Supplementary Information

Demystifying the Mechanism of Isoselective Epoxide Polymerization using the Vandenberg Catalyst

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1.1 Characterization of $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$ Initiator

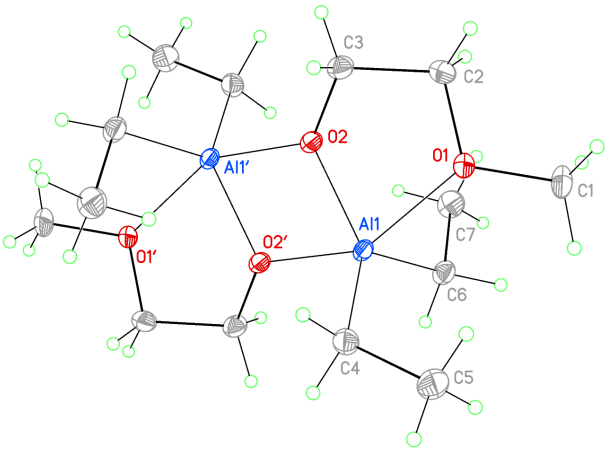


Figure S1: View of $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$ showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level. The complex resides around a crystallographic inversion center at $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$. Atoms with labels appended by a are related by 1-x, 1-y, 1-z.

Table S1: Crystal data and structure refinement for $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$.

Empirical formula	$C_{14}\,H_{34}\,Al_2\,O_4$	
Formula weight	320.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.9134(8) Å	α= 90.
	b = 7.5787(6) Å	β= 106.855(2).
	c = 14.5088(12) Å	γ= 90.
Volume	937.99(14) $Å^3$	
Z	2	
Density (calculated)	1.134 Mg/m^3	
Absorption coefficient	0.164 mm^{-1}	
F(000)	352	
Crystal size	1.170 x 0.650 x 0.480 mm^3	
Theta range for data collection	2.413 to 27.571.	
Index ranges	$-11 \leq h \leq 11$, $-9 \leq k \leq 8$, $-18 \leq l \leq 11$	
Reflections collected	13048	
Independent reflections	2152 [R(int) = 0.0317]	
Completeness to theta = 25.242	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.858	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2152 / 0 / 94	
Goodness-of-fit on F2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0259, wR2 = 0.0693	
R indices (all data)	R1 = 0.0299, wR2 = 0.0714	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.330 and -0.165 $Å^{-3}$	

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	3677(1)	9053(2)	6813(1)	20(1)
C2	5999(1)	8668(1)	6338(1)	18(1)
C3	6500(1)	7888(1)	5516(1)	16(1)
C4	1902(1)	6682(1)	4344(1)	16(1)
C5	740(1)	7903(2)	4625(1)	24(1)
C6	3452(1)	4651(1)	6525(1)	15(1)
C7	4973(1)	4099(2)	7286(1)	21(1)
O1	4330(1)	8413(1)	6079(1)	15(1)
O2	5735(1)	6236(1)	5290(1)	13(1)
Al1	3740(1)	5769(1)	5354(1)	11(1)

Table S3: Bond lengths [Å] and angles [°] for $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$.

C1-O1	1.4381(12)	O1-C1-H1A	109.5	C7-C6-Al1	115.22(7)
C1-H1A	0.98	O1-C1-H1B	109.5	C7-C6-H6A	108.5
C1-H1B	0.98	H1A-C1-H1B	109.5	Al1-C6-H6A	108.5
C1-H1C	0.98	O1-C1-H1C	109.5	C7-C6-H6B	108.5
C2-O1	1.4377(12)	H1A-C1-H1C	109.5	Al1-C6-H6B	108.5
C2-C3	1.5089(14)	H1B-C1-H1C	109.5	H6A-C6-H6B	107.5
C2-H2A	0.99	O1-C2-C3	105.21(8)	C6-C7-H7A	109.5
C2-H2B	0.99	O1-C2-H2A	110.7	C6-C7-H7B	109.5
C3-O2	1.4177(12)	C3-C2-H2A	110.7	H7A-C7-H7B	109.5
C3-H3A	0.99	O1-C2-H2B	110.7	C6-C7-H7C	109.5
C3-H3B	0.99	C3-C2-H2B	110.7	H7A-C7-H7C	109.5
C4-C5	1.5303(15)	H2A-C2-H2B	108.8	H7B-C7-H7C	109.5
C4-Al1	1.9791(10)	O2-C3-C2	107.23(8)	C2-O1-C1	111.84(8)
C4-H4A	0.99	O2-C3-H3A	110.3	C2-O1-Al1	108.96(6)
C4-H4B	0.99	C2-C3-H3A	110.3	C1-O1-Al1	123.80(6)
C5-H5A	0.98	O2-C3-H3B	110.3	C3-O2-Al1	124.36(6)
C5-H5B	0.98	C2-C3-H3B	110.3	C3-O2-Al1#1	130.22(6)
C5-H5C	0.98	H3A-C3-H3B	108.5	Al1-O2-Al1#1	104.39(3)
C6-C7	1.5377(14)	C5-C4-Al1	119.56(7)	O2-Al1-O2#1	75.61(3)
C6-Al1	1.9808(10)	C5-C4-H4A	107.4	O2-Al1-C4	119.98(4)
C6-H6A	0.99	Al1-C4-H4A	107.4	O2#1-Al1-C4	100.54(4)
C6-H6B	0.99	C5-C4-H4B	107.4	O2-Al1-C6	119.49(4)
C7-H7A	0.98	Al1-C4-H4B	107.4	O2#1-Al1-C6	100.97(4)
C7-H7B	0.98	H4A-C4-H4B	107	C4-Al1-C6	119.96(4)
C7-H7C	0.98	C4-C5-H5A	109.5	O2-Al1-O1	75.79(3)
O1-Al1	2.2535(8)	C4-C5-H5B	109.5	O2#1-Al1-O1	151.40(3)
O2-Al1	1.8419(7)	H5A-C5-H5B	109.5	C4-Al1-O1	93.79(4)
O2-Al1#1	1.9118(8)	C4-C5-H5C	109.5	C6-Al1-O1	92.89(4)
Al1-O2#1	1.9118(8)	H5A-C5-H5C	109.5	O2-Al1-Al1#1	38.63(2)
Al1-Al1#1	2.9661(6)	H5B-C5-H5C	109.5	O2#1-Al1-Al1#1	36.98(2)
C6-Al1-Al1#1	115.36(3)	O1-Al1-Al1#1	114.43(2)	C4-Al1-Al1#1	115.36(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Table S4: Anisotropic displacement parameters (Å2x 10^3) for $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	22(1)	23(1)	17(1)	-6(1)	10(1)	2(1)
C2	14(1)	19(1)	20(1)	-6(1)	4(1)	-3(1)
C3	15(1)	15(1)	20(1)	-2(1)	7(1)	-3(1)
C4	14(1)	19(1)	14(1)	-1(1)	2(1)	3(1)
C5	15(1)	31(1)	23(1)	-3(1)	3(1)	7(1)
C6	15(1)	19(1)	14(1)	2(1)	6(1)	0(1)
C7	20(1)	26(1)	16(1)	4(1)	74(1)	2(1)
O1	13(1)	19(1)	13(1)	-4(1)	5(1)	0(1)
O2	11(1)	13(1)	16(1)	-2(1)	6(1)	-1(1)
Al1	9(1)	15(1)	10(1)	1(1)	4(1)	1(1)

Table S5: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$.

	x	y	z	U(eq)
H1A	4196	8471	7426	30
H1B	2552	8795	6630	30
H1C	3838	10331	6885	30
H2A	6522	8056	6949	21
H2B	6262	9939	6413	21
H3A	6197	8680	4950	19
H3B	7651	7728	5708	19
H4A	2302	7318	3867	19
H4B	1306	5651	4008	19
H5A	355	7330	5118	35
H5B	-145	8151	4056	35
H5C	1264	9011	4880	35
H6A	2879	5485	6826	18
H6B	2785	3592	6329	18
H7A	5594	3346	6987	31
H7B	4715	3445	7803	31
H7C	5580	5153	7554	31

Table S6: Torsion angles [°] for $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$.

O1-C2-C3-O2	-45.31(11)
C3-C2-O1-C1	178.40(8)
C3-C2-O1-Al1	37.92(9)
C2-C3-O2-Al1	35.41(11)
C2-C3-O2-Al1#1	-158.07(7)
C3-O2-Al1-O2#1	169.42(9)
Al1#1-O2-Al1-O2#1	0.001(1)
C3-O2-Al1-C4	75.40(8)
Al1#1-O2-Al1-C4	-94.02(5)
C3-O2-Al1-C6	-95.96(8)
Al1#1-O2-Al1-C6	94.62(5)
C3-O2-Al1-O1	-10.75(7)
Al1#1-O2-Al1-O1	179.84(4)
C3-O2-Al1-Al1#1	169.42(9)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

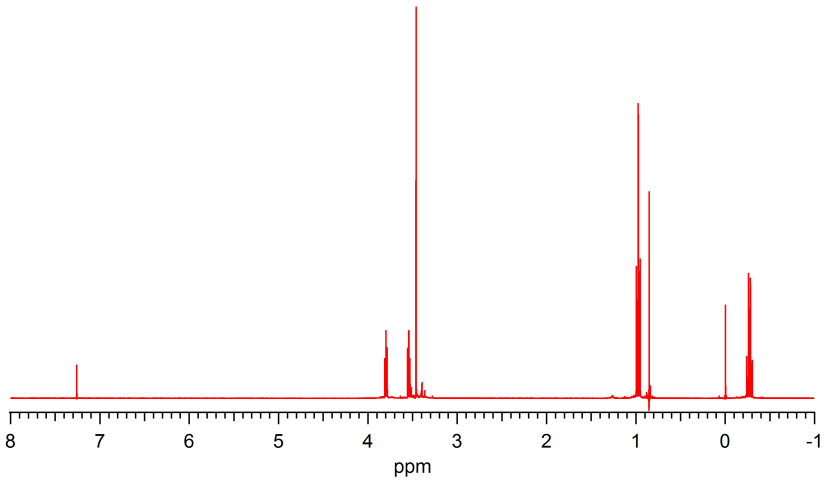


Figure S2: ^{1}H NMR Spectrum of $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.80 (t, -O-C<u>H$_2$</u>-CH$_2$-), 3.55 (t, -CH$_2$-C<u>H$_2$</u>-O-), 3.47 (s, C<u>H$_3$</u>-O-), 1.0 (t, C<u>H$_3$</u>-CH$_2$-Al-), -0.25 (q, CH$_3$-C<u>H$_2$</u>-Al-)

1.2 NMR Spectra of Synthesized Polymers

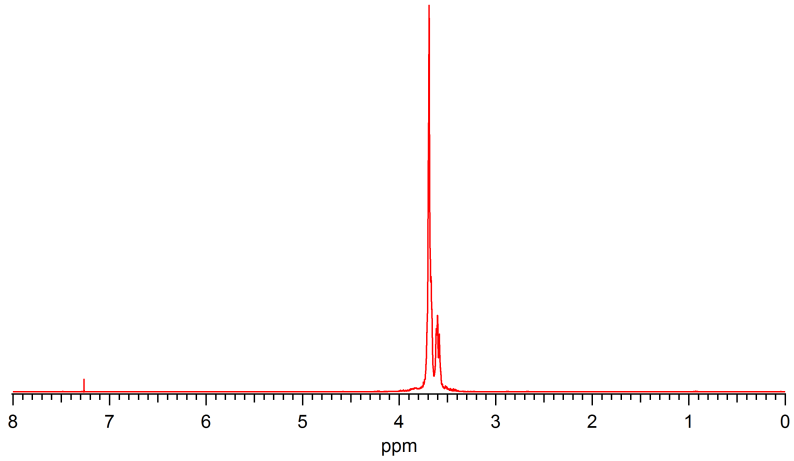


Figure S3: ^{1}H NMR Spectrum of PECH Synthesized with TAxEDA (MOD) Initiator. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.277.75 (broad m, $\underline{Ph}CH_2N$)3.373.94 (broad m, $OC\underline{H_2}C\underline{H}(C\underline{H_2}Cl)O$)

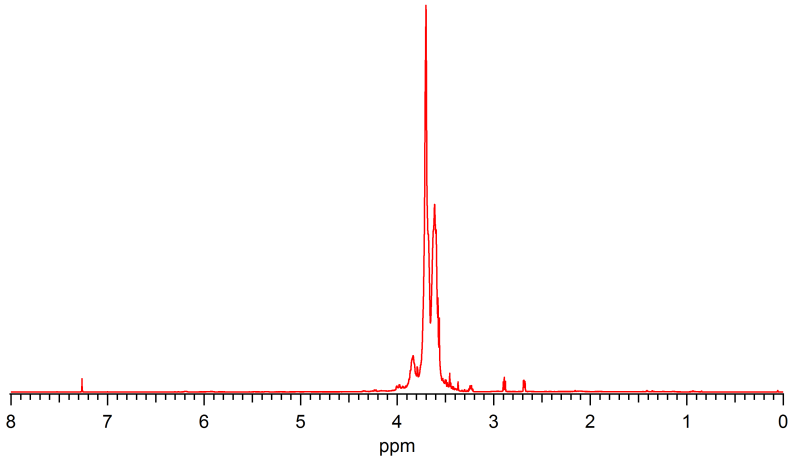


Figure S4: ^{1}H NMR Spectrum of PECH Synthesized with $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$ Initiator. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.373.94 (broad m, $OC\underline{H_2}C\underline{H}(C\underline{H_2}Cl)O$)

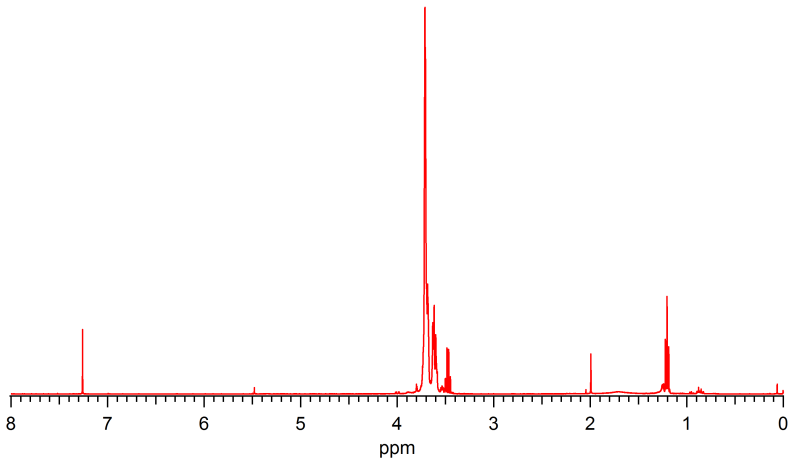


Figure S5: ^{1}H NMR Spectrum of PECH Synthesized with Vandenberg's Catalyst. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.553.78 (broad m, O$\underline{CH_2}$C$\underline{H}$(C$\underline{H_2}$Cl)O)

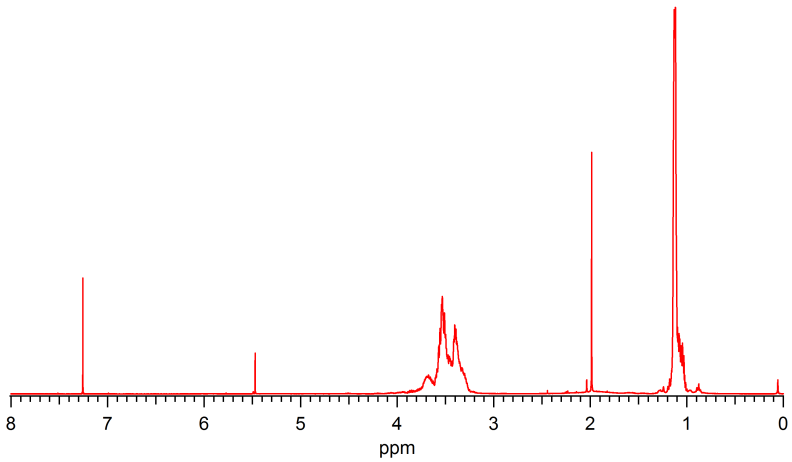


Figure S6: ^{1}H NMR Spectrum of PPO Synthesized with Vandenberg's Catalyst and Terminated with Methanol After 5 Minutes. ^{1}H NMR ($CDCl_2$, 400 MHz) δ 3.22-3.77 (broad m, $OC\underline{H_2}CH(C\underline{H_3})O$), 1.12 (m, $C\underline{H_3}$)

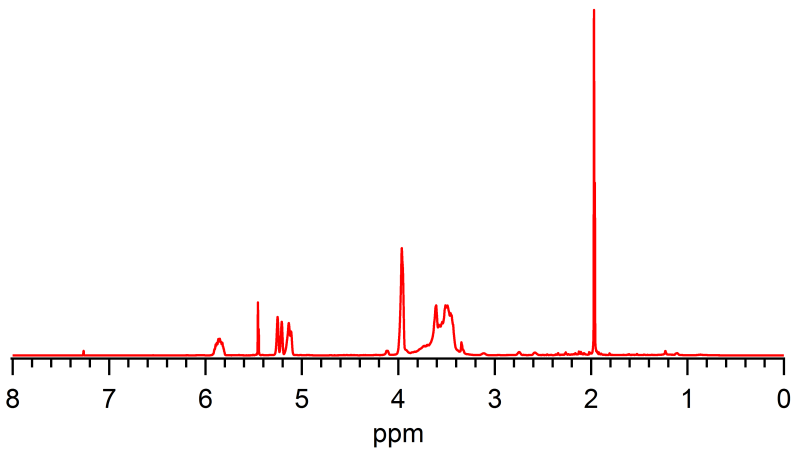


Figure S7: ^{1}H NMR Spectrum of PAGE Synthesized with $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$ Initiator. ^{1}H NMR ($CDCl_3$) δ 5.84 (m, $OCH_2C\underline{H}{=}CH_2$), 5.11/5.26 (doublet of doublets, $OCH_2CH{=}C\underline{H_2}$), 3.96 (d, $OC\underline{H^2}CH{=}CH_2$), 3.383.71 (broad m, $OC\underline{H_2}C\underline{H}(C\underline{H_2}OCH_2CH{=}CH_2)O$).

