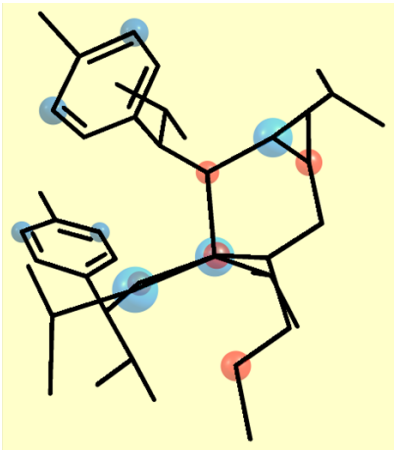

Zero-point correction= 0.868617 (Hartree/Particle)
Thermal correction to Energy= 0.927123
Thermal correction to Enthalpy= 0.928068
Thermal correction to Gibbs Free Energy= 0.768464
Sum of electronic and zero-point Energies= -2530.174447
Sum of electronic and thermal Energies= -2530.115941
Sum of electronic and thermal Enthalpies= -2530.114997
Sum of electronic and thermal Free Energies= -2530.274600

6	-1.309550000	-3.944505000	-1.130514000
6	-0.271682000	-3.208104000	-0.274806000
1	-1.311058000	-3.530718000	-2.152112000
8	-2.584872000	-3.773127000	-0.536259000
1	-1.063467000	-5.017480000	-1.197486000
8	-0.576377000	-1.846729000	-0.142579000
6	1.113412000	-3.407778000	-0.905630000
1	-0.280348000	-3.686248000	0.719074000
1	1.131950000	-2.955938000	-1.901339000
1	1.332266000	-4.481232000	-1.007682000
8	2.183519000	-2.784503000	-0.188141000
6	2.519681000	-3.420166000	1.046199000
6	-3.623594000	-4.386059000	-1.282433000
1	-4.559286000	-4.190141000	-0.756065000
1	-3.473718000	-5.473172000	-1.358495000
1	-3.687817000	-3.970211000	-2.298567000
1	1.739157000	-3.280808000	1.801196000
1	3.442904000	-2.957735000	1.400802000
1	2.693431000	-4.492601000	0.890395000
30	-2.204140000	-1.171130000	0.712471000
6	-3.666620000	-1.242307000	2.061948000
6	-4.927860000	-1.947009000	1.537412000
1	-3.925931000	-0.188370000	2.243298000
6	-3.224544000	-1.846526000	3.405243000
1	-5.308837000	-1.494556000	0.614056000
1	-5.743165000	-1.910498000	2.278177000
1	-4.736108000	-3.005765000	1.326868000
1	-2.919137000	-2.895316000	3.296215000
1	-4.048162000	-1.832445000	4.138026000
1	-2.385538000	-1.298732000	3.847635000
30	-0.119913000	-0.227993000	-1.372726000
8	-1.730128000	0.485044000	-0.398503000
6	0.559799000	-0.312632000	-3.271903000
6	0.751928000	1.069173000	-3.919595000
6	-0.267232000	-1.216658000	-4.200873000
1	-0.208298000	1.582088000	-4.067517000
1	1.216528000	0.994529000	-4.916899000

1	1.383643000	1.732218000	-3.317593000
1	-1.291313000	-0.841134000	-4.323053000
1	-0.347371000	-2.244006000	-3.825568000
1	0.168977000	-1.277721000	-5.211929000
1	1.562743000	-0.767313000	-3.191943000
6	-2.666561000	1.503328000	-0.708089000
6	-2.058772000	2.871668000	-0.434647000
1	-3.521135000	1.398987000	-0.016859000
6	-3.246051000	1.377187000	-2.142135000
1	-2.413210000	1.497145000	-2.849899000
6	-4.287638000	2.471238000	-2.428403000
6	-3.861348000	-0.010850000	-2.365673000
1	-3.129499000	-0.807825000	-2.214967000
1	-4.253141000	-0.099835000	-3.384692000
1	-4.697390000	-0.180261000	-1.674718000
1	-3.865992000	3.477192000	-2.350031000
1	-5.126444000	2.404668000	-1.724323000
1	-4.696063000	2.358253000	-3.437993000
6	-1.063455000	3.452271000	-1.230233000
6	-2.433272000	3.634873000	0.671700000
7	-0.510163000	4.638565000	-0.961977000
6	-0.954538000	5.285101000	0.132117000
7	-1.898910000	4.827697000	0.966999000
6	-0.343390000	6.628506000	0.428186000
1	-0.692683000	2.944576000	-2.118846000
1	-0.575995000	7.336162000	-0.374988000
1	0.747082000	6.550525000	0.478895000
1	-0.726167000	7.020641000	1.371055000
1	-3.201773000	3.268864000	1.353287000
8	1.598050000	0.431047000	-0.212696000
6	1.564031000	1.421838000	0.818868000
6	2.792527000	2.366570000	0.775357000
6	1.367987000	0.757462000	2.173815000
1	0.674760000	2.039083000	0.632892000
6	2.342602000	-0.010539000	2.814822000
6	0.156460000	0.847162000	2.865014000
1	3.691177000	1.752505000	0.952107000
6	2.721249000	3.431076000	1.882808000
6	2.934211000	3.040290000	-0.597563000
1	2.997822000	2.310146000	-1.408320000
1	3.838572000	3.657356000	-0.627298000
1	2.076451000	3.691550000	-0.801035000
1	2.712799000	2.991487000	2.883961000
1	1.815691000	4.040356000	1.776930000
1	3.581414000	4.105296000	1.820170000
7	-0.071384000	0.243244000	4.035945000
7	2.145709000	-0.630075000	3.984425000
6	0.936081000	-0.481238000	4.550345000
6	0.681661000	-1.183046000	5.856920000
1	3.335209000	-0.134809000	2.380637000
1	-0.664419000	1.430874000	2.450982000
1	1.608764000	-1.598345000	6.253906000
1	-0.038619000	-1.996772000	5.714626000
1	0.244009000	-0.491680000	6.582576000
30	3.124441000	-0.602664000	-0.592129000
6	4.972578000	-1.146190000	-1.028714000
6	5.934695000	0.047021000	-1.145197000
6	5.033594000	-2.038576000	-2.278288000
1	5.286825000	-1.753684000	-0.167546000
1	4.716133000	-1.500607000	-3.179848000
1	4.399577000	-2.925843000	-2.181096000
1	6.061681000	-2.386346000	-2.461069000
1	5.666765000	0.705725000	-1.979956000
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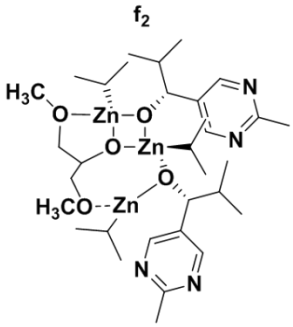
1	5.952676000	0.661240000	-0.237795000

f_2



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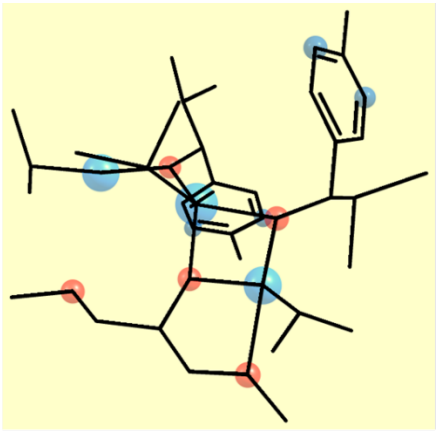

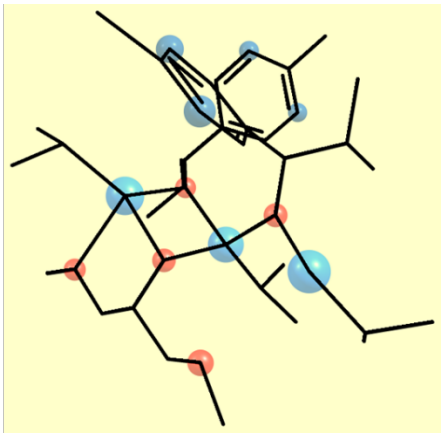

Zero-point correction= 0.868892 (Hartree/Particle)
Thermal correction to Energy= 0.926084
Thermal correction to Enthalpy= 0.927028
Thermal correction to Gibbs Free Energy= 0.771846
Sum of electronic and zero-point Energies= -2530.168555
Sum of electronic and thermal Energies= -2530.111363
Sum of electronic and thermal Enthalpies= -2530.110419
Sum of electronic and thermal Free Energies= -2530.265601

6	-0.208060000	-4.224654000	-0.851829000
6	0.827660000	-3.289362000	-0.209378000
1	-0.370324000	-3.953123000	-1.907847000
8	-1.425679000	-4.098402000	-0.129910000
1	0.141073000	-5.268334000	-0.815571000
8	0.335590000	-1.979782000	-0.090775000
6	2.120984000	-3.375040000	-1.016732000
1	1.048030000	-3.681835000	0.797456000
1	1.962849000	-2.988612000	-2.035772000
1	2.411481000	-4.434573000	-1.102328000
8	3.161052000	-2.650305000	-0.371678000
6	4.444296000	-3.033982000	-0.841863000
6	-2.442555000	-4.977037000	-0.589500000
1	-3.330847000	-4.786071000	0.014660000
1	-2.140375000	-6.026442000	-0.466696000
1	-2.678831000	-4.797353000	-1.647142000
1	4.620459000	-4.107599000	-0.680568000
1	5.184199000	-2.465863000	-0.276261000
1	4.569478000	-2.819231000	-1.913553000
30	-1.390477000	-1.749052000	0.878488000
6	-2.336622000	-2.084578000	2.602400000
6	-3.820459000	-2.440902000	2.416018000
1	-2.289067000	-1.136908000	3.155303000
6	-1.625430000	-3.154362000	3.446677000
1	-4.375333000	-1.657605000	1.886044000
1	-4.322908000	-2.594384000	3.385337000
1	-3.949389000	-3.371131000	1.847633000
1	-1.595255000	-4.122657000	2.931775000
1	-2.140050000	-3.319114000	4.407975000
1	-0.589524000	-2.877665000	3.675943000
30	0.099890000	-0.484292000	-1.489972000
8	-1.706967000	-0.356607000	-0.572084000
6	-2.979626000	0.173442000	-0.907418000
6	-2.972731000	1.692224000	-0.806707000
1	-3.705542000	-0.182259000	-0.155865000
6	-3.500433000	-0.322743000	-2.282670000
1	-2.810915000	0.049356000	-3.052935000

6	-4.904125000	0.226594000	-2.585949000
6	-3.504814000	-1.854670000	-2.350758000
1	-2.513072000	-2.267359000	-2.156012000
1	-3.832763000	-2.195932000	-3.338713000
1	-4.197150000	-2.273697000	-1.609185000
1	-4.924802000	1.319376000	-2.621769000
1	-5.623332000	-0.096550000	-1.822840000
1	-5.261466000	-0.144886000	-3.552058000
6	-2.290579000	2.525403000	-1.698063000
6	-3.641928000	2.365876000	0.219285000
7	-2.267307000	3.859832000	-1.585397000
6	-2.947356000	4.395081000	-0.557080000
7	-3.638544000	3.695855000	0.358425000
6	-2.949421000	5.894505000	-0.421498000
1	-1.737298000	2.110438000	-2.538497000
1	-3.957602000	6.287882000	-0.592684000
1	-2.267135000	6.343669000	-1.144078000
1	-2.660235000	6.187896000	0.592086000
1	-4.206660000	1.803658000	0.963836000
8	1.315891000	0.917477000	-0.268599000
6	0.756749000	1.938541000	0.566100000
6	1.514324000	3.288568000	0.430296000
6	0.634342000	1.475511000	2.011753000
1	-0.264974000	2.108503000	0.203797000
6	1.698753000	1.000677000	2.783358000
6	-0.588099000	1.522806000	2.688218000
1	2.546764000	3.128566000	0.783966000
6	0.893908000	4.385250000	1.310953000
6	1.566300000	3.747457000	-1.034895000
1	1.990215000	2.978945000	-1.686927000
1	2.176328000	4.651698000	-1.131992000
1	0.560257000	3.980555000	-1.402037000
1	0.937457000	4.137769000	2.374951000
1	-0.156703000	4.550765000	1.045895000
1	1.423227000	5.332230000	1.165145000
7	-0.747338000	1.139726000	3.959399000
7	1.572979000	0.606370000	4.054019000
6	0.344592000	0.685512000	4.594350000
6	0.175375000	0.206054000	6.010328000
1	2.707706000	0.932114000	2.376897000
1	-1.478754000	1.889035000	2.179724000
1	1.123692000	0.256986000	6.548115000
1	-0.159039000	-0.838549000	6.011172000
1	-0.585898000	0.794767000	6.526637000
30	3.144798000	0.578348000	-0.339256000
6	5.106490000	0.574763000	-0.446501000
6	5.766956000	0.296473000	0.913555000
6	5.633669000	1.879819000	-1.067004000
1	5.352113000	-0.248771000	-1.127719000
1	5.393189000	2.754093000	-0.450097000
1	5.227195000	2.060393000	-2.068005000
1	6.729477000	1.848352000	-1.159539000
1	5.547923000	1.085977000	1.642547000
1	6.861657000	0.254457000	0.811892000
1	5.441400000	-0.652226000	1.353314000
6	0.728266000	-0.461161000	-3.408319000
6	2.251956000	-0.303253000	-3.543561000
6	0.027338000	0.577436000	-4.299465000
1	0.468812000	-1.455978000	-3.803150000
1	0.221077000	1.603175000	-3.958704000
1	-1.059665000	0.440530000	-4.324687000
1	0.379714000	0.524615000	-5.343176000
1	2.582721000	0.682118000	-3.184374000
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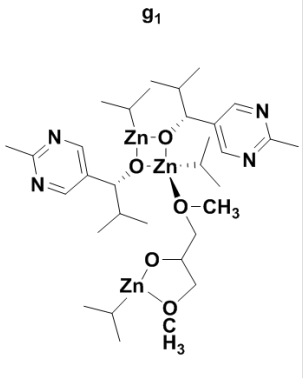
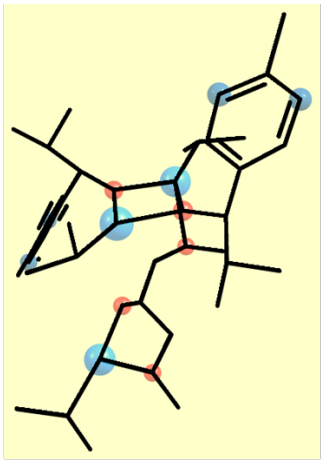
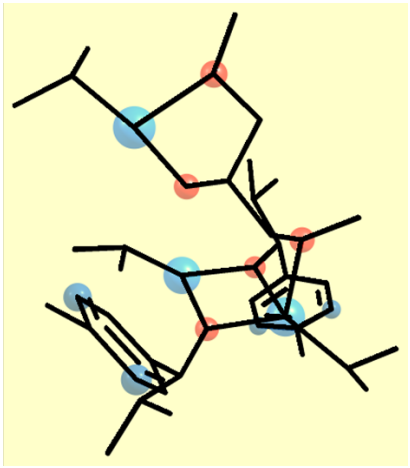
1	2.809001000	-1.063999000	-2.982180000

g_1







Zero-point correction= 0.867831 (Hartree/Particle)
Thermal correction to Energy= 0.926811
Thermal correction to Enthalpy= 0.927755
Thermal correction to Gibbs Free Energy= 0.763800
Sum of electronic and zero-point Energies= -2530.169237
Sum of electronic and thermal Energies= -2530.110257
Sum of electronic and thermal Enthalpies= -2530.109313
Sum of electronic and thermal Free Energies= -2530.273267

6	1.529325000	0.742499000	2.456909000
6	2.622896000	-0.191048000	1.920243000
1	1.842025000	1.174341000	3.418536000
8	0.227410000	0.157534000	2.592243000
1	1.421701000	1.552482000	1.733548000
8	2.342755000	-0.607889000	0.610186000
6	2.911185000	-1.400544000	2.814769000
1	3.536527000	0.436911000	1.951788000
6	-0.090853000	-0.297793000	3.903208000
1	-0.034010000	0.520544000	4.633253000
1	0.572273000	-1.108578000	4.226914000
1	-1.114236000	-0.676075000	3.872057000
30	-1.644908000	1.070705000	1.262910000
30	-0.595146000	-0.152913000	-1.329471000
8	-1.737669000	-0.642951000	0.252296000
6	-2.551359000	-1.760327000	0.560112000
6	-3.978185000	-1.514380000	0.092543000
1	-2.589186000	-1.883322000	1.656573000
6	-1.945939000	-3.071541000	-0.007143000
1	-1.836637000	-2.929036000	-1.092226000
6	-2.858361000	-4.285246000	0.228127000
6	-0.556366000	-3.326420000	0.595460000
1	0.101912000	-2.460706000	0.491537000
1	-0.081044000	-4.188701000	0.114558000
1	-0.642690000	-3.553002000	1.666328000
1	-3.819946000	-4.188910000	-0.283248000
1	-3.059891000	-4.424363000	1.297760000
1	-2.376482000	-5.198675000	-0.135502000
6	-4.286391000	-1.110507000	-1.211591000
6	-5.082814000	-1.651958000	0.932660000
7	-5.531850000	-0.887024000	-1.636314000
6	-6.519220000	-1.060372000	-0.737663000
7	-6.344540000	-1.432373000	0.538856000
6	-7.924917000	-0.792827000	-1.204249000
1	-3.493343000	-0.959757000	-1.942129000
1	-8.646394000	-1.201719000	-0.495552000
1	-8.087897000	-1.223230000	-2.195886000

