Structure–Reactivity Relationships in Lithiated Evans Enolates:
Influence of Aggregation and Solvation on the
Stereochemistry and Mechanism of Aldol Additions

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Part 2: Order of Aldehyde Addition

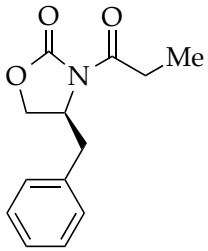
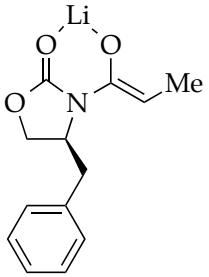
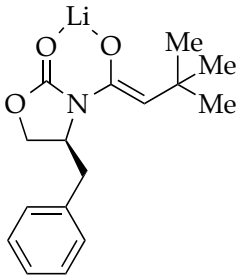
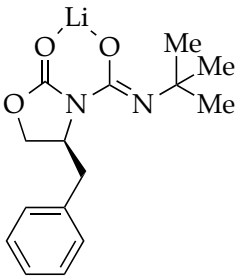
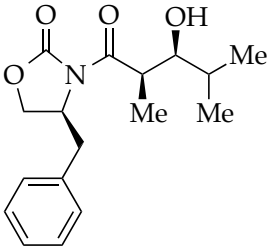
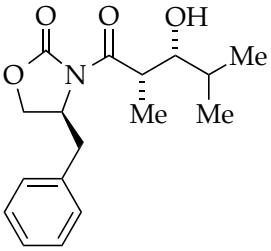
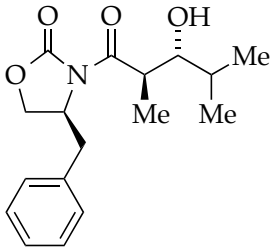
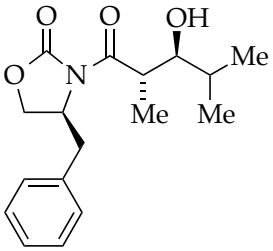
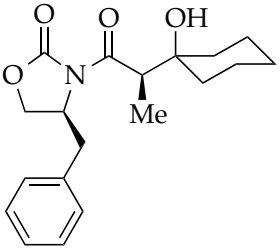
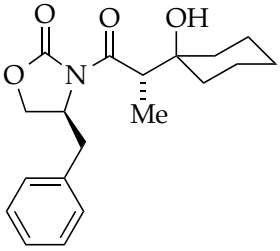
Part 3: Finding the Reactive Species of Enolate 5

Part 4: Ketone Aldol Kinetics

Part 5: Computations Overview of Enolate 5

Part 7: 5 Transition State Computations

Chart 1. Substrates

 **1**	 **5**	 **33**	 **34**
 (*R,S*)-**6**	 (*S,R*)-**6**	 (*R,R*)-**6**	 (*S,S*)-**6**
 (*R*)-**7**	 (*S*)-**7**		

Part 1: Aldol Products

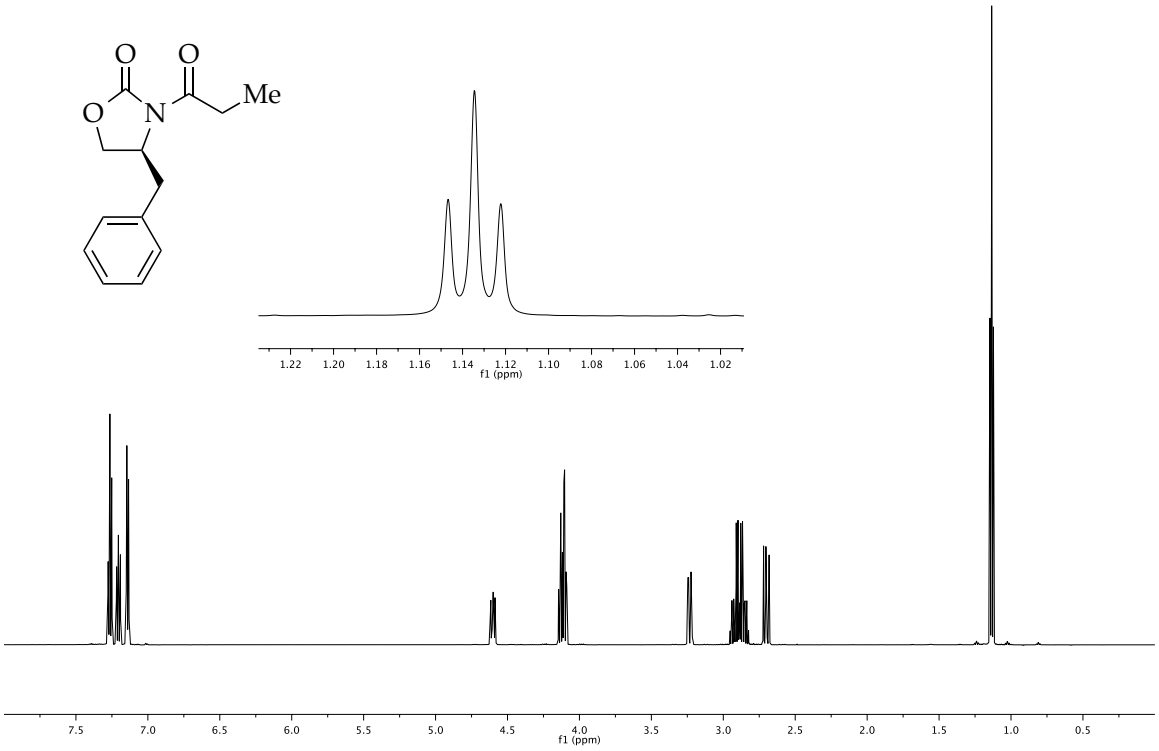


Figure 1. ^{1}H NMR spectrum of the **1** in $CDCl_3$ at 23 °C.

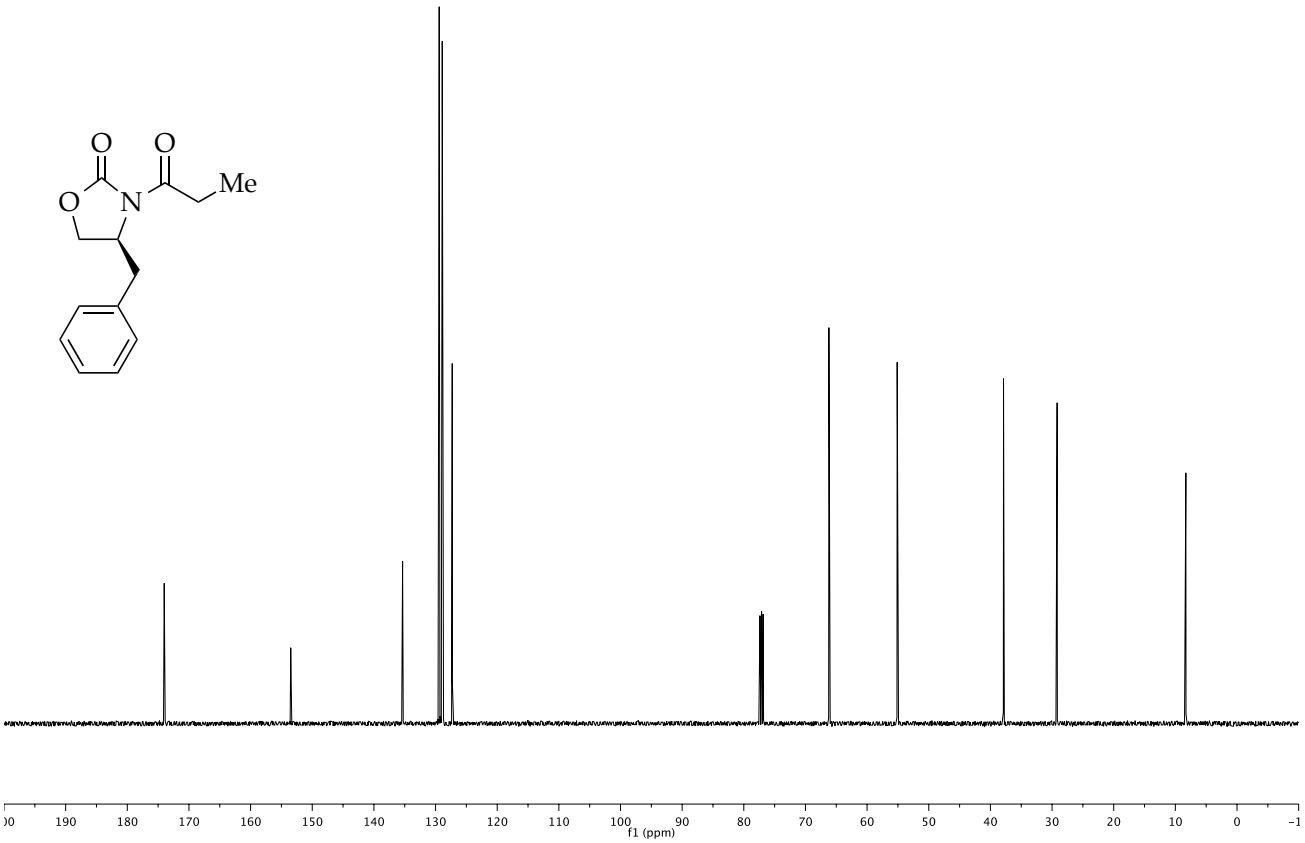


Figure 2. ^{13}C NMR spectrum of **1** in $CDCl_3$ at 23 °C.

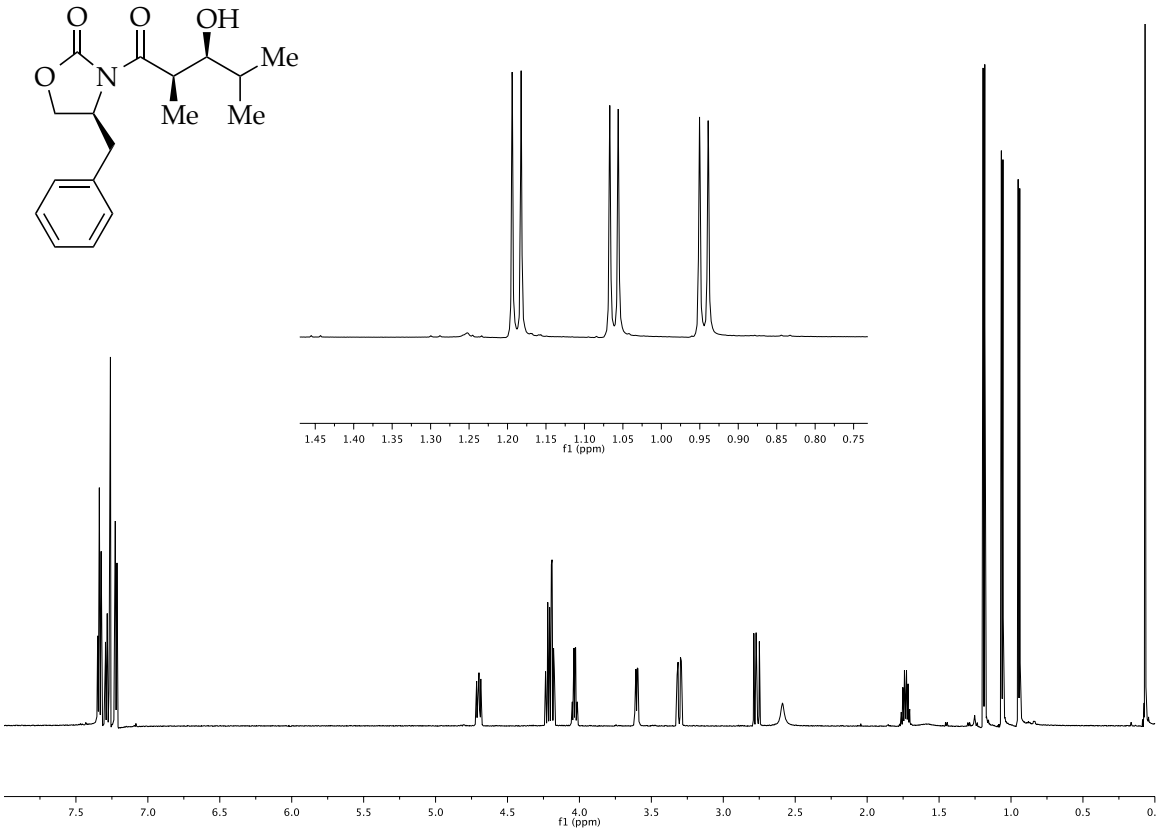


Figure 3. ^{1}H NMR spectrum of (*R,S*)-**6** aldol product in $CDCl_3$ at 23 °C.

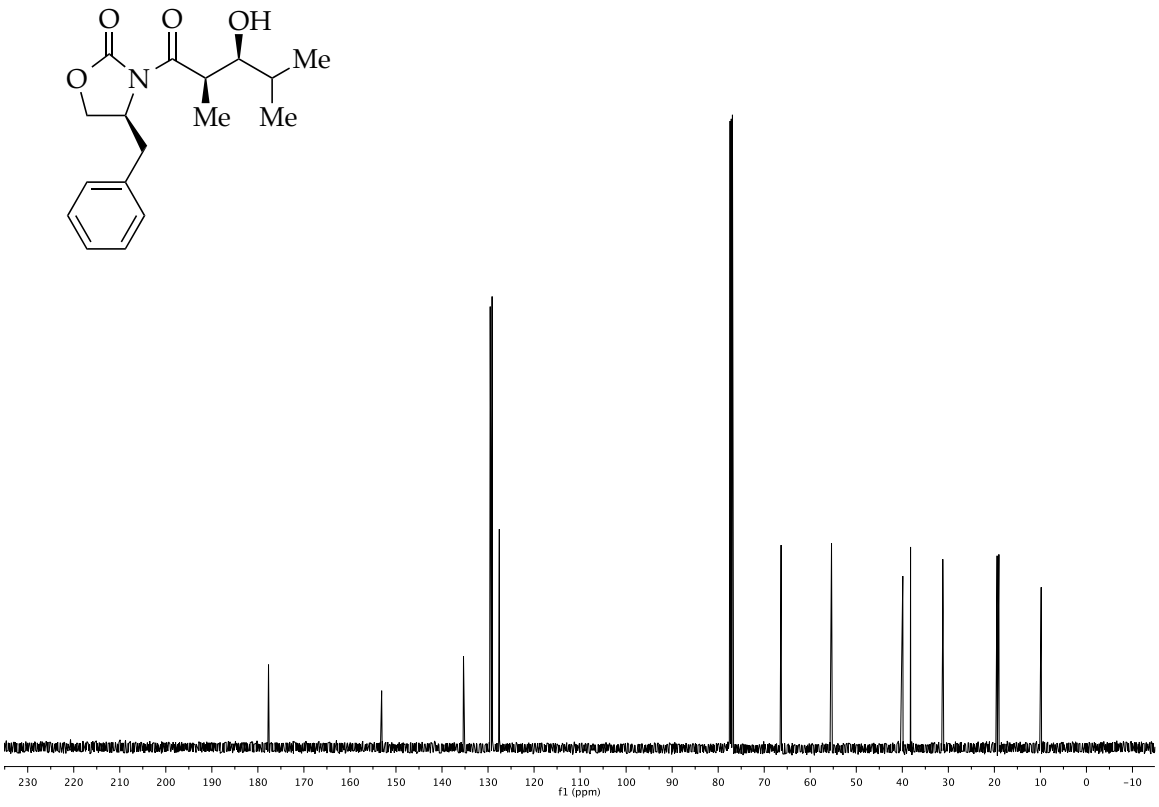


Figure 4. ^{13}C NMR spectrum of (*R,S*)-**6** aldol product in $CDCl_3$ at 23 °C.