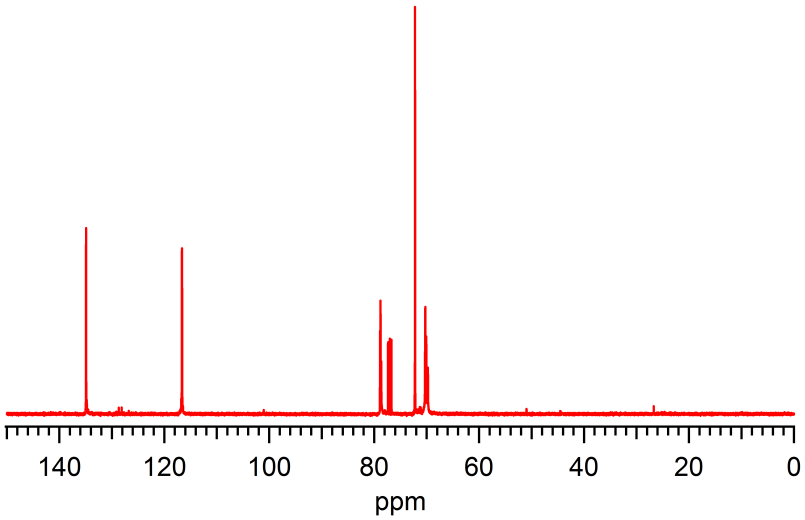


Figure S8: ^{13}C NMR Spectrum of PAGE Synthesized with $[Et_2Al(\mu\text{-}OCH_2CH_2OMe)]_2$ Initiator. ^{13}C NMR ($CDCl_3$, 125 MHz) δ 134.9 ($OCH_2\underline{C}H{=}CH_2$), 116.8 ($OCH_2CH{=}\underline{C}H_2$), 78.93 ($OCH_2\underline{C}H(CH_2OCH_2CH{=}CH_2)O$), 72.21 ($O\underline{C}H_2CH{=}CH_2$), 70.1170.25 ($O\underline{C}H_2CH(CH_2OCH_2CH{=}CH_2)O$, m), 69.75 ($O\underline{C}H_2CH(CH_2OCH_2CH{=}CH_2)O$, rrm or mrr).

1.3 SEC-MALS Trace of PPO

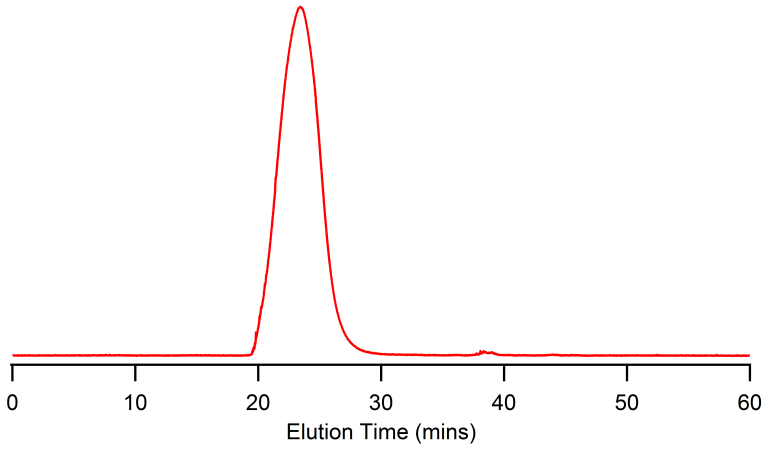


Figure S9: LS trace of PPO synthesized with Vandenberg's catalyst when terminated after 5 minutes. The M_n was determined to be 9.3x10^5 with a PDI of 2.4.

Computational Results

2.1 The structure of the catalyst A in gas phase and Et_2O

Figure S3 displays the optimized catalyst structure in gas phase. Structures optimized in diethylether (Et_2O)is similar to one optimized in gas phase.

The relevant distances has been summarized in Table S1 for the structures optimized in gas phase and Et_2O.

At the same time the solvation electronic energy (E^{solv}) and solvation free energy (G^{solv}) for the catalyst are summarized in Table S2.

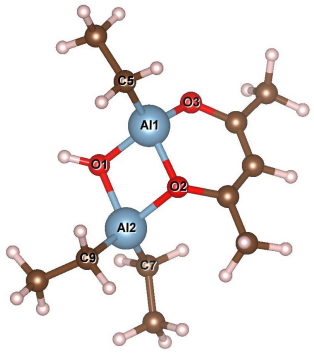


Figure S1: Catalyst-A Structure

Table S1: Selected Interatomic Distances for the Catalyst optimized in gas phase and Et_2O

Phase	Al1 - O1 (Å)	Al1 - O2 (Å)	Al1 - O3 (Å)	Al1 - C5 (Å)	Al2 - O1 (Å)	Al2 - O2 (Å)	Al2 - C7 (Å)	Al2 - C9 (Å)
Gas	1.86	1.90	1.76	1.67	1.91	1.90	1.97	1.97
Diethylether	1.85	1.86	1.76	1.96	1.93	1.91	1.97	1.97

Table S2: E^{solv} and G^{solv} for the Catalyst (w.r.t the gas optimized phase structure)

Phase	E^{solv} (kcal/mol)	G^{solv} (kcal/mol)
Gas	0 (reference)	0 (reference)
Diethylether	-2.8	-2.6

2.2 The structure of the catalyst B in gas phase and Et_2O

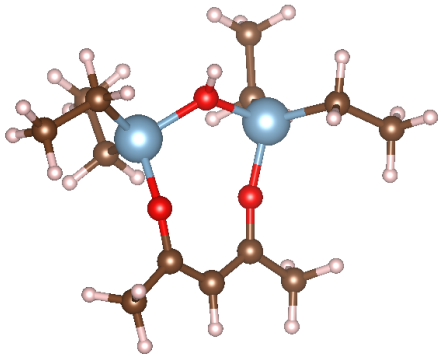


Figure S2: Catalyst-B Structure in gas phase

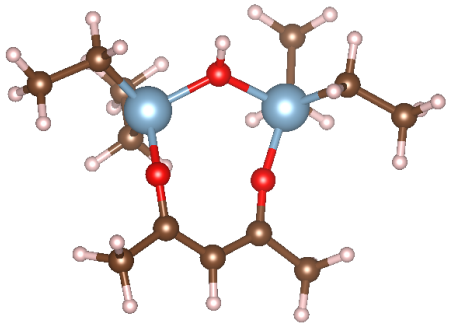
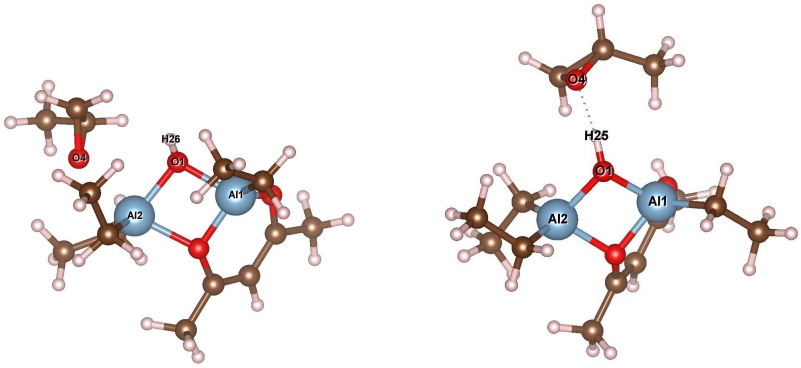


Figure S3: Catalyst-B Structure in Et_2O

2.3 Binding modes for the first epoxide-aluminum coordination (in gas phase, Et_2O and THF)

In order to investigate the binding modes of the first epoxy monomer, more than 12 binding modes were studied. The most energetically favorable binding modes are shown in Figure S4. These binding modes are named "Position 1" and "Position 2". In "Position 1", the monomer is near the Aluminum termed 'Al2'. On the other hand, in "Position 2", the monomer is near the Aluminum termed 'Al1'. The Oxygen points in general to the Aluminum atoms, this is a classic nucleophilic - electrophilic interaction. The optimization of the binding modes were carried out in implicit solvent (Et_2O and THF) and it was found that the Oxygen-Aluminum distance gets shorter compared to the gas phase (Table S3). In other words, the solvent favor the interaction of the monomer with the catalyst when compared to the gas phase structure.



(a) Position 1 (b) Position 2

Figure S4: The most favorable binding modes obtained for the addition of the first epoxy monomer

Table S3: Oxygen-Aluminum Interatomic distance for the most favorable binding modes

	Position 1	Position 2
Phase	Al2 - O4 (Å)	O4 - H25 (Å)
Gas	2.32	1.68
Diethylether	2.15	1.67
THF	2.13	1.65

2.3.1. Solvation Gibb's Free Energy of the Binding Modes

Equation 2.1 was used to calculate the total Gibb's free energy;

$$G = E^{elec} + ZPE + H^{vib} - T \cdot S^{vib} + G^{solv} \tag{2.1}$$

where E^{elec} is the electronic energy, ZPE is the zero-point energy, H^{vib} is the vibrational enthalpy, S^{vib} is the vibrational entropy, T is the temperature in Kelvin, and G^{solv} the Gibb's free energy of solvation.

The total Gibb's free energy then is used to calculate the relative binding energy (equation 2.2) between the first epoxy monomer and the catalyst;

$$\Delta G_{bind} = G_{(complex)} - [G_{(monomer)} + G_{(catalyst)}] \tag{2.2}$$

where ΔG_{bind} is the relative binding free energy, $G_{(complex)}$ is the total free energy of the optimized complex structure (or the adduct formed by the interaction between monomer and catalyst), $G_{(monomer)}$ is the total free energy of the optimized monomer, and $G_{(catalyst)}$ is the total free energy of the optimized catalyst. Both equation 2.1 and 2.2 are calculated at standard conditions (298.15 K and 1 atm pressure).

To show the effect of the solvation, we show the energies of one adduct to the two different Al atoms. The results are summarized in Table S4 and Figure S5. *The main result of the calculations is the prediction that the monomer-catalyst will be favorable in Et_2O but not in THF.*

Table S4: Gibb's free energy (ΔG_{bind}) for one of the adducts

Phase	Position 1 (kcal/mol)	Position 2 (kcal/mol)
Gas	+2.86	-1.94
Diethylether	+2.37	-1.12
THF	+4.13	+1.56

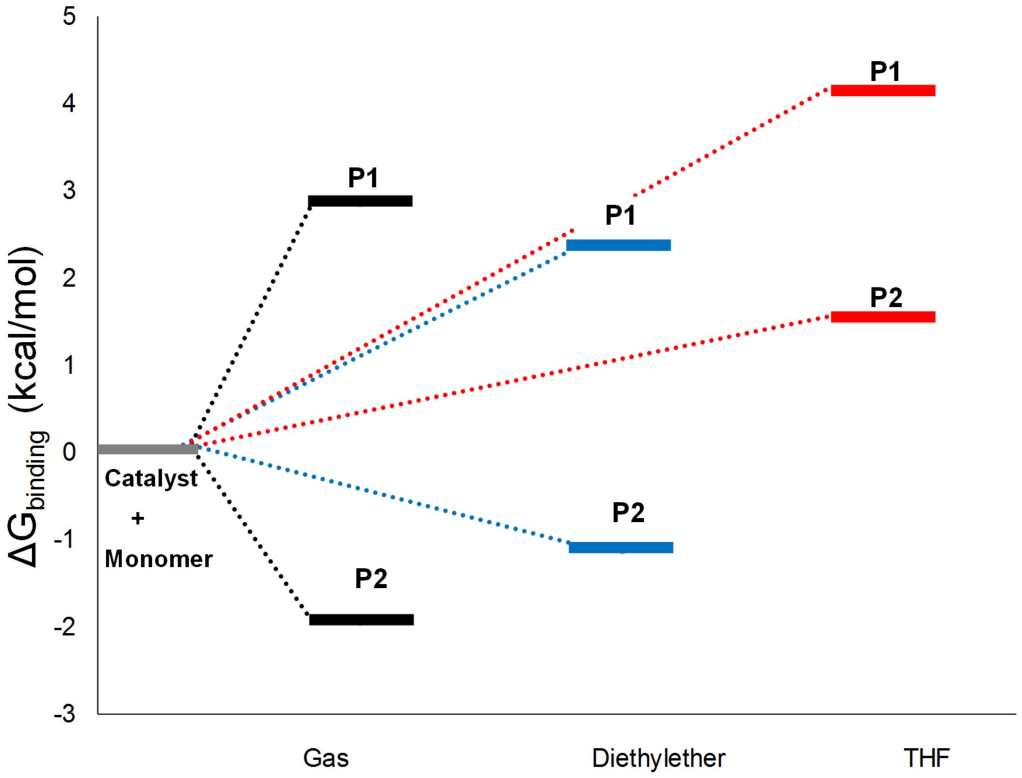


Figure S5: Gibb's Free Binding Energy Graph for one of the Adducts with P1 being position 1 and P2 being position 2. Coloring scheme: black, gas phase; blue, diethylether; red, THF

2.4 Proposed Epoxide Polymerization Mechanistic Pathways

In the following, the gas phase and solvent calculations are shown. It shows the initiation mechanism, followed by the propagation and some details about the intermediates and transition state are discussed. We also show an alternative configuration to the catalyst, which is named Catalyst B. However, the other configurations have higher barriers, thus is considered an alternative high energy route.

Initiation: There are two initiation mechanism displayed- The first is the monomer attack of the hydride and the second is the monomer attack of the chelated Al.

Propagation: There are two propagation steps presented. Firstly, the most favorable which shows no ring opening and the second which is the six-member ring opening. All the transition states were verified using the IRC method for both forward and reverse in Gaussian09 code [1]

Termination: No termination route was explored as the initiation and propagation steps are the most energetic of the reaction and as such provide the much needed results we sort to explain the regio and isoselectivity in these systems of polymers.