1	-8.095182000	0.287017000	-1.288633000
1	-4.948385000	-1.951474000	1.972550000
8	-0.580287000	1.586130000	-0.389210000
6	-0.227536000	2.893479000	-0.811889000
6	-0.696011000	3.174935000	-2.264373000
6	1.261758000	3.133500000	-0.610640000
1	-0.755101000	3.616913000	-0.167318000
6	2.251904000	2.342524000	-1.207425000
6	1.748252000	4.147639000	0.212686000
1	-0.205742000	2.431434000	-2.911683000
6	-0.283673000	4.576204000	-2.741316000
6	-2.216555000	2.999785000	-2.387792000
1	-2.543671000	2.009082000	-2.062885000
1	-2.540259000	3.141824000	-3.424246000
1	-2.740652000	3.741544000	-1.771995000
1	0.801545000	4.708298000	-2.753343000
1	-0.708968000	5.351417000	-2.091865000
1	-0.654288000	4.758362000	-3.755183000
7	3.053605000	4.369903000	0.424730000
7	3.558718000	2.539066000	-1.017751000
6	3.910112000	3.553333000	-0.204673000
6	5.382767000	3.774156000	0.017141000
1	1.056989000	4.813798000	0.730197000
1	5.912316000	3.808266000	-0.939472000
1	5.810114000	2.943804000	0.590897000
1	5.549395000	4.702526000	0.564737000
6	-0.047174000	-1.116152000	-2.988596000
6	1.196895000	-0.531892000	-3.675239000
6	-1.201660000	-1.249230000	-3.997876000
1	0.208361000	-2.128904000	-2.644269000
1	-1.545271000	-0.271634000	-4.358897000
1	-2.071298000	-1.764841000	-3.574963000
1	-0.889874000	-1.821585000	-4.885993000
1	1.029016000	0.495148000	-4.024720000
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1	2.070184000	-0.511299000	-3.013090000
1	3.193743000	-1.097388000	3.833962000
8	3.999150000	-2.101877000	2.203635000
1	2.034090000	-2.060828000	2.861664000
6	4.346343000	-3.314856000	2.860722000
1	3.492872000	-4.005294000	2.898514000
1	4.691630000	-3.119814000	3.884520000
1	5.156586000	-3.771181000	2.289139000
30	3.626277000	-1.704117000	-0.156118000
6	4.845652000	-2.770252000	-1.273186000
6	5.175478000	-2.102359000	-2.617711000
6	4.342044000	-4.209963000	-1.477459000
1	5.773348000	-2.819334000	-0.684482000
1	3.402443000	-4.236622000	-2.042646000
1	4.167888000	-4.730805000	-0.528772000
1	5.072199000	-4.805608000	-2.046670000
6	-2.667579000	2.248470000	2.509864000
6	-3.617777000	1.494137000	3.454366000
1	-3.293054000	2.861321000	1.843093000
6	-1.762440000	3.208698000	3.297466000
1	-4.330626000	0.865204000	2.908976000
1	-4.206776000	2.189152000	4.074804000
1	-3.072520000	0.842462000	4.149258000
1	-1.079916000	2.669871000	3.966555000
1	-2.351299000	3.892070000	3.930790000
1	-1.143346000	3.830400000	2.639897000
1	1.982358000	1.517160000	-1.860901000
1	4.286208000	-2.001358000	-3.251290000
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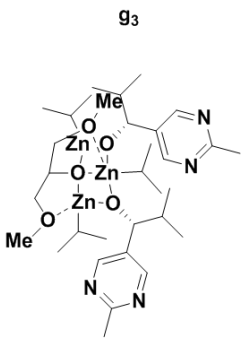
g_3



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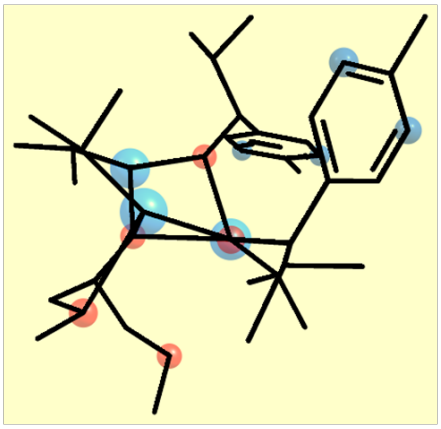

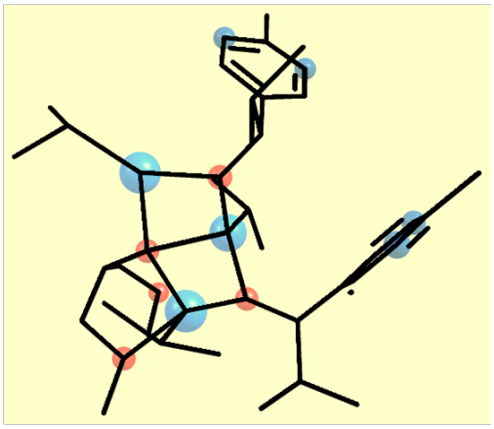

Zero-point correction= 0.868853 (Hartree/Particle)
Thermal correction to Energy= 0.927113
Thermal correction to Enthalpy= 0.928057
Thermal correction to Gibbs Free Energy= 0.769536
Sum of electronic and zero-point Energies= -2530.177152
Sum of electronic and thermal Energies= -2530.118892
Sum of electronic and thermal Enthalpies= -2530.117948
Sum of electronic and thermal Free Energies= -2530.276470

6	-1.663794000	-2.832830000	2.129408000
6	-1.939997000	-2.658771000	0.626370000
1	-2.204758000	-3.721666000	2.491126000
8	-1.936892000	-1.710215000	2.945831000
1	-0.591738000	-3.034520000	2.236582000
8	-1.190194000	-1.579885000	0.068795000
6	-3.417307000	-2.565594000	0.235251000
1	-1.599758000	-3.611517000	0.184119000
6	-3.200633000	-1.710920000	3.591124000
1	-3.356084000	-2.641403000	4.157254000
1	-4.025603000	-1.574020000	2.883153000
1	-3.196029000	-0.871617000	4.290343000
30	0.111101000	-0.054430000	1.256304000
30	-2.293277000	0.093513000	-0.719666000
8	-1.420635000	1.128125000	0.696090000
6	-1.471597000	2.495080000	1.089657000
6	-0.375274000	3.281693000	0.387745000
1	-1.249851000	2.540840000	2.168945000
6	-2.887935000	3.092590000	0.909224000
1	-3.164318000	2.966246000	-0.148387000
6	-2.927368000	4.592037000	1.244671000
6	-3.904274000	2.331446000	1.773842000
1	-3.869314000	1.255510000	1.590809000
1	-4.921682000	2.687929000	1.578737000
1	-3.695133000	2.492502000	2.838697000
1	-2.292152000	5.184845000	0.581131000
1	-2.594161000	4.769687000	2.274627000
1	-3.949653000	4.974488000	1.159511000
6	-0.363901000	3.532851000	-0.989648000
6	0.737978000	3.765213000	1.075152000
7	0.623562000	4.186132000	-1.607013000
6	1.647256000	4.608621000	-0.840192000
7	1.748192000	4.418987000	0.483456000
6	2.753713000	5.360813000	-1.529488000
1	-1.180582000	3.192637000	-1.622737000
1	3.585940000	5.526237000	-0.844423000
1	2.387090000	6.331530000	-1.882057000

1	3.100824000	4.812238000	-2.410051000
1	0.826245000	3.615981000	2.151456000
8	1.038449000	-0.326358000	-0.644749000
6	2.230376000	0.339145000	-1.051007000
6	2.472420000	0.222234000	-2.579294000
6	3.423403000	-0.138515000	-0.237257000
1	2.101524000	1.411224000	-0.832906000
6	3.913619000	-1.448206000	-0.288872000
6	4.114939000	0.705482000	0.632588000
1	2.600048000	-0.846906000	-2.809784000
6	3.752733000	0.958449000	-3.006535000
6	1.271701000	0.749230000	-3.377139000
1	0.347442000	0.230433000	-3.111282000
1	1.436899000	0.616735000	-4.451736000
1	1.122039000	1.819039000	-3.189856000
1	4.646723000	0.552203000	-2.525831000
1	3.691257000	2.024263000	-2.754446000
1	3.891514000	0.884587000	-4.089872000
7	5.157503000	0.308798000	1.374006000
7	4.948634000	-1.875437000	0.438790000
6	5.530114000	-0.973554000	1.251778000
6	6.681103000	-1.453228000	2.094671000
1	3.817998000	1.749544000	0.735544000
1	7.374834000	-2.048265000	1.494336000
1	6.313778000	-2.100162000	2.899797000
1	7.204812000	-0.606691000	2.540610000
6	-3.173443000	0.248428000	-2.514618000
6	-2.810712000	-0.900272000	-3.470518000
6	-2.958138000	1.604729000	-3.205599000
1	-4.248253000	0.165011000	-2.295030000
1	-1.902455000	1.776713000	-3.448850000
1	-3.293800000	2.445006000	-2.586161000
1	-3.512716000	1.664614000	-4.155670000
1	-1.745973000	-0.886977000	-3.736775000
1	-3.368926000	-0.828042000	-4.417749000
1	-3.025711000	-1.886825000	-3.044584000
1	-3.531546000	-2.794214000	-0.834640000
8	-3.912629000	-1.250069000	0.482823000
1	-4.004226000	-3.302807000	0.802192000
6	-5.301118000	-1.124587000	0.179293000
1	-5.578467000	-0.085083000	0.359248000
1	-5.896361000	-1.776991000	0.831017000
1	-5.503682000	-1.382064000	-0.867890000
30	0.411131000	-2.084480000	-1.141124000
6	0.727888000	-3.807328000	-2.085875000
6	-0.498532000	-4.297620000	-2.872761000
6	1.249298000	-4.903577000	-1.139806000
1	1.523731000	-3.591496000	-2.812653000
1	0.513267000	-5.162564000	-0.368206000
1	2.170298000	-4.608610000	-0.624353000
1	1.468210000	-5.831540000	-1.690771000
6	1.216296000	-0.087532000	2.928956000
6	0.478442000	0.482046000	4.150651000
1	2.058205000	0.583751000	2.703287000
6	1.812078000	-1.464938000	3.257971000
1	0.126639000	1.507850000	3.984802000
1	1.129636000	0.505189000	5.040417000
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1	1.029440000	-2.193614000	3.503501000
1	2.479190000	-1.416664000	4.134266000
1	2.400602000	-1.876442000	2.429715000
1	3.460605000	-2.185865000	-0.950447000
1	-1.347760000	-4.517020000	-2.212959000
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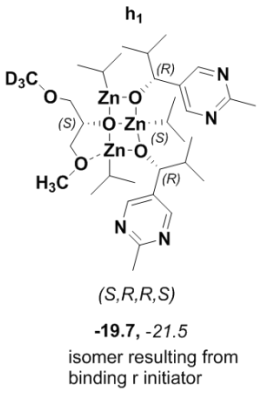
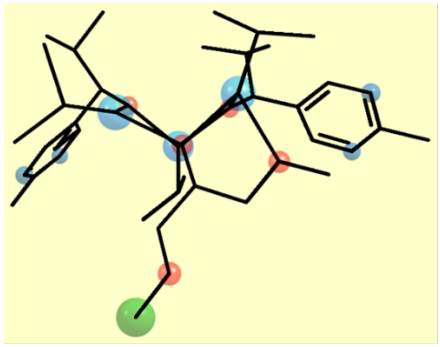
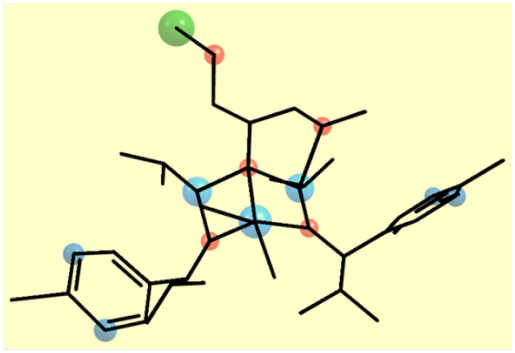
h_1







Zero-point correction= 0.859076 (Hartree/Particle)
Thermal correction to Energy= 0.917690
Thermal correction to Enthalpy= 0.918635
Thermal correction to Gibbs Free Energy= 0.758527
Sum of electronic and zero-point Energies= -2530.196387
Sum of electronic and thermal Energies= -2530.137773
Sum of electronic and thermal Enthalpies= -2530.136828
Sum of electronic and thermal Free Energies= -2530.296936

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6	0.368323000	2.214196000	1.558019000
1	1.935726000	2.561943000	2.998284000
8	2.697223000	1.818195000	1.214818000
1	1.605843000	0.834337000	2.683244000
8	0.071934000	1.313854000	0.491775000
6	-0.759819000	2.232277000	2.593754000
1	-0.861685000	1.235926000	3.054203000
1	-1.716399000	2.465785000	2.097033000
8	-0.455653000	3.211155000	3.567932000
6	-1.444337000	3.307592000	4.577657000
6	4.007989000	1.602467000	1.738512000
1	4.700508000	1.622112000	0.897462000
1	4.267180000	2.399754000	2.446020000
1	4.073930000	0.632700000	2.246583000
1 (iso=2)	-1.123339000	4.086831000	5.272316000
1 (iso=2)	-1.556402000	2.360957000	5.127178000
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30	1.814882000	1.001492000	-0.759016000
30	-0.288720000	-0.882228000	0.678048000
8	-1.625503000	-0.279701000	-0.805983000
6	-2.595741000	-1.105999000	-1.443987000
6	-3.703102000	-1.489484000	-0.474788000
1	-2.096509000	-2.040306000	-1.747062000
6	-3.142251000	-0.453307000	-2.742142000
1	-3.609490000	0.500735000	-2.452274000
6	-4.216493000	-1.323829000	-3.414384000
6	-2.009845000	-0.159540000	-3.736968000
1	-1.212420000	0.441049000	-3.291683000
1	-2.394079000	0.379961000	-4.608624000
1	-1.559968000	-1.093259000	-4.094153000
1	-5.090183000	-1.474696000	-2.775087000
1	-3.814296000	-2.311018000	-3.673273000
1	-4.557904000	-0.855089000	-4.342751000
6	-4.509619000	-0.551884000	0.181502000
6	-3.993743000	-2.818521000	-0.167456000
7	-5.477928000	-0.886949000	1.036188000
6	-5.665803000	-2.202280000	1.256373000

7	-4.959283000	-3.188087000	0.684475000
6	-6.751134000	-2.584865000	2.225911000
1	-4.373264000	0.515427000	0.011604000
1	-6.868383000	-3.668600000	2.256846000
1	-7.699546000	-2.119545000	1.940282000
1	-6.506207000	-2.222813000	3.230377000
1	-3.422722000	-3.625426000	-0.627568000
8	1.492183000	-0.899522000	-0.339461000
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1	2.650089000	-1.627526000	-2.696152000
6	0.814568000	-2.722482000	-2.534586000
6	3.129373000	-3.703383000	-2.356938000
1	4.186000000	-3.529811000	-2.135099000
1	3.054575000	-4.008993000	-3.405577000
1	2.794034000	-4.548811000	-1.743210000
1	0.187678000	-1.845844000	-2.365748000
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1	0.772855000	-2.979138000	-3.598583000
7	5.388160000	-2.116719000	1.615678000
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1	7.877265000	-0.057732000	1.316197000
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1	7.669298000	-1.418633000	2.459911000
6	-0.593924000	-2.003787000	2.320676000
6	-0.506212000	-3.512409000	2.027728000
6	-1.887858000	-1.694946000	3.090069000
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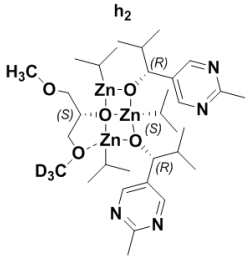
1	-2.778956000	-1.916089000	2.491709000
1	-1.957715000	-0.644512000	3.395353000
1	-1.964364000	-2.302084000	4.006938000
1	-1.306478000	-3.843390000	1.353687000
1	-0.608388000	-4.108477000	2.949404000
1	0.446449000	-3.796541000	1.565680000
6	2.502790000	2.126509000	-2.266687000
6	3.823650000	2.832355000	-1.918536000
6	1.466550000	3.143250000	-2.773002000
1	2.707474000	1.426812000	-3.090414000
1	3.703795000	3.526094000	-1.077495000
1	4.197082000	3.424063000	-2.769783000
1	4.616701000	2.125524000	-1.647424000
1	1.174014000	3.853404000	-1.989075000
1	0.551516000	2.658265000	-3.134340000
1	1.862697000	3.741721000	-3.609276000
30	-1.632135000	1.658534000	-0.653927000
6	-2.503560000	3.418177000	-0.976754000
6	-2.687237000	3.745621000	-2.466814000
1	-1.802836000	4.152573000	-0.554841000
6	-3.836605000	3.553807000	-0.221132000
1	-4.590031000	2.848340000	-0.593984000
1	-4.262170000	4.561562000	-0.346646000
1	-3.732446000	3.380687000	0.856314000
1	-1.738589000	3.739463000	-3.013887000
1	-3.134326000	4.743031000	-2.600075000
1	-3.356824000	3.031200000	-2.962065000
1	0.476367000	3.231675000	1.154338000
1	1.906112000	-2.879820000	-0.024039000

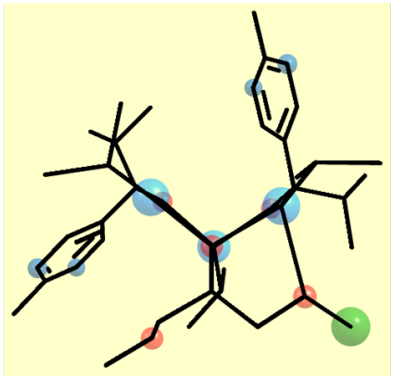
h_2

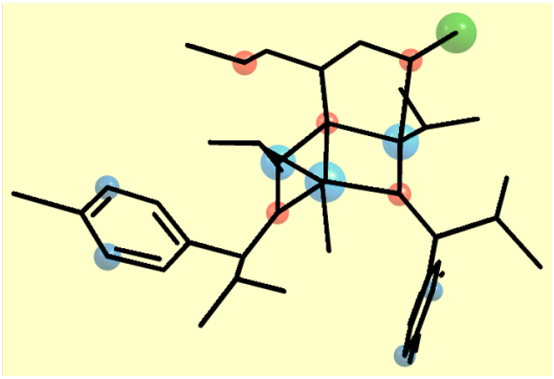


(S,R,R,S)