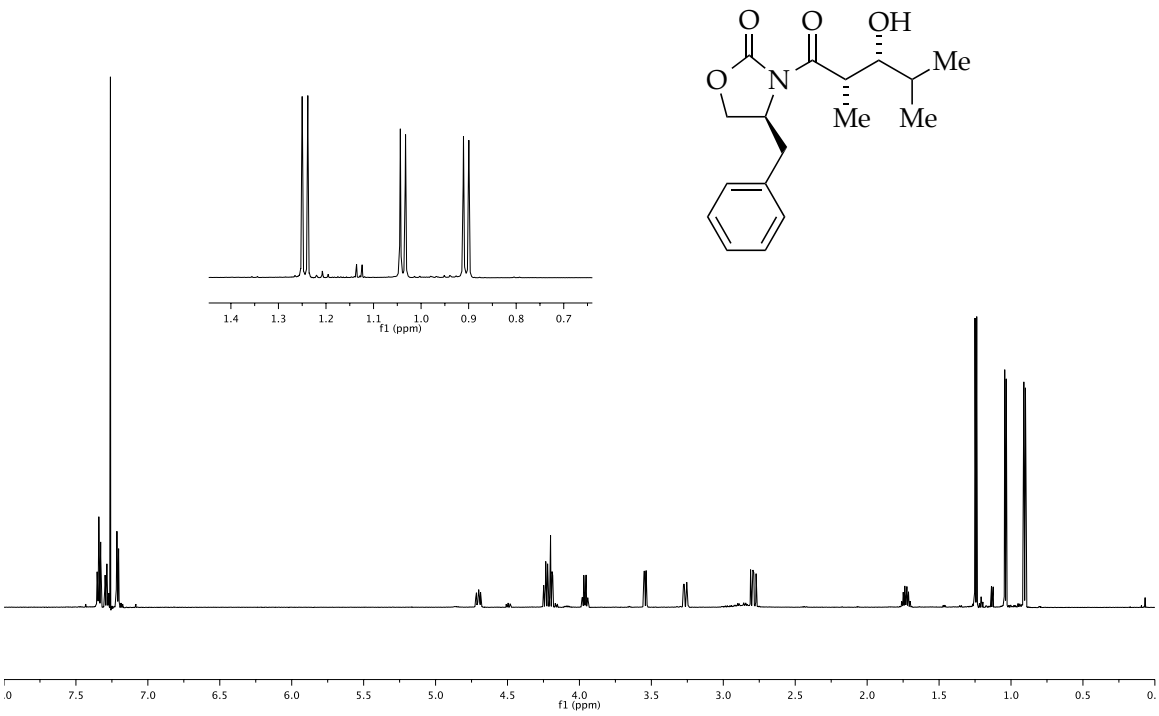


Figure 5. ^{1}H NMR spectrum of (*S,R*)-**6** aldol product in $CDCl_3$ at 23 °C.

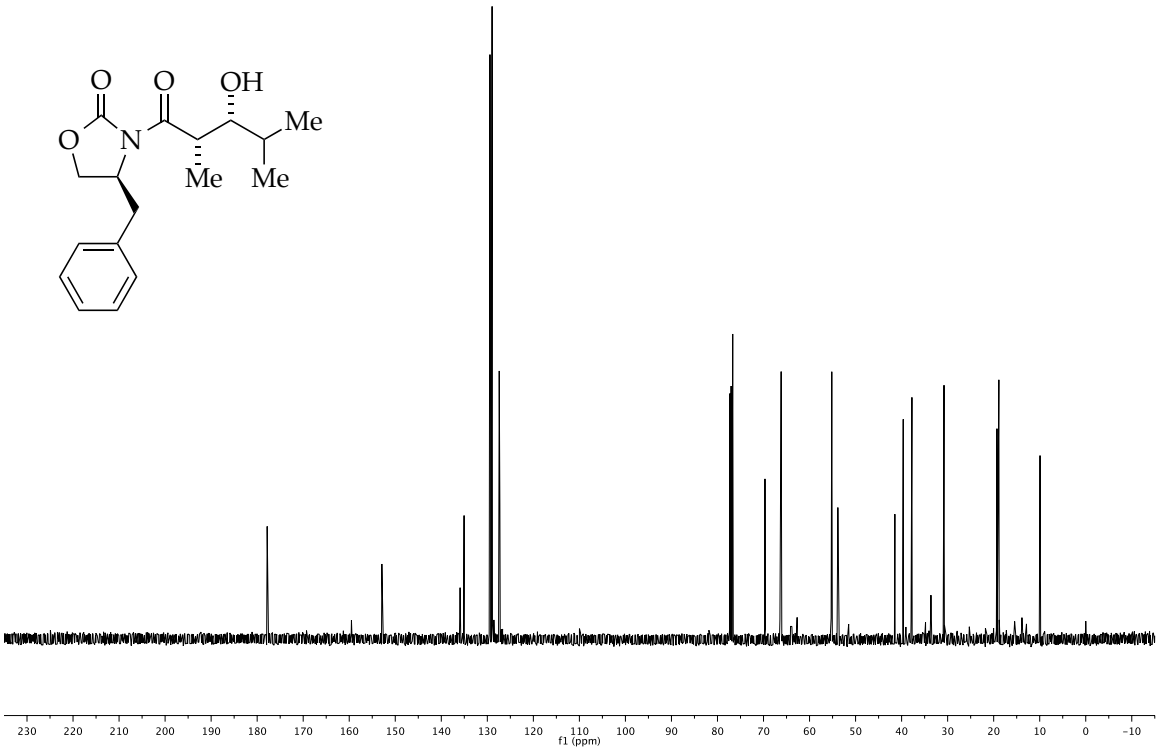


Figure 6. ^{13}C NMR spectrum of (*S*,*R*)-**6** aldol product in $CDCl_3$ at 23 °C.

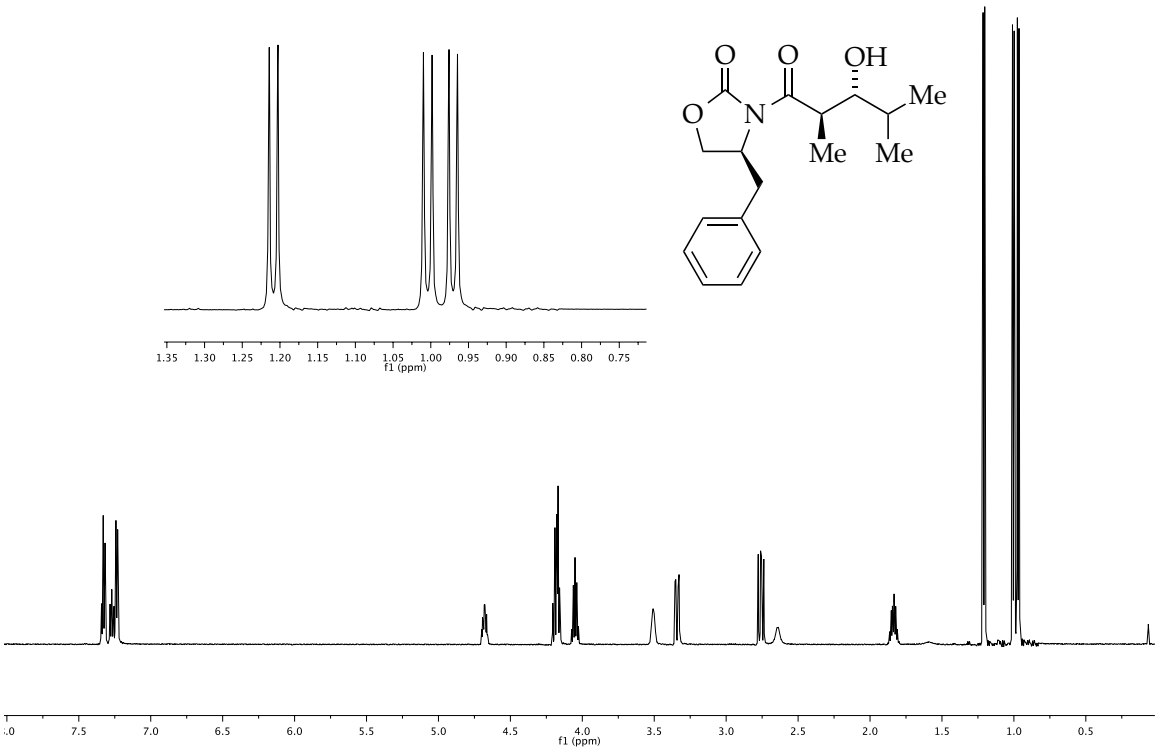


Figure 7. ^{1}H NMR spectrum of (*R,R*)-**6** aldol product in $CDCl_3$ at 23 °C.

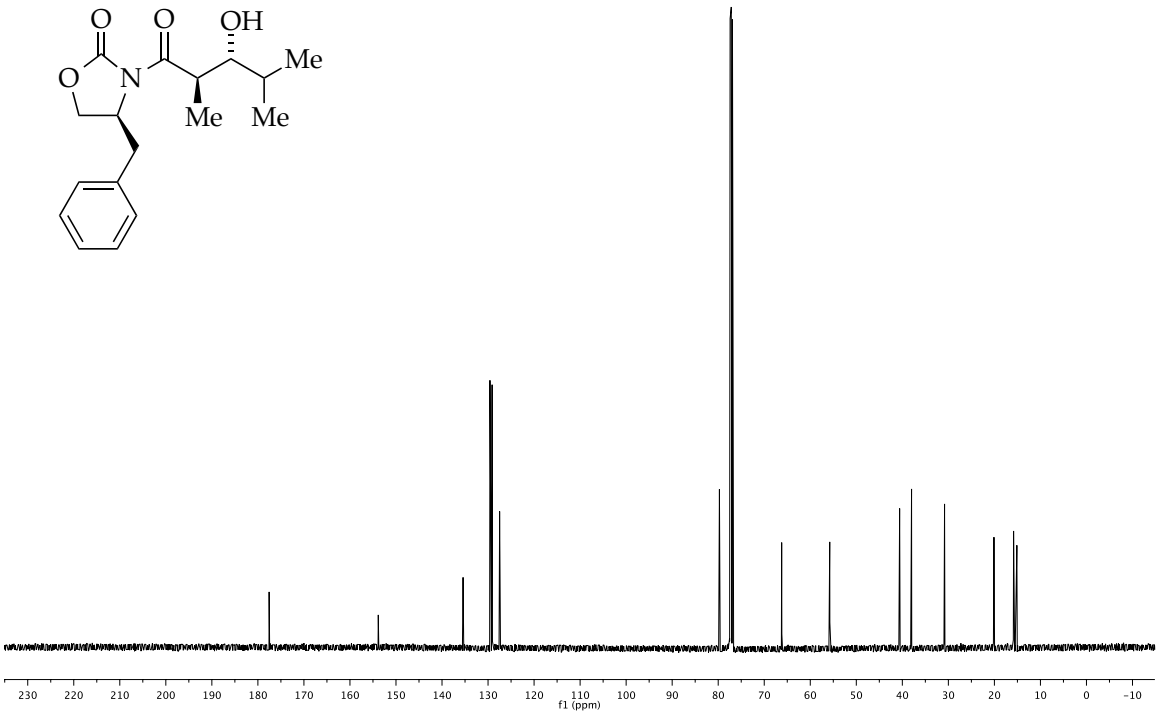


Figure 8. ^{13}C NMR spectrum of (*R,R*)-**6** aldol product in $CDCl_3$ at 23 °C.

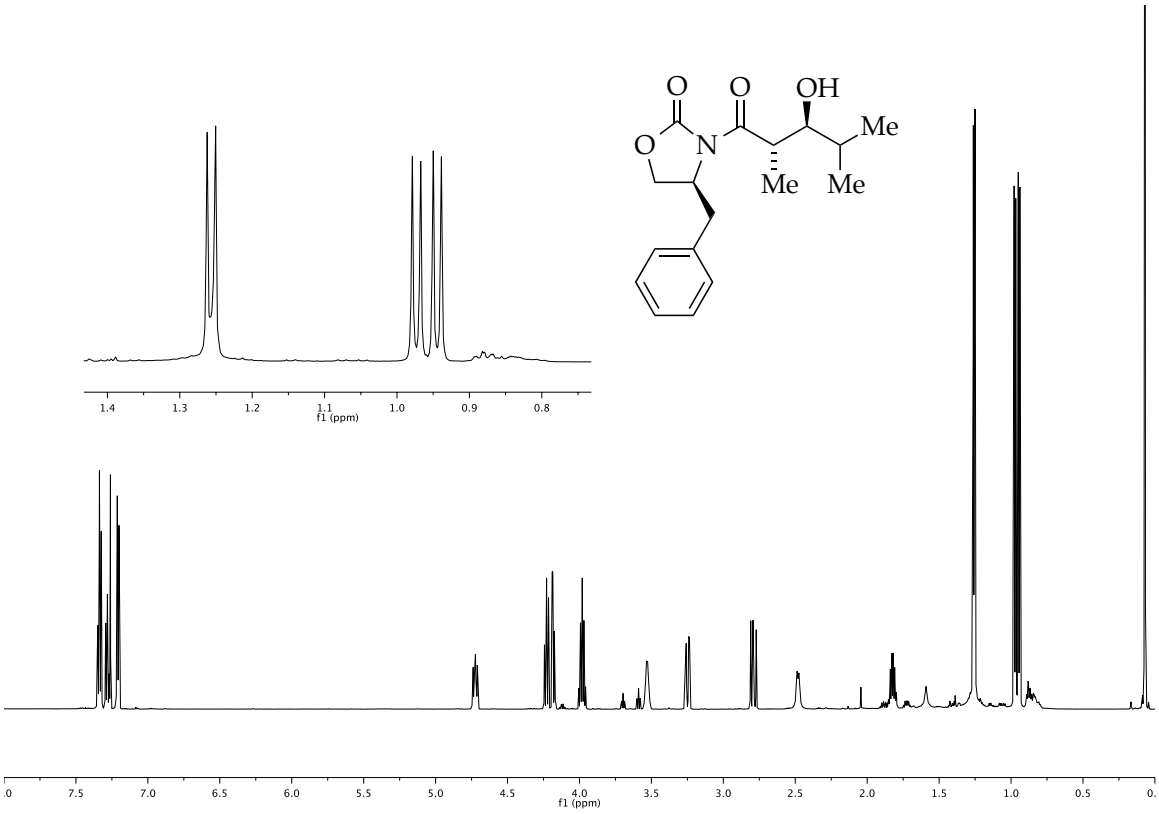


Figure 9. ^{1}H NMR spectrum of (*S,S*)-**6** aldol product in $CDCl_3$ at 23 °C.