The cationic +1 charge is shown in all the structures used in the different mechanisms for clarity as implicit charge, however, repeating the calculations with the explicit charge using small counter anion (OH^-) to obtain a neutral species gives the same results. This suggest the counter anion does not play a major role in the mechanism

2.4.1. Chemical Mechanism for the PO monomer

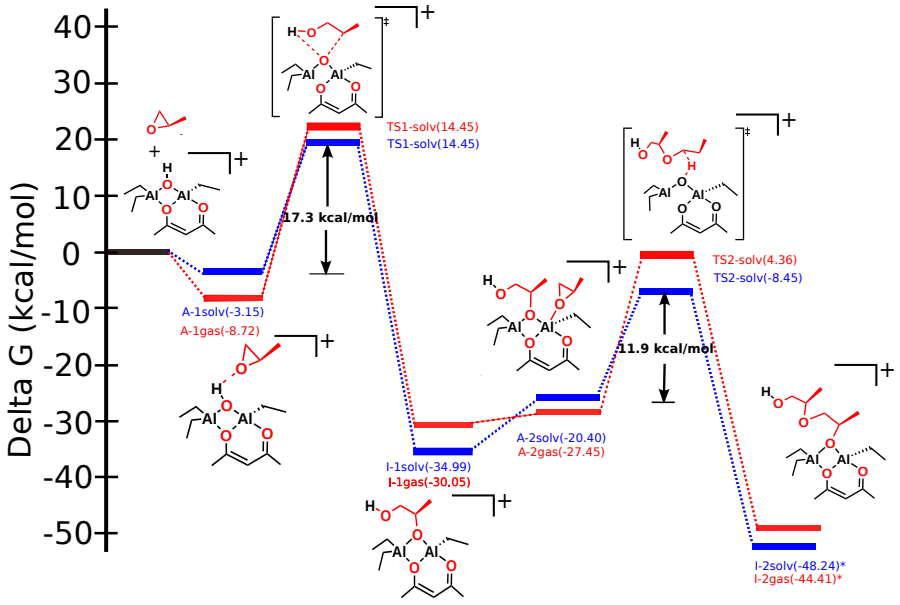


Figure S6: Catalyst A Mechanism of epoxide initiation and propagation for the PO monomer (Most favorable pathway)

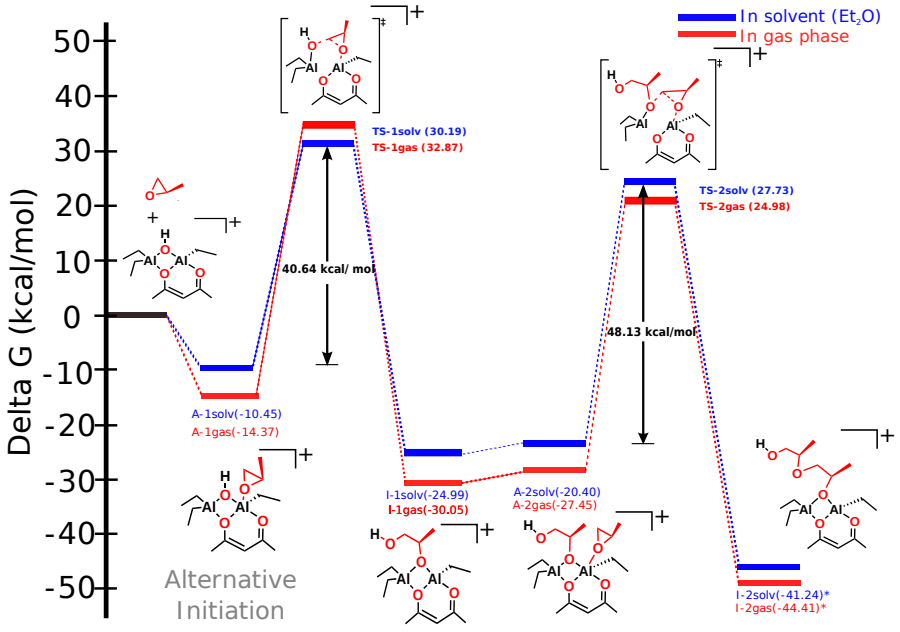


Figure S7: Catalyst A mechanism of epoxide initiation and propagation for the PO monomer (Alternative initiation and pathway)

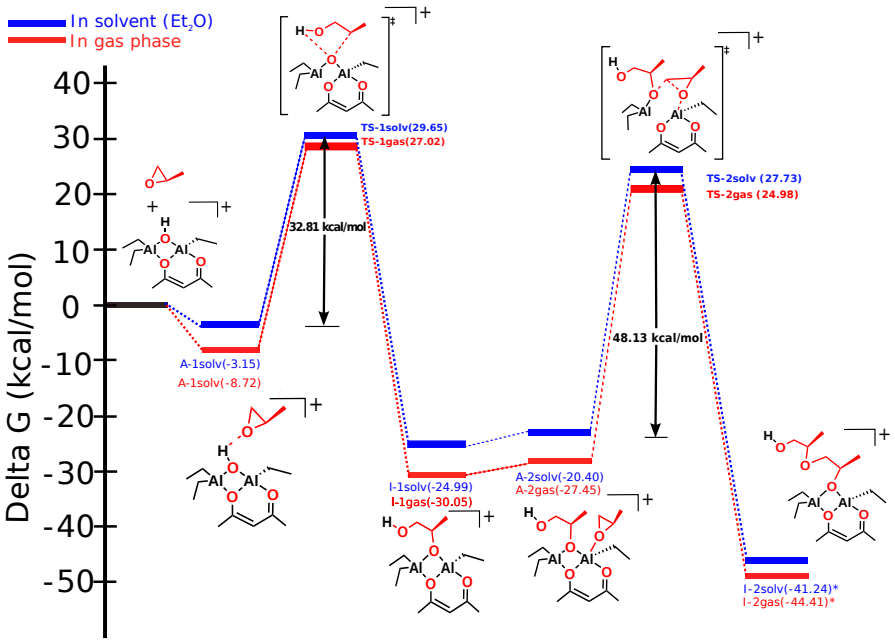


Figure S8: Catalyst A mechanism for the PO monomer (Alternative Pathway)

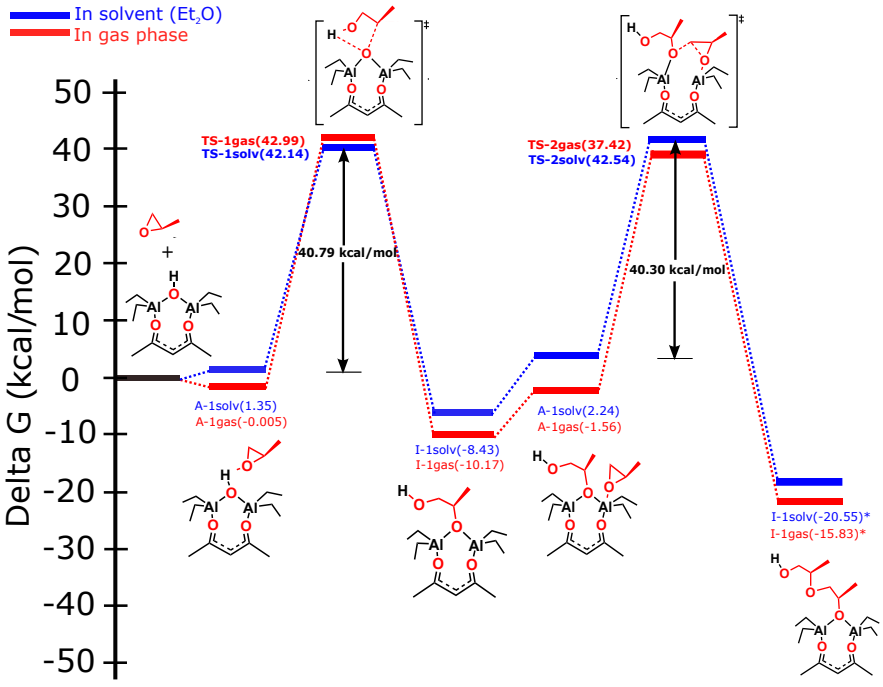


Figure S9: Catalyst B mechanism for the PO monomer. Notice how the total charge is zero. This was a path we explore to make sure the cationic species was the most favorable path.

2.4.2. Chemical Mechanism for the AGE monomer

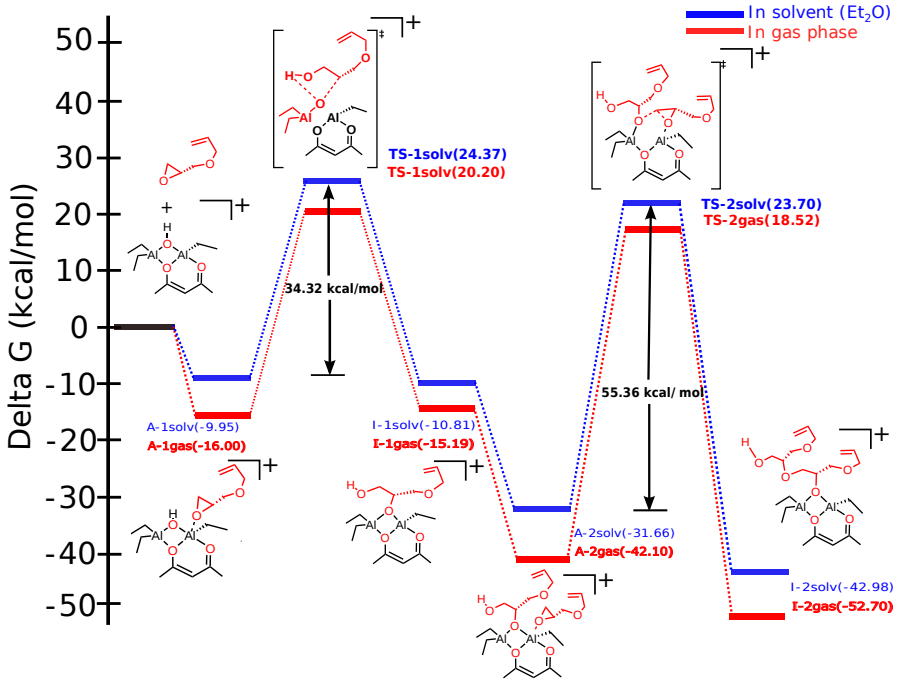


Figure S10: Catalyst A mechanism for the AGE monomer (Alternative Pathway)

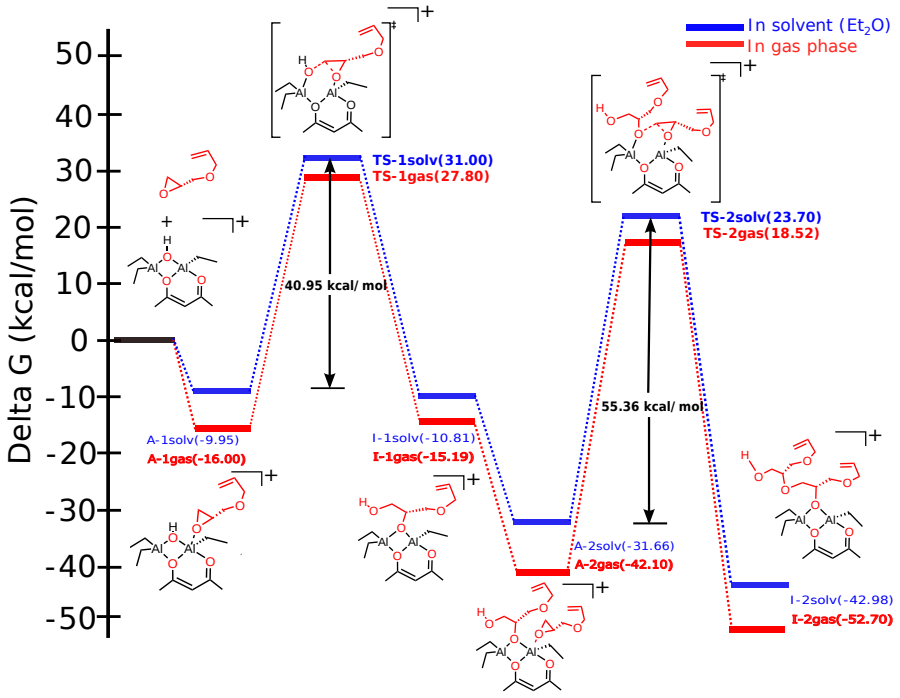


Figure S11: Catalyst A mechanism for the AGE monomer (Alternative Pathway)

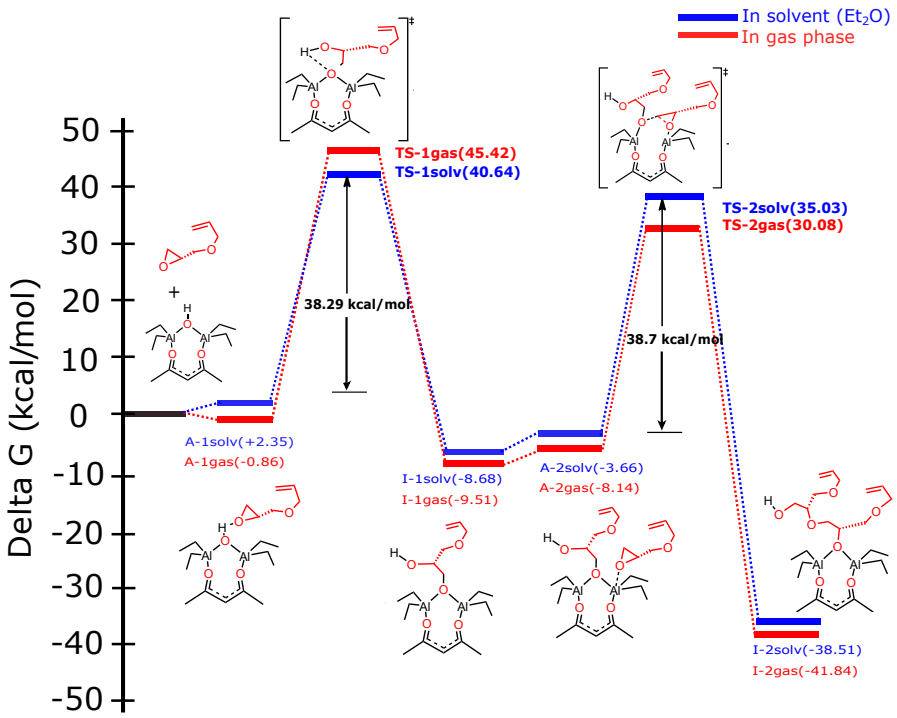


Figure S12: Catalyst B mechanism for the AGE monomer. Notice how the total charge is zero. This was a path we explore to make sure the cationic species was the most favorable path.

2.4.3. Transition States: PO system

The Transition State 1 (initiation) is shown in Figure S13 while the different possibilities for transition state 2 (propagation) is shown in Figure S14 and the energetics summarized in Table S9. It should be notice that the R-R system has an activation energy of 11.9 kcal/mol. If it is used as the reference, then at least 10.4 kcal/mol extra is needed to create the S-R and the R-S system.

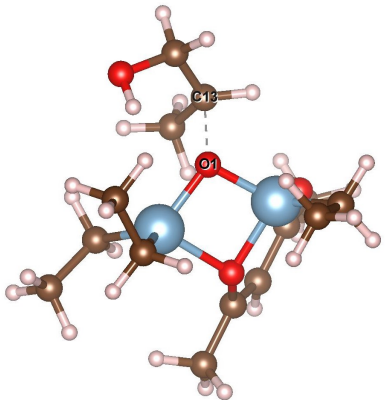
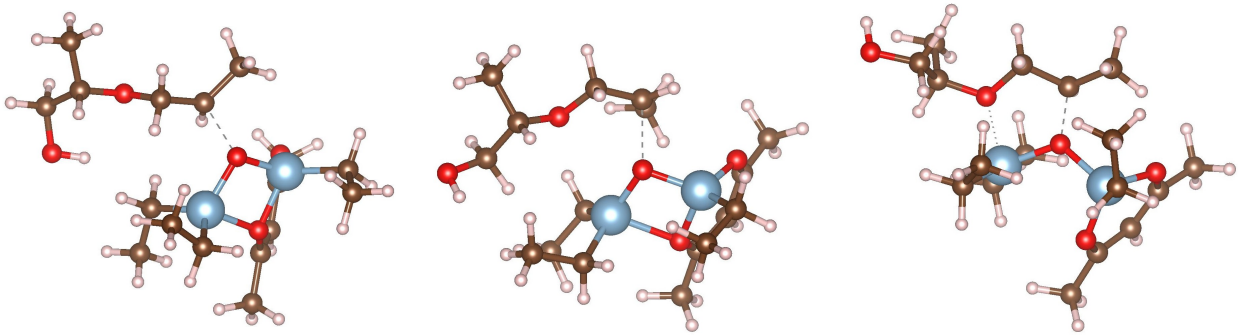


Figure S13: Transition State 1 (initiation)

Table S5: Activation energy (ΔG_{bind}) for the transition state 1 corresponding to initiation

Complex	$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta S^{\ddagger}$ (kcal/mol)
Transition State 1	+17.3	+5.26	-0.040



(a) S-R System (b) R-S System (c) R-R System

Figure S14: Transition State 2 (propagation)

Table S6: Activation energy (ΔG_{bind}) for the transition state 2 corresponding to propagation of Catalyst A and PO