-19.7, *-21.5*

isomer resulting from binding s initiator



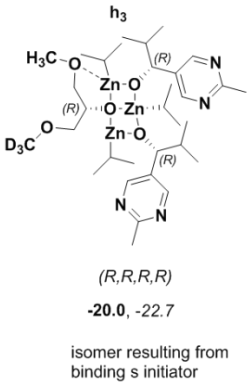


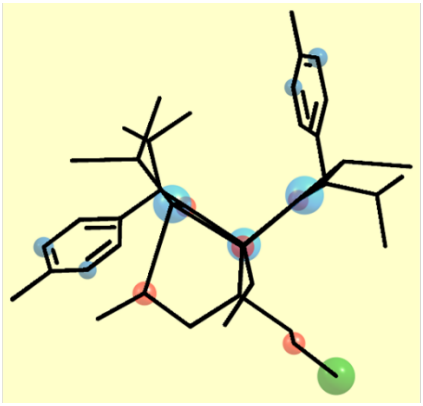
Zero-point correction= 0.858102 (Hartree/Particle)
Thermal correction to Energy= 0.916264
Thermal correction to Enthalpy= 0.917208
Thermal correction to Gibbs Free Energy= 0.757315
Sum of electronic and zero-point Energies= -2530.197385
Sum of electronic and thermal Energies= -2530.139223
Sum of electronic and thermal Enthalpies= -2530.138279
Sum of electronic and thermal Free Energies= -2530.298172

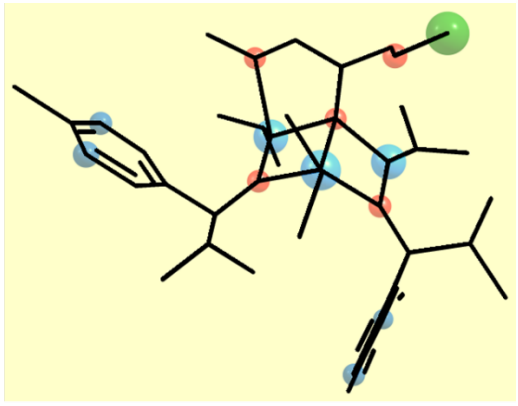
6	0.354960000	-3.822243000	-0.205706000
6	-0.259173000	-2.957347000	0.891218000
1	0.192404000	-4.886863000	0.017939000
8	1.754881000	-3.545054000	-0.232736000
1	-0.098377000	-3.593715000	-1.179117000
8	0.026785000	-1.583246000	0.633459000
6	-1.749751000	-3.244357000	1.065360000
1	0.216754000	-3.245881000	1.841695000
1	-2.140932000	-2.634215000	1.897186000
1	-1.878605000	-4.301222000	1.357437000
8	-2.447887000	-2.968435000	-0.130080000
6	-3.841954000	-3.209656000	-0.026927000
6	2.480677000	-4.388189000	-1.121044000
1	-4.278379000	-2.984895000	-1.001627000
1	-4.309388000	-2.563537000	0.729740000
1	-4.048954000	-4.259572000	0.228903000
30	2.138322000	-1.281299000	0.561370000
30	-0.337394000	-0.438468000	-1.276074000
8	-1.099851000	0.827197000	0.155742000
6	-1.898422000	1.973791000	-0.122902000
6	-3.329975000	1.558251000	-0.427586000
1	-1.496853000	2.449779000	-1.031975000
6	-1.818355000	3.030941000	1.009588000
1	-2.222839000	2.562933000	1.920686000
6	-2.675403000	4.266469000	0.689203000
6	-0.367960000	3.451532000	1.282629000
1	0.273234000	2.595675000	1.505717000
1	-0.323831000	4.139943000	2.133190000
1	0.058557000	3.968076000	0.415280000
1	-3.733943000	4.019782000	0.570550000
1	-2.335334000	4.747005000	-0.236191000
1	-2.592008000	5.005619000	1.492281000
6	-4.134973000	0.870772000	0.488369000
6	-3.943429000	1.821842000	-1.651798000
7	-5.384508000	0.483584000	0.224278000
6	-5.869502000	0.791202000	-0.993971000
7	-5.197027000	1.451488000	-1.947004000
6	-7.274847000	0.349461000	-1.301930000
1	-3.760875000	0.622888000	1.481238000
1	-7.604564000	0.767316000	-2.253707000

1	-7.956583000	0.660634000	-0.504838000
1	-7.325165000	-0.743744000	-1.358579000
1	-3.403047000	2.356682000	-2.432925000
8	1.715422000	-0.204344000	-1.008890000
6	2.552301000	0.636841000	-1.790784000
6	3.805579000	-0.113562000	-2.312605000
6	2.889739000	1.915359000	-1.039291000
1	1.980537000	0.940840000	-2.682961000
6	3.668748000	1.951698000	0.124276000
6	2.423369000	3.159909000	-1.460902000
1	4.350942000	-0.490761000	-1.433281000
6	4.747460000	0.807679000	-3.104159000
6	3.386847000	-1.311214000	-3.176341000
1	2.681208000	-1.954293000	-2.647973000
1	4.258273000	-1.909370000	-3.463941000
1	2.901408000	-0.967330000	-4.098038000
1	5.145282000	1.622288000	-2.493120000
1	4.227905000	1.254207000	-3.961071000
1	5.596536000	0.238242000	-3.496163000
7	2.679296000	4.306772000	-0.816961000
7	3.941225000	3.076640000	0.789658000
6	3.430068000	4.217682000	0.290670000
6	3.726621000	5.486305000	1.044220000
1	4.094130000	1.039162000	0.538655000
1	1.814178000	3.239287000	-2.361783000
1	4.803015000	5.587605000	1.212707000
1	3.249307000	5.462201000	2.030111000
1	3.357733000	6.351570000	0.492347000
6	-0.932438000	-0.886810000	-3.143793000
6	-0.839475000	0.321557000	-4.093125000
6	-2.317144000	-1.542035000	-3.250701000
1	-0.189180000	-1.624072000	-3.484677000
1	-3.112647000	-0.863646000	-2.917670000
1	-2.388466000	-2.447636000	-2.641126000
1	-2.553341000	-1.817036000	-4.292562000
1	-1.536966000	1.119380000	-3.806680000
1	-1.094983000	0.042028000	-5.128687000
1	0.164230000	0.762185000	-4.118223000
6	3.431736000	-1.518637000	2.063328000
6	4.814255000	-1.996300000	1.587115000
6	2.888513000	-2.446055000	3.162392000
1	3.562372000	-0.520972000	2.507478000
1	4.761919000	-2.985986000	1.115253000
1	5.520562000	-2.085060000	2.427905000
1	5.266610000	-1.312681000	0.858648000
1	2.711322000	-3.460895000	2.784857000
1	1.942664000	-2.083025000	3.582031000
1	3.599106000	-2.537948000	3.999439000
30	-0.905702000	-0.143872000	1.818683000
6	-1.137249000	-0.254066000	3.790746000
6	-0.197218000	0.705430000	4.540728000
1	-0.840624000	-1.280961000	4.049369000
6	-2.592984000	-0.058091000	4.244770000
1	-2.963523000	0.946018000	4.002108000
1	-2.688434000	-0.173147000	5.335769000
1	-3.278225000	-0.779310000	3.783527000
1	0.857515000	0.527808000	4.301988000
1	-0.306630000	0.594755000	5.630904000
1	-0.413033000	1.754948000	4.305789000
1(iso=2)	3.526821000	-4.082210000	-1.075601000
1(iso=2)	2.116828000	-4.288586000	-2.151814000
1(iso=2)	2.396154000	-5.438385000	-0.811761000

h_3





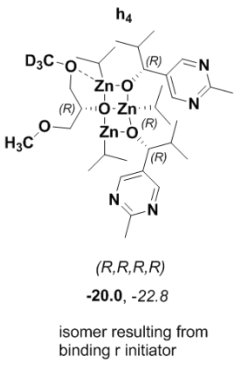


Zero-point correction= 0.858551 (Hartree/Particle)
Thermal correction to Energy= 0.917365
Thermal correction to Enthalpy= 0.918310
Thermal correction to Gibbs Free Energy= 0.756279
Sum of electronic and zero-point Energies= -2530.197850
Sum of electronic and thermal Energies= -2530.139036
Sum of electronic and thermal Enthalpies= -2530.138092
Sum of electronic and thermal Free Energies= -2530.300122

6	-1.944972000	-3.064610000	0.254840000
6	-0.470628000	-3.005760000	0.646700000
1	-2.071233000	-2.793263000	-0.800736000
8	-2.658723000	-2.147737000	1.084486000
1	-2.336941000	-4.080847000	0.406758000
8	0.009959000	-1.670469000	0.510274000
6	0.342766000	-4.025541000	-0.150607000
1	-0.391413000	-3.306078000	1.703197000
1	-0.022958000	-5.038811000	0.090186000
1	1.399855000	-3.984876000	0.161895000
8	0.220464000	-3.769352000	-1.534385000
6	0.899851000	-4.719667000	-2.336565000
6	-4.061054000	-2.140396000	0.821449000
1	-4.515505000	-1.403370000	1.483270000
1	-4.264917000	-1.865084000	-0.220669000
1	-4.492172000	-3.129197000	1.024479000
1(iso=2)	0.745566000	-4.431147000	-3.377875000
1(iso=2)	0.503476000	-5.734138000	-2.180103000
1(iso=2)	1.978996000	-4.730367000	-2.123675000
30	2.016176000	-1.222940000	0.916031000
30	-0.084481000	-0.459210000	-1.344864000
8	-1.183040000	0.700486000	-0.042058000
6	-1.836518000	1.924160000	-0.366260000
6	-3.325295000	1.682300000	-0.569512000
1	-1.433827000	2.273519000	-1.330512000
6	-1.546087000	3.039231000	0.671251000
1	-1.925179000	2.691030000	1.643863000
6	-2.267046000	4.349479000	0.313949000
6	-0.039053000	3.287235000	0.808606000
1	0.503228000	2.369665000	1.044541000
1	0.160053000	4.016859000	1.600582000
1	0.374578000	3.690563000	-0.123137000
1	-3.354652000	4.238031000	0.296580000
1	-1.951271000	4.711102000	-0.672446000
1	-2.022672000	5.129383000	1.042278000
6	-4.207431000	1.400363000	0.479782000
6	-3.916500000	1.693950000	-1.833233000
7	-5.507174000	1.150244000	0.302336000
6	-5.963390000	1.183515000	-0.963901000

7	-5.216362000	1.448119000	-2.045537000
6	-7.429815000	0.914010000	-1.170499000
1	-3.853914000	1.373706000	1.510085000
1	-7.658601000	0.850932000	-2.234904000
1	-8.028488000	1.716471000	-0.725246000
1	-7.722708000	-0.015958000	-0.673950000
1	-3.316971000	1.911729000	-2.716921000
8	1.889445000	-0.197356000	-0.711299000
6	2.907219000	0.453347000	-1.461789000
6	4.133969000	-0.466172000	-1.696484000
6	3.277010000	1.781878000	-0.821332000
1	2.489608000	0.682561000	-2.455461000
6	3.837638000	1.894313000	0.456884000
6	3.064941000	2.998995000	-1.467966000
1	4.532361000	-0.732117000	-0.705222000
6	5.244705000	0.247877000	-2.483260000
6	3.719920000	-1.755796000	-2.419563000
1	2.914393000	-2.278653000	-1.898831000
1	4.572426000	-2.437123000	-2.512435000
1	3.363409000	-1.529225000	-3.432094000
1	5.631899000	1.122537000	-1.953904000
1	4.877212000	0.582616000	-3.461157000
1	6.082764000	-0.433181000	-2.662887000
7	3.357732000	4.188562000	-0.925553000
7	4.140356000	3.063063000	1.025676000
6	3.883585000	4.172791000	0.307830000
6	4.211837000	5.493493000	0.950399000
1	4.055704000	1.006898000	1.050264000
1	2.637681000	3.018928000	-2.471020000
1	5.255322000	5.508888000	1.279967000
1	3.592765000	5.645639000	1.841228000
1	4.036570000	6.311090000	0.250328000
6	-0.424335000	-0.693043000	-3.310241000
6	-0.392240000	0.631912000	-4.091161000
6	-1.705525000	-1.477661000	-3.630210000
1	0.426993000	-1.298086000	-3.654843000
1	-2.605036000	-0.958146000	-3.274460000
1	-1.695118000	-2.472500000	-3.171629000
1	-1.835796000	-1.619134000	-4.716585000
1	-1.203395000	1.306613000	-3.788419000
1	-0.512375000	0.468807000	-5.175282000
1	0.547724000	1.179663000	-3.950969000
6	3.082699000	-1.841563000	2.479112000
6	4.439236000	-2.444751000	2.079210000
6	2.298991000	-2.805739000	3.384867000
1	3.283017000	-0.929593000	3.059959000
1	4.320440000	-3.353585000	1.475635000
1	5.024125000	-2.729438000	2.967529000
1	5.052634000	-1.746151000	1.498993000
1	2.048749000	-3.740761000	2.867047000
1	1.360740000	-2.369222000	3.744734000
1	2.889273000	-3.085658000	4.271180000
30	-1.234620000	-0.316251000	1.626713000
6	-1.336875000	-0.224077000	3.616012000
6	-0.303100000	0.724831000	4.244628000
1	-1.094144000	-1.246257000	3.942614000
6	-2.749454000	0.097977000	4.130140000
1	-3.067885000	1.109409000	3.844448000
1	-2.795538000	0.057525000	5.230299000
1	-3.502192000	-0.602076000	3.750238000
1	0.726073000	0.460607000	3.973696000
1	-0.359931000	0.709917000	5.344832000
1	-0.462020000	1.765602000	3.935209000

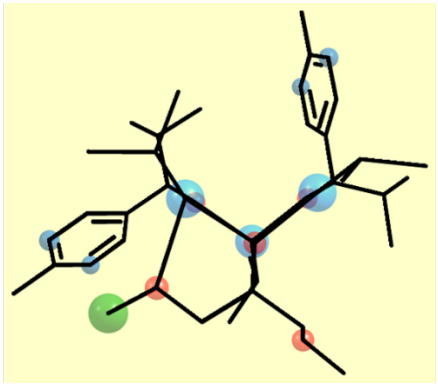
h_4

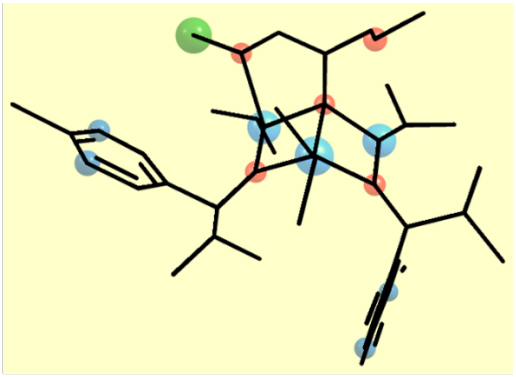


(R,R,R,R)

-20.0, *-22.8*

isomer resulting from binding r initiator



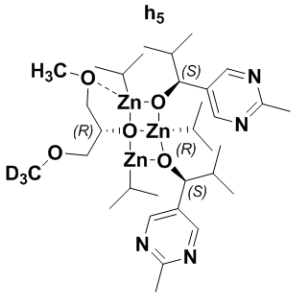


Zero-point correction= 0.858457 (Hartree/Particle)
Thermal correction to Energy= 0.917289
Thermal correction to Enthalpy= 0.918233
Thermal correction to Gibbs Free Energy= 0.756213
Sum of electronic and zero-point Energies= -2530.197945
Sum of electronic and thermal Energies= -2530.139113
Sum of electronic and thermal Enthalpies= -2530.138169
Sum of electronic and thermal Free Energies= -2530.300189

6	-1.944972000	-3.064610000	0.254840000
6	-0.470628000	-3.005760000	0.646700000
1	-2.071233000	-2.793263000	-0.800736000
8	-2.658723000	-2.147737000	1.084486000
1	-2.336941000	-4.080847000	0.406758000
8	0.009959000	-1.670469000	0.510274000
6	0.342766000	-4.025541000	-0.150607000
1	-0.391413000	-3.306078000	1.703197000
1	-0.022958000	-5.038811000	0.090186000
1	1.399855000	-3.984876000	0.161895000
8	0.220464000	-3.769352000	-1.534385000
6	0.899851000	-4.719667000	-2.336565000
6	-4.061054000	-2.140396000	0.821449000
1(iso=2)	-4.515505000	-1.403370000	1.483270000
1(iso=2)	-4.264917000	-1.865084000	-0.220669000
1(iso=2)	-4.492172000	-3.129197000	1.024479000
1	0.745566000	-4.431147000	-3.377875000
1	0.503476000	-5.734138000	-2.180103000
1	1.978996000	-4.730367000	-2.123675000
30	2.016176000	-1.222940000	0.916031000
30	-0.084481000	-0.459210000	-1.344864000
8	-1.183040000	0.700486000	-0.042058000
6	-1.836518000	1.924160000	-0.366260000
6	-3.325295000	1.682300000	-0.569512000
1	-1.433827000	2.273519000	-1.330512000
6	-1.546087000	3.039231000	0.671251000
1	-1.925179000	2.691030000	1.643863000
6	-2.267046000	4.349479000	0.313949000
6	-0.039053000	3.287235000	0.808606000
1	0.503228000	2.369665000	1.044541000
1	0.160053000	4.016859000	1.600582000
1	0.374578000	3.690563000	-0.123137000
1	-3.354652000	4.238031000	0.296580000
1	-1.951271000	4.711102000	-0.672446000
1	-2.022672000	5.129383000	1.042278000
6	-4.207431000	1.400363000	0.479782000
6	-3.916500000	1.693950000	-1.833233000
7	-5.507174000	1.150244000	0.302336000
6	-5.963390000	1.183515000	-0.963901000
7	-5.216362000	1.448119000	-2.045537000