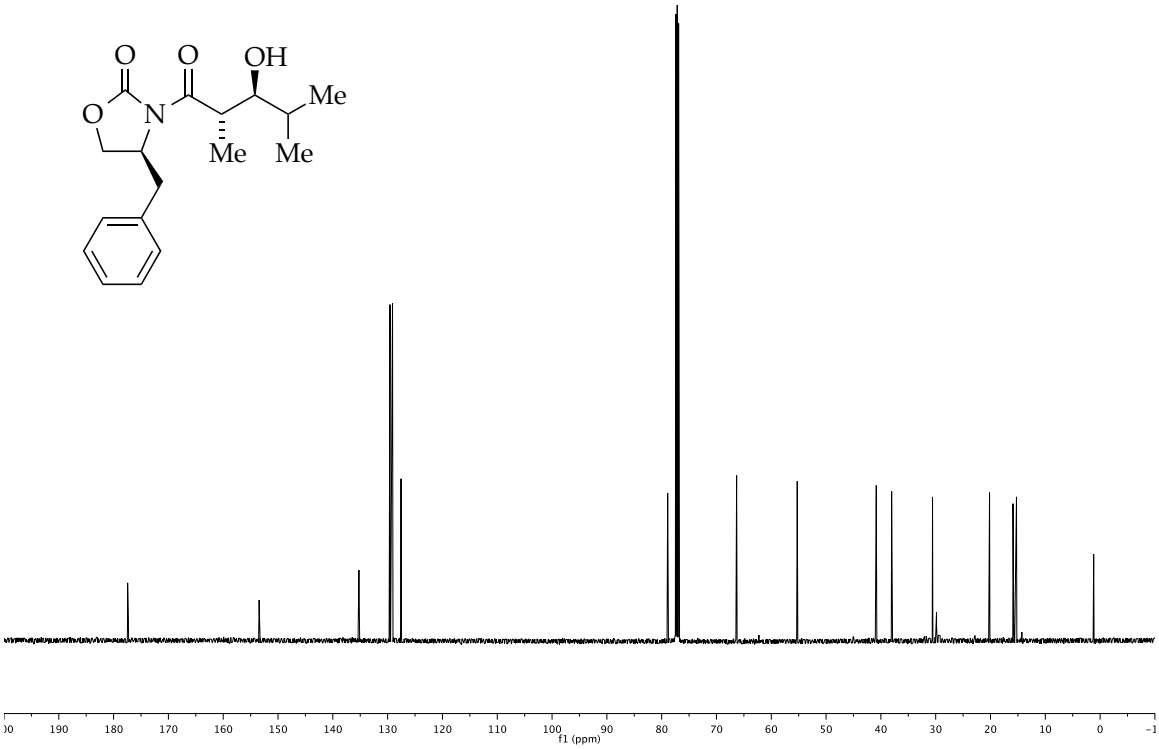


Figure 10. ^{13}C NMR spectrum of (*S,S*)-**6** aldol product in $CDCl_3$ at 23 °C.

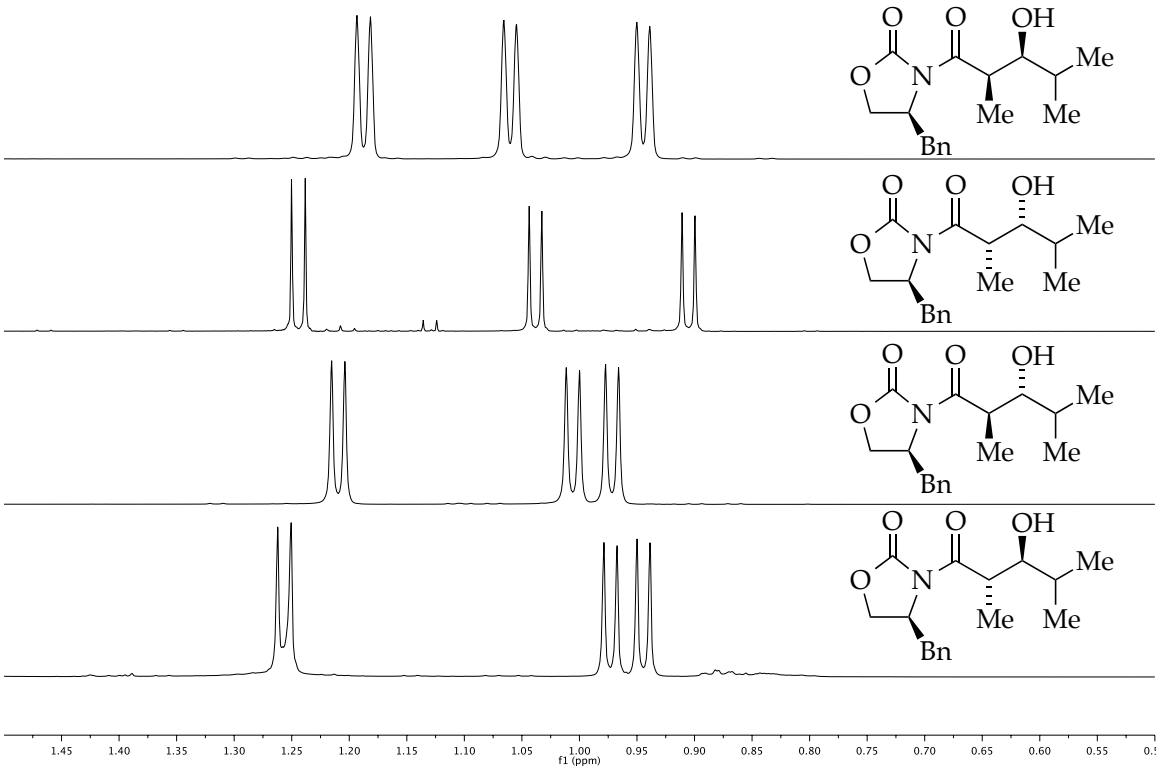


Figure 11. ^{1}H NMR spectrum of (*R,S*)-**6**, (*S,R*)-**6**, (*R,R*)-**6**, and (*S,S*)-**6** aldol products in $CDCl_3$ at 23 °C.

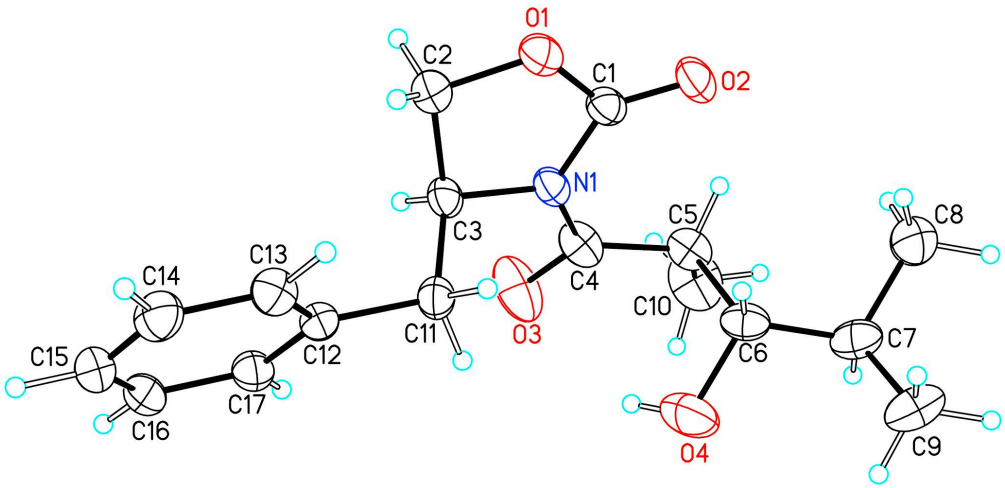


Figure 12. X-ray crystal structure of (*R*,*S*)-**6**.

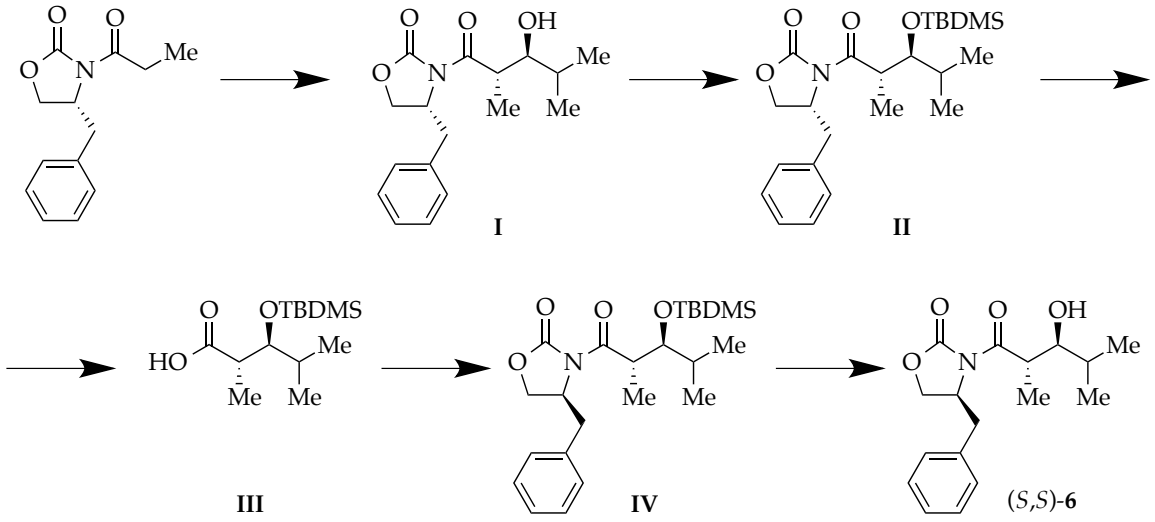
Table 1. Crystal data and structural refinement of recrystallized (*R,S*)-**6** aldol product

Empirical formula	C17 H23 N O4
Formula weight	305.36
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 11.4134(4) Å α= 90°.
	b = 6.2066(2) Å β= 103.613(2)°.
	c = 11.8551(4) Å γ = 90°.
Volume	816.20(5) Å 3
Z	2
Density (calculated)	1.243 Mg/m3
Absorption coefficient	0.088 mm-1
F(000)	328
Crystal size	0.50 x 0.20 x 0.10 mm3
Theta range for data collection	1.77 to 29.13°.
Index ranges	-14<=h<=15, -7<=k<=8, -16<=l<=13
Reflections collected	7975
Independent reflections	4023 [R(int) = 0.0222]
Completeness to theta = 29.13°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9912 and 0.9573
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	4023 / 1 / 276
Goodness-of-fit on F2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0941
R indices (all data)	R1 = 0.0466, wR2 = 0.1012
Absolute structure parameter	0.6(9)
Largest diff. peak and hole	0.166 and -0.173 e. Å -3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4766(1)	6317(2)	5459(1)	45(1)
O(2)	6528(1)	5057(2)	6463(1)	46(1)
O(3)	4191(1)	822(2)	7613(2)	68(1)
O(4)	5655(1)	3080(4)	9782(1)	76(1)
N(1)	4699(1)	3764(2)	6750(1)	33(1)
C(1)	5448(1)	5024(3)	6256(1)	35(1)
C(2)	3515(1)	5669(4)	5245(1)	49(1)
C(3)	3429(1)	4370(3)	6304(1)	34(1)
C(4)	4998(1)	1993(2)	7491(1)	41(1)
C(5)	6295(1)	1705(2)	8148(1)	38(1)
C(6)	6555(1)	3363(3)	9138(1)	41(1)
C(7)	7817(2)	3212(3)	9932(1)	49(1)
C(8)	8794(2)	3249(5)	9257(2)	64(1)
C(9)	8036(2)	5042(5)	10813(2)	66(1)
C(10)	6501(2)	-620(3)	8565(2)	67(1)
C(11)	2983(1)	5632(3)	7228(1)	35(1)
C(12)	1646(1)	6115(3)	6861(1)	32(1)
C(13)	1228(1)	8089(3)	6383(1)	39(1)
C(14)	-2(1)	8524(3)	6060(1)	45(1)
C(15)	-819(1)	6976(3)	6212(1)	45(1)
C(16)	-416(1)	4992(3)	6668(1)	44(1)
C(17)	812(1)	4568(3)	6993(1)	38(1)

Figure 13. Synthesis of (*S*,*S*)-6



(*R*)-4-benzyl-3-((2*S*,3*S*)-3-hydroxy-2,4-dimethylpentanoyl)oxazolidin-2-one (I). Following a procedure from Evans *et al.* (*JACS* **2001**, *123*, 10840) to a solution of titanium(IV) chloride (2.10 mL of 1.0 M solution in CH_2Cl_2, 2.10 mmol) at 0 °C was added titanium(IV) isopropoxide (215 μL, 0.706 mmol) in 9.4 mL CH_2Cl_2. After 5 min (R)-4-benzyl-3-propionyl-2-oxazolidinone (500 mg, 2.14 mmol) in 2.0 mL CH_2Cl_2 was added. After 5 min diisopropylethylamine (500 μL, 2.83 mmol) was added, and the resulting deep red solution was stirred for 1 h at 0 °C to insure the complete conversion to the titanium enolate. In a separate flask, freshly distilled isobutyraldehyde (430 μL, 4.71 mmol) was added to a solution of diethylaluminum chloride (5.9 mL of 1 M solution in hexanes, 5.90 mmol) in 2.0 mL of CH_2Cl_2 at -78 °C. After 15 min the enolate solution was cooled to -78 °C, and the aldehyde solution was added *via* cannula. After 1.5 h the reaction was quenched at -78 °C with 2.0 mL sat. aqueous NH_4Cl. 40 mL of 3.0 M aqueous HCl was added to dissolve the aluminum salts. The aqueous layer was extracted three times with CH_2Cl_2. The combined layers were washed with sat. aqueous $NaHCO_3$, dried over $MgSO_4$, filtered, and concentrated. The product was

purified by flash chromatography (15% EtOAc/hexanes), affording 290 mg (44% yield) of a white crystalline solid showing spectral data as described in the main text.

(*R*)-4-benzyl-3-((2*S*,3*S*)-3-((*tert*-butyldimethylsilyl)oxy)-2,4-dimethylpentanoyl)oxazolidin-2-one (II). To a solution of **I** (250 mg, 0.82 mmol) in 3.5 mL freshly distilled THF at 0 °C was added freshly distilled 2,6-lutidine (114 μL, 0.98 mmol) and *tert*-butyldimethylsilyl trifluoromethanesulfonate (207 μL, 0.90 mmol). After 30 min at 0 °C the reaction was quenched by addition of 0.2 mL MeOH. After an additional 5 min the reaction was washed with a solution of $NaHSO_4$ (5.0 mL) and sat. aqueous $NaHCO_3$ (5 mL). The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure. The product was purified by flash chromatography (10% EtOAc/hexanes) to provide affording 295 mg (86% yield) of product **II** as white crystalline solid. ^{1}H NMR (600 MHz; $CDCl_3$): δ 7.34 (dd, *J* = 8.0, 6.7 Hz, 2H), 7.30 – 7.21 (m, 3H), 4.67 (ddt, *J* = 10.7, 7.1, 3.6 Hz, 1H), 4.17 – 4.10 (m, 2H), 4.09 – 4.01 (m, 2H), 3.44 (dd, *J* = 13.3, 3.5 Hz, 1H), 2.63 (dd, *J* = 13.2, 10.4 Hz, 1H), 1.81 (heptd, *J* = 6.9, 2.5 Hz, 1H), 1.16 (d, *J* = 6.7 Hz, 3H), 0.97 (d, *J* = 7.0 Hz, 3H), 0.95 (d, *J* = 6.7 Hz, 4H), 0.90 (s, 9H), 0.11 (s, 3H), 0.09 (s, 3H). ^{13}C NMR (151 MHz, CDCl3) δ 175.7, 153.2, 135.7, 129.5, 129.1, 127.4, 76.5, 66.1, 55.9, 43.9, 38.6, 31.3, 26.3, 20.9, 18.6, 16.9, 13.6, -3.8, -4.3. HRMS *m*/*z* calculated for $C_{23}H_{38}NO_4Si$ $(M+H)^+$ 420.25646, found 420.25482.