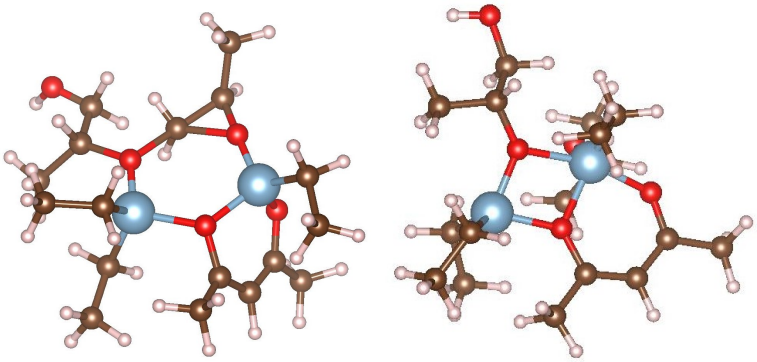
Transition State 2	$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G^{\ddagger}_{rel}$ (kcal/mol)
R-R System	+27.73	0
S-R System	+29.00	+1.27
R-S System	+29.94	+2.21

Table S7: Activation energy (ΔG_{bind}) for the transition state 2 corresponding to propagation of Catalyst B and PO

Transition State 2	$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G^{\ddagger}_{rel}$ (kcal/mol)
R-R System	+42.54	0
S-R System	+42.86	+0.32
R-S System	+46.30	+3.76

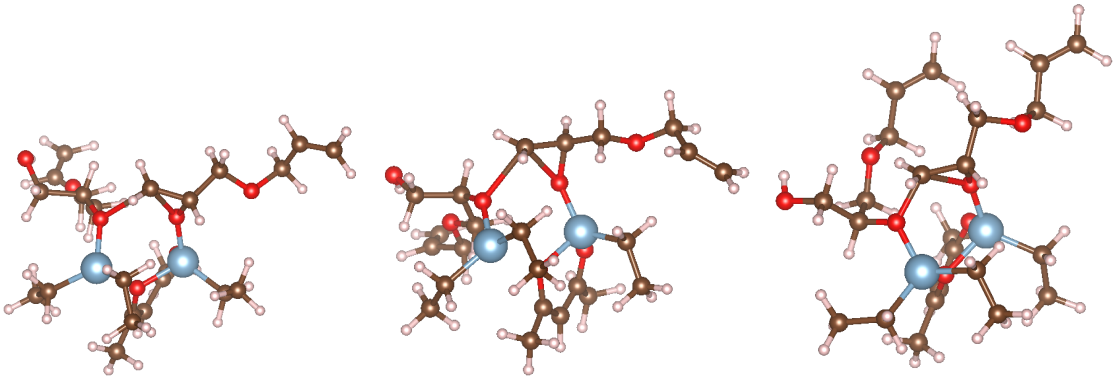
2.4.4. Transition State: AGE system

The initial proposed mechanism for the catalysis suggested the catalyst ring opening intermediate in the transition state. However, this did not occur as originally proposed. During the transition state search, the catalyst optimized 4-member ring transition state with lower energy than the 6-member ring transition state. This can be seen in Figure S17. The search for a 6-member ring was extended to the 20 other possibilities with success. The six-member ring could have more stability in water instead of Et_2O. Saukkoriipi et. al suggests that open structures, i.e. six-member ring, are more favorable in water. There are more atoms that can interact with the solvent and have a more stable structure.[2]



(a) Initial (b) Final

Figure S15: The search for an elusive 6-Member Ring transition state

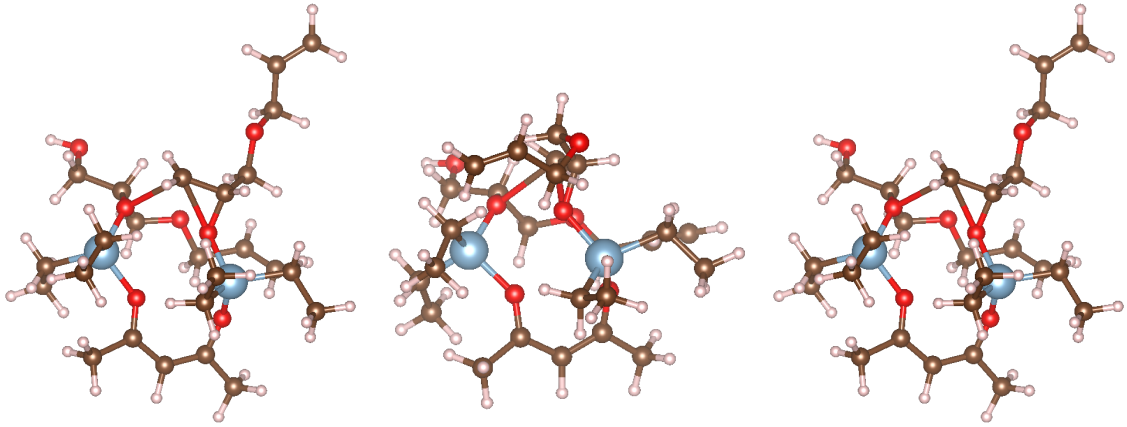


(a) RR System (b) RS System (c) SR System

Figure S16: 6-member ring transition state structures for all propagation configurations of Catalyst A and AGE

Table S8: Activation energy (ΔG) for the transition state 2 corresponding to propagation for Catalyst A and AGE

Transition State 2	$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G^{\ddagger}_{rel}$ (kcal/mol)
R-R System	+25.33	+0
S-R System	+27.32	+1.99
R-S System	+27.54	+2.21



(a) RR System (b) RS System (c) SR System

Figure S17: 6-member ring transition state structures for all propagation configurations of Catalyst B and AGE

Table S9: Activation energy (ΔG) for the transition state 2 corresponding to propagation for Catalyst B and AGE

Transition State 2	$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G^{\ddagger}_{rel}$ (kcal/mol)
S-R System	+35.04	-2.59
R-S System	+36.20	-1.43
R-R System	+37.63	+0

2.5 Theoretical Calculations of the Nuclear Magnetic Resonances (NMR) shifts

The excess electron density in the ACAC ligand allows us to compare theoretical and experimental data. **We found experimentally a 0.5 NMR shift when the monomer binds with the catalyst**. Using the optimized structures, Gaussian09 was implemented for all theoretical NMR calculations. There are different ways to estimate the NMR at the quantum mechanical level. Table S10shows the options for the two different GIAO methods. The Simple GIAO method uses the 6-31+G** basis set. The Advanced GIAO method uses the same basis also with spin-spin couple and NMR mixing. The advanced GIAO gives more accurate and consistent results, however it is more computationally demanding. **The theoretical NMR shifts are intended to predict the relative NMR shift**, because the absolute value requires other variables and less approximation to be considered.

Table S10: Methods used for calculating NMR

Option	**Simple GIAO**	**Advanced GIAO**
Basis Set: 6-31G + (d,p)	X	X
No Symmetry	X	X
Spin-spin coupling		X
NMR mix		X

The theoretical shifts for catalyst A are more consistent with experiments and the relative shift of less than 0.5 ppm (see Table S11 and Table S12). However, the relative NMR shift for the mechanism involving catalysts are larger than 0.5 ppm (see Table S13 and Table S14). This another evidence against the possibility of catalyst B being a major species.

2.5.1. ^{1}H−NMR for Catalyst A and PO

From the two GIAO methods explained in Table S10, we obtained the NMR shift for the different components described in Figure S18 and the numerical results are presented in Table S11. The simple GIAO Method did not yield the same experimental result for the H_c shift, while the advanced GIAO Method did. **The most accurate method is the advanced GIAO to calculate the relative NMR shift, indicated with bold in the tables.**

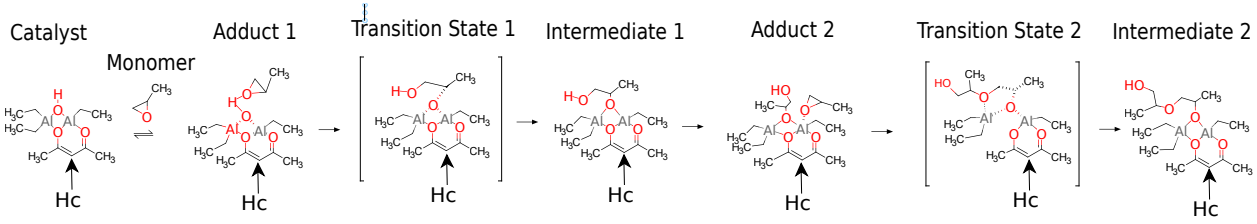


Figure S18: NMR Hc explanation

Table S11: ^{1}H−NMR shifts for H_c. The Δ is the shift with respect to the catalyst

Complex	H_c - shift (ppm)		H_c - shift (ppm)	
	Simple GIAO		**Advanced GIAO**	
	Absolute	Δ	Absolute	**Δ**
Catalyst	5.52	N/A	5.35	N/A
Adduct 1	5.66	+0.14	5.42	+0.07
Transition State 1	5.82	+0.30	5.80	+0.45
Intermediate 1	5.35	-0.17	5.40	+0.05
Adduct 2	5.24	-0.28	5.30	-0.05
Transition State 2	5.62	+0.1	5.59	+0.23
Intermediate 2	5.37	-0.18	5.39	+0.04

2.5.2. ^{27}Al-NMR for Catalyst A and PO

Table S12 displays the shift from the aluminum-2 attached to the ACAC ligand and the Aluminum-1 has 2 ethyl groups attached.

Table S12: ^{27}Al−NMR shifts for Al. The Δ is the shift with respect to the Al1

Complex	Al - shift (ppm)					
	Simple GIAO			**Advanced GIAO**		
	Al1	Al2	Δ	Al1	Al2	**Δ**
Catalyst	449	507	57.9	454	509	55
Adduct 1	433	474	41.3	457	501	44
Transition State 1	459	493	34.5	460	495	35
Intermediate 1	482	508	25.3	482	506	24
Adduct 2	456	533	77	457	533	76
Transition State 2	449	504	55	451	505	54
Intermediate 2	462	504	42	462	504	42

2.5.3. ^{1}H−NMR for Catalyst B and PO

The most accurate method is the advanced GIAO to calculate the relative NMR shift, indicated with bold in the tables. The relative NMR shift for the mechanism involving catalysts are larger than 0.5 ppm (see Table S13). This another evidence against the possibility of catalyst B being a major species.

Table S13: ^{1}H−NMR shifts for H_c. The Δ is the shift with respect to the catalyst at 298K

Complex	H_c - shift (ppm)		H_c - shift (ppm)	
	Simple GIAO		**Advanced GIAO**	
	Absolute	Δ	Absolute	**Δ**
Catalyst B	26.0415	N/A	25.9878	N/A
Adduct 1	26.1132	- 0.0717	26.0517	- 0.0639
Transition State 1	25.7326	0.3089	25.7783	0.2095
Intermediate 1	25.7326	0.3089	25.7550	0.2328
Adduct 2	25.8280	0.2135	25.7359	0.2519
Transition State 2	25.8382	0.2033	22.8281	3.160

2.5.4. ^{27}Al−NMR for Catalyst B and PO

Table S14: ^{27}Al−NMR shifts for Al. The Δ is the shift with respect to the Al1

Complex	Al - shift (ppm)					
	Simple GIAO			**Advanced GIAO**		
	Al1	Al2	Δ	Al1	Al2	**Δ**
Catalyst B	474.899	475.846	0.9470	475.073	475.811	0.7380
Adduct 1	469.746	474.575	4.829	470.091	474.313	4.222
Transition State 1	474.872	480.085	5.213	474.451	480.580	6.129
Intermediate 1	468.071	470.671	2.600	467.935	471.711	3.776
Adduct 2	466.831	473.377	6.546	468.891	473.976	5.085
Transition State 2	469.119	473.433	4.314	468.789	473.707	4.918

2.6 Geometries of the Optimized Structures

The geometries here included correspond to the Transition state, adducts and intermediate structures. Note that all atoms the final structures are given in the standard x,y,z format:

```
Atom  X  Y  Z
Atom1 X1 Y1 Z1
Atom2 X2 Y2 Z2
...
```

2.6.1. Catalyst-A

```
O  -0.00842500   -0.01106900   -0.00039400
O   0.00657300   -0.00684100    2.45534600
C   0.78508600    0.00339800    3.54817900
C   2.22887000    1.83226300    2.69485300
O   1.57372000    2.02605100    1.60104700
C   3.45795400    2.65677900    2.87334800
H   3.15217600    3.69845500    3.03311400
H   4.06354200    2.32850000    3.71765500
H   4.04525200    2.63434900    1.95068900
C   0.46823400   -1.04455000    4.55607600
H  -0.60081700   -1.01603000    4.78955400
H   0.68514100   -2.03346200    4.13337800
H   1.05238000   -0.92121500    5.46760200
Al -0.06331900    1.37780500    1.17172700
C  -1.53722900    2.63413400    1.08603000
H  -1.29804700    3.40651500    0.34188400
H  -1.57857300    3.16538400    2.04760600
C  -2.91354200    2.00413900    0.76924400
H  -3.70253000    2.76414300    0.74782400
H  -2.91846700    1.50485700   -0.20617300
H  -3.20337700    1.25698100    1.51661400
C   1.40985600   -2.59675000    1.26309700
H   1.84268900   -2.64295400    0.25244100
H   2.15491000   -2.04805500    1.85917500
C   1.24485600   -4.03110500    1.81298300
H   2.19968800   -4.56936300    1.84142800
H   0.84051500   -4.03978200    2.83250000
H   0.55786700   -4.62111600    1.19584300
C  -2.12043600   -2.05217800    1.10772300
H  -2.23200100   -3.03717000    1.58147600
H  -2.68169700   -1.35242800    1.74433500
C  -2.75730000   -2.08023700   -0.30203400
H  -2.25650800   -2.79801300   -0.96274300
H  -3.81628000   -2.36222000   -0.26564300
H  -2.70799500   -1.09767900   -0.78789000
Al -0.23136200   -1.52658400    1.13489600
C   1.82039500    0.90342100    3.68985900
H   2.40891100    0.85137500    4.59629700
H  -0.34690900    0.02362100   -0.90466800
```

2.6.2. PO Monomer

```
C  -0.00071800   -0.00435500    0.00257400
C  -0.00047000    0.00187700    1.47392500
O   1.23644900   -0.00317400    0.73814300
C  -0.30711700   -1.24468000   -0.79794200
H  -0.20289100    0.94349400   -0.50171200
H  -0.22099600   -0.92117300    2.01104800
H  -0.21183300    0.92177100    2.01904200
H  -0.07849500   -2.14332000   -0.21720500
H   0.29109300   -1.26702900   -1.71529000
H  -1.36608600   -1.26689500   -1.08024500
```

2.6.3. AGE Monomer

```
C   0.01648800    0.07586700   -0.04502200
C   0.49459600    0.14849700    1.34500200
O   1.41112200   -0.07936600    0.26111200
C  -0.65858600   -1.16240400   -0.60318000
H  -0.23688000    1.00629200   -0.55705100
H   0.34307300   -0.70474100    2.00698900
H   0.59068000    1.11579100    1.83735900
H  -0.37015500   -2.03901800   -0.00092900
H  -0.31492300   -1.32781300   -1.62907000
C  -2.73884300   -1.06508000    0.57817800
C  -4.21445100   -0.96632300    0.33481900
H  -2.40769800   -0.21954000    1.20281800
H  -2.49256200   -1.99527200    1.11581700
H  -4.52686600   -0.12984700   -0.28866200
O  -2.07062800   -1.03087600   -0.68515200
C  -5.11799700   -1.80792200    0.84178700
H  -4.82515500   -2.65694500    1.45578100
H  -6.18112400   -1.67650500    0.66354100
```