6	-7.429815000	0.914010000	-1.170499000
1	-3.853914000	1.373706000	1.510085000
1	-7.658601000	0.850932000	-2.234904000
1	-8.028488000	1.716471000	-0.725246000
1	-7.722708000	-0.015958000	-0.673950000
1	-3.316971000	1.911729000	-2.716921000
8	1.889445000	-0.197356000	-0.711299000
6	2.907219000	0.453347000	-1.461789000
6	4.133969000	-0.466172000	-1.696484000
6	3.277010000	1.781878000	-0.821332000
1	2.489608000	0.682561000	-2.455461000
6	3.837638000	1.894313000	0.456884000
6	3.064941000	2.998995000	-1.467966000
1	4.532361000	-0.732117000	-0.705222000
6	5.244705000	0.247877000	-2.483260000
6	3.719920000	-1.755796000	-2.419563000
1	2.914393000	-2.278653000	-1.898831000
1	4.572426000	-2.437123000	-2.512435000
1	3.363409000	-1.529225000	-3.432094000
1	5.631899000	1.122537000	-1.953904000
1	4.877212000	0.582616000	-3.461157000
1	6.082764000	-0.433181000	-2.662887000
7	3.357732000	4.188562000	-0.925553000
7	4.140356000	3.063063000	1.025676000
6	3.883585000	4.172791000	0.307830000
6	4.211837000	5.493493000	0.950399000
1	4.055704000	1.006898000	1.050264000
1	2.637681000	3.018928000	-2.471020000
1	5.255322000	5.508888000	1.279967000
1	3.592765000	5.645639000	1.841228000
1	4.036570000	6.311090000	0.250328000
6	-0.424335000	-0.693043000	-3.310241000
6	-0.392240000	0.631912000	-4.091161000
6	-1.705525000	-1.477661000	-3.630210000
1	0.426993000	-1.298086000	-3.654843000
1	-2.605036000	-0.958146000	-3.274460000
1	-1.695118000	-2.472500000	-3.171629000
1	-1.835796000	-1.619134000	-4.716585000
1	-1.203395000	1.306613000	-3.788419000
1	-0.512375000	0.468807000	-5.175282000
1	0.547724000	1.179663000	-3.950969000
6	3.082699000	-1.841563000	2.479112000
6	4.439236000	-2.444751000	2.079210000
6	2.298991000	-2.805739000	3.384867000
1	3.283017000	-0.929593000	3.059959000
1	4.320440000	-3.353585000	1.475635000
1	5.024125000	-2.729438000	2.967529000
1	5.052634000	-1.746151000	1.498993000
1	2.048749000	-3.740761000	2.867047000
1	1.360740000	-2.369222000	3.744734000
1	2.889273000	-3.085658000	4.271180000
30	-1.234620000	-0.316251000	1.626713000
6	-1.336875000	-0.224077000	3.616012000
6	-0.303100000	0.724831000	4.244628000
1	-1.094144000	-1.246257000	3.942614000
6	-2.749454000	0.097977000	4.130140000
1	-3.067885000	1.109409000	3.844448000
1	-2.795538000	0.057525000	5.230299000
1	-3.502192000	-0.602076000	3.750238000
1	0.726073000	0.460607000	3.973696000
1	-0.359931000	0.709917000	5.344832000
1	-0.462020000	1.765602000	3.935209000

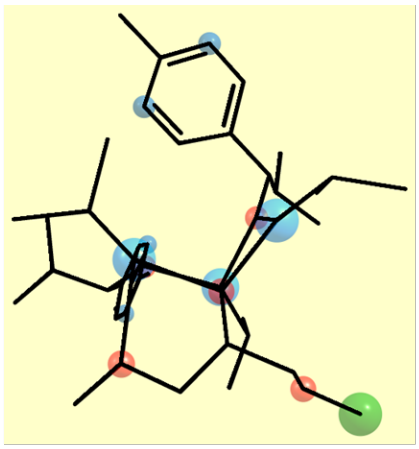
h_5

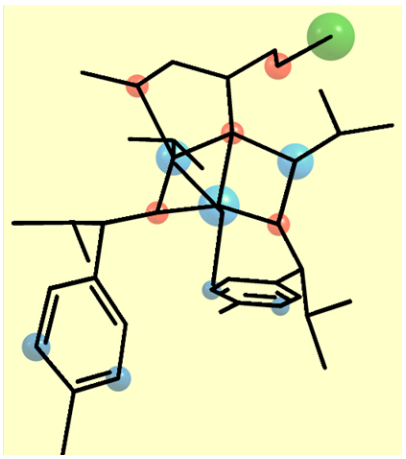


(R,S,S,R)

-17.5, *-20.7*

isomer resulting from binding S initiator



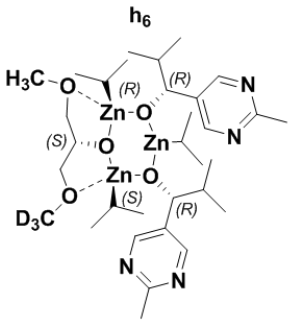


Zero-point correction= 0.858276 (Hartree/Particle)
Thermal correction to Energy= 0.917271
Thermal correction to Enthalpy= 0.918215
Thermal correction to Gibbs Free Energy= 0.755403
Sum of electronic and zero-point Energies= -2530.193966
Sum of electronic and thermal Energies= -2530.134971
Sum of electronic and thermal Enthalpies= -2530.134027
Sum of electronic and thermal Free Energies= -2530.296839

6	1.393307000	-3.444193000	1.141749000
6	2.344582000	-2.428409000	0.513240000
1	0.615109000	-3.744137000	0.430122000
8	0.801553000	-2.830810000	2.289774000
1	1.951502000	-4.339488000	1.451528000
8	1.641038000	-1.230349000	0.191747000
6	3.089180000	-3.029392000	-0.678352000
1	3.116081000	-2.197005000	1.265276000
1	3.702679000	-3.876869000	-0.325415000
1	3.785244000	-2.278158000	-1.087721000
8	2.175647000	-3.453684000	-1.667607000
6	2.811734000	-4.029559000	-2.794967000
6	-0.056632000	-3.702761000	3.019721000
1	-0.446288000	-3.136966000	3.867372000
1	-0.890209000	-4.053112000	2.397080000
1	0.501953000	-4.571373000	3.391263000
1(iso=2)	2.026638000	-4.313869000	-3.498150000
1(iso=2)	3.389813000	-4.924299000	-2.518661000
1(iso=2)	3.490625000	-3.315032000	-3.284015000
30	2.637993000	0.335459000	-0.696864000
30	-0.294991000	-0.924427000	-1.012306000
8	-1.008759000	-0.401061000	0.870750000
6	-2.223901000	-0.941099000	1.384202000
6	-3.390491000	-0.652760000	0.455137000
1	-2.137857000	-2.039209000	1.445367000
6	-2.493849000	-0.453527000	2.842056000
1	-1.576582000	-0.693832000	3.399789000
6	-3.636340000	-1.243125000	3.499199000
6	-2.727969000	1.057250000	2.968975000
1	-1.925609000	1.646042000	2.517339000
1	-2.788113000	1.337460000	4.026187000
1	-3.672495000	1.355568000	2.501126000
1	-3.469255000	-2.324935000	3.443209000
1	-4.599501000	-1.027047000	3.024553000
1	-3.724493000	-0.974294000	4.556783000
6	-3.586365000	0.572048000	-0.193969000
6	-4.380782000	-1.605223000	0.204940000

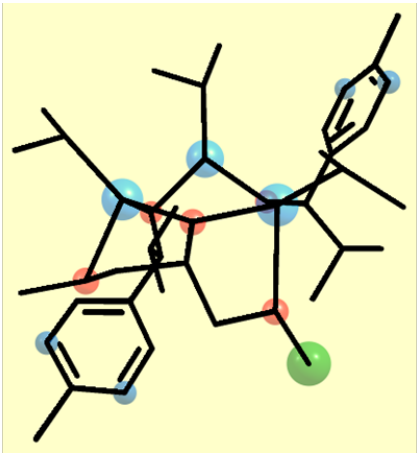
7	-4.634252000	0.823219000	-0.983953000
6	-5.530764000	-0.166698000	-1.139887000
7	-5.445231000	-1.381202000	-0.574923000
6	-6.707947000	0.107096000	-2.036468000
1	-2.868369000	1.379032000	-0.076967000
1	-7.483565000	-0.645504000	-1.888373000
1	-6.394711000	0.080499000	-3.086799000
1	-7.111248000	1.104833000	-1.844721000
1	-4.312615000	-2.598086000	0.649900000
8	0.879238000	0.774545000	-1.401849000
6	0.654541000	2.039456000	-2.018762000
6	-0.460115000	1.935809000	-3.093134000
6	0.400164000	3.106295000	-0.965392000
1	1.569771000	2.340382000	-2.557411000
6	0.921158000	4.397869000	-1.061482000
6	-0.347434000	2.862546000	0.191308000
1	-1.328427000	1.472330000	-2.602450000
6	0.008335000	1.028747000	-4.241387000
6	-0.895445000	3.301812000	-3.645004000
1	-1.332312000	3.942848000	-2.875074000
1	-1.645710000	3.166740000	-4.430617000
1	-0.048593000	3.838502000	-4.090670000
1	0.318721000	0.046094000	-3.880374000
1	0.858987000	1.486459000	-4.762591000
1	-0.790228000	0.885020000	-4.976396000
7	-0.581074000	3.795996000	1.120935000
7	0.705435000	5.351638000	-0.146812000
6	-0.051178000	5.013620000	0.908858000
6	-0.308282000	6.067085000	1.952576000
1	1.545567000	4.679629000	-1.909867000
1	-0.748365000	1.870593000	0.387208000
1	-0.007692000	7.048941000	1.584527000
1	0.260813000	5.844685000	2.862659000
1	-1.366005000	6.080580000	2.229791000
6	-1.049637000	-2.170242000	-2.402558000
6	-2.312717000	-1.648022000	-3.104999000
6	-1.285802000	-3.600185000	-1.889682000
1	-0.248035000	-2.222440000	-3.153397000
1	-2.031488000	-3.630891000	-1.083939000
1	-0.363447000	-4.055797000	-1.517341000
1	-1.670792000	-4.253320000	-2.690756000
1	-3.166770000	-1.601629000	-2.420692000
1	-2.610708000	-2.313906000	-3.931704000
1	-2.179817000	-0.647992000	-3.529424000
6	4.542800000	0.905464000	-0.686182000
6	5.228526000	0.670250000	-2.043641000
6	5.353449000	0.274783000	0.457328000
1	4.510750000	1.990467000	-0.513477000
1	5.273368000	-0.395857000	-2.300916000
1	6.267358000	1.035512000	-2.032063000
1	4.713451000	1.181526000	-2.864854000
1	5.414619000	-0.817062000	0.362022000
1	4.924187000	0.493322000	1.441462000
1	6.389482000	0.648083000	0.463213000
30	0.662158000	-0.485446000	1.943213000
6	1.689145000	0.311769000	3.456177000
6	2.081120000	1.782413000	3.235910000
1	2.615853000	-0.280695000	3.488112000
6	0.985188000	0.137214000	4.811729000
1	0.040214000	0.693032000	4.853560000
1	1.609070000	0.513747000	5.638331000
1	0.758476000	-0.912850000	5.032299000
1	2.686641000	1.921197000	2.331681000
1	2.675149000	2.168583000	4.079956000
1	1.203038000	2.431686000	3.139151000

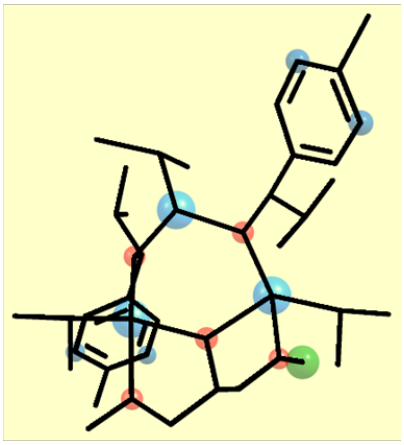
h_6



(R,R,R,S) - Start

-9.6, *-9.9*



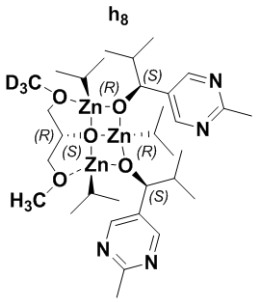


Zero-point correction= 0.858779 (Hartree/Particle)
Thermal correction to Energy= 0.917258
Thermal correction to Enthalpy= 0.918203
Thermal correction to Gibbs Free Energy= 0.760462
Sum of electronic and zero-point Energies= -2530.181375
Sum of electronic and thermal Energies= -2530.122895
Sum of electronic and thermal Enthalpies= -2530.121951
Sum of electronic and thermal Free Energies= -2530.279691

6	-1.895266000	3.054450000	-0.248506000
6	-1.680270000	2.238311000	-1.524898000
1	-2.448123000	3.977141000	-0.483030000
8	-0.607527000	3.386982000	0.264812000
1	-2.467237000	2.482491000	0.493884000
8	-0.859863000	1.114160000	-1.261962000
6	-3.008734000	1.829435000	-2.159933000
1	-1.185094000	2.900584000	-2.252184000
1	-2.842042000	1.480690000	-3.188524000
1	-3.696204000	2.687065000	-2.195760000
8	-3.586606000	0.776530000	-1.384806000
6	-4.878559000	0.389631000	-1.857556000
6	-0.651471000	4.323324000	1.333161000
1	-5.245498000	-0.388581000	-1.188679000
1	-4.826647000	0.008768000	-2.884864000
1	-5.564011000	1.246558000	-1.827045000
30	1.006232000	1.703677000	-0.682026000
30	0.920024000	-1.588161000	-0.103876000
8	-1.030585000	-1.571243000	0.348185000
6	-1.401914000	-1.330988000	1.705107000
6	-2.804100000	-0.756978000	1.787541000
1	-0.717288000	-0.588381000	2.145431000
6	-1.296825000	-2.630608000	2.558784000
1	-2.035267000	-3.339397000	2.158454000
6	-1.631982000	-2.357009000	4.034581000
6	0.085077000	-3.287003000	2.452255000
1	0.308687000	-3.604227000	1.430458000
1	0.137070000	-4.178814000	3.085946000
1	0.875074000	-2.604148000	2.793448000
1	-2.644648000	-1.966696000	4.166457000
1	-0.933860000	-1.628355000	4.465632000
1	-1.550580000	-3.277003000	4.622218000
6	-3.926859000	-1.417891000	1.274932000
6	-3.078952000	0.463661000	2.402645000
7	-5.165826000	-0.925094000	1.355177000
6	-5.309165000	0.263869000	1.970403000
7	-4.309971000	0.983117000	2.501737000

6	-6.704406000	0.820483000	2.065905000
1	-3.820981000	-2.378506000	0.772908000
1	-6.700314000	1.765601000	2.609998000
1	-7.363829000	0.110357000	2.574980000
1	-7.121023000	0.981754000	1.065919000
1	-2.270544000	1.050811000	2.838274000
8	1.404123000	0.234261000	0.659720000
6	2.440007000	0.245369000	1.648410000
6	2.450456000	1.572556000	2.447118000
6	3.793426000	-0.118221000	1.055919000
1	2.205287000	-0.545555000	2.382294000
6	4.481562000	0.676184000	0.131017000
6	4.449912000	-1.299469000	1.404341000
1	2.601404000	2.389733000	1.725995000
6	3.595471000	1.620447000	3.471638000
6	1.102492000	1.782952000	3.150796000
1	0.272881000	1.749247000	2.441976000
1	1.079700000	2.748491000	3.666879000
1	0.939557000	1.002480000	3.904948000
1	4.579653000	1.572527000	2.998653000
1	3.523004000	0.785857000	4.180070000
1	3.547259000	2.547740000	4.051590000
7	5.629790000	-1.672497000	0.893771000
7	5.659462000	0.332545000	-0.396686000
6	6.186264000	-0.839993000	0.000937000
6	7.494640000	-1.250264000	-0.618632000
1	4.070840000	1.627362000	-0.196778000
1	4.005838000	-1.978585000	2.133198000
1	8.162430000	-0.389954000	-0.709802000
1	7.324528000	-1.638134000	-1.630101000
1	7.968737000	-2.034092000	-0.026189000
6	2.202991000	2.910258000	-1.758740000
6	2.718182000	4.127118000	-0.974675000
6	1.546268000	3.365885000	-3.072616000
1	3.071949000	2.295547000	-2.034016000
1	1.892104000	4.769760000	-0.646025000
1	3.384842000	4.752774000	-1.589851000
1	3.283782000	3.845069000	-0.078031000
1	0.683755000	4.020105000	-2.891004000
1	1.195807000	2.522843000	-3.679082000
1	2.249441000	3.944077000	-3.693740000
30	-1.708613000	-0.714210000	-1.400979000
6	-1.965718000	-2.014412000	-2.911272000
6	-3.049269000	-3.060047000	-2.599620000
1	-1.006278000	-2.549461000	-2.965256000
6	-2.200108000	-1.365654000	-4.283685000
1	-3.139882000	-0.798901000	-4.317320000
1	-2.265515000	-2.121338000	-5.083541000
1	-1.395804000	-0.672988000	-4.557846000
1	-2.848287000	-3.590902000	-1.662152000
1	-3.121615000	-3.819334000	-3.395417000
1	-4.044908000	-2.606318000	-2.510089000
1(iso=2)	0.378263000	4.515629000	1.637723000
1(iso=2)	-1.216139000	3.929358000	2.188605000
1(iso=2)	-1.113335000	5.265233000	1.006837000
6	2.080744000	-2.853728000	-1.127069000
1	2.939606000	-3.034129000	-0.465612000
6	2.621558000	-2.218493000	-2.420457000
6	1.416053000	-4.208042000	-1.416399000
1	1.089946000	-4.717771000	-0.502508000
1	2.109807000	-4.887809000	-1.936284000
1	0.534519000	-4.101678000	-2.059653000
1	3.171920000	-1.290262000	-2.229158000
1	1.817665000	-1.984173000	-3.129871000
1	3.310755000	-2.902136000	-2.941126000

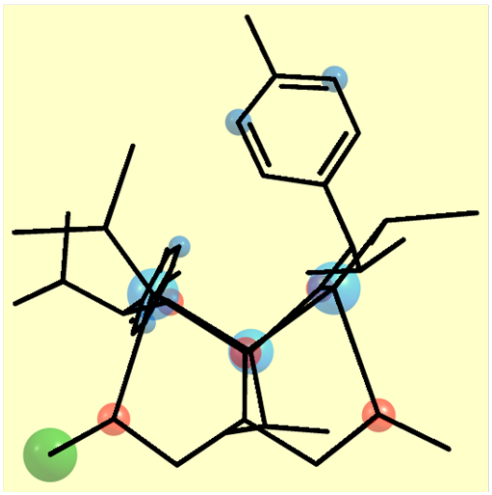
h_8

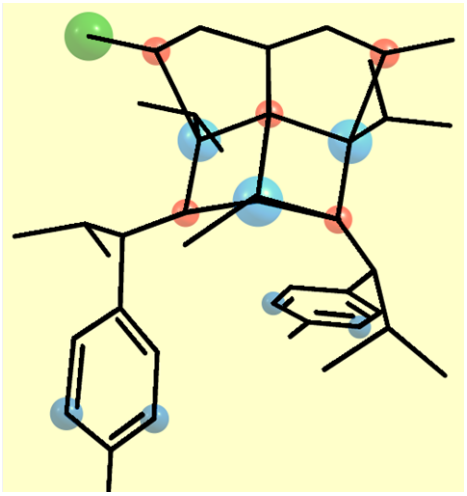


(S,S,S,S) - start

-18.9, *-20.3*

isomer resulting from binding r initiator



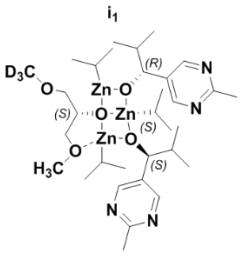


Zero-point correction= 0.858794 (Hartree/Particle)
Thermal correction to Energy= 0.917414
Thermal correction to Enthalpy= 0.918358
Thermal correction to Gibbs Free Energy= 0.758713
Sum of electronic and zero-point Energies= -2530.196163
Sum of electronic and thermal Energies= -2530.137543
Sum of electronic and thermal Enthalpies= -2530.136599
Sum of electronic and thermal Free Energies= -2530.296244