(2*S*,3*S*)-3-((*tert*-butyldimethylsilyl)oxy)-2,4-dimethylpentanoic acid (III). To a solution of **II** (200 mg, 0.48 mmol) in 6.0 mL of a 5:1 THF/water mixture was added 0.80 M aqueous LiOH (0.90 mL, 0.72 mmol) at 0 °C, followed by 30% aq.

H_2O_2 (250 μL, 2.2 mmol), which was added dropwise. The reaction was monitored by TLC (*p*-anisaldehyde stain) and quenched after stirring the mixture 1 h at 0 °C. The reaction was quenched by addition of 1.33 M Na_2SO_3 and saturated aqueous NH_4Cl. The resulting mixture was extracted with ether and the combined organic extracts were dried over $MgSO_4$. The concentrated mixture was purified by flash chromatography (CH_2Cl_2 90%, MeOH 10%). affording 45 mg (36%) of product **III** as a colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 11.09 (s, 1H), 3.69 (t, *J* = 4.4 Hz, 1H), 2.66 (qd, *J* = 7.3, 4.1 Hz, 1H), 1.85 (heptd, *J* = 6.9, 4.7 Hz, 1H), 1.23 (d, *J* = 7.3 Hz, 3H), 0.93-0.90 (m, 14H), 0.12 (s, 3H), 0.10 (s, 3H). ^{13}C NMR (151 MHz, CDCl3) δ 178.9, 79.7, 43.0, 32.6, 26.1, 18.4, 18.2, 15.5, -4.0, -4.3. HRMS *m*/*z* calcd for $C_{13}H_{29}O_3Si$ $(M+H)^+$ 261.18805, found 261.18793. HRMS *m*/*z* calculated for $C_{13}H_{27}O_3Si$ $(M-H)^-$ 259.17240, found 259.17311.

(*S*)-4-benzyl-3-((2*S*,3*S*)-3-((*tert*-butyldimethylsilyl)oxy)-2,4-dimethylpentanoyl)oxazolidin-2-one (IV). To a solution of **III** (38 mg, 0.15 mmol) in 2.0 mL benzene was added DMF (34 μL, 0.44 mmol). Oxalyl chloride (39 μL, 45 mmol) was then added dropwise to the solution, and the reaction mixture was stirred for 2 h at room temperature. The solvent was then evaporated, and the resulting acid chloride was used directly in the next step. 1.6 M *n*-BuLi in hexanes (95 μL, 0.15 mmol) was added dropwise to a solution of (*S*)-4-benzyl-3-propionyloxazolidin-2-one (27 mg, 0.15 mmol) in 1.0 mL freshly distilled THF under inert atmosphere at -78 °C. A solution of the freshly prepared acid chloride in 0.50 mL THF was then added dropwise at -78 °C. The resulting mixture was stirred for 30 min at -78 °C and then allowed to warm to room temperature over 1 h. Following quenching with saturated aqueous NH_4Cl

(1 mL) and water, the resulting mixture was extracted with EtOAc and the organic extracts were combined and dried over $MgSO_4$. The concentrated mixture was purified by flash chromatography (10% EtOAc/hexanes), affording 34 mg (56% yield) of product **IV** as a white crystalline solid. ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.39 – 7.23 (m, 5H), 4.69 (ddd, *J* = 10.0, 6.7, 3.3 Hz, 1H), 4.24 – 4.08 (m, 3H), 3.99 (dd, *J* = 9.0, 1.8 Hz, 1H), 3.26 (dd, *J* = 13.4, 3.3 Hz, 1H), 2.81 (dd, *J* = 13.4, 9.5 Hz, 1H), 1.88 (heptd, *J* = 8.1, 7.0, 2.7 Hz, 1H), 1.16 (d, *J* = 6.9 Hz, 3H), 1.02 (d, *J* = 6.9 Hz, 3H), 0.94 (d, *J* = 6.8 Hz, 3H), 0.88 (s, 9H), 0.12 (s, 3H), 0.00 (s, 3H). ^{13}C NMR (126 MHz, CDCl3): δ 176.5, 153.0, 135.5, 129.6, 129.1, 127.5, 78.4, 65.9, 55.5, 42.4, 37.9, 30.6, 26.2, 20.5, 18.6, 15.4, 14.9, -4.1, -4.2. HRMS *m*/*z* calcd for $C_{23}H_{38}NO_4Si$ $(M+H)^+$ 420.25646, found 420.25576.

(*S*)-4-benzyl-3-((2*S*,3*S*)-3-hydroxy-2,4-dimethylpentanoyl)oxazolidin-2-one [**(*S*,*S*)-6**] To a solution of **IV** (34 mg, 81 μmol) in 3 mL of THF was added 1.0 mL of concentrated HCl. The solution was stirred for 5 min. The resulting mixture was diluted with ether, extracted, and dried over $MgSO_4$. The concentrated mixture was purified by flash chromatography (30% EtOAc/hexanes), affording 14 mg (57% yield) of [(*S*,*S*)-**6**] was obtained as a white crystalline solid. ^{1}H NMR (600 MHz; $CDCl_3$): δ 7.36 – 7.26 (m, 3H), 7.22 – 7.19 (m, 2H), 4.72 (ddt, *J* = 9.3, 7.7, 3.1 Hz, 1H), 4.26 – 4.16 (m, 2H), 3.98 (p, *J* = 7.0 Hz, 1H), 3.53 (q, *J* = 6.2 Hz, 1H), 3.25 (dd, *J* = 13.4, 3.4 Hz, 1H), 2.79 (dd, *J* = 13.4, 9.4 Hz, 1H), 2.51 – 2.44 (m, 1H), 1.82 (pd, *J* = 6.8, 4.6 Hz, 1H), 1.26 (d, *J* = 6.9 Hz, 3H), 0.97 (d, *J* = 6.9 Hz, 3H), 0.94 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.4, 153.5, 135.2, 129.6, 129.1, 127.6, 78.9, 66.3, 55.3, 40.8, 38.0, 30.6, 20.2, 15.9, 15.3. HRMS *m*/*z* calcd for $C_{17}H_{24}NO_4$ $(M+H)^+$ 306.16998, found 306.16913.

Part 2: Order of Aldehyde Addition

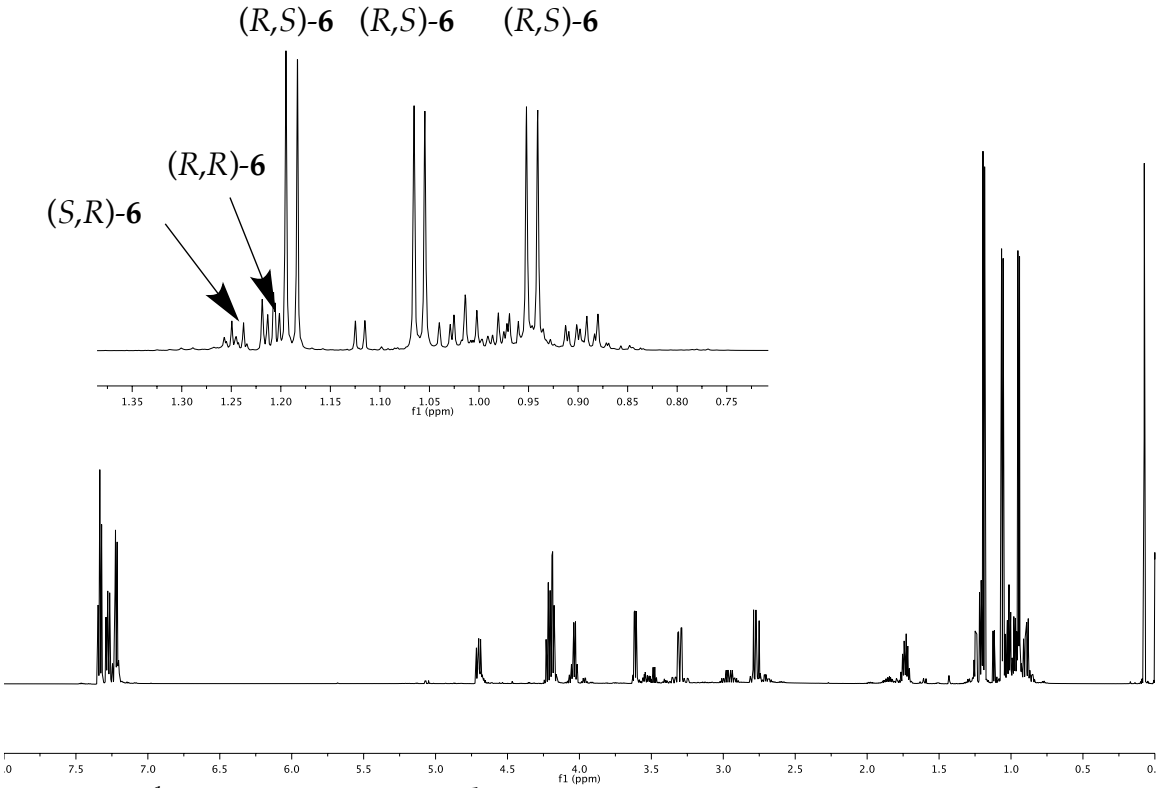


Figure 14. ^{1}H NMR spectrum of the aldol between enolate **5** and isobutyrlaldehyde. The major product, (*R*,*S*)-**6**, and the two minor products (*S*,*R*)-**6** and (*R*,*R*)-**6** are highlighted.

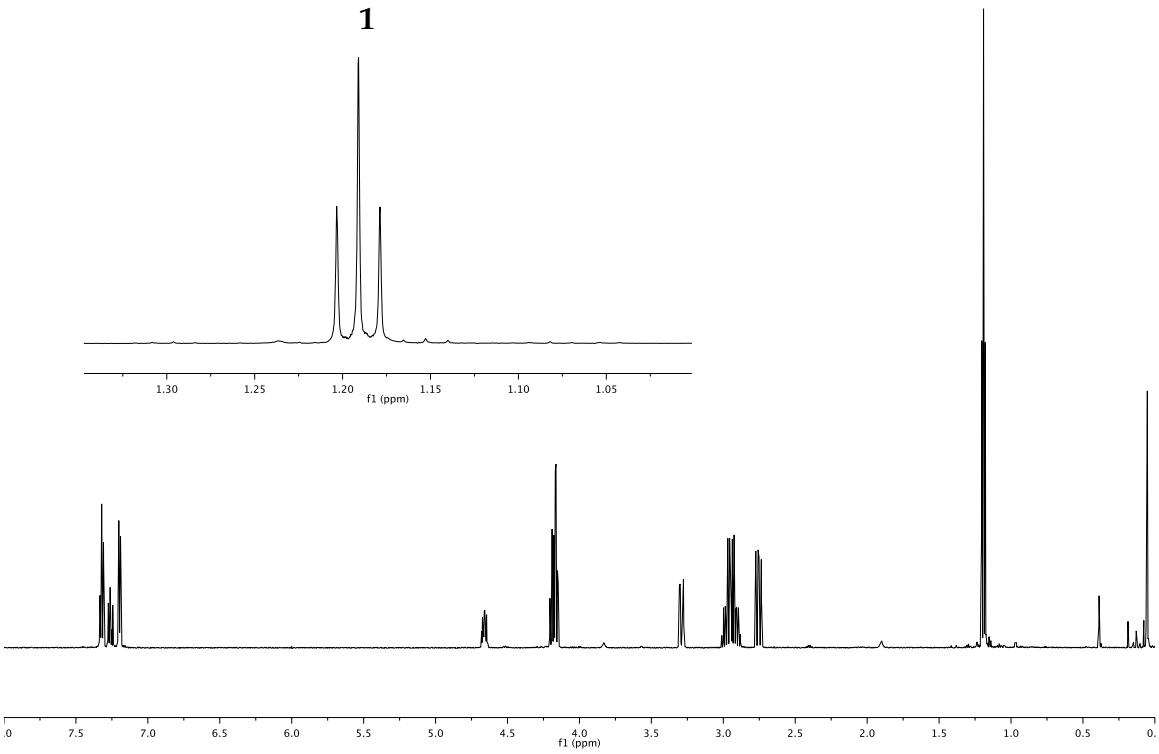


Figure 15. ^{1}H NMR spectrum of the aldol reaction between enolate **5** and isobutyraldehyde, pre-mixing LDA and aldehyde before adding the oxazolidinone **1**. Due to pre-reacting with the aldehyde, no LDA is available to lithiate **1**, so upon quench and workup only unreacted **1** is recovered.

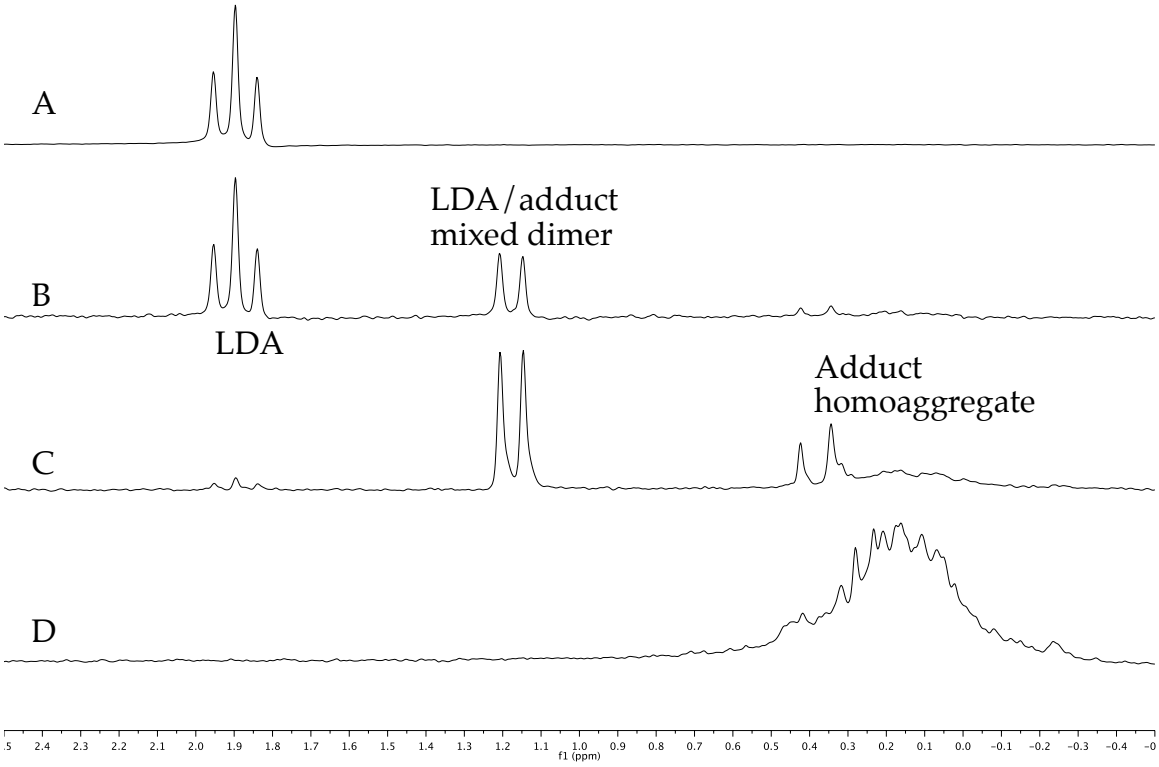


Figure 16. ^{6}Li NMR spectra of 0.10 M [^{6}Li^{15}N]LDA with varying equiv of isobutyraldehyde: A) 0.0 equiv; B) 0.50 equiv; C) 1.0 equiv; D) 2.0 equiv. The isobutyraldehyde first forms a 1,2-mixed adduct/LDA dimer before forming an undecipherable oligomer that is presumably a laddered 1,2-adduct homoaggregate.