2.6.4. Adduct 1*

```
O   1.4954593762  0.5624707792 -2.3438441776
O   0.2924808336  2.1741735592 -0.9026428654
C   0.0458215503  2.5364543379  0.4349727317
C   2.3916840003  2.0704818333  1.1766957958
O   2.9086546510  1.8343254648 -0.0544031795
C   3.3816234360  1.9364009521  2.2920708545
H   3.7949947257  0.9168836781  2.3220832612
H   4.2305727180  2.6190169479  2.1391238758
H   2.9215807078  2.1545715633  3.2612134573
C  -1.3684931517  2.9281197492  0.6923414924
H  -1.6570842054  3.8000351721  0.0868694204
```

```
H  -2.0633061347  2.1137730037  0.4305864804
H  -1.5129406163  3.1713473897  1.7497542533
Al  2.0371597465  2.1309823679 -1.5689301667
C   2.7315917683  3.5500838660 -2.7255245063
H   1.9708661613  3.8301991943 -3.4697558515
H   3.5814099070  3.1649734727 -3.3111893584
C   3.1807740053  4.8043729743 -1.9359744927
H   3.5830074373  5.5858021105 -2.5952440663
H   2.3445720189  5.2450204835 -1.3775690980
H   3.9588875732  4.5516554255 -1.2053089123
C  -0.0570408525 -0.8312129357  0.0328573208
H   0.1090419660 -1.8560903167 -0.3384588556
H   0.8334881825 -0.5751026672  0.6289568569
C  -1.2967066981 -0.8296641677  0.9590253049
H  -1.2207049944 -1.5725107558  1.7656452386
H  -1.4282877537  0.1508577477  1.4328914381
H  -2.2160458840 -1.0486923559  0.3987657993
C  -1.7243904177  0.4014122531 -2.7259543655
H  -2.6057847783  0.8122167891 -2.2073734476
H  -1.5462351120  1.0741587464 -3.5787680741
C  -2.0629227182 -1.0184781617 -3.2451989919
H  -2.2527617273 -1.7111931656 -2.4140624513
H  -2.9533133345 -1.0288432188 -3.8892377540
H  -1.2344852025 -1.4375454146 -3.8323001959
Al -0.1799340505  0.4173825649 -1.4987876960
C   1.0574081922  2.4350609719  1.3836998983
H   0.7732917551  2.6714763303  2.4050869490
C   2.9978208128 -2.2545249107 -1.2401457414
C   4.2033557116 -1.7944307544 -1.9471180678
O   2.8948096784 -1.6828476396 -2.5722828454
H   2.7550884854 -3.3153942650 -1.1928588006
H   4.8186201742 -2.5517037831 -2.4351328494
H   2.0589557163 -0.2266206003 -2.5445891182
H   2.5758547964 -1.6287565886 -0.4543923556
C   4.8960876102 -0.5054654710 -1.5859222673
H   4.2442444462  0.1488064106 -0.9980832889
H   5.7874286720 -0.7265409913 -0.9857295595
H   5.2230334161  0.0213401239 -2.4909432278
```

2.6.5. Transition State 1*

```
O   1.8387527866  0.7450169106 -2.2331625751
O   0.3115846652  2.0612930667 -0.6659806058
C   0.2396598514  2.2659616997  0.6772452923
C   2.6960721351  2.6311489642  0.9442451886
O   2.9958447718  2.7049643889 -0.3353016305
C   3.8635283639  2.7365638348  1.8769735261
H   4.4579169068  3.6279792490  1.6370990462
H   3.5459685876  2.7783918044  2.9226286028
H   4.5227354346  1.8656745161  1.7436655715
C  -1.1320194429  2.1369254620  1.2482840918
H  -1.8103631096  2.8604412164  0.7761148080
H  -1.5298078424  1.1348729033  1.0365517025
H  -1.1302755020  2.2966614968  2.3300923995
Al  1.8614834685  2.4372629991 -1.7192524997
C   1.7394145290  3.9103028206 -3.0047827637
H   2.7280833613  4.1070327423 -3.4485298907
H   1.4691497889  4.8390969601 -2.4785631204
C   0.7146188764  3.6324836899 -4.1325723609
H   0.6610711694  4.4591432119 -4.8541282783
H   0.9718429453  2.7211102313 -4.6863548349
H  -0.2939892459  3.4838504111 -3.7260180793
C   0.1336888831 -1.0886012025 -0.0665183365
H   0.7943813304 -1.9340571242 -0.3094577784
H   0.5216270407 -0.6805328879  0.8799706567
C  -1.2986845768 -1.6357533223  0.1445876837
H  -1.3442533498 -2.3988687001  0.9343049230
H  -2.0072558840 -0.8425651441  0.4202275699
H  -1.6850715037 -2.0900662676 -0.7766716543
C  -1.1343093749  0.2548513657 -2.9459478956
H  -2.1162150763 -0.0515481988 -2.5536073574
H  -1.2684921719  1.2701563068 -3.3488343808
C  -0.7229144640 -0.6936540721 -4.1004833214
H  -0.6100877680 -1.7302906100 -3.7512170871
H  -1.4570314876 -0.7103442013 -4.9186514649
H   0.2392577918 -0.3872063265 -4.5333372059
Al  0.2406925644  0.2572704528 -1.5217912099
C   1.3745451286  2.5000662179  1.4316790897
H   1.2404930614  2.5791220090  2.5051786296
C   3.9179085980 -0.8963534923 -2.6490236331
C   3.7365233450  0.0026107098 -1.4667172024
O   2.8498606354 -1.8059935699 -2.8515819751
H   4.0979969216 -0.2861672816 -3.5445510488
H   4.2709818542  0.9485069998 -1.5023537893
H   2.0912726208 -1.2430245292 -3.0690694272
H   4.8153329892 -1.5148398437 -2.4784299140
C   3.4159165913 -0.5251515639 -0.1218307524
H   4.3501307712 -0.6245002526  0.4601899282
H   2.7802439790  0.1675472260  0.4486066965
H   2.9246090518 -1.4982412763 -0.1799133327
```

2.6.6. Intermediate 1*

```
O   1.8387527866  0.7450169106 -2.2331625751
O   0.3115846652  2.0612930667 -0.6659806058
C   0.2396598514  2.2659616997  0.6772452923
C   2.6960721351  2.6311489642  0.9442451886
O   2.9958447718  2.7049643889 -0.3353016305
C   3.8635283639  2.7365638348  1.8769735261
H   4.4579169068  3.6279792490  1.6370990462
H   3.5459685876  2.7783918044  2.9226286028
H   4.5227354346  1.8656745161  1.7436655715
C  -1.1320194429  2.1369254620  1.2482840918
H  -1.8103631096  2.8604412164  0.7761148080
H  -1.5298078424  1.1348729033  1.0365517025
H  -1.1302755020  2.2966614968  2.3300923995
Al  1.8614834685  2.4372629991 -1.7192524997
C   1.7394145290  3.9103028206 -3.0047827637
H   2.7280833613  4.1070327423 -3.4485298907
H   1.4691497889  4.8390969601 -2.4785631204
C   0.7146188764  3.6324836899 -4.1325723609
H   0.6610711694  4.4591432119 -4.8541282783
H   0.9718429453  2.7211102313 -4.6863548349
H  -0.2939892459  3.4838504111 -3.7260180793
C   0.1336888831 -1.0886012025 -0.0665183365
H   0.7943813304 -1.9340571242 -0.3094577784
```

```
H   0.5216270407 -0.6805328879  0.8799706567
C  -1.2986845768 -1.6357533223  0.1445876837
H  -1.3442533498 -2.3988687001  0.9343049230
H  -2.0072558840 -0.8425651441  0.4202275699
H  -1.6850715037 -2.0900662676 -0.7766716543
C  -1.1343093749  0.2548513657 -2.9459478956
H  -2.1162150763 -0.0515481988 -2.5536073574
H  -1.2684921719  1.2701563068 -3.3488343808
C  -0.7229144640 -0.6936540721 -4.1004833214
H  -0.6100877680 -1.7302906100 -3.7512170871
H  -1.4570314876 -0.7103442013 -4.9186514649
H   0.2392577918 -0.3872063265 -4.5333372059
Al  0.2406925644  0.2572704528 -1.5217912099
C   1.3745451286  2.5000662179  1.4316790897
H   1.2404930614  2.5791220090  2.5051786296
C   3.9179085980 -0.8963534923 -2.6490236331
C   3.7365233450  0.0026107098 -1.4667172024
O   2.8498606354 -1.8059935699 -2.8515819751
H   4.0979969216 -0.2861672816 -3.5445510488
H   4.2709818542  0.9485069998 -1.5023537893
H   2.0912726208 -1.2430245292 -3.0690694272
H   4.8153329892 -1.5148398437 -2.4784299140
C   3.4159165913 -0.5251515639 -0.1218307524
H   4.3501307712 -0.6245002526  0.4601899282
H   2.7802439790  0.1675472260  0.4486066965
H   2.9246090518 -1.4982412763 -0.1799133327
```

2.6.7. Adduct 2*

```
O   0.4384467478 -0.3173631251 -1.7051969136
C  -0.3099212296  3.3634620138  1.2254989109
H   0.3865275246  4.0668708185  0.7439705178
H  -1.2568967788  3.4165111783  0.6645104418
H  -0.5027990650  3.7055758733  2.2473418980
C  -2.4048483978  0.2476097044 -0.3454202420
H  -2.9939812925 -0.3509444995 -1.0600301177
H  -2.0581730031 -0.4611850063  0.4229218049
C  -3.3340091353  1.2953476058  0.3143911307
H  -4.2233386017  0.8399501679  0.7731573022
H  -2.8067423834  1.8433396406  1.1052926776
H  -3.6890234048  2.0361213362 -0.4157659021
C  -1.0325629489  2.2425976522 -2.7992846849
H  -1.1727086439  3.2701034709 -2.4265216252
H  -0.1023095851  2.2770180187 -3.3886036041
C  -2.2186562508  1.8841663544 -3.7276361371
H  -3.1640225071  1.8537109888 -3.1696994432
H  -2.3436984821  2.6026173014 -4.5496908796
H  -2.0875037178  0.8935158597 -4.1858153928
Al -0.8289262627  1.0092874100 -1.2643575937
O   0.4932414430  1.4633435498 -0.0405091822
C   0.2443368306  1.9787699629  1.2281169453
C   1.0522054335 -0.0815131536  2.3613334640
O   1.4758617438 -0.7154420916  1.2418540931
C   1.2423625795 -0.8735912993  3.6188256304
H   0.6919907851 -1.8257910651  3.5677710903
H   2.3037805831 -1.1272410320  3.7683683768
H   0.8919174298 -0.3193929587  4.4954165215
Al  1.7304547285 -0.0073989741 -0.3836400689
C   3.3633210153  1.0013422788 -0.8493070012
H   3.1187941843  1.7049732162 -1.6600345805
H   4.1657438713  0.3612595283 -1.2455148357
C   3.8833855487  1.8094964947  0.3639345025
H   3.0960087259  2.4620545090  0.7617230984
H   4.1879887982  1.1465968476  1.1845492258
H   4.7465647795  2.4429651630  0.1141557743
C   0.5048234587  1.2024006220  2.3488074899
H   0.2586048030  1.6413198230  3.3112729174
C   3.7651862238 -2.4876730313 -0.3114485707
C   2.4422521885 -3.1111063246 -0.1366749895
O   2.5693242452 -1.8724198183 -0.8963582830
H   4.4047198385 -2.8922683634 -1.0962862676
H   1.9231441487 -2.9699475057  0.8080003005
H   2.1511561285 -3.9615084765 -0.7514129412
C   4.4659452212 -1.7495570728  0.7977334364
H   5.0581088871 -0.9227649517  0.3950665683
H   3.7379826328 -1.3534481786  1.5091470980
H   5.1410933513 -2.4463269825  1.3099877679
C   0.4920299588 -0.8479550276 -3.0462725122
H  -0.3242054824 -0.3812921992 -3.6115615387
C   0.2844811553 -2.3583780870 -3.0347671705
H   1.1338154040 -2.8601257893 -2.5615713216
H   0.1715201872 -2.7300036647 -4.0605150461
H  -0.6277523773 -2.6066958379 -2.4823008140
C   1.8078485291 -0.4162222474 -3.7017908273
O   1.8607645592 -0.7952601903 -5.0755242646
H   2.6530439194 -0.8319227423 -3.1373925347
H   1.8778935785  0.6745233390 -3.6772391147
H   1.9475504783 -1.7553226327 -5.1246361838
```

2.6.8. TS 2: R-R System*

```
O   1.6325840457  0.5692806790 -1.5138678459
O  -0.0880562917  2.5529902866 -0.6493441464
C  -0.1769861193  2.6009520222  0.6699183550
C   2.2678106408  2.8772888782  1.0793152161
O   2.6269439535  2.9275019717 -0.1985581493
C   3.3994601603  3.0353973268  2.0511329521
H   3.9246572566  3.9822902845  1.8640096405
H   3.0497821602  3.0164414332  3.0877145496
H   4.1355271261  2.2303503763  1.9069642122
C  -1.5700717587  2.5089035394  1.2167436346
H  -2.1756457565  3.3480900996  0.8467164556
H  -2.0539207791  1.5872392803  0.8652062019
H  -1.5752795390  2.5206557918  2.3109391610
Al  1.5046804853  2.3510789513 -1.5006189538
C   1.6400240453  3.2317143948 -3.2560874246
H   1.8752867784  4.2994089198 -3.1274430306
H   0.6350755722  3.2099522938 -3.7084828951
C   2.6449857214  2.6036607113 -4.2499511182
H   2.5992974873  3.0735942338 -5.2426953269
H   3.6775855561  2.7051122221 -3.8909767731
H   2.4478615610  1.5318103519 -4.3851148334
C  -0.2936628494 -1.0513205567  0.4673002234
H  -1.0453857430 -0.3451269731  0.8474083679
H  -0.7968775035 -2.0329722387  0.4657815507
C   0.9039680335 -1.0875780175  1.4461919660
```

```
H   0.6093784358 -1.3717161423  2.4668077234
H   1.6647214024 -1.8086820872  1.1140320467
H   1.3857453344 -0.1033194985  1.5030607815
C  -0.8754730700 -0.6452149654 -2.9956489068
H  -1.2349686707 -1.6745240377 -3.1652959314
H  -1.7871872986 -0.0426097527 -2.8678994619
C  -0.1120135510 -0.1490639613 -4.2472999026
H   0.8212184491 -0.7108152500 -4.3989488307
H  -0.7015450744 -0.2400426694 -5.1706345114
H   0.1792180137  0.9016574335 -4.1377003771
Al  0.2581885833 -0.5643898918 -1.3718248260
C   2.9208296166 -1.5852157298 -2.1030624512
C   3.2525482485 -0.3916257990 -1.2742794875
O   1.5838418272 -2.0302292501 -1.7152811438
H   2.9171827801 -1.3278935510 -3.1690292773
C   4.3107866060  0.5392562781 -1.7638171275
C   1.1756230428 -3.3953733339 -2.0039817717
H   3.6111977608 -2.4222035971 -1.9311794879
H   3.1840191391 -0.5466052831 -0.2006878973
C   1.9612524294 -4.3862536020 -1.1545228328
C   1.2565652290 -3.6543473507 -3.5122715616
O   0.6985642407 -4.9197772956 -3.8451906358
H   0.1229581518 -3.4153446902 -1.7083617039
H   1.5148766987 -5.3818019046 -1.2511129329
H   1.9179408806 -4.0933562916 -0.1009718665
H   3.0112112569 -4.4470456502 -1.4655990583
H   2.3008260559 -3.5789488008 -3.8510188529
H   0.6648530024 -2.8993564839 -4.0355486879
H   1.3137873736 -5.6145054802 -3.5800827548
C   0.9451494922  2.7187388803  1.5072382564
H   4.1830203045  0.7434548288 -2.8326653667
H   5.3195851761  0.1246043813 -1.6093345846
H   4.2560788619  1.4852210582 -1.2099151823
H   0.7679033280  2.7149381274  2.5771382157
```

2.6.9. TS 2: R-S System*

```
O   1.9888727437  0.6592021047 -2.0603802573
O   0.3706231809  2.1845851970 -0.8149704069
C   0.1979868688  2.5803983247  0.4667004374
C   2.6352371093  2.9331608493  0.8835746924
O   3.0415090609  2.8305336617 -0.3626840828
C   3.7261902238  3.1392345453  1.8884445803
H   3.3297042573  3.3131343501  2.8926643350
H   4.3728506581  2.2486048943  1.9106816219
H   4.3583664436  3.9855335429  1.5895914609
C  -1.2169717054  2.5532103034  0.9397975812
H  -1.8367079993  3.2143540567  0.3190741294
H  -1.6201903830  1.5372276990  0.8336235594
H  -1.2960838683  2.8611779084  1.9861830584
Al  1.9954394701  2.3976260229 -1.7777821156
C   1.9977175099  3.6998954642 -3.2444244849
H   2.9781894246  3.6987068265 -3.7463279265
H   1.8767973297  4.7183821282 -2.8442706042
C   0.8894500084  3.4137189802 -4.2882404563
H   0.9000103989  4.1391695416 -5.1134995528
H   1.0055717885  2.4130613402 -4.7234268188
H  -0.1076283451  3.4496415735 -3.8303783290
C   0.0825038970 -0.7638653317  0.3060198335
H   0.7881303946 -1.6000473090  0.3819594109
H   0.3120545703 -0.1029513786  1.1572204507
C  -1.3611978369 -1.3013115403  0.4498230619
H  -1.5334739799 -1.7965322316  1.4160185466
H  -2.1096952649 -0.5025329765  0.3545680698
H  -1.5926616073 -2.0335967125 -0.3350548783
C  -1.0277256204  0.1421430327 -2.8100609089
H  -1.9846021085  0.4476876021 -2.3561180996
H  -0.7917549697  0.9203065418 -3.5519710927
C  -1.2455023361 -1.1992573514 -3.5481631774
H  -1.6004072506 -1.9743089492 -2.8554858979
H  -1.9900870967 -1.1209642583 -4.3529283209
H  -0.3113277294 -1.5559587590 -4.0066833940
Al  0.3778715927  0.2052186885 -1.4052507007
H   1.0595388496  3.1309305239  2.3127062557
C   3.5858961229 -1.4106476818 -1.8646255675
C   3.6670969121 -0.1878291039 -1.0172868231
O   2.4359327052 -2.1626161041 -1.5116851527
H   3.5503272103 -1.1167366958 -2.9220456812
H   4.3415401150  0.5845825447 -1.3747100900
C   1.9574630585 -3.0407271560 -2.5321752302
H   4.4948784990 -2.0246492864 -1.7083358009
C   3.3885873108 -0.2277889783  0.4381143579
H   4.3092816950 -0.0076458271  1.0036961124
H   2.6676747898  0.5480788719  0.7463299994
H   2.9829731711 -1.1948186783  0.7428828202
C   2.9470467720 -4.1516156638 -2.8715158736
C   0.6366200534 -3.5948718066 -1.9905213189
O  -0.0670415202 -4.3373941209 -2.9796969904
H   1.7458114239 -2.4426599124 -3.4355801899
H   3.2101481296 -4.7026743342 -1.9600508042
H   3.8632422559 -3.7530131396 -3.3210841235
H   2.4809603988 -4.8446194277 -3.5799168278
H   0.0313489981 -2.7670964154 -1.6041259057
H   0.8413916415 -4.2819267511 -1.1624794721
H  -0.5080649251 -3.7055373755 -3.5629139033
C   1.2746375031  2.9016881363  1.2747968850
```