6	1.740624000	-3.529838000	-0.987961000
6	2.519175000	-2.222463000	-0.853443000
1	2.415531000	-4.354299000	-1.260965000
8	1.129264000	-3.799539000	0.271436000
1	0.966966000	-3.438702000	-1.764087000
8	1.671605000	-1.191313000	-0.374118000
6	3.137221000	-1.817156000	-2.192737000
1	3.333515000	-2.381406000	-0.130065000
1	2.363225000	-1.760205000	-2.971154000
1	3.895091000	-2.551175000	-2.505027000
8	3.738874000	-0.538327000	-2.018522000
6	4.323493000	-0.021935000	-3.210162000
6	0.366572000	-5.002930000	0.278845000
1(iso=2)	-0.048987000	-5.113692000	1.281509000
1(iso=2)	1.003467000	-5.868213000	0.054150000
1(iso=2)	-0.450122000	-4.959726000	-0.454179000
1	3.572000000	0.096272000	-4.001944000
1	4.746951000	0.952451000	-2.962364000
1	5.122671000	-0.683013000	-3.570130000
30	2.580942000	0.672156000	-0.229122000
30	-0.143954000	-0.470170000	-1.437075000
8	-1.008657000	-1.033131000	0.376928000
6	-2.246467000	-1.739858000	0.444759000
6	-3.407567000	-0.889188000	-0.045182000
1	-2.200107000	-2.615909000	-0.225084000
6	-2.501085000	-2.315396000	1.871795000
1	-1.600383000	-2.902130000	2.107091000
6	-2.655508000	-1.245941000	2.960823000
6	-3.685535000	-3.293512000	1.886559000
1	-4.632325000	-2.780372000	1.687229000
1	-3.568727000	-4.085331000	1.137771000
1	-3.771052000	-3.772585000	2.867270000
1	-1.846145000	-0.511398000	2.931000000
1	-3.604479000	-0.708813000	2.861770000
1	-2.648545000	-1.713143000	3.951196000
6	-3.632716000	0.435672000	0.348196000
6	-4.373383000	-1.406060000	-0.912229000

7	-4.682556000	1.153521000	-0.064825000
6	-5.547433000	0.547244000	-0.895646000
7	-5.435325000	-0.714232000	-1.340376000
6	-6.720527000	1.356150000	-1.380339000
1	-2.944448000	0.940136000	1.019551000
1	-7.079449000	2.020321000	-0.590747000
1	-6.419031000	1.986304000	-2.225949000
1	-7.524860000	0.700124000	-1.717450000
1	-4.286749000	-2.427836000	-1.281166000
8	0.855119000	1.286520000	-0.983181000
6	0.589111000	2.683511000	-0.979131000
6	-0.386030000	3.093474000	-2.121777000
6	0.152025000	3.151754000	0.402721000
1	1.531302000	3.210114000	-1.204025000
6	0.433254000	4.427882000	0.895131000
6	-0.529079000	2.320367000	1.298780000
1	0.026867000	2.602747000	-3.012325000
6	-1.826844000	2.607186000	-1.930252000
6	-0.362892000	4.609420000	-2.372959000
1	-0.948042000	4.855157000	-3.265185000
1	-0.798355000	5.165062000	-1.535196000
1	0.656222000	4.980213000	-2.531439000
1	-1.887977000	1.523349000	-1.796288000
1	-2.302183000	3.077568000	-1.063447000
1	-2.429326000	2.855798000	-2.810608000
7	-0.928202000	2.718525000	2.511849000
7	0.049688000	4.854035000	2.105922000
6	-0.633160000	3.982197000	2.863773000
6	-1.090567000	4.439800000	4.222865000
1	1.003244000	5.139165000	0.297605000
1	-0.744213000	1.289276000	1.030155000
1	-2.169151000	4.288988000	4.332232000
1	-0.603716000	3.849459000	5.006672000
1	-0.852287000	5.493838000	4.369643000
6	-0.536655000	-1.106189000	-3.313220000
6	-1.975112000	-1.580212000	-3.568999000
6	-0.117869000	-0.081701000	-4.379610000
1	0.113770000	-1.986555000	-3.439810000
1	-0.734256000	0.823992000	-4.330657000
1	0.926244000	0.235306000	-4.269560000
1	-0.232079000	-0.486387000	-5.398754000
1	-2.269962000	-2.392878000	-2.895479000
1	-2.703921000	-0.771784000	-3.436467000
1	-2.100638000	-1.952601000	-4.599117000
6	4.090262000	1.402944000	0.845945000
6	5.068683000	0.304177000	1.291172000
6	4.839492000	2.541782000	0.133220000
1	3.630135000	1.826850000	1.750116000
1	5.882482000	0.716654000	1.909323000
1	4.574817000	-0.474123000	1.884807000
1	5.539683000	-0.189297000	0.432032000
1	4.178793000	3.375697000	-0.131137000
1	5.642385000	2.951557000	0.766923000
1	5.318593000	2.197568000	-0.792752000
30	0.607729000	-1.672710000	1.369610000
6	1.440931000	-1.878906000	3.171570000
6	0.853380000	-3.044997000	3.981564000
1	2.488379000	-2.130259000	2.946986000
6	1.439268000	-0.581323000	3.996291000
1	0.422294000	-0.238195000	4.221516000
1	1.949976000	-0.721417000	4.962696000
1	1.948899000	0.240120000	3.479539000
1	-0.202158000	-2.879073000	4.230490000
1	0.918409000	-3.997572000	3.442617000
1	1.384969000	-3.176617000	4.937759000

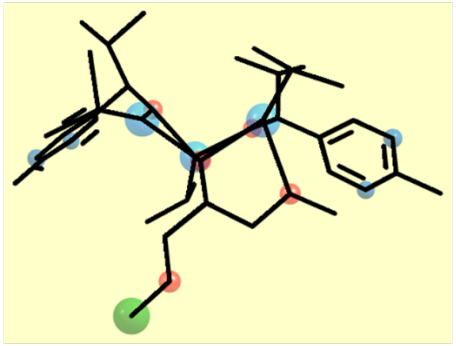
i_1

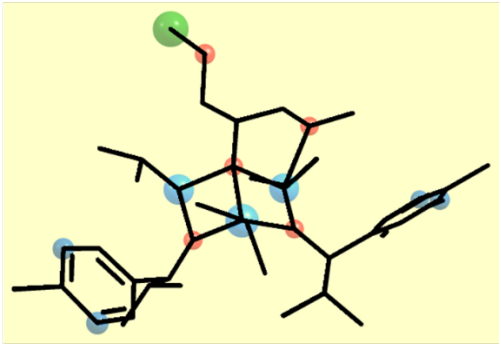


(S,S,R,S)

-19.0, *-20.7*

isomer resulting from binding r initiator



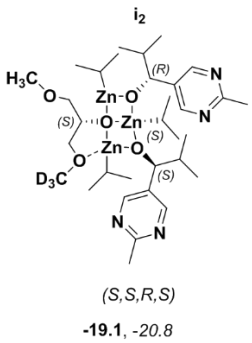


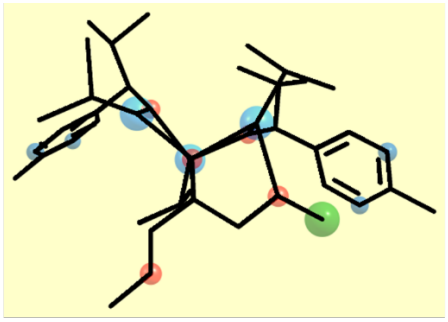
Zero-point correction= 0.859076 (Hartree/Particle)
Thermal correction to Energy= 0.917690
Thermal correction to Enthalpy= 0.918635
Thermal correction to Gibbs Free Energy= 0.758527
Sum of electronic and zero-point Energies= -2530.196387
Sum of electronic and thermal Energies= -2530.137773
Sum of electronic and thermal Enthalpies= -2530.136828
Sum of electronic and thermal Free Energies= -2530.296936

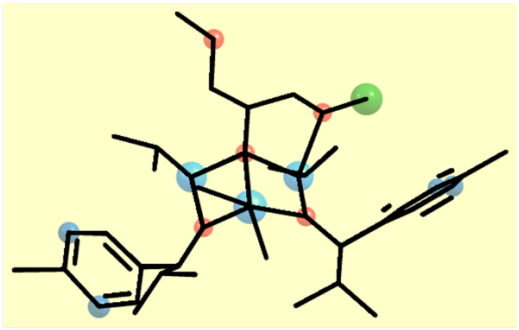
6	1.684626000	1.830185000	2.221594000
6	0.368323000	2.214196000	1.558019000
1	1.935726000	2.561943000	2.998284000
8	2.697223000	1.818195000	1.214818000
1	1.605843000	0.834337000	2.683244000
8	0.071934000	1.313854000	0.491775000
6	-0.759819000	2.232277000	2.593754000
1	-0.861685000	1.235926000	3.054203000
1	-1.716399000	2.465785000	2.097033000
8	-0.455653000	3.211155000	3.567932000
6	-1.444337000	3.307592000	4.577657000
6	4.007989000	1.602467000	1.738512000
1	4.700508000	1.622112000	0.897462000
1	4.267180000	2.399754000	2.446020000
1	4.073930000	0.632700000	2.246583000
1(iso=2)	-1.123339000	4.086831000	5.272316000
1(iso=2)	-1.556402000	2.360957000	5.127178000
1(iso=2)	-2.423618000	3.583535000	4.158399000
30	1.814882000	1.001492000	-0.759016000
30	-0.288720000	-0.882228000	0.678048000
8	-1.625503000	-0.279701000	-0.805983000
6	-2.595741000	-1.105999000	-1.443987000
6	-3.703102000	-1.489484000	-0.474788000
1	-2.096509000	-2.040306000	-1.747062000
6	-3.142251000	-0.453307000	-2.742142000
1	-3.609490000	0.500735000	-2.452274000
6	-4.216493000	-1.323829000	-3.414384000
6	-2.009845000	-0.159540000	-3.736968000
1	-1.212420000	0.441049000	-3.291683000
1	-2.394079000	0.379961000	-4.608624000
1	-1.559968000	-1.093259000	-4.094153000
1	-5.090183000	-1.474696000	-2.775087000
1	-3.814296000	-2.311018000	-3.673273000
1	-4.557904000	-0.855089000	-4.342751000
6	-4.509619000	-0.551884000	0.181502000
6	-3.993743000	-2.818521000	-0.167456000
7	-5.477928000	-0.886949000	1.036188000
6	-5.665803000	-2.202280000	1.256373000
7	-4.959283000	-3.188087000	0.684475000

6	-6.751134000	-2.584865000	2.225911000
1	-4.373264000	0.515427000	0.011604000
1	-6.868383000	-3.668600000	2.256846000
1	-7.699546000	-2.119545000	1.940282000
1	-6.506207000	-2.222813000	3.230377000
1	-3.422722000	-3.625426000	-0.627568000
8	1.492183000	-0.899522000	-0.339461000
6	2.308061000	-2.034620000	-0.606448000
6	2.260510000	-2.462353000	-2.095568000
6	3.722913000	-1.796016000	-0.098367000
6	4.670911000	-1.011557000	-0.766341000
6	4.165295000	-2.330266000	1.113239000
1	2.650089000	-1.627526000	-2.696152000
6	0.814568000	-2.722482000	-2.534586000
6	3.129373000	-3.703383000	-2.356938000
1	4.186000000	-3.529811000	-2.135099000
1	3.054575000	-4.008993000	-3.405577000
1	2.794034000	-4.548811000	-1.743210000
1	0.187678000	-1.845844000	-2.365748000
1	0.386559000	-3.564927000	-1.975055000
1	0.772855000	-2.979138000	-3.598583000
7	5.388160000	-2.116719000	1.615678000
7	5.898718000	-0.779357000	-0.291808000
6	6.211759000	-1.346832000	0.887282000
6	7.601134000	-1.110960000	1.415644000
1	4.436781000	-0.550311000	-1.724703000
1	3.503234000	-2.961680000	1.706468000
1	7.877265000	-0.057732000	1.316197000
1	8.327846000	-1.690063000	0.834014000
1	7.669298000	-1.418633000	2.459911000
6	-0.593924000	-2.003787000	2.320676000
6	-0.506212000	-3.512409000	2.027728000
6	-1.887858000	-1.694946000	3.090069000
1	0.250977000	-1.751048000	2.980183000
1	-2.778956000	-1.916089000	2.491709000
1	-1.957715000	-0.644512000	3.395353000
1	-1.964364000	-2.302084000	4.006938000
1	-1.306478000	-3.843390000	1.353687000
1	-0.608388000	-4.108477000	2.949404000
1	0.446449000	-3.796541000	1.565680000
6	2.502790000	2.126509000	-2.266687000
6	3.823650000	2.832355000	-1.918536000
6	1.466550000	3.143250000	-2.773002000
1	2.707474000	1.426812000	-3.090414000
1	3.703795000	3.526094000	-1.077495000
1	4.197082000	3.424063000	-2.769783000
1	4.616701000	2.125524000	-1.647424000
1	1.174014000	3.853404000	-1.989075000
1	0.551516000	2.658265000	-3.134340000
1	1.862697000	3.741721000	-3.609276000
30	-1.632135000	1.658534000	-0.653927000
6	-2.503560000	3.418177000	-0.976754000
6	-2.687237000	3.745621000	-2.466814000
1	-1.802836000	4.152573000	-0.554841000
6	-3.836605000	3.553807000	-0.221132000
1	-4.590031000	2.848340000	-0.593984000
1	-4.262170000	4.561562000	-0.346646000
1	-3.732446000	3.380687000	0.856314000
1	-1.738589000	3.739463000	-3.013887000
1	-3.134326000	4.743031000	-2.600075000
1	-3.356824000	3.031200000	-2.962065000
1	0.476367000	3.231675000	1.154338000
1	1.906112000	-2.879820000	-0.024039000

i_2





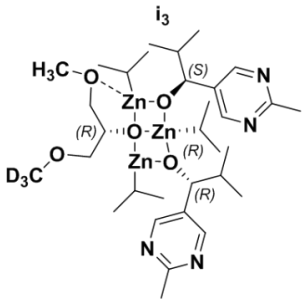


Zero-point correction= 0.858955 (Hartree/Particle)
Thermal correction to Energy= 0.917593
Thermal correction to Enthalpy= 0.918537
Thermal correction to Gibbs Free Energy= 0.758416
Sum of electronic and zero-point Energies= -2530.196507
Sum of electronic and thermal Energies= -2530.137870
Sum of electronic and thermal Enthalpies= -2530.136925
Sum of electronic and thermal Free Energies= -2530.297047

6	1.684863000	1.830353000	2.221339000
6	0.368421000	2.214246000	1.557972000
1	1.936018000	2.562141000	2.997977000
8	2.697320000	1.818459000	1.214402000
1	1.606260000	0.834498000	2.682999000
8	0.071934000	1.313901000	0.491749000
6	-0.759543000	2.232180000	2.593908000
1	-0.861197000	1.235807000	3.054351000
1	-1.716255000	2.465582000	2.097390000
8	-0.455306000	3.211070000	3.568052000
6	-1.443722000	3.307245000	4.578065000
6	4.008229000	1.603128000	1.737928000
1(iso=2)	4.700635000	1.623031000	0.896793000
1(iso=2)	4.267238000	2.400473000	2.445432000
1(iso=2)	4.074530000	0.633365000	2.245957000
1	-1.122661000	4.086474000	5.272705000
1	-1.555467000	2.360538000	5.127530000
1	-2.423170000	3.583056000	4.159109000
30	1.814912000	1.001383000	-0.759032000
30	-0.288881000	-0.882475000	0.677919000
8	-1.625557000	-0.279650000	-0.806009000
6	-2.595853000	-1.105855000	-1.444020000
6	-3.703351000	-1.489120000	-0.474883000
1	-2.096738000	-2.040257000	-1.747000000
6	-3.142159000	-0.453180000	-2.742275000
1	-3.609316000	0.500936000	-2.452517000
6	-4.216428000	-1.323623000	-3.414568000
6	-2.009593000	-0.159616000	-3.736974000
1	-1.212173000	0.440934000	-3.291624000
1	-2.393654000	0.379848000	-4.608730000
1	-1.559756000	-1.093410000	-4.094018000
1	-5.090209000	-1.474329000	-2.775356000
1	-3.814329000	-2.310884000	-3.673333000
1	-4.557678000	-0.854915000	-4.343011000
6	-4.509701000	-0.551375000	0.181390000
6	-3.994280000	-2.818110000	-0.167591000
7	-5.478075000	-0.886266000	1.036080000
6	-5.666201000	-2.201552000	1.256262000
7	-4.959893000	-3.187499000	0.684326000