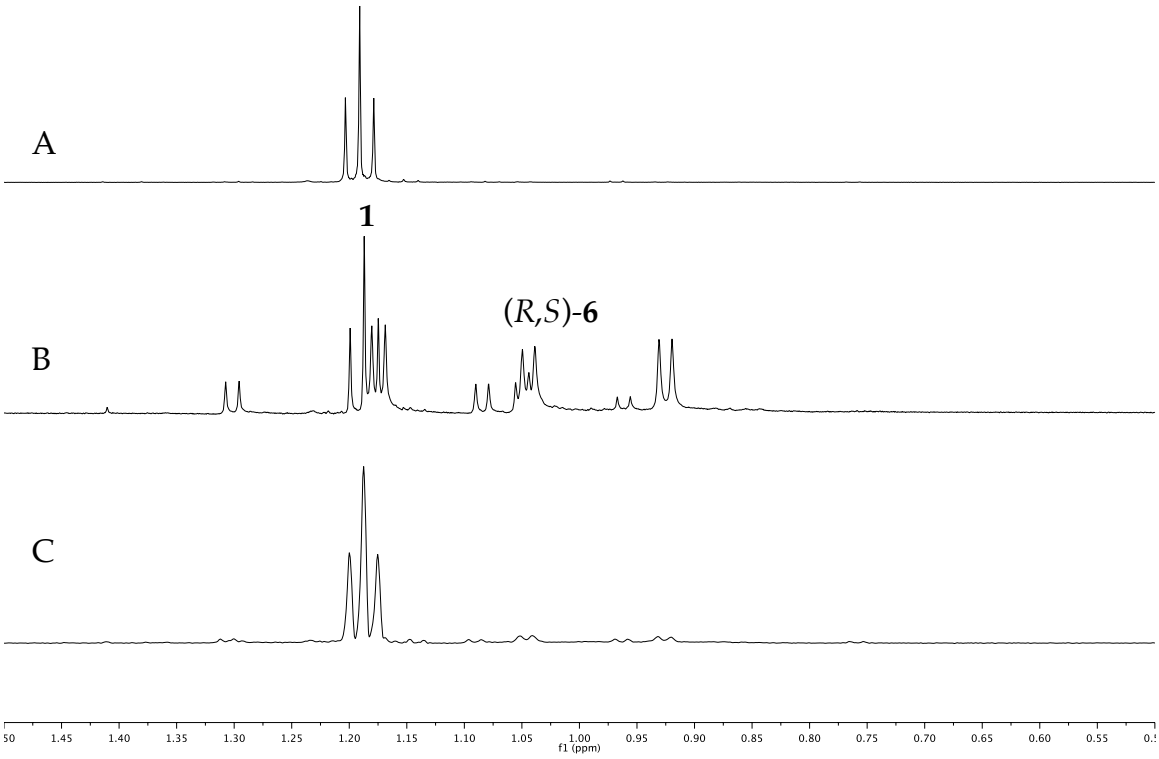


Figure 17. A) ^{1}H NMR spectrum of 1.0 equiv LDA treated sequentially with 0.50 equiv isobutyraldehyde and 1.0 equiv of oxazolidinone **1** followed by standard workup. Owing to the aldehyde pre-reacting with the LDA, it is inaccessible to the 0.50 equiv of **5** formed by the 0.50 equiv LDA remaining and 1.0 equiv of **1**. This resulted in only unreacted starting material being recovered. B) ^{1}H NMR spectrum of 1.0 equiv LDA, then add 0.50 equiv isobutyraldehyde, then 1.0 equiv of oxazolidinone **1**, then add 1.50 equiv isobutyraldehyde, followed by standard workup. As in A, 0.50 equiv of **5** is produced but the subsequent addition of excess isobutyraldehyde uses this to react and form **6** in approximately the same diasteriomeric ratio as previously seen. C) ^{1}H NMR spectrum of 1.0 equiv LDA, then add 2.0 equiv isobutyraldehyde, then 1.0 equiv of oxazolidinone **1**, followed by standard workup. The isobutyraldehyde has consumed all of the LDA, leaving none for the enolization of **1**, resulting in no aldol reaction.

Part 3: Finding the Reactive Species of Enolate 5

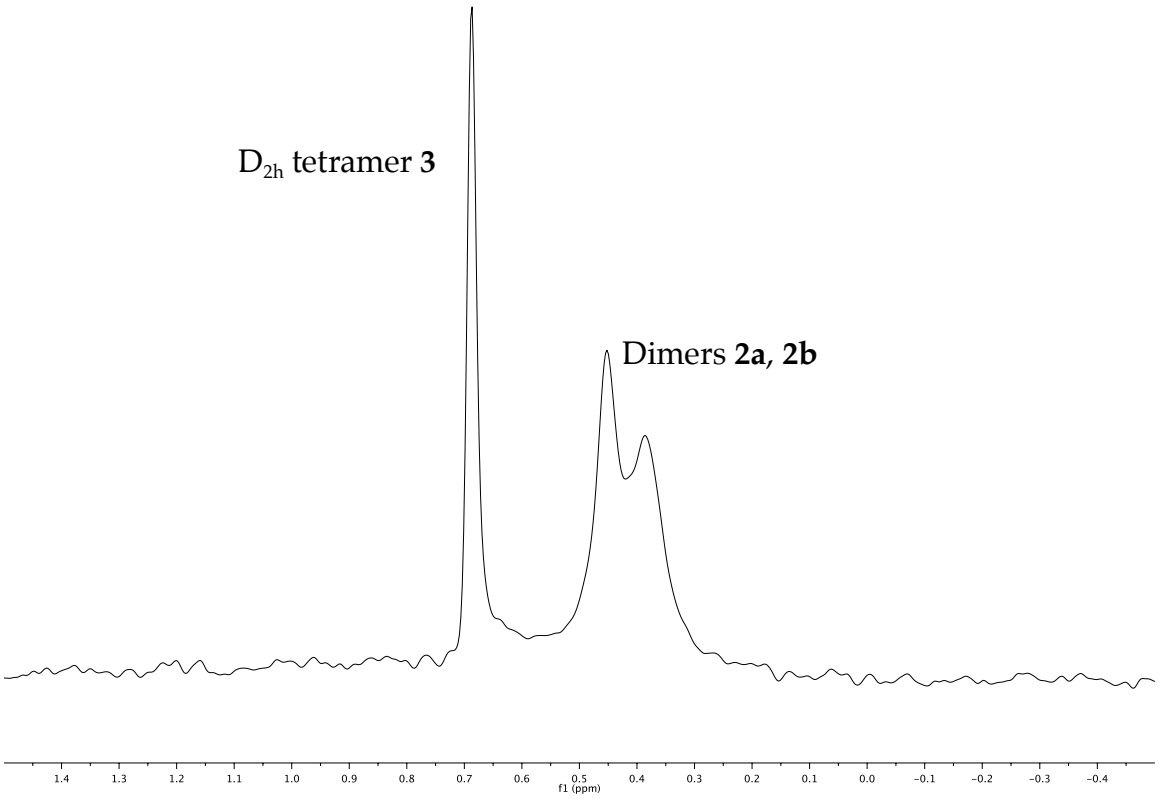


Figure 18. ^{6}Li NMR spectrum of 0.10 M enolate **5** in THF previously aged at 0 °C and recorded at -80 °C.

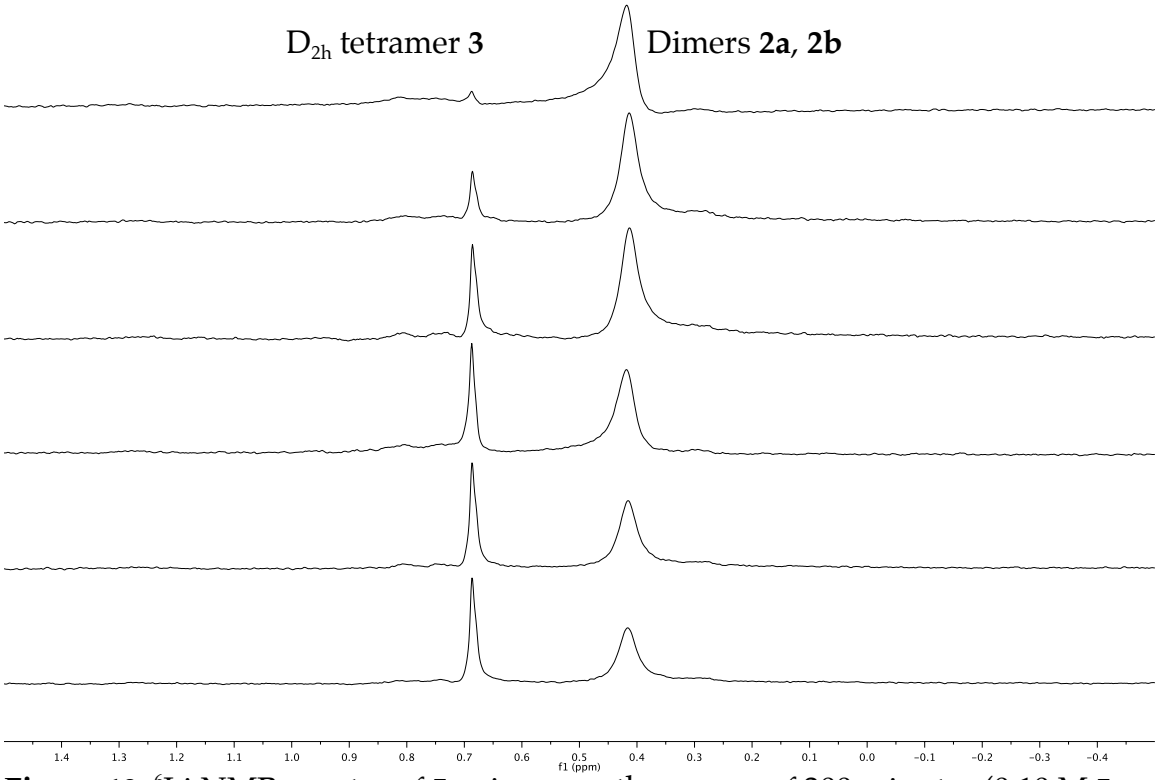


Figure 19. ^{6}Li NMR spectra of **5** aging over the course of 200 minutes (0.10 M **5**, THF, -60 °C)

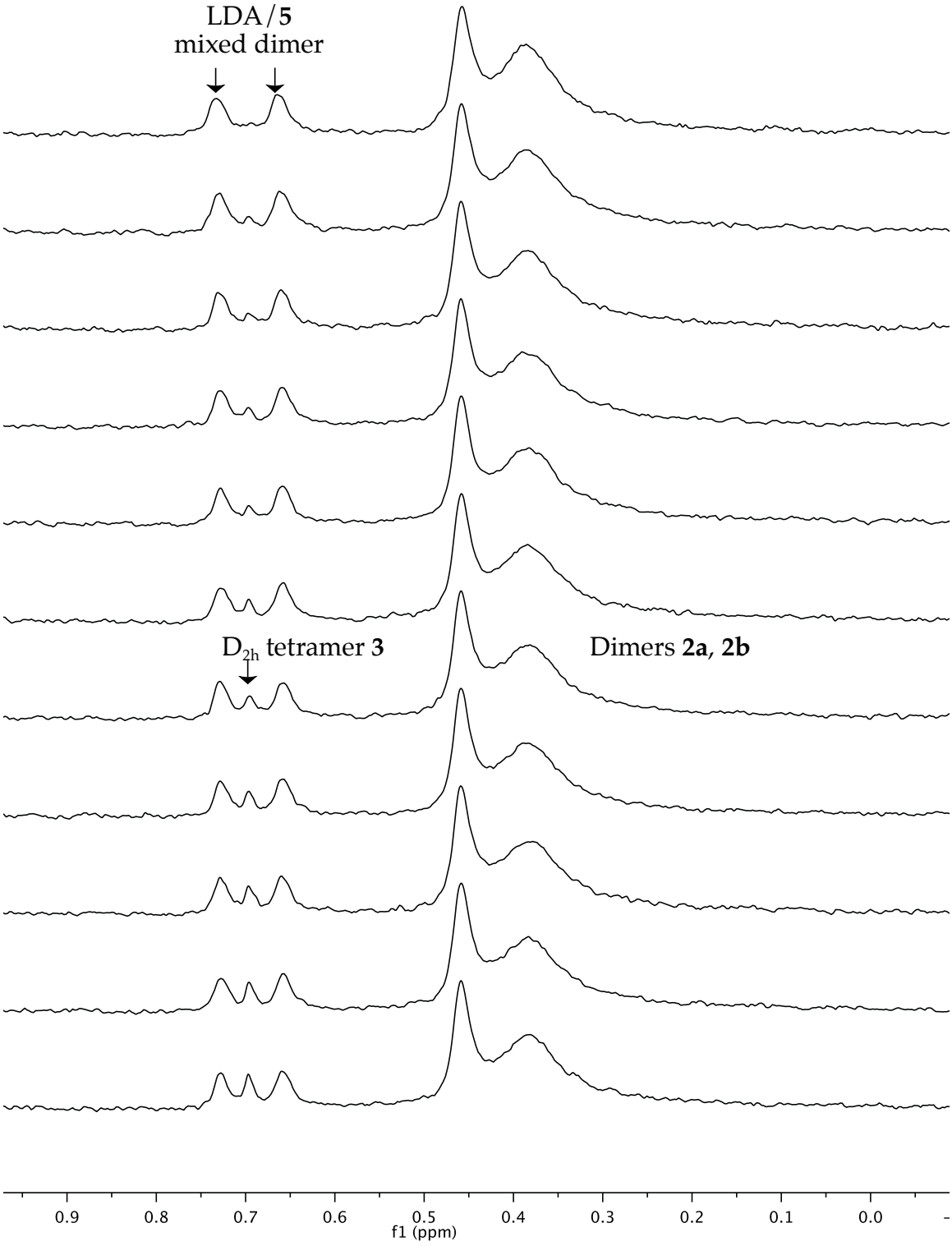


Figure 20. ^{6}Li NMR spectra of enolate **5** aging over the course of 388 minutes (0.10 M **5**, 0.010 M excess [^{6}Li^{15}N]LDA, THF, -80 °C)