2.6.10. TS 2: S-R System*

```
O   1.6650221749  0.9397875752 -2.6337511214
O   0.1797037433  1.9790294752 -0.8444113941
C  -0.0439605176  2.1812751114  0.4747792935
C   2.3838643862  2.3082746387  1.0278516560
O   2.8324951034  2.2151943628 -0.2035779771
C   3.4406388171  2.3840080705  2.0889040123
H   3.0068052898  2.4590313438  3.0898235491
H   4.0802388130  1.4924068641  2.0409019994
H   4.0890591526  3.2521671388  1.9076559553
C  -1.4830831004  2.2121925841  0.8678382220
H  -1.9887166663  3.0545948569  0.3751519296
H  -1.9830911161  1.2942536749  0.5322881065
H  -1.5988986389  2.3073440927  1.9510491199
Al  1.8248179154  2.4262862399 -1.7083203998
C   1.9659277795  4.2041330225 -2.5231997244
H   2.9748628160  4.3439102496 -2.9421380456
H   1.8666962343  4.9772849278 -1.7451051547
```

```
C   0.9121723661  4.4410834977 -3.6330251509
H   1.0055554155  5.4375757278 -4.0865489773
H   1.0106496819  3.6992528985 -4.4352136766
H  -0.1085943407  4.3538641266 -3.2381331180
C   0.2758518613 -1.2216534528 -0.7170677396
H   0.1967895564 -2.1403155711 -1.3202874822
H   1.2845025120 -1.2465589494 -0.2766338433
C  -0.7734740480 -1.2908140874  0.4168267434
H  -0.7255726779 -2.2364033204  0.9745820755
H  -0.6251173628 -0.4777727664  1.1388811989
H  -1.7961452177 -1.1990683101  0.0252204978
C  -1.4526455181  0.4293770157 -3.1706414921
H  -2.3896934517  0.2573574950 -2.6169987138
H  -1.5359254604  1.4411413548 -3.5962644806
C  -1.3478045259 -0.6021570859 -4.3218702919
H  -1.3006892856 -1.6297925450 -3.9347140884
H  -2.2037466497 -0.5561242860 -5.0104547447
H  -0.4405728026 -0.4361936342 -4.9187438783
Al  0.1035284445  0.3258327441 -1.9547135496
H   0.7601675237  2.4857744769  2.4048426921
C   2.9475155821 -1.5651606564 -2.7250780393
C   3.3312503246 -0.2911012480 -2.0443264824
O   3.2163190061 -2.6392813355 -1.8226591420
H   1.8796269334 -1.5799645867 -2.9897933499
C   4.4384149738  0.5390053341 -2.5883595366
C   2.8826675998 -3.9353906004 -2.3437015144
H   3.5214307381 -1.6844109943 -3.6573987027
H   3.1250666466 -0.2416134159 -0.9817748441
C   2.6119888515 -4.8093165203 -1.1240306632
C   4.0106941287 -4.4882978352 -3.2124001820
H   3.7251591724 -5.4566436793 -3.6403075638
H   1.9512684316 -3.8525027978 -2.9264657903
O   1.4817483192 -4.3713469800 -0.3863592036
H   3.5191082892 -4.8198045020 -0.4978538425
H   2.4016245026 -5.8344917339 -1.4471492330
H   4.9171988856 -4.6200765727 -2.6100982928
H   4.2393547613 -3.8055976478 -4.0378160331
C   1.0109116680  2.3454603153  1.3593194270
H   1.5692460525 -3.4145953947 -0.2572252892
H   4.2620844921  0.7788267012 -3.6442559943
H   5.3862798224 -0.0250474676 -2.5329303991
H   4.5708213120  1.4645068603 -2.0188726354
```

2.6.11. Intermediate 2*

```
O   1.6639175943  0.2132411314 -1.2241011691
C  -0.8150966174  3.1462402593  1.5995568512
H  -0.3192071151  4.1179164961  1.4515066874
H  -1.5448528369  3.0363632948  0.7827574492
H  -1.3630949634  3.1755460729  2.5467219281
C  -1.4346873643 -0.0576211308 -0.4762594067
H  -1.4915136288 -0.9745153690 -1.0802816814
H  -1.1065999574 -0.3832887809  0.5231897477
C  -2.8491658145  0.5564986595 -0.3587080761
H  -3.5899285254 -0.1701183872  0.0037572586
H  -2.8580424693  1.4004298534  0.3416141184
H  -3.2130118873  0.9369573336 -1.3229209588
C  -0.1109471577  2.6372993798 -2.4473423742
H  -0.6730787070  3.4342333769 -1.9323198820
H   0.9131719955  3.0356523554 -2.5362623802
C  -0.7070970341  2.4385386324 -3.8558660030
H  -1.7617978934  2.1454114102 -3.7980757037
H  -0.6528863519  3.3544716296 -4.4609733417
H  -0.1894059479  1.6410012592 -4.4019367099
C   1.3483555100 -1.4435135404 -2.9250433314
C   2.3090931957 -0.4190573809 -2.3429037685
O   0.1937283444 -0.7554451832 -3.3931515256
H   1.8509175373 -1.9806541163 -3.7412579631
H   3.1790283791 -0.9668446827 -1.9583636887
C  -0.9346861681 -1.5971979415 -3.6735042085
H   1.0624814616 -2.1642105026 -2.1436548146
H   3.2686148524  0.1560636494 -4.1966343556
Al -0.0085018104  1.1144875933 -1.1892809180
C   2.7586773868  0.6339225829 -3.3517647170
H   1.8928657047  1.1859092130 -3.7263705978
H   3.4497004913  1.3338185681 -2.8721439296
O   0.8513248856  1.8803918763  0.3799798765
C   0.1718312246  2.0300142824  1.6006093812
C   1.3824024935  0.1405516946  2.7115807224
O   2.2885485446 -0.0731910603  1.7247838990
C   1.5225656147 -0.7821092447  3.8823507173
H   1.3850064395 -1.8275896943  3.5686858412
H   2.5324875102 -0.7095736301  4.3121475910
H   0.7881459165 -0.5511590370  4.6608122954
Al  2.4343004562  0.9322526643  0.2865583641
C   4.1681158549  1.7682308146 -0.0903172229
H   4.0301494289  2.5462430834 -0.8574493542
H   4.8411016261  1.0259108851 -0.5504163002
C   4.8600749624  2.3798471042  1.1518189408
H   5.8333320864  2.8257248626  0.9051340282
H   4.2433138449  3.1686647028  1.6017934756
H   5.0268566843  1.6194610264  1.9244909778
C   0.4260493366  1.1595067678  2.6555402425
H  -0.1877770203  1.2968482267  3.5411929943
C  -0.6615649651 -2.4923231809 -4.8940541343
O  -1.7432569279 -3.3881462327 -5.1383725430
C  -2.1377366949 -0.6996506432 -3.9031663992
H  -1.1083274852 -2.2442677439 -2.7951774974
H   0.2778490807 -3.0477270638 -4.7671656020
H  -0.5726310787 -1.8650662763 -5.7870040021
H  -1.7811688986 -4.0304219368 -4.4179060060
H  -1.9442773939 -0.0340854957 -4.7501219569
H  -2.3412215252 -0.0940533025 -3.0181013398
H  -3.0109233035 -1.3177416847 -4.1315597247
```

2.6.12. Adduct 1: Catalyst A-PO

```
O  -0.22065900   -0.37776600   -0.29851700
O   0.09023300   -0.20939100    2.06619300
C   0.75750900   -0.06736500    3.19309900
C   1.97702700    1.90810900    2.35819300
O   1.40531400    1.94519500    1.20233400
C   3.08128300    2.89727600    2.56191100
H   2.68686200    3.90858600    2.41480200
H   3.53487700    2.82235400    3.55015300
H   3.84700100    2.73589000    1.79515300
```

C	0.54086600	-1.12069300	4.22735000
H	-0.52661600	-1.18246100	4.46241500
H	0.84238400	-2.09527600	3.82550300
H	1.10682100	-0.92362600	5.13740900
Al	-0.19598100	1.21516400	0.64341200
C	-1.84797800	2.04598400	1.29004900
H	-2.58283300	2.02306400	0.47144400
H	-1.64612700	3.11377700	1.45918400
C	-2.47877000	1.44017200	2.56243300
H	-3.40354400	1.95610700	2.84768600
H	-2.72609900	0.38187600	2.42753500
H	-1.79755100	1.50243700	3.41947200
C	1.24034300	-2.94366200	0.97378300
H	1.52741700	-3.11757600	-0.07486500
H	2.09771500	-2.41149200	1.41360800
C	1.04762000	-4.30636000	1.67617900
H	1.94558000	-4.93387700	1.61701200
H	0.80754400	-4.19147200	2.74058300
H	0.22445200	-4.87547400	1.22863700
C	-2.19524600	-2.34200000	1.23217500
H	-2.87862900	-1.54877000	0.89630000
H	-2.37535200	-3.18758500	0.55048700
C	-2.56878000	-2.77023700	2.67002200
H	-2.51175100	-1.92663800	3.36836000
H	-3.59142200	-3.16275600	2.73036200
H	-1.90077800	-3.55267400	3.05002300
Al	-0.33448000	-1.75872800	0.96554600
C	1.62959600	0.99470800	3.37693600
H	2.14716200	1.06882800	4.32377300
C	1.20367100	2.59546200	-1.79655000
C	0.11296000	3.54412600	-1.53462700
O	-0.00262600	2.12939300	-1.09360500
H	1.31701200	2.14456200	-2.77751500
H	-0.58574200	3.72648300	-2.34777600
H	-0.53387000	-0.41354300	-1.21054900
H	2.08392500	2.62348300	-1.16096300
C	0.19427400	4.60269600	-0.47456300
H	0.57167300	5.52121300	-0.93611600
H	-0.79482900	4.81383900	-0.06031700
H	0.87095700	4.30947600	0.33014900

2.6.13. Adduct 1: Catalyst A-AGE

O	0.23417100	0.31545500	0.39842000
O	0.22496600	-0.25796100	2.71787700
C	0.74211200	-0.48274900	3.90622600
C	1.88805300	1.70494700	3.96204200
O	1.47268200	2.10813700	2.80909700
C	2.84897100	2.62150000	4.65368900
H	2.35396800	3.58181600	4.83891100
H	3.21495100	2.21688400	5.59756300
H	3.69473100	2.82047100	3.98685300
C	0.49692800	-1.83356500	4.49245800
H	-0.57603100	-2.05000300	4.47991900
H	0.99009300	-2.59277800	3.87307900
H	0.87577100	-1.91362500	5.51148600
Al	0.05728600	1.52402000	1.78290000
C	-1.71778800	2.11136900	2.37080100
H	-2.40436700	2.10325300	1.51061900
H	-1.66326800	3.16630000	2.68302500
C	-2.34569100	1.28515600	3.51665900
H	-3.33089600	1.66729600	3.80477700
H	-2.47568800	0.23659500	3.22916500
H	-1.71911800	1.30064600	4.41678100
C	1.48948400	-2.58877900	0.95971700
H	1.89735700	-2.46139000	-0.05492900
H	2.29740000	-2.24180700	1.62262500
C	1.21223800	-4.09051900	1.20225500
H	2.11145500	-4.70093300	1.06224800
H	0.84641300	-4.28790100	2.21769100
H	0.45043100	-4.47528000	0.51500800
C	-1.96462500	-1.87217300	1.02564200
H	-2.56660500	-0.95274100	0.98589600
H	-2.13318000	-2.36675300	0.05692400
C	-2.49826300	-2.78788200	2.15227200
H	-2.46958800	-2.28639900	3.12776800
H	-3.54055500	-3.08007200	1.98198600
H	-1.91630500	-3.71279300	2.24109600
Al	-0.06380400	-1.39826700	1.13963300
C	1.50045400	0.48390300	4.55279100
H	1.88937000	0.24937000	5.53470500
C	-0.27764700	4.06605400	-0.02329200
C	0.85633100	4.35475500	0.85747800
O	0.56036400	2.96078300	0.49168500
H	-1.28717900	4.07485700	0.37586700
H	0.64574400	4.57759400	1.90059600
H	0.27238200	0.56297300	-0.53146800
H	-0.16954800	4.19829000	-1.09608200
C	2.17473200	4.86622500	0.33443700
H	2.99438800	4.43175800	0.92997300
H	2.31310900	4.55377700	-0.71358300
O	2.11286500	6.26625600	0.47062900
C	3.32739400	6.93706100	0.08311000
C	3.10996600	8.41347400	0.19610900
H	3.56739300	6.65959100	-0.95663100
H	4.15724100	6.60751100	0.72621600
H	2.27591100	8.81106600	-0.37952000
C	3.88200100	9.22424500	0.92257400
H	4.71906000	8.84675900	1.50583000
H	3.71105900	10.29587200	0.95066800

2.6.14. TS 1: Catalyst A - PO

O	-0.52453500	0.19278000	0.85474300
O	-0.06415400	-0.21635700	3.23686900
C	0.55864400	-0.11840000	4.39176400
C	0.38082700	2.34634000	4.40959500
O	-0.27593200	2.45145300	3.30686000
C	0.76688700	3.64178300	5.05161600
H	1.39892500	3.50462900	5.92917100
H	1.28335100	4.26410500	4.31375400
H	-0.14552600	4.17754800	5.33782400
C	1.06635100	-1.39067800	4.98826700
H	0.23544300	-2.09483300	5.10514200
H	1.79409300	-1.85002900	4.30932300
H	1.54070900	-1.22821200	5.95589600

Al	-1.26829500	1.26636600	2.32782500
C	-2.96972200	0.59227200	3.05309400
H	-3.48509100	-0.01212000	2.29110000
H	-3.60968100	1.47815500	3.18765400
C	-2.92080400	-0.20436800	4.37314000
H	-3.92245700	-0.47235100	4.73029900
H	-2.35960500	-1.13671400	4.25606300
H	-2.43468300	0.36589700	5.17380800
C	1.90116500	-1.81142500	1.32015500
H	2.07814500	-1.54673900	0.26586000
H	2.55242900	-1.13622300	1.89514400
C	2.33489600	-3.27831300	1.54809900
H	3.38383400	-3.44381500	1.27394600
H	2.22524800	-3.58073800	2.59665000
H	1.73021800	-3.97304400	0.95383100
C	-1.48891700	-2.67905900	1.75109200
H	-2.42611600	-2.12861900	1.90954900
H	-1.56575200	-3.10403600	0.73830800
C	-1.38871500	-3.83255700	2.77570800
H	-1.39684100	-3.45999900	3.80714900
H	-2.22773600	-4.53346400	2.68702200
H	-0.46744500	-4.41290900	2.64791100
Al	0.01640100	-1.42081700	1.73938500
C	0.74316900	1.11419900	4.99800100
H	1.26185800	1.13989800	5.94673300
C	-2.02919400	1.11484800	-0.60313200
C	-2.73837800	2.19057200	0.11374400
O	-1.69159900	2.50108000	1.02486300
H	-2.35171000	0.07905500	-0.62962100
H	-3.63504700	1.82296700	0.62583200
H	0.23430700	0.63826200	0.44339000
H	-1.19323500	1.40069300	-1.23444300
C	-3.08398400	3.38146400	-0.77497200
H	-3.86026500	3.12520800	-1.50234800
H	-3.45939400	4.17769200	-0.12480200
H	-2.19428100	3.74235500	-1.29784500