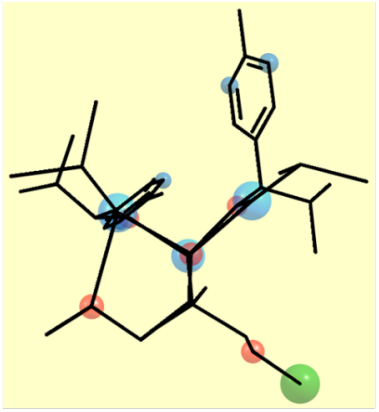
6	-6.751582000	-2.583944000	2.225819000
1	-4.373151000	0.515912000	0.011507000
1	-6.868846000	-3.667670000	2.256942000
1	-7.699980000	-2.118668000	1.940062000
1	-6.506707000	-2.221696000	3.230226000
1	-3.423419000	-3.625117000	-0.627725000
8	1.492123000	-0.899599000	-0.339273000
6	2.307961000	-2.034847000	-0.605780000
6	2.260296000	-2.463260000	-2.094709000
6	3.722872000	-1.796054000	-0.097956000
6	4.670687000	-1.011683000	-0.766271000
6	4.165522000	-2.330024000	1.113690000
1	2.649929000	-1.628737000	-2.695679000
6	0.814316000	-2.723452000	-2.533568000
6	3.129041000	-3.704484000	-2.355531000
1	4.185678000	-3.530917000	-2.133733000
1	3.054249000	-4.010532000	-3.404043000
1	2.793604000	-4.549621000	-1.741456000
1	0.187538000	-1.846638000	-2.365220000
1	0.386207000	-3.565537000	-1.973574000
1	0.772567000	-2.980694000	-3.597422000
7	5.388447000	-2.116278000	1.615862000
7	5.898560000	-0.779256000	-0.291987000
6	6.211852000	-1.346435000	0.887155000
6	7.601276000	-1.110312000	1.415278000
1	4.436378000	-0.550695000	-1.724709000
1	3.503599000	-2.961369000	1.707154000
1	7.877208000	-0.057040000	1.315740000
1	8.327987000	-1.689314000	0.833547000
1	7.669663000	-1.417924000	2.459549000
6	-0.594339000	-2.003869000	2.320618000
6	-0.507046000	-3.512551000	2.027849000
6	-1.888244000	-1.694623000	3.089917000
1	0.250598000	-1.751277000	2.980133000
1	-2.779358000	-1.915626000	2.491531000
1	-1.957882000	-0.644141000	3.395083000
1	-1.964936000	-2.301644000	4.006847000
1	-1.307391000	-3.843370000	1.353823000
1	-0.609429000	-4.108471000	2.949596000
1	0.445541000	-3.797037000	1.565865000
6	2.502949000	2.125667000	-2.267173000
6	3.824193000	2.831078000	-1.919619000
6	1.466933000	3.142660000	-2.773455000
1	2.707102000	1.425656000	-3.090765000
1	3.704889000	3.525126000	-1.078752000
1	4.197616000	3.422368000	-2.771159000
1	4.617028000	2.123983000	-1.648538000
1	1.174895000	3.853131000	-1.989631000
1	0.551614000	2.657897000	-3.134381000
1	1.863030000	3.740755000	-3.610022000
30	-1.631965000	1.658631000	-0.653876000
6	-2.503246000	3.418325000	-0.976872000
6	-2.686978000	3.745824000	-2.466905000
1	-1.802426000	4.152645000	-0.554979000
6	-3.836247000	3.554091000	-0.221178000
1	-4.589755000	2.848690000	-0.593990000
1	-4.261723000	4.561885000	-0.346678000
1	-3.732051000	3.380970000	0.856264000
1	-1.738372000	3.739549000	-3.014052000
1	-3.133943000	4.743296000	-2.600106000
1	-3.356694000	3.031503000	-2.962128000
1	0.476299000	3.231747000	1.154300000
1	1.906033000	-2.879764000	-0.022945000

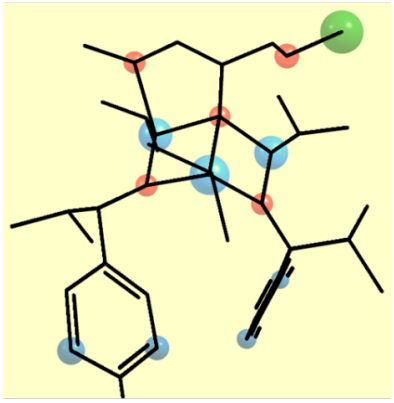
i_3



(R,R,S,R)

-19.9, *-21.5*



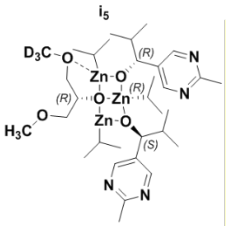


Zero-point correction= 0.858492 (Hartree/Particle)
Thermal correction to Energy= 0.917195
Thermal correction to Enthalpy= 0.918140
Thermal correction to Gibbs Free Energy= 0.757978
Sum of electronic and zero-point Energies= -2530.197673
Sum of electronic and thermal Energies= -2530.138969
Sum of electronic and thermal Enthalpies= -2530.138025
Sum of electronic and thermal Free Energies= -2530.298186

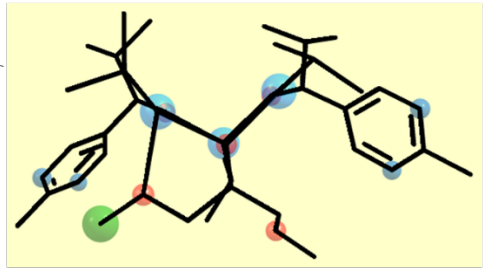
6	3.298108000	-2.133555000	-0.965593000
6	3.334954000	-0.656905000	-0.576544000
1	2.654415000	-2.279276000	-1.841518000
8	2.787701000	-2.862125000	0.152355000
1	4.309704000	-2.490783000	-1.207508000
8	2.031400000	-0.234695000	-0.182821000
6	3.934567000	0.194266000	-1.695736000
1	4.018964000	-0.556755000	0.281374000
1	4.969707000	-0.140831000	-1.882259000
1	3.992383000	1.245475000	-1.366065000
8	3.156059000	0.082240000	-2.869349000
6	3.698673000	0.802994000	-3.962113000
6	2.645648000	-4.257926000	-0.095023000
1	2.258808000	-4.708744000	0.820366000
1	1.947367000	-4.445438000	-0.920610000
1	3.616775000	-4.708987000	-0.336520000
1(iso=2)	3.027632000	0.656194000	-4.810531000
1(iso=2)	4.701513000	0.436236000	-4.227800000
1(iso=2)	3.768900000	1.878753000	-3.742373000
30	1.630414000	1.756353000	0.208572000
30	0.119136000	-0.586445000	-1.307978000
8	-0.290811000	-1.615784000	0.451896000
6	-1.209594000	-2.694051000	0.539688000
6	-2.535806000	-2.298585000	-0.087845000
1	-0.827725000	-3.554795000	-0.035925000
6	-1.362173000	-3.191645000	2.008762000
1	-0.332430000	-3.386151000	2.345417000
6	-2.125444000	-4.521712000	2.086101000
6	-1.975190000	-2.147533000	2.950799000
1	-1.456488000	-1.187162000	2.883507000
1	-1.913644000	-2.490571000	3.988879000
1	-3.033027000	-1.977280000	2.723304000
1	-1.674889000	-5.286949000	1.443827000
1	-3.171595000	-4.401954000	1.783695000
1	-2.122755000	-4.904407000	3.111832000
6	-3.058262000	-1.004812000	0.015302000
6	-3.319675000	-3.184544000	-0.827778000

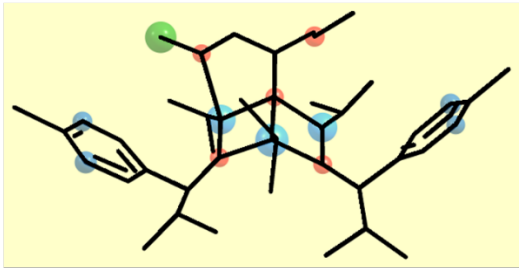
7	-4.213375000	-0.634023000	-0.543110000
6	-4.892460000	-1.577175000	-1.221725000
7	-4.488800000	-2.845474000	-1.387913000
6	-6.197494000	-1.165452000	-1.847705000
1	-2.506196000	-0.238853000	0.552996000
1	-6.670686000	-2.018527000	-2.335069000
1	-6.031171000	-0.374895000	-2.587197000
1	-6.871980000	-0.756829000	-1.088518000
1	-2.991807000	-4.211609000	-0.987707000
8	-0.072844000	1.363073000	-0.632396000
6	-1.098251000	2.292299000	-0.983985000
6	-0.562377000	3.438960000	-1.882150000
6	-1.795778000	2.811393000	0.265927000
1	-1.853615000	1.747690000	-1.570829000
6	-1.165291000	3.633238000	1.208623000
6	-3.123116000	2.495709000	0.564814000
1	0.181376000	3.994784000	-1.289776000
6	-1.680905000	4.415516000	-2.280155000
6	0.134868000	2.893694000	-3.136626000
1	0.932455000	2.187991000	-2.892854000
1	0.567249000	3.714009000	-3.719894000
1	-0.582592000	2.373003000	-3.782199000
1	-2.146669000	4.889516000	-1.412051000
1	-2.467955000	3.898096000	-2.842320000
1	-1.284878000	5.208586000	-2.922746000
7	-3.752219000	2.932302000	1.665981000
7	-1.764668000	4.079236000	2.314848000
6	-3.045211000	3.706998000	2.500184000
6	-3.726851000	4.203629000	3.746936000
1	-0.132769000	3.950050000	1.069469000
1	-3.706837000	1.855522000	-0.097516000
1	-3.667210000	5.295002000	3.805815000
1	-3.226112000	3.807672000	4.637121000
1	-4.772353000	3.893676000	3.756926000
6	-0.228014000	-1.276437000	-3.163261000
6	-1.583822000	-0.835274000	-3.739059000
6	-0.077224000	-2.800493000	-3.292500000
1	0.560600000	-0.813484000	-3.772112000
1	-0.819175000	-3.336122000	-2.686579000
1	0.913096000	-3.154072000	-2.981108000
1	-0.223818000	-3.135464000	-4.332935000
1	-2.424109000	-1.259455000	-3.176316000
1	-1.706144000	-1.169296000	-4.783002000
1	-1.705651000	0.253635000	-3.733340000
6	2.804649000	3.078955000	1.122030000
6	3.218772000	4.240735000	0.202099000
6	4.036145000	2.428262000	1.772379000
1	2.186733000	3.498465000	1.928595000
1	3.821511000	3.894701000	-0.647501000
1	3.830888000	4.978277000	0.743830000
1	2.355401000	4.776787000	-0.208538000
1	4.699310000	1.971025000	1.026746000
1	3.763985000	1.646624000	2.490252000
1	4.639435000	3.172966000	2.314424000
30	1.378796000	-1.451202000	1.460383000
6	2.277986000	-1.413794000	3.240710000
6	1.590570000	-0.498516000	4.267401000
1	3.271163000	-0.990004000	3.028443000
6	2.494764000	-2.819603000	3.824324000
1	1.543586000	-3.318424000	4.052806000
1	3.061498000	-2.779476000	4.768494000
1	3.050943000	-3.470587000	3.140112000
1	1.501220000	0.535271000	3.912577000
1	2.149794000	-0.466439000	5.216270000
1	0.578309000	-0.845315000	4.509015000

i_5



(*R,S,R,R*)
-19.1, *-19.9*
isomer resulting from
binding r initiator



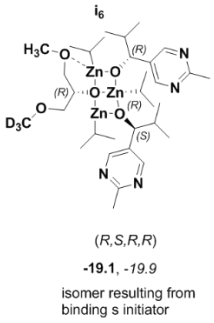


Zero-point correction= 0.858384 (Hartree/Particle)
Thermal correction to Energy= 0.916351
Thermal correction to Enthalpy= 0.917296
Thermal correction to Gibbs Free Energy= 0.759326
Sum of electronic and zero-point Energies= -2530.196541
Sum of electronic and thermal Energies= -2530.138574
Sum of electronic and thermal Enthalpies= -2530.137630
Sum of electronic and thermal Free Energies= -2530.295600

6	0.938959000	0.619784000	-3.047804000
6	-0.347327000	1.065572000	-2.355999000
1	1.072600000	-0.464171000	-2.950013000
8	2.033798000	1.307348000	-2.442684000
1	0.894178000	0.870389000	-4.117806000
8	-0.252247000	0.838574000	-0.950682000
6	-1.554171000	0.385539000	-3.006123000
1	-1.643808000	0.745641000	-4.045960000
1	-2.479454000	0.681286000	-2.485252000
8	-1.387811000	-1.016424000	-2.982079000
6	-2.432151000	-1.717260000	-3.638434000
6	3.284915000	0.999072000	-3.056581000
1(iso=2)	4.051912000	1.577690000	-2.542047000
1(iso=2)	3.516538000	-0.068943000	-2.969349000
1(iso=2)	3.267955000	1.281295000	-4.117107000
1	-2.181737000	-2.778897000	-3.592722000
1	-2.515858000	-1.412620000	-4.692597000
1	-3.401352000	-1.560299000	-3.145471000
30	-1.867340000	1.403349000	0.276261000
30	0.023737000	-1.125596000	0.031300000
8	1.650915000	-0.062558000	0.732943000
6	2.673942000	-0.596713000	1.565345000
6	3.842722000	-1.091379000	0.725526000
1	2.261067000	-1.474020000	2.089155000
6	3.127681000	0.405700000	2.659576000
1	3.530370000	1.290186000	2.143913000
6	4.238668000	-0.181582000	3.546065000
6	1.945561000	0.852498000	3.527435000
1	1.136556000	1.268307000	2.923378000
1	2.260475000	1.615551000	4.246893000
1	1.543336000	0.005276000	4.095293000
1	5.140915000	-0.427110000	2.979447000
1	3.896432000	-1.096837000	4.044876000
1	4.519021000	0.532276000	4.327308000
6	4.643561000	-0.240460000	-0.044428000
6	4.202894000	-2.437319000	0.660380000
7	5.665339000	-0.665382000	-0.790977000
6	5.916215000	-1.988394000	-0.777494000
7	5.223309000	-2.896886000	-0.076633000
6	7.062655000	-2.475910000	-1.622093000
1	4.455767000	0.832814000	-0.059273000

1	7.246319000	-3.535042000	-1.438353000
1	7.968097000	-1.900988000	-1.405819000
1	6.838851000	-2.333712000	-2.685306000
1	3.647005000	-3.181742000	1.229904000
8	-1.598770000	-0.327523000	1.102806000
6	-2.598295000	-1.147728000	1.711008000
6	-2.856041000	-0.757607000	3.186520000
6	-3.857253000	-1.163729000	0.852930000
6	-4.868709000	-0.197308000	0.918905000
6	-4.060042000	-2.146038000	-0.118846000
1	-3.243117000	0.272121000	3.202401000
6	-1.547703000	-0.776521000	3.985643000
6	-3.894564000	-1.682583000	3.842419000
1	-4.870960000	-1.634921000	3.352447000
1	-4.035833000	-1.413002000	4.894007000
1	-3.557346000	-2.726118000	3.812799000
1	-0.803493000	-0.116050000	3.540223000
1	-1.127388000	-1.790040000	4.016828000
1	-1.721149000	-0.458179000	5.019129000
7	-5.116488000	-2.168057000	-0.941367000
7	-5.936684000	-0.194471000	0.115023000
6	-6.017256000	-1.183669000	-0.792241000
6	-7.215508000	-1.182591000	-1.702560000
1	-4.823943000	0.609190000	1.648661000
1	-3.334962000	-2.949915000	-0.241950000
1	-7.251914000	-0.255358000	-2.283902000
1	-8.138349000	-1.226960000	-1.115230000
1	-7.178345000	-2.034710000	-2.382054000
6	0.010491000	-3.077411000	-0.445036000
6	0.296257000	-3.997423000	0.754211000
6	0.929869000	-3.427119000	-1.625292000
1	-1.022056000	-3.273572000	-0.769267000
1	1.984186000	-3.222596000	-1.398758000
1	0.666795000	-2.858537000	-2.523929000
1	0.868431000	-4.497547000	-1.884942000
1	1.308730000	-3.850355000	1.151526000
1	0.223881000	-5.062112000	0.476073000
1	-0.400057000	-3.833917000	1.585990000
6	-2.850105000	3.132387000	0.163695000
6	-3.947817000	3.107703000	-0.914509000
6	-1.914206000	4.333926000	-0.042600000
1	-3.343875000	3.253585000	1.138167000
1	-3.527993000	2.971612000	-1.919653000
1	-4.501129000	4.059737000	-0.933161000
1	-4.681120000	2.310615000	-0.752639000
1	-1.365496000	4.265290000	-0.990187000
1	-1.170574000	4.429231000	0.755668000
1	-2.482622000	5.276739000	-0.073528000
30	1.549377000	1.689688000	-0.152645000
6	2.032682000	3.617375000	0.078135000
6	1.943840000	4.116668000	1.528968000
1	1.276122000	4.159716000	-0.506564000
6	3.406705000	3.958878000	-0.521936000
1	4.222579000	3.437215000	-0.003937000
1	3.623498000	5.036047000	-0.437940000
1	3.470752000	3.699416000	-1.583935000
1	0.950624000	3.964439000	1.967399000
1	2.165322000	5.193934000	1.596159000
1	2.663464000	3.606372000	2.181057000
1	-0.467863000	2.146514000	-2.529959000
1	-2.207425000	-2.177380000	1.718925000

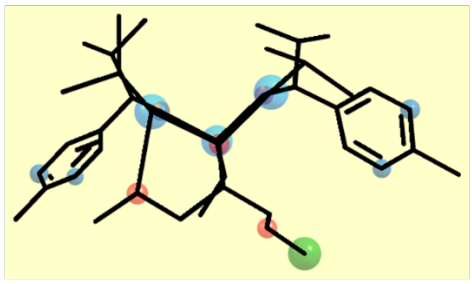
i_6

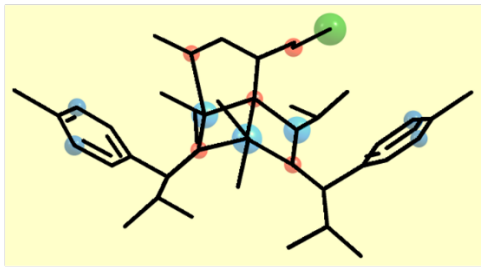


(*R,S,R,R*)

-19.1, *-19.9*

isomer resulting from binding s initiator



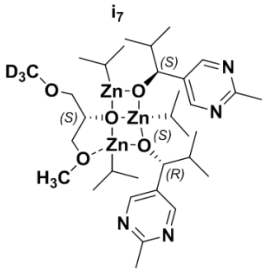


Zero-point correction= 0.858429 (Hartree/Particle)
Thermal correction to Energy= 0.916389
Thermal correction to Enthalpy= 0.917334
Thermal correction to Gibbs Free Energy= 0.759363
Sum of electronic and zero-point Energies= -2530.196496
Sum of electronic and thermal Energies= -2530.138536
Sum of electronic and thermal Enthalpies= -2530.137592
Sum of electronic and thermal Free Energies= -2530.295562