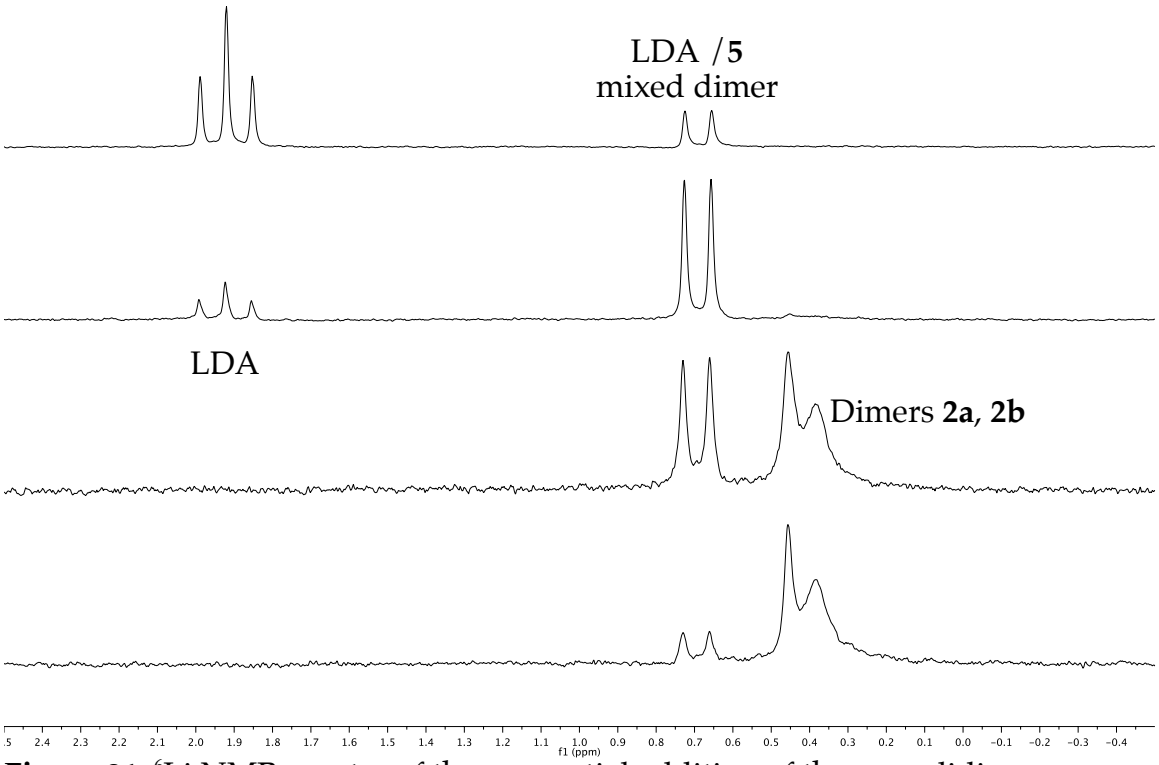


Figure 21. ^{6}Li NMR spectra of the sequential addition of the oxazolidinone precursor of **5** to [^{6}Li^{15}N]LDA, (0.16, 0.50, 0.84, 1.0 eq of the oxazolidinone of **5**, 0.10 M [^{6}Li^{15}N]LDA, THF, -60 °C)

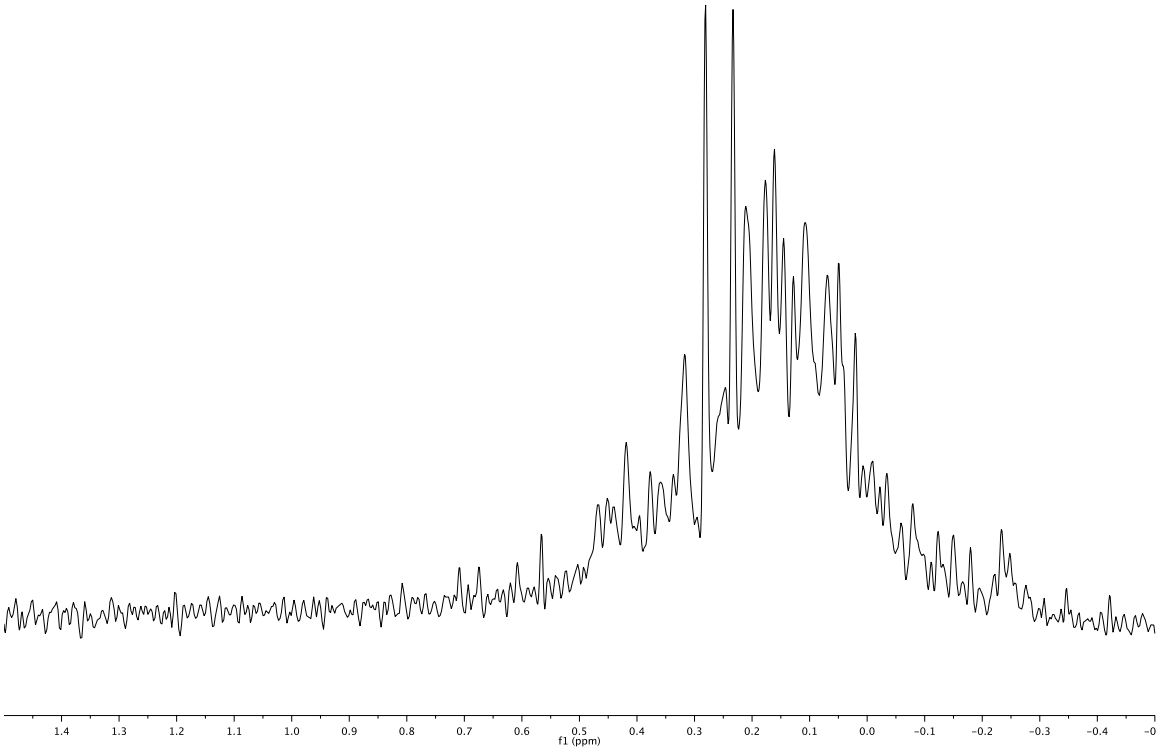


Figure 22. ^{6}Li NMR spectrum of (*R*,*S*)-**6** (0.10 M **5**, 0.20 M isobutyraldehyde, THF, -80 °C)

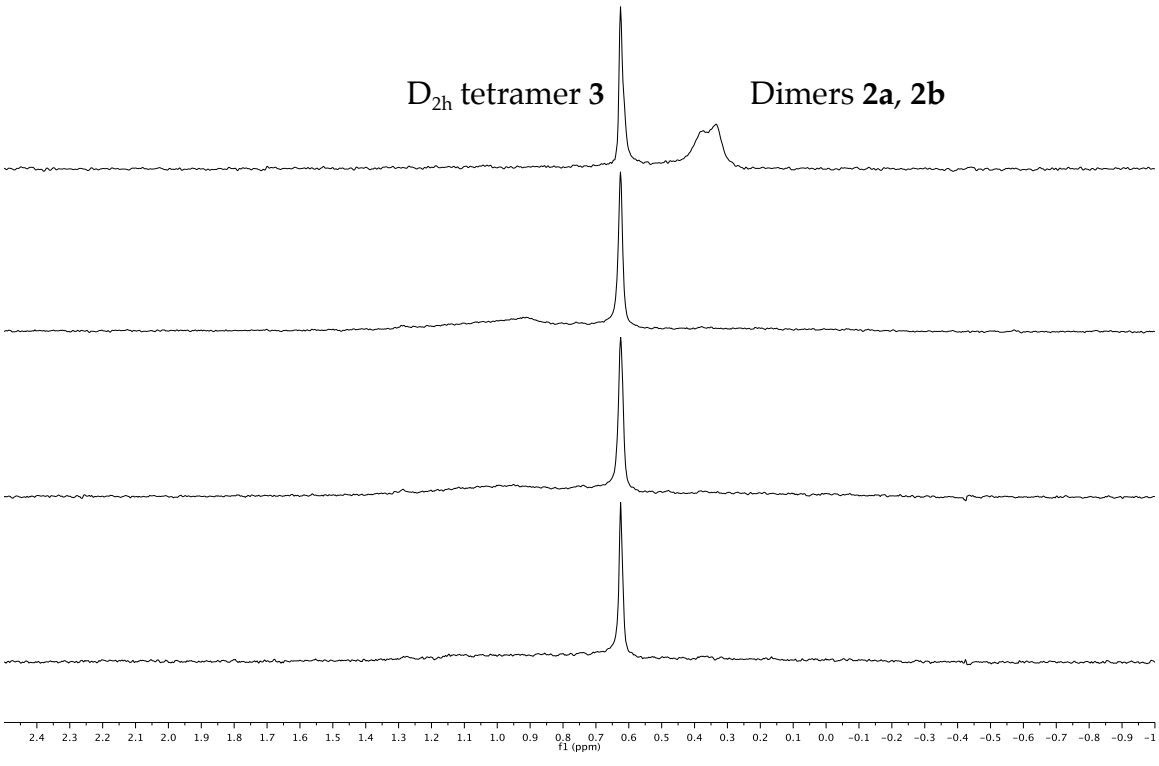


Figure 23. ^{6}Li NMR spectra of equilibrated enolate **5**, followed by aging with the addition of isobutyraldehyde at -70 °C for 4, 20, and 44 minutes (0.10 M **5**, 0.20 M isobutyraldehyde, THF, -80 °C). The resulting peaks corresponding to (*R*,*S*)-**6** are too broad to be seen.

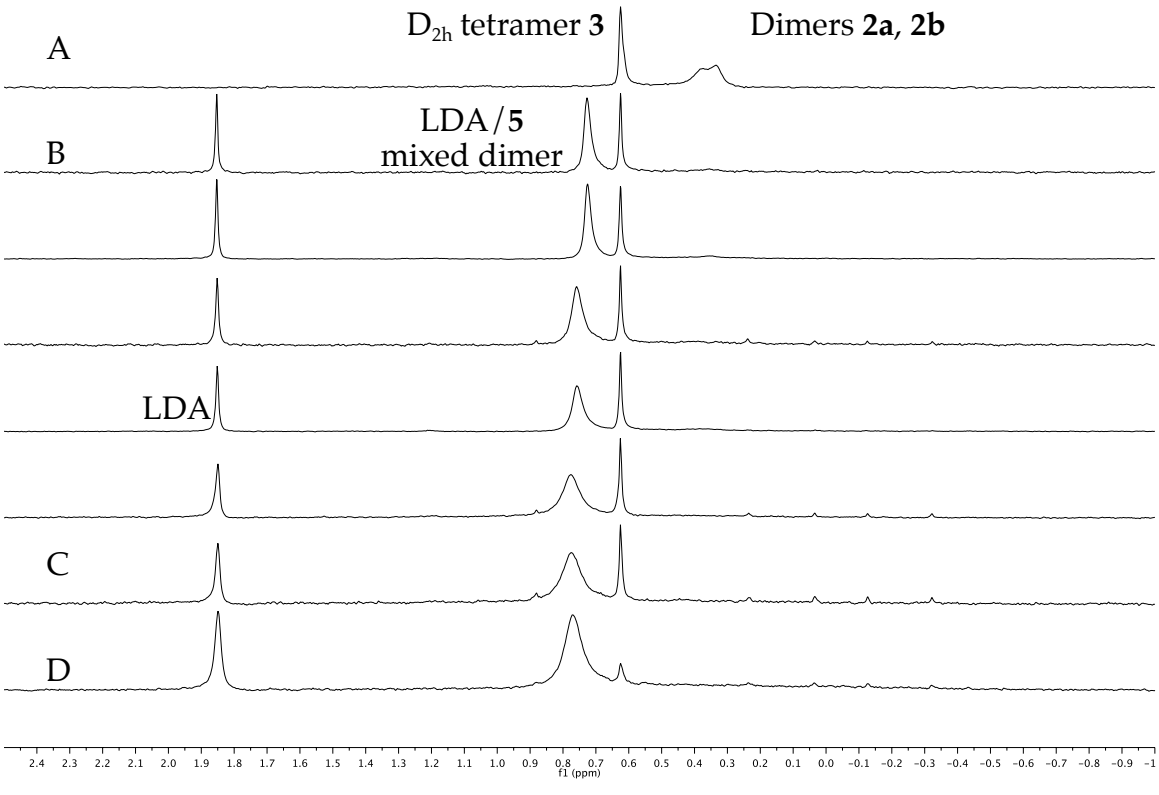


Figure 24. ^{6}Li NMR spectra of the addition of LDA to an equilibrated sample of **5** (A) aged for 160 minutes (B-C), followed by aging at 0 °C for 10 min (D) (0.10 **5**, 0.20 M isobutyraldehyde, THF, -70 °C), illustrating the extraordinarily slow equilibration out of tetramer to the energetically more favorable LDA mixed dimer.

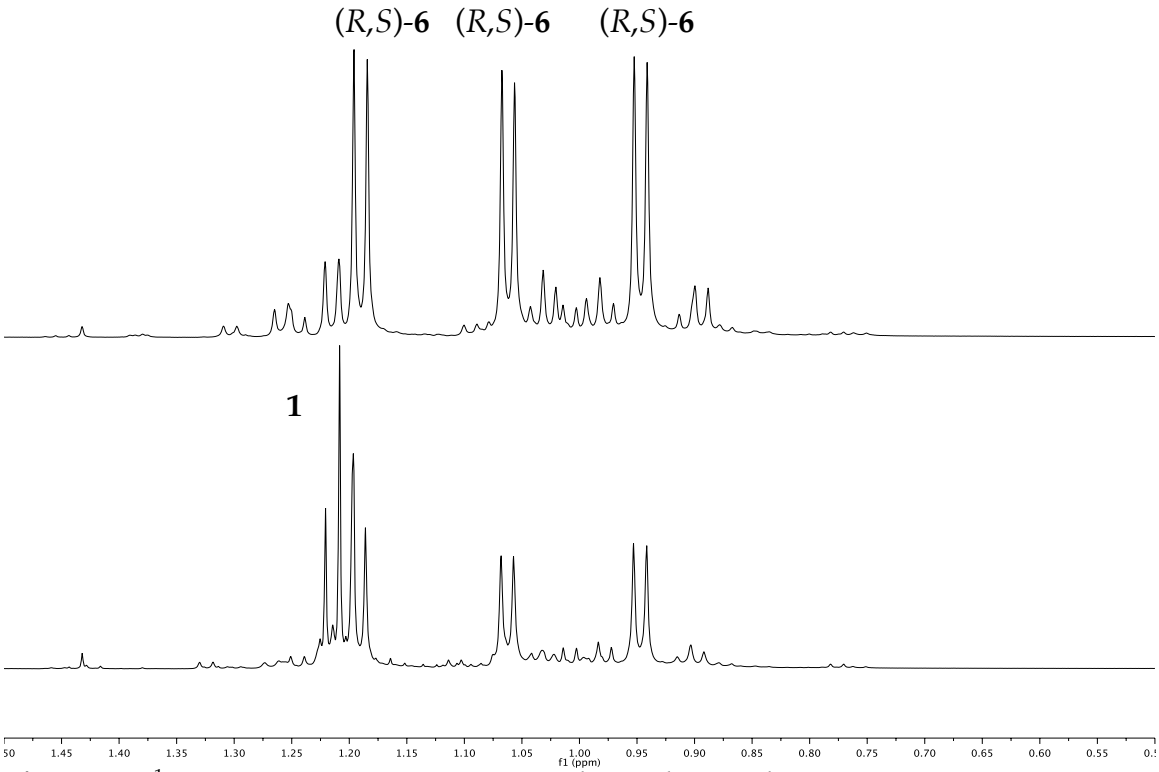


Figure 25. ^{1}H NMR spectra on an unaged **5** and **5** aged 30 minutes at 0° C prior to the aldol in neat THF on the aldol product distribution (0.10 M **5**, 0.20 M isobutyraldehyde, THF, -80 °C). Tetramer is present in the aged sample, resulting in the recovery of significant amounts of unreacted starting material **1** corresponding to the amount of **5** in tetramer. Some dimer does exist in the equilibrated sample in neat THF, resulting in some reactivity.