2.6.15. TS 1: AGE - Catalyst A

O	-0.52453500	0.19278000	0.85474300
O	-0.06415400	-0.21635700	3.23686900
C	0.55864400	-0.11840000	4.39176400
C	0.38082700	2.34634000	4.40959500
O	-0.27593200	2.45145300	3.30686000
C	0.76688700	3.64178300	5.05161600
H	1.39892500	3.50462900	5.92917100
H	1.28335100	4.26410500	4.31375400
H	-0.14552600	4.17754800	5.33782400
C	1.06635100	-1.39067800	4.98826700
H	0.23544300	-2.09483300	5.10514200
H	1.79409300	-1.85002900	4.30932300
H	1.54070900	-1.22821200	5.95589600
Al	-1.26829500	1.26636600	2.32782500
C	-2.96972200	0.59227200	3.05309400
H	-3.48509100	-0.01212000	2.29110000
H	-3.60968100	1.47815500	3.18765400
C	-2.92080400	-0.20436800	4.37314000
H	-3.92245700	-0.47235100	4.73029900
H	-2.35960500	-1.13671400	4.25606300
H	-2.43468300	0.36589700	5.17380800
C	1.90116500	-1.81142500	1.32015500
H	2.07814500	-1.54673900	0.26586000
H	2.55242900	-1.13622300	1.89514400
C	2.33489600	-3.27831300	1.54809900
H	3.38383400	-3.44381500	1.27394600
H	2.22524800	-3.58073800	2.59665000
H	1.73021800	-3.97304400	0.95383100
C	-1.48891700	-2.67905900	1.75109200
H	-2.42611600	-2.12861900	1.90954900
H	-1.56575200	-3.10403600	0.73830800
C	-1.38871500	-3.83255700	2.77570800
H	-1.39684100	-3.45999900	3.80714900
H	-2.22773600	-4.53346400	2.68702200
H	-0.46744500	-4.41290900	2.64791100
Al	0.01640100	-1.42081700	1.73938500
C	0.74316900	1.11419900	4.99800100
H	1.26185800	1.13989800	5.94673300
C	-2.02919400	1.11484800	-0.60313200
C	-2.73837800	2.19057200	0.11374400
O	-1.69159900	2.50108000	1.02486300
H	-2.35171000	0.07905500	-0.62962100
H	-3.63504700	1.82296700	0.62583200
H	0.23430700	0.63826200	0.44339000
H	-1.19323500	1.40069300	-1.23444300
C	-3.08398400	3.38146400	-0.77497200
H	-3.86026500	3.12520800	-1.50234800
H	-3.45939400	4.17769200	-0.12480200
H	-2.19428100	3.74235500	-1.29784500

2.6.16. Int. 1: Catalyst A - PO

O	-0.00349700	-0.05973600	-0.07383000
O	-0.00192500	-0.10958800	2.38974900
C	0.73664000	-0.12750100	3.50908100
C	2.24848100	1.68128700	2.73437400
O	1.65769300	1.88081900	1.60519100
C	3.50201000	2.45619100	2.96044200
H	3.26191900	3.52567700	2.94959000
H	3.99078600	2.19845600	3.89941400
H	4.18416500	2.27472700	2.12290800
C	0.38425600	-1.19877100	4.47913500
H	-0.67852100	-1.12843500	4.73248700
H	0.54115800	-2.17855400	4.01092600
H	0.98677500	-1.14119700	5.38491500
Al	0.00908100	1.29361100	1.12773800
C	-1.39900600	2.62420600	1.04215400
H	-1.18174200	3.31649100	0.21652500
H	-1.34339600	3.23711000	1.95258000
C	-2.82288900	2.04338400	0.88070300
H	-3.57711700	2.83786900	0.85564400
H	-2.92562700	1.47054400	-0.04763200
H	-3.08628700	1.37160000	1.70546800
C	1.24675800	-2.77595200	1.07482800
H	1.08587200	-3.56769800	1.82044800
H	1.23796900	-3.30458400	0.10860700
C	2.62981200	-2.12392000	1.28756000

H	3.44629300	-2.84373000	1.15659700
H	2.80583000	-1.30198100	0.58395900
H	2.73221100	-1.71015200	2.29729800
C	-2.21151900	-2.01986300	1.11614700
H	-2.79863700	-1.13453900	0.83434500
H	-2.42510600	-2.77032100	0.34100300
C	-2.69879900	-2.54581700	2.48573900
H	-2.58569200	-1.78792000	3.27006400
H	-3.75881100	-2.82556900	2.46258700
H	-2.13910800	-3.43234000	2.80768400
Al	-0.30299700	-1.57500800	1.03708500
C	1.76740000	0.76762100	3.71010500
H	2.31254600	0.69998600	4.64195700
C	0.03120300	0.05046300	-1.53803900
C	-1.19288000	-0.68304100	-2.10013100
O	-1.27297100	-0.54109600	-3.51182300
H	-1.10073100	-1.75786800	-1.90464400
H	-1.65913800	0.31889300	-3.72681200
H	-0.06314300	1.11736300	-1.77489800
C	1.35421700	-0.48491400	-2.05468000
H	2.19130600	0.08220100	-1.63870400
H	1.47468500	-1.53951600	-1.78666200
H	1.37718700	-0.40292700	-3.14422900
H	-2.09999100	-0.32376700	-1.59910100

2.6.17. Int. 1: Catalyst A- AGE

O	-0.77450200	-0.42601200	0.38189000
O	0.02662800	-0.31963200	2.70803500
C	1.03572600	-0.02272800	3.54454300
C	1.59747800	2.08117300	2.35855300
O	0.63992800	2.00963500	1.49891700
C	2.55219400	3.21184000	2.17920700
H	3.34626900	3.21353800	2.92490600
H	2.98627900	3.14888800	1.17509300
H	1.99570200	4.15460900	2.22592600
C	1.31163200	-1.05141000	4.58342000
H	0.40480200	-1.21751800	5.17530100
H	1.56180300	-2.00546400	4.10381300
H	2.13275500	-0.75938300	5.23741900
Al	-0.82152800	0.93028600	1.58478900
C	-2.48622600	1.80892100	2.04435000
H	-3.25565000	1.03704800	2.17910100
H	-2.81808000	2.40440900	1.18223900
C	-2.40927000	2.70926700	3.29946900
H	-3.37581100	3.18034100	3.51004700
H	-2.12611300	2.14079000	4.19304400
H	-1.67698500	3.51491400	3.17540700
C	1.76941600	-2.23829800	0.83383400
H	2.43198700	-2.19068600	1.71134500
H	1.83051900	-3.28101500	0.49324700
C	2.31096000	-1.29986800	-0.26849800
H	3.35692000	-1.51905400	-0.51328800
H	1.73751400	-1.40097800	-1.19692200
H	2.26141000	-0.24465100	0.02543500
C	-1.50226600	-3.03292200	2.06290100
H	-1.94373600	-3.56473700	1.20687000
H	-1.05076900	-3.82043400	2.68366900
C	-2.61307100	-2.31617200	2.86176500
H	-3.13367700	-1.56434000	2.25655200
H	-3.37657400	-3.01668500	3.21976100
H	-2.20937800	-1.79874900	3.73978000
Al	-0.07116000	-1.86590600	1.41109600
C	1.76175400	1.14148500	3.41355000
H	2.56168300	1.31583500	4.12075500
H	-3.04673000	-0.43602700	-2.83623200
C	-2.82041900	-0.69621500	-0.92295700
C	-1.29354400	-0.55790400	-0.97146900
O	-3.34925600	-1.08656300	-2.18047300
H	-3.08348200	-1.47925700	-0.20656800
H	-0.87138400	-1.47395200	-1.39809000
H	-3.26544800	0.24763100	-0.57103700
C	-0.81407100	0.66294700	-1.76831200
H	-1.22019600	1.57368000	-1.30786000
H	0.28155900	0.72230300	-1.73881700
O	-1.30295100	0.63907200	-3.10321800
C	-0.42533100	-0.01930200	-4.04606100
C	-1.16687600	-0.19623400	-5.33455200
H	-0.12675500	-0.99883700	-3.64594600
H	0.47794200	0.58946600	-4.18354000
H	-2.06757000	-0.80707000	-5.28363200
C	-0.76935600	0.32394800	-6.49845400
H	0.12606600	0.93712800	-6.57192500
H	-1.32145600	0.14789600	-7.41678700

2.6.18. Adduct 2: Catalyst A - PO

O	0.4384467478	-0.3173631251	-1.7051969136
C	-0.3099212296	3.3634620138	1.2254989109
H	0.3865275246	4.0668708185	0.7439705178
H	-1.2568967788	3.4165111783	0.6645104418
H	-0.5027990650	3.7055758733	2.2473418980
C	-2.4048483978	0.2476097044	-0.3454202420
H	-2.9939812925	-0.3509444995	-1.0600301177
H	-2.0581730031	-0.4611850063	0.4229218049
C	-3.3340091353	1.2953476058	0.3143911307
H	-4.2233386017	0.8399501679	0.7731573022
H	-2.8067423834	1.8433396406	1.1052926776
H	-3.6890234048	2.0361213362	-0.4157659021
C	-1.0325629489	2.2425976522	-2.7992846849
H	-1.1727086439	3.2701034709	-2.4265216252
H	-0.1023095851	2.2770180187	-3.3886036041
C	-2.2186562508	1.8841663544	-3.7276361371
H	-3.1640225071	1.8537109888	-3.1696994432
H	-2.3436984821	2.6026173014	-4.5496908796
H	-2.0875037178	0.8935158597	-4.1858153928
Al	-0.8289262627	1.0092874100	-1.2643575937
O	0.4932414430	1.4633435498	-0.0405091822
C	0.2443368306	1.9787699629	1.2281169453
C	1.0522054335	-0.0815131536	2.3613334640
O	1.4758617438	-0.7154420916	1.2418540931
C	1.2423625795	-0.8735912993	3.6188256304
H	0.6919907851	-1.8257910651	3.5677710903
H	2.3037805831	-1.1272410320	3.7683683768
H	0.8919174298	-0.3193929587	4.4954165215
Al	1.7304547285	-0.0073989741	-0.3836400689

C	3.3633210153	1.0013422788	-0.8493070012
H	3.1187941843	1.7049732162	-1.6600345805
H	4.1657438713	0.3612595283	-1.2455148357
C	3.8833855487	1.8094964947	0.3639345025
H	3.0960087259	2.4620545090	0.7617230984
H	4.1879887982	1.1465968476	1.1845492258
H	4.7465647795	2.4429651630	0.1141557743
C	0.5048234587	1.2024006220	2.3488074899
H	0.2586048030	1.6413198230	3.3112729174
C	3.7651862238	-2.4876730313	-0.3114485707
C	2.4422521885	-3.1111063246	-0.1366749895
O	2.5693242452	-1.8724198183	-0.8963582830
H	4.4047198385	-2.8922683634	-1.0962862676
H	1.9231441487	-2.9699475057	0.8080003005
H	2.1511561285	-3.9615084765	-0.7514129412
C	4.4659452212	-1.7495570728	0.7977334364
H	5.0581088871	-0.9227649517	0.3950665683
H	3.7379826328	-1.3534481786	1.5091470980
H	5.1410933513	-2.4463269825	1.3099877679
C	0.4920299588	-0.8479550276	-3.0462725122
H	-0.3242054824	-0.3812921992	-3.6115615387
C	0.2844811553	-2.3583780870	-3.0347671705
H	1.1338154040	-2.8601257893	-2.5615713216
H	0.1715201872	-2.7300036647	-4.0605150461
H	-0.6277523773	-2.6066958379	-2.4823008140
C	1.8078485291	-0.4162222474	-3.7017908273
O	1.8607645592	-0.7952601903	-5.0755242646
H	2.6530439194	-0.8319227423	-3.1373925347
H	1.8778935785	0.6745233390	-3.6772391147
H	1.9475504783	-1.7553226327	-5.1246361838

* Structures of most energetically favorable PES

2.6.19. TS2: PO-Catalyst A- RR

O	-0.11874600	-0.07580700	-0.01290100
O	-0.04220900	0.05127900	2.85348100
C	1.09536900	0.00660100	3.58398800
C	1.96063600	2.11436300	2.60651500
O	0.84629200	2.48170200	2.08472500
C	3.16076900	2.93057300	2.26531600
H	3.43562500	2.70193100	1.22714200
H	2.91230800	3.99422200	2.30878300
H	4.01209400	2.70620200	2.90811000
C	1.20343700	-1.13638100	4.53038900
H	0.43155800	-1.00770500	5.29964000
H	0.99146700	-2.08152100	4.02646500
H	2.18285500	-1.18047700	5.00649600
A	-0.76671800	1.76836000	2.61810700
C	-1.44594200	2.56434400	4.26346500
H	-2.31247600	1.96964500	4.58642800
H	-1.85433600	3.55354300	4.01040500
C	-0.44178900	2.70228800	5.42922100
H	-0.90281400	3.17609400	6.30395000
H	-0.05922800	1.72857400	5.75639300
H	0.42465400	3.31340500	5.15027600
C	0.95949900	-2.71234100	1.42411800
H	0.68500700	-3.34490000	2.28236000
H	0.72660400	-3.34804800	0.55338400
C	2.47962800	-2.44845700	1.44712600
H	2.82217700	-1.95475600	0.53208500
H	2.77914000	-1.80463800	2.28208500
H	3.05497000	-3.37806100	1.54128100
C	-2.29213300	-1.71424500	1.59770200
H	-2.88250100	-0.79649800	1.71890000
H	-2.68531300	-2.20587800	0.69405200
C	-2.52545300	-2.63577500	2.81681300
H	-2.18294700	-2.16583700	3.74773900
H	-3.58541900	-2.88438800	2.95582000
H	-1.98323300	-3.58389900	2.71836500
A	-0.39254800	-1.26840000	1.30920200
C	1.15418700	0.20959300	-0.60495900
C	1.42686600	-0.81967600	-1.70473000
O	2.75140000	-0.59803200	-2.19372600
H	0.67890800	-0.69551800	-2.50210700
H	1.32402200	-1.83051200	-1.29167700
H	2.96411700	-1.27370400	-2.85043600
C	2.06552400	0.97615900	3.45940000
H	2.98622500	0.84509600	4.01250600
C	-2.06635000	1.14548600	-0.62753000
C	-2.61490000	2.21094600	0.23093800
O	-1.93659700	1.59855100	1.32198100
H	-2.52103400	0.16302400	-0.59071200
H	-1.31080800	1.33004500	-1.37392900
C	1.22228300	1.63901700	-1.14235600
H	0.58411600	1.76834000	-2.02411600
H	2.24537100	1.86264500	-1.45483100
H	0.92504700	2.35501700	-0.37299500
H	1.93735400	0.10204200	0.16023400
H	-2.20272700	3.19795400	0.00115500
C	-4.11722700	2.25193700	0.42223700
H	-4.60748400	2.63091300	-0.47996900
H	-4.34965200	2.92544800	1.25255500
H	-4.50323700	1.25564700	0.65429300

2.6.20. TS 2: PO-Catalyst A- RS

O	0.00751500	0.00690000	0.01560000
O	0.04240200	-0.04802800	2.85471200
C	0.99454400	-0.03485100	3.81215500
C	1.42626400	2.39047500	3.53789300
O	0.35969100	2.63237200	2.86524700
C	2.39483100	3.51580800	3.67491200
H	1.88620100	4.37773100	4.11972000
H	3.26790900	3.24795500	4.26922300
H	2.71310100	3.81735300	2.67017300
C	1.22889900	-1.32603700	4.51604800
H	0.32090600	-1.56431200	5.08429700
H	1.38584700	-2.14364900	3.81090400
H	2.07401400	-1.26541000	5.20146600
Al	-1.06911000	1.48188800	2.79651400
C	-2.26207800	1.47452300	4.33874200
H	-2.63895000	2.49418100	4.49849800
H	-1.65499200	1.24509300	5.22701700
C	-3.44988900	0.48819400	4.25366400
H	-4.05678200	0.50685600	5.16646800