6	0.938958000	0.619784000	-3.047804000
6	-0.347328000	1.065572000	-2.355999000
1	1.072600000	-0.464172000	-2.950014000
8	2.033798000	1.307348000	-2.442684000
1	0.894177000	0.870388000	-4.117806000
8	-0.252247000	0.838573000	-0.950682000
6	-1.554171000	0.385538000	-3.006123000
1	-1.643809000	0.745640000	-4.045960000
1	-2.479454000	0.681285000	-2.485252000
8	-1.387811000	-1.016425000	-2.982079000
6	-2.432151000	-1.717262000	-3.638434000
6	3.284914000	0.999072000	-3.056582000
1	4.051911000	1.577690000	-2.542047000
1	3.516538000	-0.068943000	-2.969349000
1	3.267955000	1.281295000	-4.117107000
1(iso=2)	-2.181736000	-2.778898000	-3.592722000
1(iso=2)	-2.515858000	-1.412621000	-4.692597000
1(iso=2)	-3.401351000	-1.560301000	-3.145471000
30	-1.867340000	1.403349000	0.276261000
30	0.023737000	-1.125596000	0.031301000
8	1.650915000	-0.062558000	0.732942000
6	2.673942000	-0.596713000	1.565345000
6	3.842723000	-1.091379000	0.725526000
1	2.261068000	-1.474019000	2.089155000
6	3.127681000	0.405700000	2.659576000
1	3.530369000	1.290187000	2.143913000
6	4.238668000	-0.181580000	3.546065000
6	1.945561000	0.852499000	3.527435000
1	1.136555000	1.268307000	2.923378000
1	2.260475000	1.615552000	4.246892000
1	1.543336000	0.005277000	4.095293000
1	5.140915000	-0.427108000	2.979447000
1	3.896432000	-1.096836000	4.044876000
1	4.519021000	0.532278000	4.327308000
6	4.643561000	-0.240459000	-0.044428000
6	4.202894000	-2.437318000	0.660380000
7	5.665339000	-0.665380000	-0.790977000
6	5.916216000	-1.988393000	-0.777494000
7	5.223310000	-2.896885000	-0.076633000
6	7.062655000	-2.475908000	-1.622093000

1	4.455767000	0.832815000	-0.059273000
1	7.246323000	-3.535040000	-1.438350000
1	7.968097000	-1.900984000	-1.405822000
1	6.838850000	-2.333715000	-2.685306000
1	3.647006000	-3.181741000	1.229904000
8	-1.598770000	-0.327523000	1.102807000
6	-2.598295000	-1.147728000	1.711009000
6	-2.856041000	-0.757606000	3.186520000
6	-3.857252000	-1.163729000	0.852930000
6	-4.868708000	-0.197307000	0.918904000
6	-4.060042000	-2.146038000	-0.118845000
1	-3.243117000	0.272121000	3.202402000
6	-1.547703000	-0.776520000	3.985644000
6	-3.894564000	-1.682583000	3.842420000
1	-4.870959000	-1.634921000	3.352447000
1	-4.035833000	-1.413001000	4.894008000
1	-3.557345000	-2.726117000	3.812800000
1	-0.803493000	-0.116049000	3.540224000
1	-1.127387000	-1.790039000	4.016830000
1	-1.721149000	-0.458178000	5.019130000
7	-5.116487000	-2.168057000	-0.941366000
7	-5.936682000	-0.194470000	0.115022000
6	-6.017254000	-1.183668000	-0.792242000
6	-7.215506000	-1.182591000	-1.702561000
1	-4.823942000	0.609191000	1.648660000
1	-3.334962000	-2.949916000	-0.241948000
1	-7.251910000	-0.255358000	-2.283904000
1	-8.138347000	-1.226958000	-1.115231000
1	-7.178344000	-2.034710000	-2.382054000
6	0.010492000	-3.077412000	-0.445035000
6	0.296258000	-3.997423000	0.754212000
6	0.929870000	-3.427119000	-1.625292000
1	-1.022055000	-3.273573000	-0.769266000
1	1.984186000	-3.222596000	-1.398757000
1	0.666796000	-2.858537000	-2.523929000
1	0.868432000	-4.497547000	-1.884942000
1	1.308731000	-3.850355000	1.151526000
1	0.223883000	-5.062113000	0.476074000
1	-0.400055000	-3.833917000	1.585990000
6	-2.850107000	3.132385000	0.163694000
6	-3.947819000	3.107700000	-0.914509000
6	-1.914208000	4.333925000	-0.042600000
1	-3.343876000	3.253583000	1.138166000
1	-3.527994000	2.971610000	-1.919653000
1	-4.501131000	4.059734000	-0.933161000
1	-4.681120000	2.310611000	-0.752639000
1	-1.365498000	4.265290000	-0.990188000
1	-1.170576000	4.429231000	0.755668000
1	-2.482625000	5.276738000	-0.073529000
30	1.549377000	1.689688000	-0.152645000
6	2.032680000	3.617375000	0.078135000
6	1.943838000	4.116668000	1.528968000
1	1.276120000	4.159715000	-0.506564000
6	3.406703000	3.958879000	-0.521938000
1	4.222577000	3.437217000	-0.003938000
1	3.623495000	5.036048000	-0.437941000
1	3.470750000	3.699417000	-1.583936000
1	0.950623000	3.964439000	1.967398000
1	2.165320000	5.193934000	1.596158000
1	2.663463000	3.606373000	2.181056000
1	-0.467864000	2.146513000	-2.529959000
1	-2.207424000	-2.177380000	1.718926000

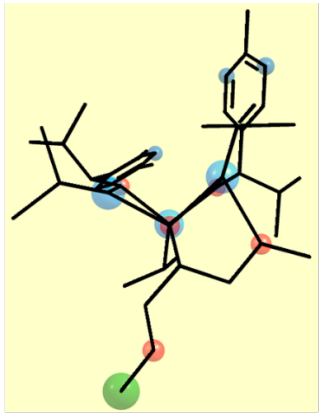
i_7

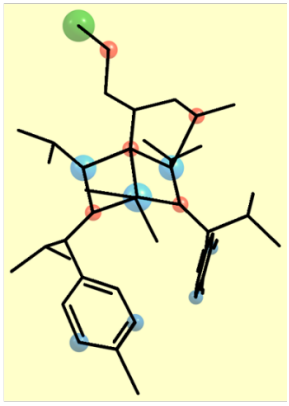


(*S,R,S,S*)

-18.8, *-19.8*

isomer resulting from binding r initiator



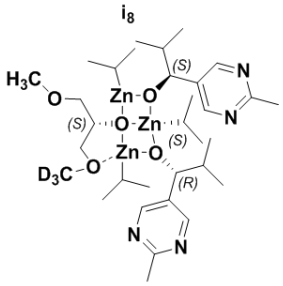


Zero-point correction= 0.858702 (Hartree/Particle)
Thermal correction to Energy= 0.917426
Thermal correction to Enthalpy= 0.918370
Thermal correction to Gibbs Free Energy= 0.759159
Sum of electronic and zero-point Energies= -2530.195971
Sum of electronic and thermal Energies= -2530.137247
Sum of electronic and thermal Enthalpies= -2530.136303
Sum of electronic and thermal Free Energies= -2530.295514

6	-2.984127000	-1.828816000	-1.771256000
6	-3.193194000	-0.741044000	-0.721558000
1	-3.957829000	-2.197318000	-2.114762000
8	-2.240536000	-2.890333000	-1.171962000
1	-2.434059000	-1.429796000	-2.637017000
8	-1.944439000	-0.324128000	-0.173200000
6	-3.943087000	0.444500000	-1.337883000
1	-3.819014000	-1.160370000	0.079592000
1	-3.360196000	0.864302000	-2.174051000
1	-4.059270000	1.239625000	-0.582436000
8	-5.207675000	-0.008721000	-1.780222000
6	-5.987401000	1.019037000	-2.364552000
6	-2.133431000	-4.048880000	-1.996870000
1	-1.549113000	-4.784792000	-1.443166000
1	-3.128467000	-4.459962000	-2.208331000
1	-1.630276000	-3.816076000	-2.942969000
1(iso=2)	-6.936516000	0.572752000	-2.669229000
1(iso=2)	-5.493879000	1.450442000	-3.248392000
1(iso=2)	-6.187736000	1.830280000	-1.648417000
30	-0.728315000	-2.013435000	0.379778000
30	-0.267739000	0.654503000	-1.265720000
8	-0.244301000	1.642559000	0.581459000
6	0.311730000	2.936933000	0.793684000
6	1.655131000	3.045573000	0.095839000
1	-0.343455000	3.699972000	0.341048000
6	0.387210000	3.275595000	2.312400000
1	-0.641580000	3.142956000	2.678332000
6	0.770214000	4.743447000	2.550350000
6	1.295137000	2.329655000	3.108602000
1	1.057511000	1.280419000	2.911131000
1	1.178073000	2.506055000	4.182856000
1	2.350981000	2.488491000	2.864120000
1	0.106212000	5.429300000	2.012113000
1	1.797243000	4.945909000	2.227654000
1	0.706352000	4.986625000	3.615783000
6	2.580648000	1.996957000	0.073642000
6	2.060735000	4.194158000	-0.585693000

7	3.761215000	2.075910000	-0.546414000
6	4.052499000	3.237508000	-1.159829000
7	3.243342000	4.306595000	-1.204645000
6	5.380326000	3.329179000	-1.861415000
1	2.347065000	1.053358000	0.559259000
1	5.566985000	4.351992000	-2.190460000
1	5.392168000	2.668967000	-2.736073000
1	6.185811000	2.999300000	-1.198961000
1	1.404040000	5.062064000	-0.644418000
8	0.605084000	-1.129146000	-0.776193000
6	1.889384000	-1.588783000	-1.198790000
6	1.772930000	-2.740518000	-2.233219000
6	2.757481000	-1.970672000	-0.007681000
1	2.395526000	-0.753039000	-1.706494000
6	2.484352000	-3.069481000	0.815926000
6	3.902303000	-1.251859000	0.343379000
1	1.255066000	-3.573584000	-1.733388000
6	3.152658000	-3.236774000	-2.694861000
6	0.934200000	-2.313049000	-3.444381000
1	-0.044584000	-1.936995000	-3.140254000
1	0.786194000	-3.155020000	-4.129487000
1	1.440343000	-1.518267000	-4.005209000
1	3.748080000	-3.639697000	-1.871347000
1	3.725314000	-2.421679000	-3.154210000
1	3.043597000	-4.025706000	-3.446346000
7	4.679266000	-1.571820000	1.389364000
7	3.237384000	-3.410949000	1.863498000
6	4.313110000	-2.640165000	2.110836000
6	5.166041000	-3.017932000	3.292085000
1	1.621286000	-3.704469000	0.625913000
1	4.207441000	-0.375841000	-0.229945000
1	5.519931000	-4.049173000	3.192578000
1	4.579727000	-2.969293000	4.215832000
1	6.021325000	-2.346262000	3.372780000
6	-0.407831000	1.603748000	-3.034029000
6	0.941774000	1.792156000	-3.746502000
6	-1.140089000	2.951812000	-2.927743000
1	-1.021889000	0.943530000	-3.665915000
1	-0.584097000	3.666009000	-2.307107000
1	-2.141265000	2.855276000	-2.490694000
1	-1.263868000	3.426049000	-3.915093000
1	1.610774000	2.451198000	-3.180060000
1	0.813319000	2.254458000	-4.738991000
1	1.470492000	0.844750000	-3.898287000
6	-0.983250000	-3.132988000	2.015066000
6	-1.090229000	-4.633024000	1.694296000
6	-2.202076000	-2.682634000	2.836981000
1	-0.086567000	-2.987343000	2.632752000
1	-1.966622000	-4.849505000	1.070931000
1	-1.198923000	-5.231315000	2.612701000
1	-0.209090000	-5.018987000	1.167233000
1	-3.135891000	-2.788707000	2.270014000
1	-2.132683000	-1.635391000	3.152194000
1	-2.316703000	-3.288297000	3.750158000
30	-1.916793000	1.055084000	1.393760000
6	-3.299422000	1.300972000	2.806452000
6	-2.724225000	1.317979000	4.231499000
1	-3.949039000	0.419397000	2.716565000
6	-4.159522000	2.551311000	2.553437000
1	-3.565525000	3.472351000	2.610675000
1	-4.957687000	2.643371000	3.306573000
1	-4.644417000	2.536064000	1.570392000
1	-2.167432000	0.404988000	4.469370000
1	-3.526603000	1.413702000	4.979433000
1	-2.044566000	2.164957000	4.388069000

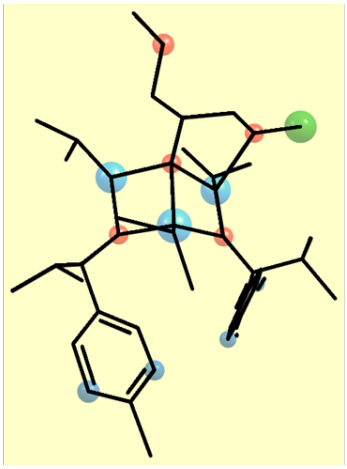
i_8

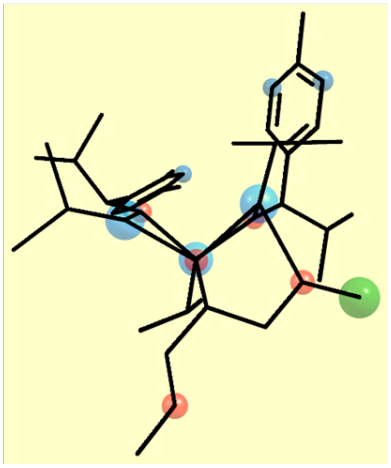


(*S,R,S,S*)

-18.5, *-18.7*

isomer resulting from binding s initiator



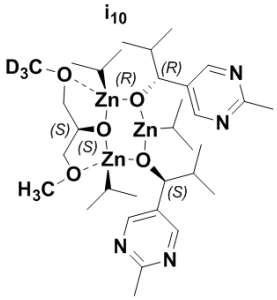


Zero-point correction= 0.859293 (Hartree/Particle)
Thermal correction to Energy= 0.917722
Thermal correction to Enthalpy= 0.918666
Thermal correction to Gibbs Free Energy= 0.761166
Sum of electronic and zero-point Energies= -2530.195501
Sum of electronic and thermal Energies= -2530.137073
Sum of electronic and thermal Enthalpies= -2530.136129
Sum of electronic and thermal Free Energies= -2530.293629

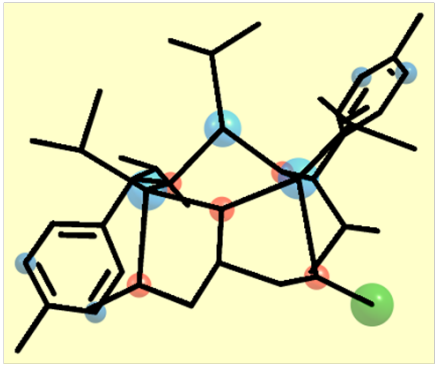
6	-2.833500000	-2.057440000	-1.719733000
6	-3.126050000	-0.939945000	-0.722785000
1	-3.776673000	-2.499325000	-2.061769000
8	-2.038420000	-3.044559000	-1.063036000
1	-2.292987000	-1.662445000	-2.593328000
8	-1.914681000	-0.422027000	-0.176672000
6	-3.939958000	0.164648000	-1.406059000
1	-3.737493000	-1.361340000	0.088267000
1	-3.376178000	0.572779000	-2.261048000
1	-4.111675000	0.992470000	-0.697995000
8	-5.170195000	-0.390015000	-1.830040000
6	-6.002020000	0.549774000	-2.485958000
6	-1.822280000	-4.217603000	-1.845082000
1(iso=2)	-1.212730000	-4.894840000	-1.245464000
1(iso=2)	-2.778651000	-4.701588000	-2.079298000
1(iso=2)	-1.299449000	-3.980365000	-2.779529000
1	-6.919743000	0.029162000	-2.768149000
1	-5.524488000	0.951458000	-3.392303000
1	-6.258105000	1.392498000	-1.826115000
30	-0.573000000	-2.015025000	0.429305000
30	-0.300725000	0.633551000	-1.271397000
8	-0.335867000	1.630940000	0.573803000
6	0.138554000	2.959090000	0.777064000
6	1.488638000	3.136172000	0.107279000
1	-0.549368000	3.676019000	0.298337000
6	0.157472000	3.322625000	2.291788000
1	-0.868709000	3.126857000	2.636255000
6	0.437361000	4.815534000	2.515543000
6	1.105765000	2.447788000	3.121286000
1	0.936270000	1.382928000	2.936790000
1	0.956649000	2.633580000	4.189974000
1	2.154556000	2.667029000	2.894038000
1	-0.257088000	5.447851000	1.950696000
1	1.456446000	5.081296000	2.214054000
1	0.331275000	5.069599000	3.575056000
6	2.468659000	2.138415000	0.114043000
6	1.845860000	4.298092000	-0.578767000