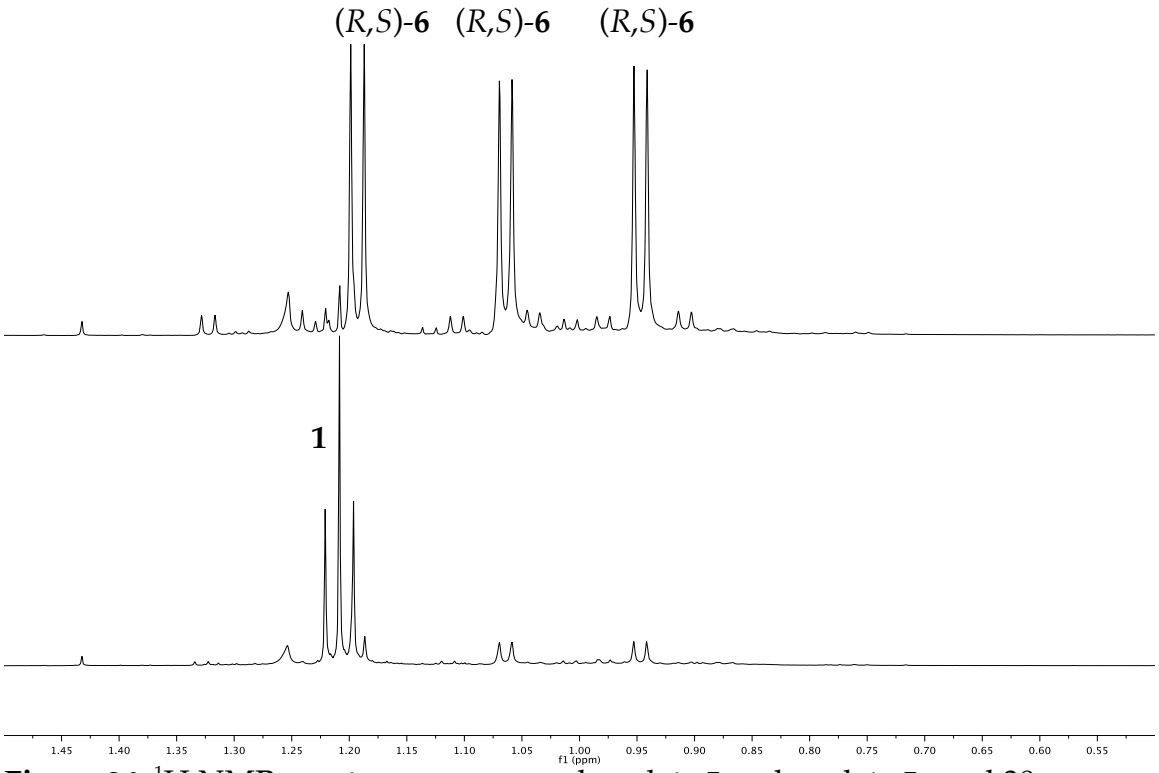


Figure 26. ^{1}H NMR spectra on an unaged enolate **5** and enolate **5** aged 30 minutes at 0° C prior to the aldol in low THF on the aldol product distribution (0.10 M **5**, 0.20 M isobutyraldehyde, 0.20 M THF, toluene, -80 °C). In the aged sample in low THF there is minimal dimer present, resulting in minimal reactivity.

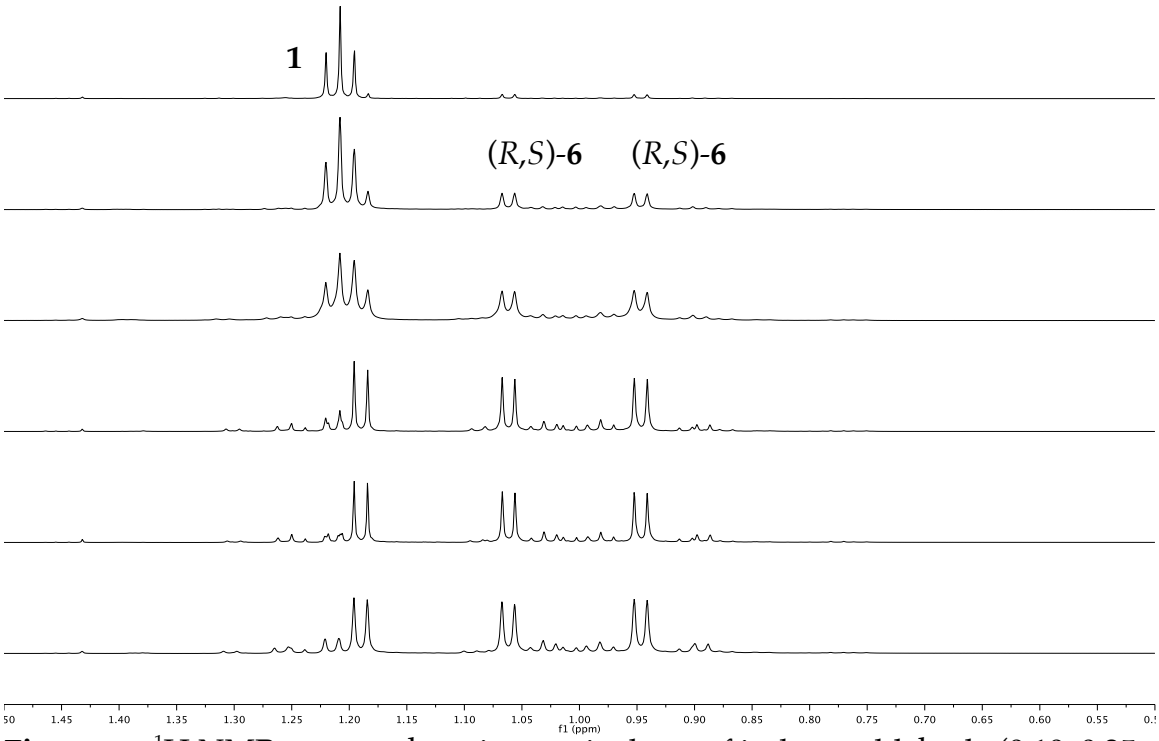


Figure 27. ^{1}H NMR spectra changing equivalents of isobutyraldehyde (0.10, 0.25, 0.50, 1.0, 1.5, 2.0) on the aldol product distribution in neat THF with an unaged enolate (0.10 M **5**, changing isobutyraldehyde, THF, -80 °C). The amount of recovered starting material corresponds to the deficit of aldehyde as expected. Notibly no erosion of selectivity is observed.

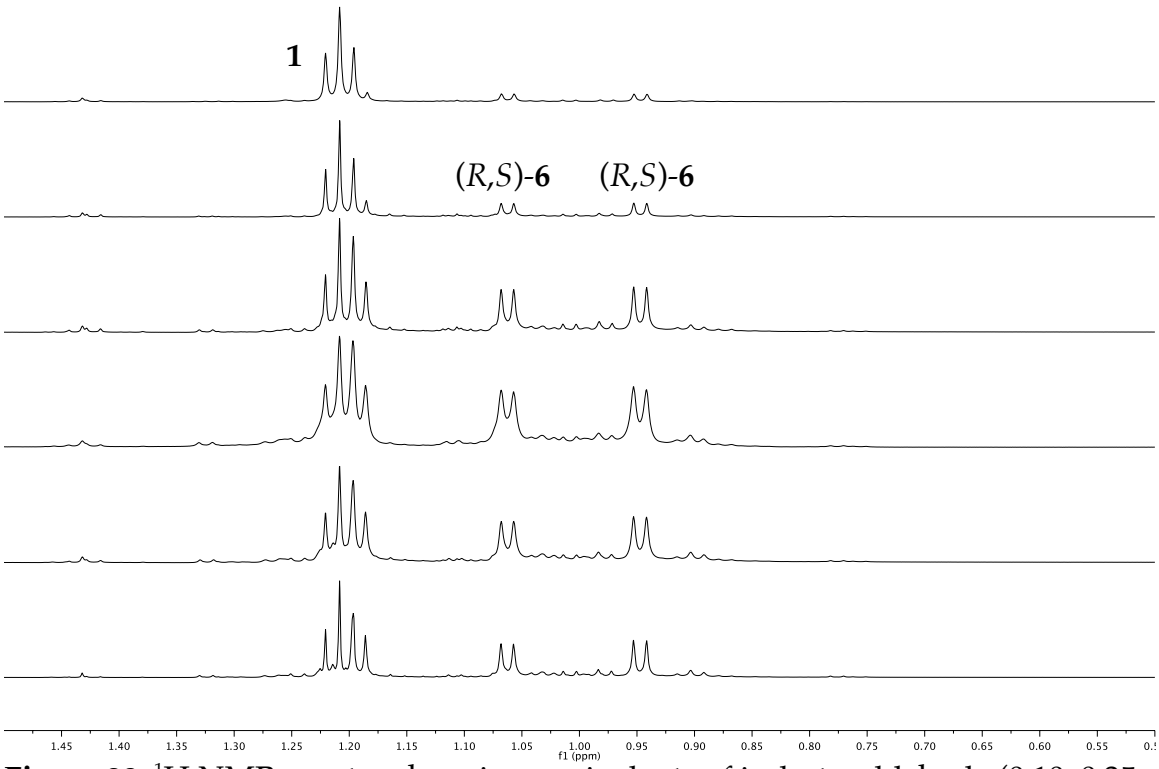


Figure 28. ^{1}H NMR spectra changing equivalents of isobutyraldehyde (0.10, 0.25, 0.50, 1.0, 1.5, 2.0) on the aldol product distribution in neat THF with enolate 5 aged 30 minutes at 0 °C (0.10 M **5**, changing isobutyraldehyde, THF, -80 °C). The amount of recovered starting material corresponds to the deficit of aldehyde until the dimer is used up, after which no further reactivity is observed. Notibly no erosion of selectivity is observed.

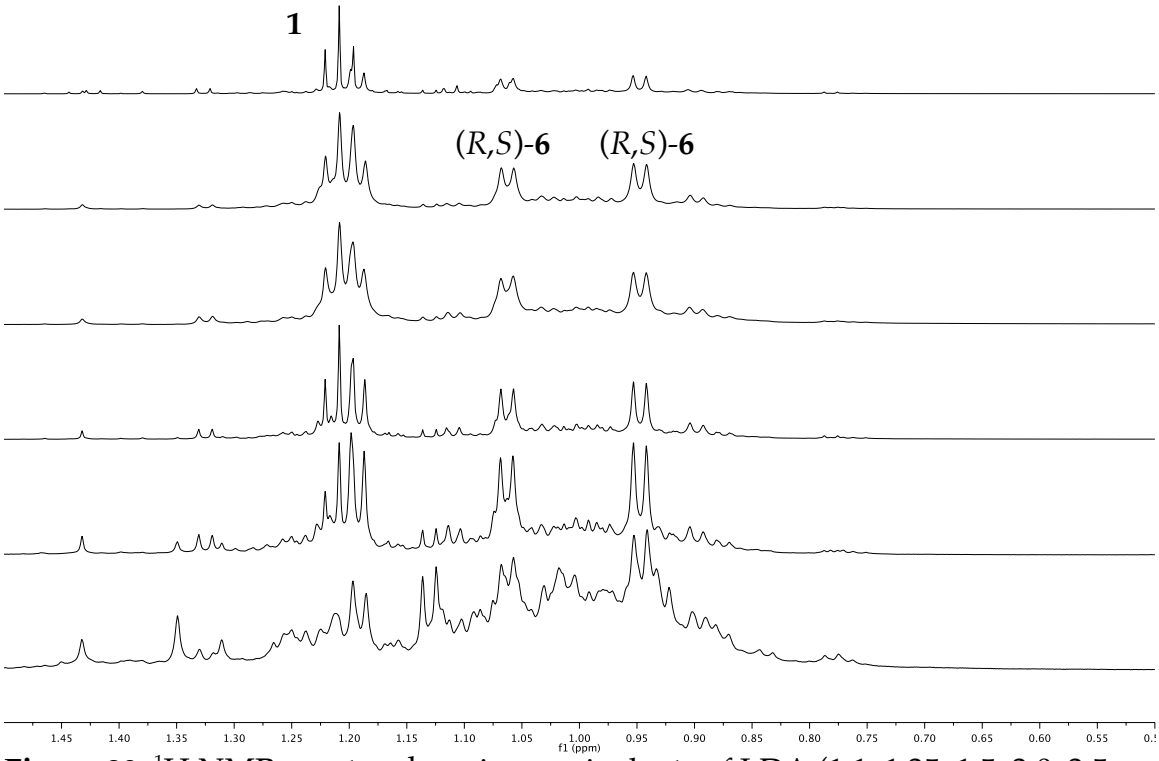


Figure 29. ^{1}H NMR spectra changing equivalents of LDA (1.1, 1.25, 1.5, 2.0, 2.5, 3.0) on the aldol product distribution in neat THF with an enolate aged 30 minutes at 0 °C (0.10 M **5**, 0.20 M isobutyraldehyde, THF, -80 °C). Additional LDA does not improve either the selectivity or the percent conversion but does lead to degradation of the sample.