H	-4.11963000	0.73328900	3.42132000
H	-3.11753300	-0.54566000	4.10829900
C	1.51431900	-2.51039200	1.24467500
H	1.33912700	-3.30397800	1.98662200
H	1.42851300	-3.03315900	0.27760200
C	2.95559200	-1.97545400	1.38657600
H	3.69472100	-2.78629100	1.37959600
H	3.22029400	-1.29743600	0.56908200
H	3.10675700	-1.41897900	2.31951400
C	-1.88395100	-1.98622600	1.48700100
H	-2.60213900	-1.16998900	1.66197700
H	-2.22342700	-2.47214500	0.55962200
C	-1.99896500	-2.99331500	2.65451700
H	-1.69831200	-2.54164100	3.60826800
H	-3.02250100	-3.36527700	2.78665000
H	-1.35438200	-3.86590700	2.49682400
Al	-0.04543400	-1.29461400	1.24951400
C	1.21137900	0.67831700	-0.37900100
C	0.98329900	2.16629700	-0.63127700
C	1.76955300	-0.03666200	-1.61136100
O	3.04567400	0.53302700	-1.91139000
H	1.95438900	0.58773600	0.42846100
H	1.93824700	2.64103500	-0.87095200
H	0.55237000	2.65092600	0.24623000
H	0.31473600	2.32502000	-1.48480200
H	1.06673200	0.09127100	-2.44824700
H	1.85731800	-1.10936200	-1.39589400
H	3.43239300	0.06592300	-2.66315400
C	1.67532400	1.11974500	4.13183900
H	2.48532600	1.04608400	4.84583600
C	-2.13205400	0.83326300	-0.50956400
C	-2.96465100	1.53372800	0.48650800
O	-1.75540500	1.79669200	1.19913500
H	-2.13162100	-0.24230400	-0.61034000
H	-1.61144500	1.41435900	-1.25855600
H	-3.63203000	0.86229800	1.03507000
C	-3.67185000	2.79715200	0.04569800
H	-2.98010100	3.45855300	-0.48264300
H	-4.05759000	3.31666700	0.92793900
H	-4.51470500	2.55453400	-0.60942200

2.6.21. TS 2: PO-Catalyst A- SR

O	0.00260600	0.03714900	0.01068100
O	0.01013000	0.00090300	2.91912900
C	1.15764100	-0.00323900	3.64135600
C	1.85272700	2.21543100	2.77551600
O	0.70557800	2.53788900	2.30351100
C	2.99080100	3.14639000	2.52441100
H	2.72353600	3.87964000	1.76352900
H	3.22346100	3.67227000	3.45967800
H	3.88863200	2.59435500	2.23239400
C	1.34081600	-1.17141900	4.54481100
H	0.57994100	-1.10432100	5.33265900
H	1.16614200	-2.10919000	4.01531900
H	2.33030100	-1.18073200	5.00166600
Al	-0.83852200	1.66628600	2.83390000
C	-1.56138500	2.32147400	4.51999700
H	-2.40745100	1.67342400	4.78951300
H	-2.00434700	3.31065200	4.33324100
C	-0.57590000	2.41241600	5.70666700
H	-1.06623500	2.80084000	6.60697600
H	-0.15916600	1.43263500	5.96643900
H	0.26829200	3.07646500	5.48729600
C	1.08513900	-2.65479700	1.40883900
H	0.75369900	-3.27645600	2.25635800
H	0.87577700	-3.29225700	0.53446000
C	2.60779500	-2.43151100	1.50598800
H	3.01501200	-2.01000900	0.58182700
H	2.88449800	-1.73874400	2.30880400
H	3.14907900	-3.36791000	1.69072000
C	-2.15540900	-1.77713800	1.48721000
H	-2.78892100	-1.23259200	0.77488300
H	-2.19518800	-2.83156000	1.17183100
C	-2.75957300	-1.65841300	2.90254000
H	-2.84651300	-0.61079800	3.21491200
H	-3.76672300	-2.09036200	2.96472800
H	-2.14332900	-2.16847200	3.65375100
Al	-0.27400000	-1.21219900	1.29221800
C	0.97323000	0.18087600	-1.01960100
C	1.17859000	-1.13786300	-1.77365500
O	1.89185300	-0.82827200	-2.97303400
H	0.19205200	-1.56785700	-1.99789600
H	1.73975900	-1.85111700	-1.15999700
H	2.11752800	-1.65030700	-3.42746700
C	2.05352200	1.03532900	3.55727200
H	2.99057000	0.94525800	4.09284100
C	-1.52938000	1.66404300	-0.48031400
C	-2.54446700	2.20096700	0.44662300
O	-1.94585900	1.42370300	1.48819100
H	-1.76068700	0.83837200	-1.13997700
H	-0.60402400	2.20560800	-0.61898400
C	2.26641700	0.79311500	-0.48558500
H	2.69083400	0.17011400	0.30648000
H	2.07106000	1.78941100	-0.07890900
H	3.00013700	0.88241100	-1.29135400
H	0.55619600	0.87147000	-1.77235800
H	-2.43430400	3.27734500	0.62065200
C	-3.98708700	1.81457900	0.21023500
H	-4.37976000	2.34324200	-0.66428500
H	-4.58589000	2.09210700	1.08199800
H	-4.07560400	0.73680900	0.04988400

2.6.22. TS 2: AGE-Catalyst A- RR

O	0.05645500	0.08561600	0.20252300
O	0.07392200	0.09775300	3.09146700
C	0.90375900	0.17086300	4.14302100
C	0.69532800	2.63367100	4.35298200
O	-0.27745500	2.74789300	3.52113500
C	1.26263800	3.90210300	4.89791600
H	2.25119400	3.76071100	5.33605600
H	1.29575200	4.65619200	4.10755500
H	0.58323400	4.27534300	5.67515600

C	1.47553100	-1.12035400	4.61411500
H	0.65211800	-1.80286100	4.85162500
H	2.06008600	-1.59062300	3.82095400
H	2.10438500	-0.98586500	5.49397500
Al	-1.36034000	1.33915800	3.06110900
C	-2.71085200	0.91755800	4.40648800
H	-2.85918200	1.83606300	4.99313700
H	-2.26210900	0.19751400	5.10654200
C	-4.08320100	0.39163500	3.93315800
H	-4.74103700	0.17119300	4.78211300
H	-4.59634900	1.12792100	3.30589400
H	-3.98712900	-0.53490600	3.35616300
C	1.56918000	-2.53142200	1.41455200
H	1.28252500	-3.30760200	2.14126000
H	1.33674200	-2.98798800	0.43597300
C	3.08917300	-2.29601200	1.49099900
H	3.65287400	-3.19733400	1.21905600
H	3.41677900	-1.48144300	0.84070600
H	3.41606200	-2.01530200	2.49778800
C	-1.67980400	-1.92083000	1.74902500
H	-2.48176200	-1.17122800	1.67971000
H	-1.87946600	-2.61374700	0.91703400
C	-1.84282800	-2.67686000	3.08675900
H	-1.71907900	-2.00338700	3.94392900
H	-2.83110900	-3.14204600	3.19050500
H	-1.09891300	-3.47566700	3.19254100
Al	0.13939900	-1.16672400	1.47993400
C	1.02452900	0.82788800	-0.51575500
C	1.84522000	1.73241500	0.39666700
C	1.88428000	-0.07590400	-1.39646100
O	1.02806500	-0.63993100	-2.39440700
H	0.49250600	1.50303700	-1.20397900
H	1.16534500	2.39064500	0.95804100
H	2.50203600	2.36532900	-0.21946200
H	2.34892000	-0.85720000	-0.78882500
H	2.67915400	0.52655100	-1.85900600
H	1.52342700	-1.30217700	-2.89340800
C	1.19939500	1.37038000	4.76048100
H	1.91983700	1.35297900	5.56805200
C	-2.08927500	0.80725000	-0.34692800
C	-2.99291800	1.43059200	0.63181600
O	-1.81524000	1.71223000	1.38785300
H	-2.04759900	-0.26208300	-0.49227300
H	-3.66255200	0.72550700	1.13033000
C	-3.74289800	2.68863200	0.24430000
H	-4.48605900	2.44572300	-0.52970100
H	-3.03553300	3.42842700	-0.16027600
H	-1.56021400	1.44304700	-1.04511200
O	-4.34703900	3.15209100	1.43731800
C	-4.90992400	4.47544800	1.35880800
C	-6.16858000	4.53671400	0.53704600
H	-4.14899400	5.16160800	0.95472500
H	-5.11254500	4.75907300	2.39481800
H	-6.07244300	4.32368100	-0.52703900
C	-7.36479200	4.85418000	1.04079100
H	-7.49486400	5.08004500	2.09718200
H	-8.25130000	4.90767700	0.41538200
O	2.62011700	0.93962800	1.29070500
C	3.57135400	1.72064100	2.02230900
C	4.35502900	0.82913600	2.93514600
H	3.03506100	2.48506800	2.60953100
H	4.24161200	2.24617100	1.32652100
H	3.77162200	0.22407700	3.62418100
C	5.68843600	0.76950500	2.95948700
H	6.29799200	1.35796200	2.27743900
H	6.21524900	0.13162900	3.66295900

2.6.23. TS 2: AGE-Catalyst A- RS

O	0.02466600	0.06768100	0.06211600
O	0.03214600	0.14302900	2.92629200
C	0.86212300	0.21393900	3.97368100
C	0.61196200	2.67089300	4.25073000
O	-0.37702400	2.78832100	3.44113500
C	1.15085700	3.94072000	4.82437600
H	0.37030200	4.41409600	5.43162800
H	2.04179100	3.78484700	5.43311300
H	1.37389000	4.63257900	4.00529400
C	1.47405200	-1.06712800	4.43387600
H	0.70523800	-1.84339400	4.48804600
H	2.23082800	-1.40672900	3.72212600
H	1.94434900	-0.94881800	5.41050200
Al	-1.41321800	1.39993500	2.84588100
C	-2.81919100	0.80839000	4.04957500
H	-3.30579200	-0.07629800	3.61621100
H	-3.59939300	1.57732000	4.07871200
C	-2.34652000	0.47676000	5.48252500
H	-3.17900700	0.14456600	6.11255500
H	-1.59986400	-0.32676200	5.49507400
H	-1.89770500	1.34572800	5.97806300
C	1.58480400	-2.45185300	1.36400600
H	1.44199800	-3.10513600	2.23742200
H	1.33952000	-3.10486500	0.50936300
C	3.07048200	-2.05888300	1.24680400
H	3.72582900	-2.93642200	1.28068400
H	3.27891800	-1.54252500	0.30523400
H	3.40205200	-1.38644700	2.04894100
C	-1.74051000	-1.97518800	1.61024400
H	-2.55120300	-1.23145200	1.61006900
H	-1.96539800	-2.63961200	0.76157700
C	-1.83733600	-2.78873500	2.92234800
H	-1.69202800	-2.14859600	3.80129400
H	-2.81311800	-3.27322500	3.04220900
H	-1.08098900	-3.58106400	2.96418900
Al	0.06008700	-1.19872900	1.32991900
C	1.00882600	0.95297800	-0.47055800
C	1.94669600	1.43440700	0.64250800
C	1.74346800	0.29564100	-1.65230300
O	2.33403500	1.25078800	-2.51325800
H	0.50073800	1.84085100	-0.87105300
H	2.39062300	0.57001100	1.16193400
H	1.37518400	2.02218800	1.37641800
H	1.00566800	-0.25262600	-2.24646500
H	2.47884000	-0.43451600	-1.28237200
H	2.94670400	1.78572500	-1.98542800
C	1.15859700	1.41072500	4.60216200

H	1.88683500	1.38427800	5.40248300
C	-2.05384700	0.82499200	-0.51264000
C	-2.76201500	1.89029800	0.22015600
O	-1.68216100	1.84856900	1.14727200
H	-2.29435400	-0.21415000	-0.32947900
H	-2.77614600	2.86349700	-0.27878000
C	-4.13543000	1.56207000	0.77978700
H	-4.11251700	0.58686400	1.29124400
H	-4.84670900	1.49052800	-0.06078100
H	-1.43592200	1.05954800	-1.36813800
O	-4.47018000	2.61049700	1.65707000
C	-5.86378800	2.67870100	2.03195400
C	-6.28274900	1.58934700	2.97891600
H	-6.47383700	2.65428000	1.11521600
H	-5.98194400	3.66170500	2.49380100
H	-6.21997700	0.56541800	2.61160300
C	-6.75103900	1.81993200	4.20789100
H	-6.83949700	2.82966000	4.60305600
H	-7.07652400	1.01153900	4.85567000
O	2.96836300	2.22178100	0.05787100
C	3.89866200	2.75836100	1.00827600
C	5.01238400	3.43034900	0.26660300
H	4.29028800	1.93318300	1.62687500
H	3.38134900	3.46892900	1.67220900
H	5.57936000	2.79270600	-0.40992200
C	5.33029400	4.71854600	0.40889300
H	4.77318800	5.37428700	1.07458200
H	6.16092300	5.16232400	-0.13090300

2.6.24. TS 2: AGE-Catalyst A- SR

O	0.22568100	-0.18294700	0.08328800
O	-0.07212500	-0.14566400	2.92282100
C	0.77387200	-0.04409700	3.95865900
C	0.41773600	2.39619600	4.28067400
O	-0.54428200	2.49775500	3.43405400
C	0.87901100	3.66772100	4.91222600
H	1.12873100	4.38539000	4.12378900
H	0.04747500	4.09762600	5.48245200
H	1.73676700	3.52406500	5.56894500
C	1.47209800	-1.29299300	4.37748100
H	0.75077500	-2.11116600	4.45594100
H	2.21806700	-1.57957000	3.63104000
H	1.97555300	-1.15605300	5.33435500
Al	-1.51300300	1.09117800	2.77675500
C	-3.02857200	0.57318900	3.88236100
H	-3.59694400	-0.22273600	3.38417300
H	-3.71294800	1.43179000	3.93504100
C	-2.64567300	0.12180600	5.31098700
H	-3.53026600	-0.14488700	5.90087500
H	-1.99255600	-0.75891200	5.29829100
H	-2.11683600	0.90903600	5.86147700
C	1.31423400	-2.86812200	1.41007500
H	1.23293900	-3.39483900	2.37058800
H	0.93202800	-3.59537700	0.67397800
C	2.79623700	-2.58965400	1.08395700
H	3.40880000	-3.49710000	1.15105200
H	2.91569800	-2.19917100	0.06760800
H	3.24795700	-1.85161400	1.75907300
C	-1.95255000	-2.01216100	1.34470300
H	-2.68174500	-1.19179500	1.29275900
H	-2.11781000	-2.58230600	0.41674600
C	-2.30123800	-2.90892900	2.55501200
H	-2.19398300	-2.36631400	3.50148600
H	-3.33249400	-3.28056700	2.51493600
H	-1.64445600	-3.78515500	2.60939000
Al	-0.05625300	-1.44966700	1.30795300
C	1.46124200	0.44809100	-0.23531800
C	1.44823400	1.94232200	0.07774600
C	1.76846800	0.15950000	-1.71446200
O	2.90001300	0.87862100	-2.19812900
H	2.26477300	0.02298800	0.38307100
H	2.48273300	2.31397400	0.10869200
H	0.99167900	2.10784500	1.06202400
H	0.87365800	0.38248600	-2.30779500
H	1.99173600	-0.90437700	-1.83050500
H	2.62624500	1.79639700	-2.33828600
C	1.00727100	1.15199900	4.61323300
H	1.73331800	1.14155300	5.41496100
C	-1.75435100	0.84595600	-0.76573800
C	-2.75937100	1.42203100	0.14012300
O	-1.71302700	1.59512500	1.09192100
H	-1.74496200	-0.20470900	-1.02091400
H	-3.52248100	0.71356700	0.47514200
C	-3.40372900	2.75554600	-0.22688000
H	-4.14673000	2.60275700	-1.01755700
H	-2.63809800	3.44899500	-0.59351400
H	-1.05163800	1.51918400	-1.24857000
O	-4.05696000	3.24397000	0.93442800
C	-3.41827600	4.35811400	1.59082800
C	-3.85752600	5.66787300	0.99955200
H	-2.32800100	4.24083700	1.52830300
H	-3.70428600	4.29096900	2.64464400
H	-3.71426500	5.77801300	-0.07490200
C	-4.39480800	6.66595700	1.70632600
H	-4.55939700	6.57897300	2.77826400
H	-4.68440400	7.60304300	1.23999300
O	0.71932000	2.64366700	-0.93022600
C	0.65553400	4.05419900	-0.68667100
C	-0.10712400	4.70006600	-1.80345000
H	1.68207600	4.45427700	-0.64408500
H	0.17692500	4.24769600	0.28477700
H	0.18369600	4.39218000	-2.80713900
C	-1.05580700	5.62340600	-1.62642900
H	-1.35276000	5.95214100	-0.63331200
H	-1.55126600	6.09784900	-2.46813300

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