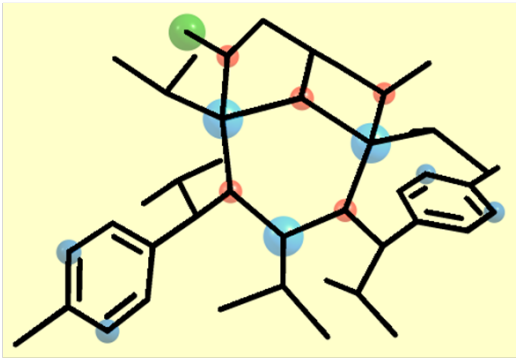
7	3.654963000	2.273375000	-0.484744000
6	3.895666000	3.442138000	-1.106455000
7	3.032406000	4.466527000	-1.177256000
6	5.228419000	3.595982000	-1.787503000
1	2.275612000	1.188791000	0.605446000
1	5.370479000	4.625707000	-2.117279000
1	5.285210000	2.935204000	-2.660037000
1	6.038441000	3.306563000	-1.111916000
1	1.145385000	5.129248000	-0.659484000
8	0.681216000	-1.096988000	-0.780627000
6	1.981856000	-1.497368000	-1.216039000
6	1.910539000	-2.627578000	-2.277524000
6	2.863552000	-1.869831000	-0.031795000
1	2.453162000	-0.629877000	-1.703426000
6	2.684408000	-3.036867000	0.720952000
6	3.928373000	-1.067503000	0.385300000
1	1.434019000	-3.496161000	-1.798178000
6	3.309775000	-3.047298000	-2.756834000
6	1.046683000	-2.211633000	-3.474901000
1	0.051078000	-1.893322000	-3.159422000
1	0.938668000	-3.042340000	-4.180939000
1	1.509816000	-1.378318000	-4.016374000
1	3.928841000	-3.439200000	-1.945510000
1	3.840154000	-2.195891000	-3.200635000
1	3.234040000	-3.823846000	-3.525114000
7	4.706987000	-1.367348000	1.435650000
7	3.441137000	-3.360089000	1.771901000
6	4.425936000	-2.500646000	2.093753000
6	5.272652000	-2.848072000	3.288696000
1	1.902094000	-3.749293000	0.464484000
1	4.169030000	-0.142917000	-0.140938000
1	5.652255000	-3.870797000	3.204336000
1	4.672107000	-2.803879000	4.204183000
1	6.106904000	-2.151391000	3.378378000
6	-0.485930000	1.567780000	-3.043480000
6	0.858302000	1.859101000	-3.731082000
6	-1.321432000	2.855522000	-2.953694000
1	-1.035331000	0.860600000	-3.684123000
1	-0.834408000	3.610270000	-2.323129000
1	-2.321093000	2.682841000	-2.537270000
1	-1.460723000	3.318957000	-3.944192000
1	1.463350000	2.568786000	-3.153914000
1	0.713710000	2.308262000	-4.727422000
1	1.461281000	0.955042000	-3.869050000
6	-0.774812000	-3.066732000	2.116081000
6	-0.788898000	-4.584768000	1.871634000
6	-2.029198000	-2.648488000	2.900850000
1	0.103972000	-2.837013000	2.734034000
1	-1.635588000	-4.883449000	1.241297000
1	-0.886612000	-5.140083000	2.817907000
1	0.126435000	-4.944764000	1.387005000
1	-2.947123000	-2.836533000	2.329259000
1	-2.025939000	-1.584642000	3.164210000
1	-2.121628000	-3.213890000	3.841968000
30	-2.000135000	0.980080000	1.358051000
6	-3.436342000	1.195313000	2.721388000
6	-2.907814000	1.298710000	4.160732000
1	-4.027872000	0.272343000	2.646152000
6	-4.363266000	2.379742000	2.397528000
1	-3.829183000	3.337754000	2.435470000
1	-5.187300000	2.449369000	3.124844000
1	-4.817893000	2.298243000	1.403305000
1	-2.300813000	0.433090000	4.447543000
1	-3.737442000	1.367135000	4.881460000
1	-2.289862000	2.193625000	4.306199000

$\dot{i}_{10}$



(R,S,R,S) start





-9.3, *-11.3*

Zero-point correction= 0.858023 (Hartree/Particle)
Thermal correction to Energy= 0.915991
Thermal correction to Enthalpy= 0.916935
Thermal correction to Gibbs Free Energy= 0.757129
Sum of electronic and zero-point Energies= -2530.180909
Sum of electronic and thermal Energies= -2530.122941
Sum of electronic and thermal Enthalpies= -2530.121996
Sum of electronic and thermal Free Energies= -2530.281802

6	2.035884000	2.869191000	-0.993150000
6	0.978924000	3.239387000	0.054437000
1	1.567382000	2.324788000	-1.817302000
8	3.002569000	1.983322000	-0.405276000
1	2.543326000	3.756119000	-1.392408000
8	0.391639000	2.057648000	0.559680000
6	-0.067899000	4.194195000	-0.521583000
1	1.486522000	3.790550000	0.866191000
1	0.419942000	5.007131000	-1.078700000
1	-0.666119000	4.641639000	0.284559000
8	-0.919704000	3.446977000	-1.392417000
6	-1.780400000	4.267123000	-2.179921000
6	4.201182000	2.626749000	0.035876000
1	4.823327000	1.858420000	0.496045000
1	4.732095000	3.060277000	-0.819359000
1	3.994278000	3.410928000	0.774056000
1(iso=2)	-2.401788000	3.599850000	-2.778792000
1(iso=2)	-1.191408000	4.909270000	-2.847289000
1(iso=2)	-2.423101000	4.893796000	-1.550280000
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8	1.343674000	-0.917585000	0.111374000
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6	3.586830000	-1.579772000	-0.531007000
1	2.507386000	-2.299020000	1.147959000
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6	2.526424000	-4.504980000	-0.376847000
6	1.307837000	-3.043547000	-2.049735000
1	0.732319000	-2.125364000	-2.196661000
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1	2.210182000	-2.978319000	-2.667012000
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1	3.476938000	-4.418449000	-0.914660000
1	2.011756000	-5.392250000	-0.759647000
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6	3.654933000	-0.778050000	-1.675285000
7	5.994848000	-1.653502000	-0.589123000

6	5.935756000	-0.905267000	-1.703029000
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6	7.240355000	-0.570019000	-2.375984000
1	4.881666000	-2.578282000	0.884106000
1	7.104451000	0.245234000	-3.088096000
1	7.618895000	-1.443639000	-2.919978000
1	7.996952000	-0.299752000	-1.634802000
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6	-2.233638000	-0.671132000	-1.638726000
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6	-3.544673000	-1.231051000	-1.108782000
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6	-4.530779000	-0.449455000	-0.493342000
6	-3.854187000	-2.587727000	-1.198632000
1	-2.895589000	1.211681000	-2.425667000
6	-3.332459000	-0.274867000	-3.920178000
6	-1.054676000	0.684312000	-3.421214000
1	-0.383751000	1.074383000	-2.654978000
1	-1.167007000	1.442171000	-4.204177000
1	-0.581404000	-0.193757000	-3.878144000
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6	-7.142106000	-2.848408000	0.382887000
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1	-8.000929000	-2.281278000	0.011787000
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1	-4.509011000	3.015653000	-0.251583000
1	-1.960308000	4.020385000	2.453009000
1	-1.923421000	2.434949000	3.223235000
1	-3.380911000	3.433119000	3.318451000
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6	2.736076000	0.900045000	2.972188000
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1	3.247138000	1.875026000	2.956602000
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1	2.178710000	1.110069000	5.089676000
1	1.138307000	0.008286000	4.188788000
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6	-2.656098000	-2.464659000	2.464958000
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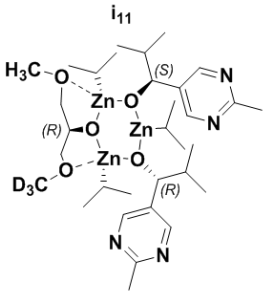
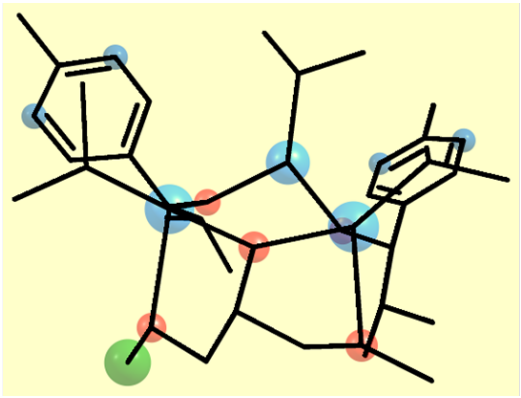
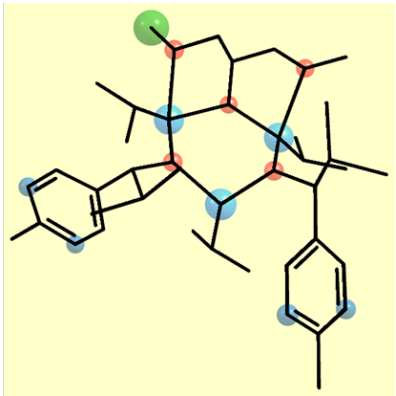
i_{11}



(R,R,S,S) start

-9.4, *-11.6*





Zero-point correction= 0.857976 (Hartree/Particle)
Thermal correction to Energy= 0.916915
Thermal correction to Enthalpy= 0.917859
Thermal correction to Gibbs Free Energy= 0.756672
Sum of electronic and zero-point Energies= -2530.181039
Sum of electronic and thermal Energies= -2530.122099
Sum of electronic and thermal Enthalpies= -2530.121155
Sum of electronic and thermal Free Energies= -2530.282342

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1	-0.365724000	-3.027251000	2.298694000
8	1.662115000	-2.934578000	1.850093000
1	0.484852000	-4.598279000	2.223542000
8	0.024506000	-2.439844000	-0.323018000
6	-1.255199000	-4.473386000	0.062304000
8	-2.340565000	-3.617481000	0.432786000
6	-3.612372000	-4.252170000	0.313802000
6	2.093415000	-2.703973000	3.185346000
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1(iso=2)	2.195901000	-3.651891000	3.730352000
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1	-3.795516000	-4.585962000	-0.715100000
1	-4.367867000	-3.517821000	0.596314000
30	-1.766935000	-1.670781000	-0.817344000
30	-0.226954000	1.043473000	-0.395657000
8	1.325718000	0.211934000	0.625304000
6	2.277331000	0.901374000	1.438425000
6	3.458040000	1.419085000	0.631395000
1	2.692227000	0.180328000	2.163437000
6	1.589822000	2.005871000	2.282278000
1	1.079110000	2.679245000	1.574960000
6	2.594952000	2.840591000	3.091328000
6	0.543887000	1.384385000	3.218735000
1	-0.160442000	0.753224000	2.673564000
1	-0.015645000	2.163116000	3.749053000
1	1.036057000	0.762479000	3.977323000
1	3.289359000	3.391424000	2.452207000
1	3.186654000	2.201125000	3.758064000
1	2.066308000	3.566925000	3.716903000
6	3.340094000	2.336544000	-0.419678000
6	4.765495000	1.016730000	0.903777000
7	4.384605000	2.789319000	-1.116953000
6	5.598289000	2.322496000	-0.768836000
7	5.833979000	1.451140000	0.223045000
6	6.775191000	2.816864000	-1.565662000
1	2.366142000	2.721924000	-0.710645000

1	7.709203000	2.477975000	-1.115936000
1	6.765966000	3.909350000	-1.623360000
1	6.719252000	2.441076000	-2.593399000
1	4.964665000	0.310275000	1.710150000
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6	-3.230778000	0.301658000	2.352516000
6	-3.215212000	1.995072000	0.467794000
6	-2.467489000	3.030890000	1.042205000
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1	-2.495025000	0.926232000	2.876519000
6	-2.970098000	-1.155215000	2.745359000
6	-4.636605000	0.734094000	2.800443000
1	-4.828471000	1.794210000	2.612624000
1	-4.766235000	0.557701000	3.873123000
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1	-3.703326000	-1.824262000	2.278900000
1	-3.054296000	-1.280691000	3.830401000
7	-4.395472000	3.704289000	-0.754168000
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6	-3.796404000	6.055915000	-0.517127000
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1	-3.732841000	6.685741000	0.373832000
1	-4.757304000	6.200760000	-1.012635000
6	-2.722315000	-1.716217000	-2.584685000
6	-4.246233000	-1.529411000	-2.505804000
6	-2.373393000	-2.963969000	-3.412757000
1	-2.318490000	-0.846923000	-3.125200000
1	-4.734017000	-2.343653000	-1.954265000
1	-4.703825000	-1.513003000	-3.508381000
1	-4.525397000	-0.591522000	-2.012380000
1	-2.749511000	-3.884394000	-2.946017000
1	-1.292264000	-3.086650000	-3.543844000
1	-2.822464000	-2.920849000	-4.418335000
30	1.876717000	-1.564654000	-0.129104000
6	3.406945000	-2.377546000	-1.134044000
6	3.822638000	-1.586495000	-2.384475000
1	2.988951000	-3.337493000	-1.475801000
6	4.631011000	-2.698361000	-0.261925000
1	5.115611000	-1.786939000	0.109512000
1	5.398261000	-3.247555000	-0.832182000
1	4.370208000	-3.312392000	0.607758000
1	2.984911000	-1.426195000	-3.073019000
1	4.612149000	-2.109165000	-2.949250000
1	4.222891000	-0.597958000	-2.127143000
1	0.844849000	-4.331167000	-0.189511000
6	0.012803000	2.109994000	-2.082323000
1	0.558536000	3.019384000	-1.793358000
6	-1.297709000	2.554215000	-2.746528000
6	0.888326000	1.334116000	-3.084229000
1	1.862749000	1.055504000	-2.669510000
1	1.081467000	1.932881000	-3.988135000
1	0.397977000	0.411302000	-3.420607000
1	-1.894427000	3.203816000	-2.100294000
1	-1.929012000	1.700504000	-3.022618000
1	-1.098633000	3.113108000	-3.674786000
1	-1.353793000	-4.754953000	-0.994863000
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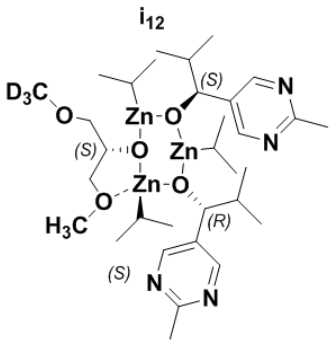
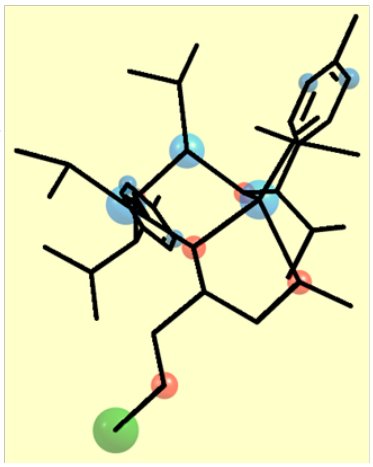
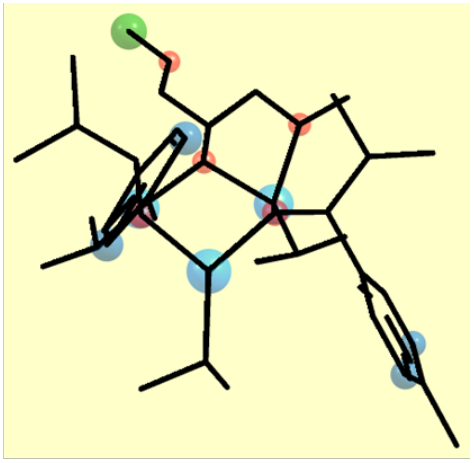
i_{12}



(S,R,S,R) at start

-8.5, *-11.5*





Zero-point correction= 0.858217 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.918143
Thermal correction to Gibbs Free Energy= 0.755666
Sum of electronic and zero-point Energies= -2530.179633
Sum of electronic and thermal Energies= -2530.120652
Sum of electronic and thermal Enthalpies= -2530.119708
Sum of electronic and thermal Free Energies= -2530.282184

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1	-3.454109000	-2.898385000	-2.535605000
8	-1.469849000	-2.960562000	-1.922005000
1	-2.493536000	-1.433437000	-2.888317000
8	-2.052903000	-0.872893000	-0.263780000
6	-4.347600000	-0.734754000	-1.034050000
1	-3.408661000	-2.450218000	-0.148583000
1	-4.078542000	0.109993000	-1.691691000
1	-4.671427000	-0.316506000	-0.066663000
8	-5.381653000	-1.510999000	-1.607181000
6	-6.565686000	-0.768687000	-1.833385000
6	-1.056142000	-3.742452000	-3.038654000
1	-0.143586000	-4.264361000	-2.747489000
1	-1.827116000	-4.479462000	-3.296214000
1	-0.856736000	-3.110538000	-3.913024000
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1(iso=2)	-6.393681000	0.067189000	-2.528711000
1(iso=2)	-6.972993000	-0.361274000	-0.895746000
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30	0.992060000	0.771326000	0.989722000
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6	-1.002060000	2.272543000	-0.572064000
6	0.186362000	3.171840000	-0.870353000
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1	-2.640498000	2.767400000	-2.760289000
1	-1.980463000	4.347538000	-2.307677000
1	-3.688476000	3.994015000	-2.033026000
6	0.796590000	3.984376000	0.095290000
6	0.766703000	3.243070000	-2.139215000

7	1.844720000	4.771360000	-0.166890000
6	2.313969000	4.761509000	-1.427398000
7	1.815726000	4.021706000	-2.431103000
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1	3.654756000	5.720930000	-2.800134000
1	4.407791000	5.201930000	-1.277760000
1	3.370660000	6.624953000	-1.282180000
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6	2.185314000	-0.534331000	-1.375361000
6	1.962358000	-1.290263000	-2.709598000
6	3.341452000	-1.097756000	-0.563073000
1	2.466061000	0.496218000	-1.651929000
6	3.354192000	-2.392348000	-0.028886000
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1	1.632346000	-2.309104000	-2.454862000
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6	6.558505000	-2.601061000	1.711217000
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6	0.182392000	-4.851970000	0.415707000
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1	-0.696531000	-5.123912000	-0.181213000
1	0.349132000	-5.671403000	1.133107000
1	1.044589000	-4.844424000	-0.263169000
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1	-1.278066000	-2.709852000	2.757541000
1	-0.992849000	-4.450435000	2.862138000
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6	-3.251532000	1.661373000	3.751512000
1	-2.512569000	-0.350963000	3.698629000
6	-4.544149000	-0.396734000	3.024623000
1	-5.255110000	0.171848000	2.411106000
1	-4.989752000	-0.477466000	4.028587000
1	-4.492106000	-1.409754000	2.610070000
1	-2.267768000	2.131245000	3.860723000
1	-3.693982000	1.588591000	4.757636000
1	-3.880485000	2.355291000	3.179630000
6	2.186239000	0.950030000	2.580628000
1	3.203886000	1.025591000	2.173616000
6	2.137061000	-0.303981000	3.472311000
6	1.910036000	2.218605000	3.401916000
1	2.399579000	-1.216327000	2.925463000
1	1.142116000	-0.457600000	3.909791000
1	2.839861000	-0.216707000	4.315887000
1	2.040118000	3.132069000	2.811494000
1	2.593210000	2.289822000	4.263225000
1	0.889715000	2.231838000	3.805704000

9. References

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