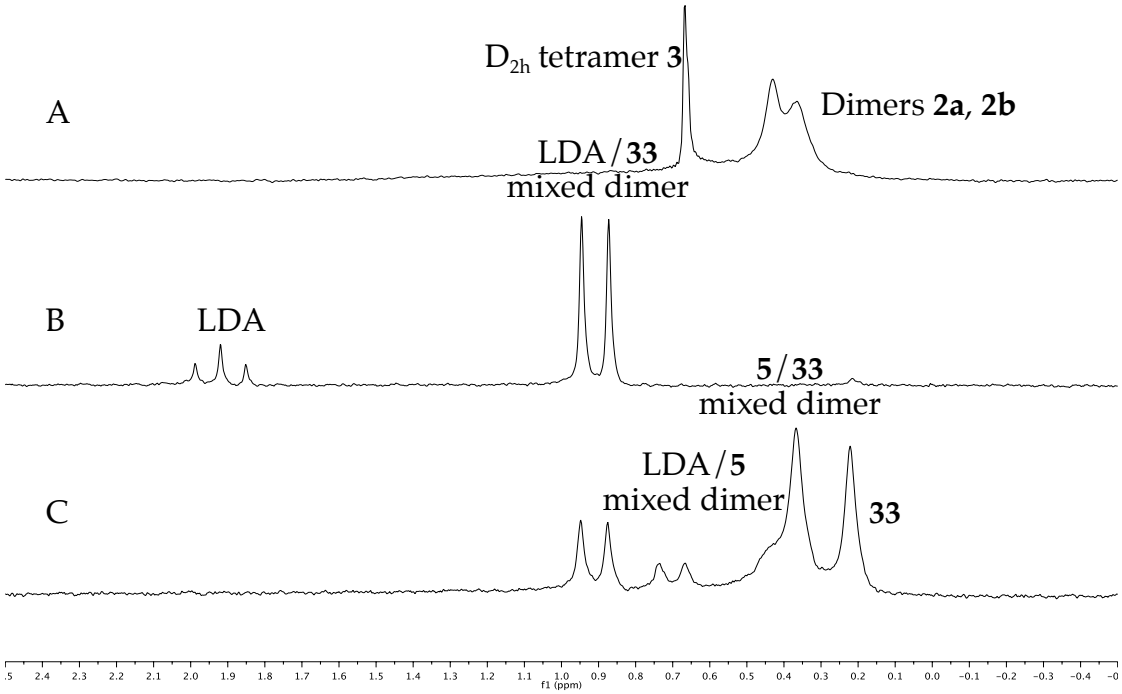


Figure 30. Kinetic mixed dimer formation. Spectrum A is an equilibrated sample of **5**. Spectrum B is **33** with 1 additional equivalent of [^{6}Li]LDA. Spectrum C is spectra 2 plus one equivalent of oxazolidinone **1** unaged. (0.10 M **5**, 0.10 M **33**, THF, -78 °C)

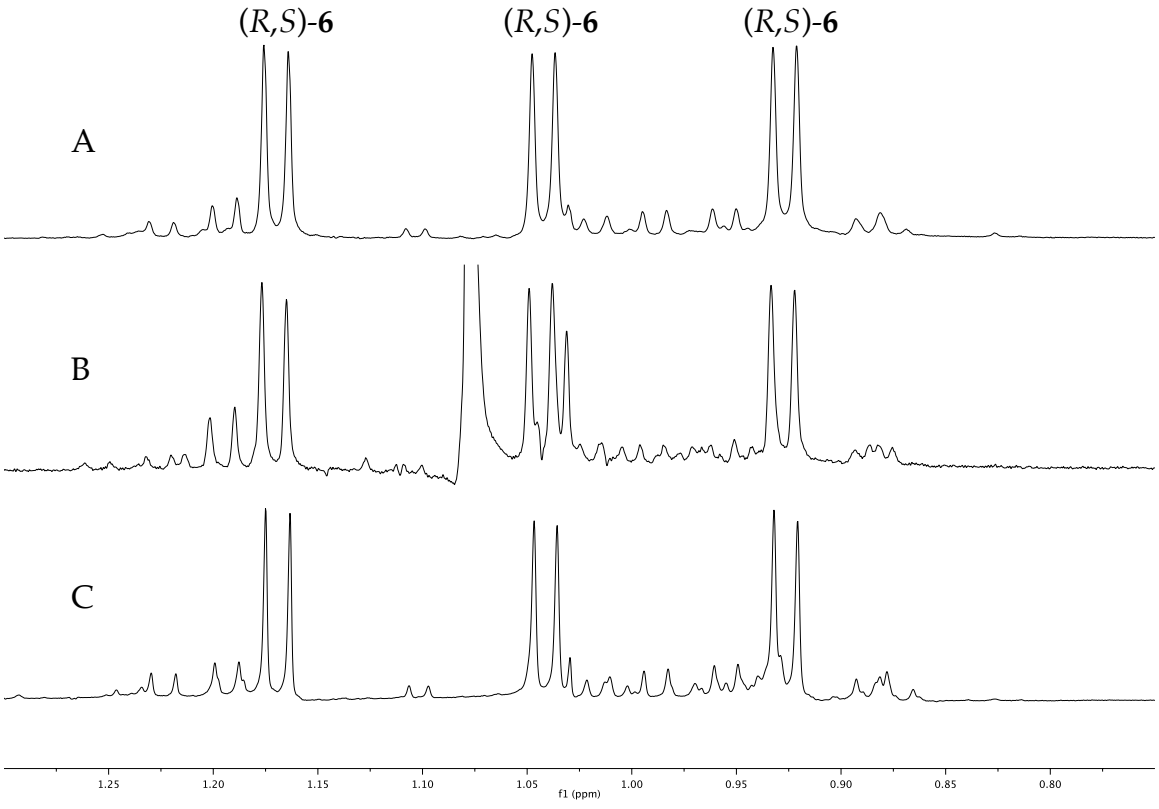


Figure 31. Kinetic mixed dimer selectivities. Spectrum A is enolate **5** alone. Spectrum B is enolate **5** plus one equivalent of enolate **33**. Spectrum C is enolate **5** plus one equivalent of enolate **34**. (0.10 M **5**, 0.10 M **33**/**34**, 0.20 M isobutyrlaldehyde, THF, -78 °C). No change in selectivity or percent conversion is noted.

Part 4: Ketone Aldol Kinetics

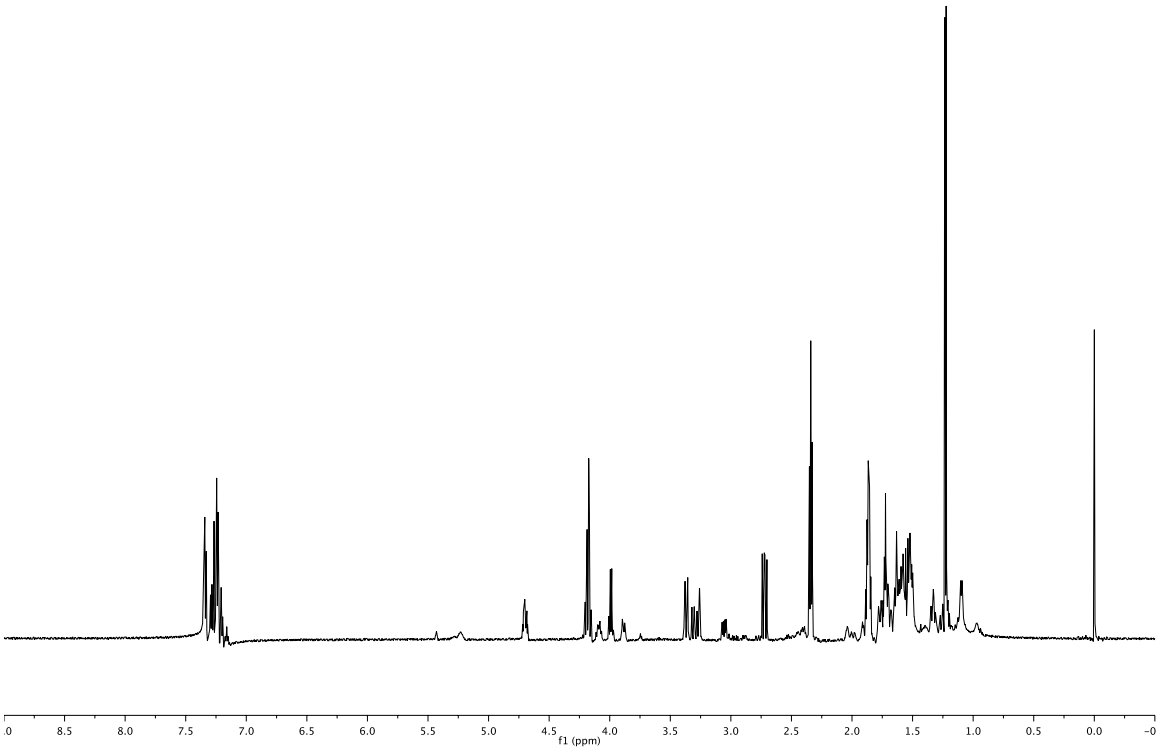


Figure 32. ^{1}H NMR spectra of crude aldol product of the aldol reaction between cyclohexanone and enolate **5**.

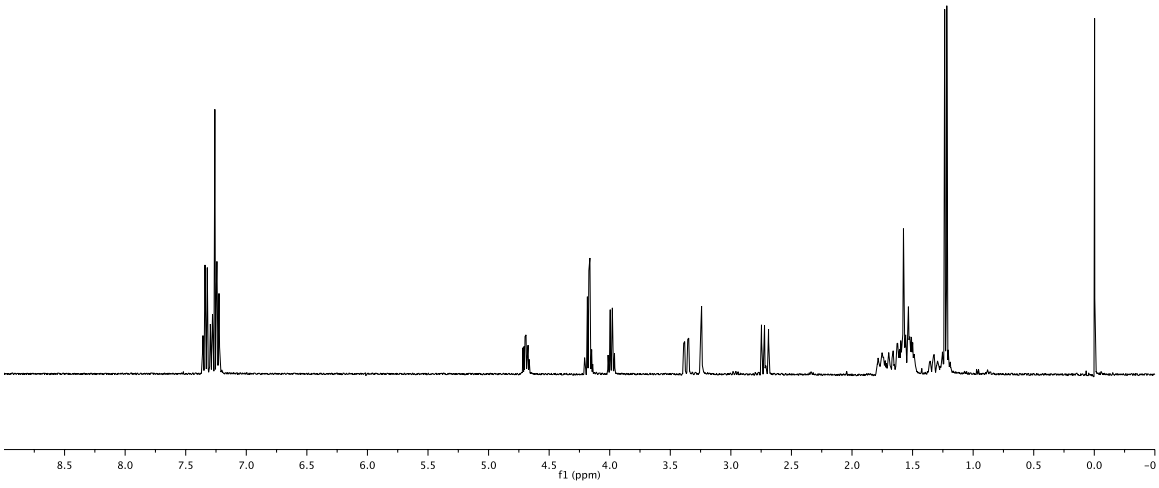


Figure 33. ^{1}H NMR spectrum of recrystallized (*R*)-**7**

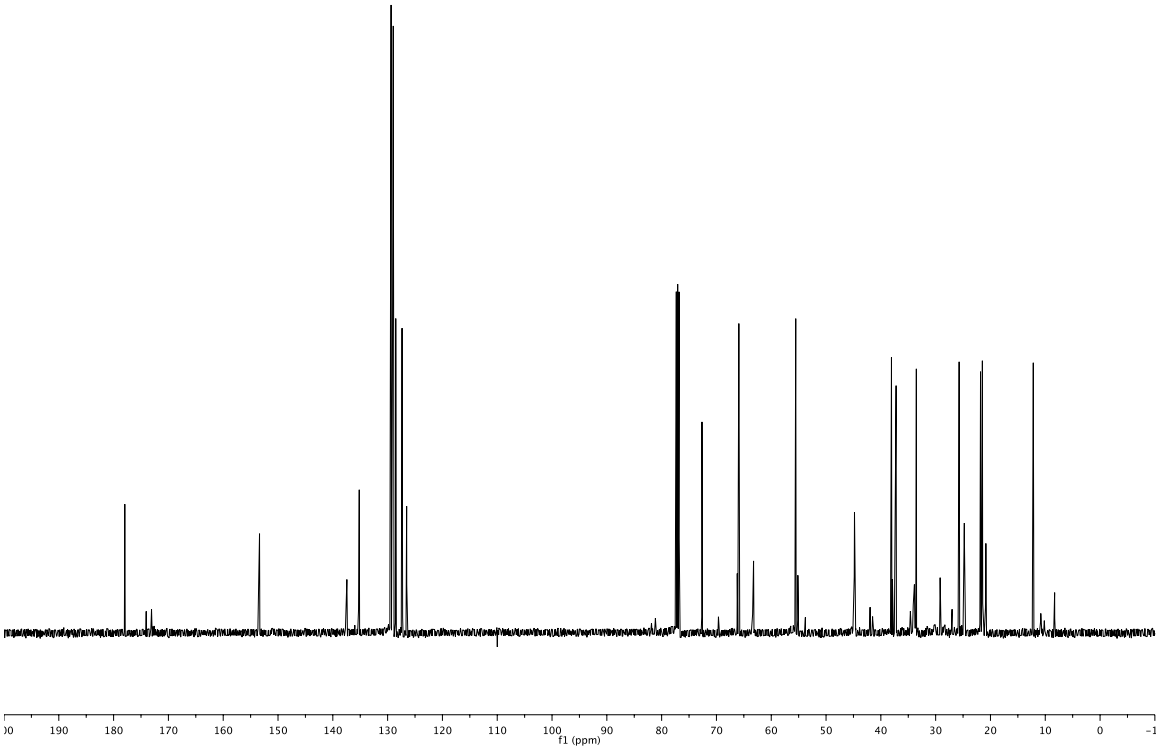


Figure 34. ^{13}C NMR spectrum of recrystallized (*R*)-**7**

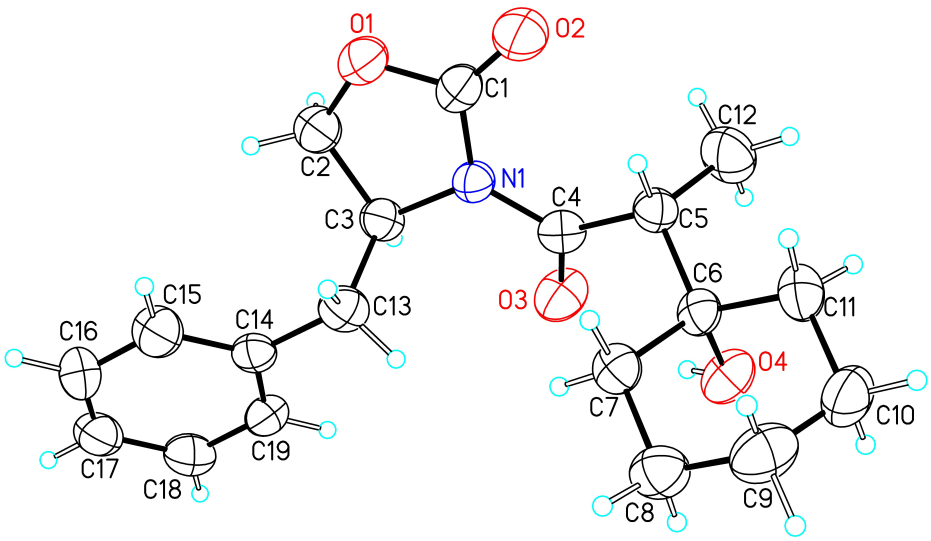


Figure 35. X-ray crystal structure of (*R*)-**7**.

Table 3. Crystal data and structural refinement of recrystallized (*R*)-**7** aldol product

Empirical formula	C19 H25 N O4	
Formula weight	331.40	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 5.7701(6) Å	a= 90°.
	b = 13.3976(12) Å	b= 90°.
	c = 22.752(2) Å	g = 90°.
Volume	1758.8(3) $Å^3$	
Z	4	
Density (calculated)	1.252 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	712	
Crystal size	0.60 x 0.05 x 0.03 mm^3	
Theta range for data collection	1.76 to 23.84°.	
Index ranges	-6<=h<=5, -14<=k<=15, -25<=l<=18	
Reflections collected	5883	
Independent reflections	2552 [R(int) = 0.0270]	
Completeness to theta = 23.84°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9978 and 0.9495	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2552 / 0 / 217	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0662	
R indices (all data)	R1 = 0.0812, wR2 = 0.0808	
Absolute structure parameter	0.8(16)	
Largest diff. peak and hole	0.118 and -0.168 $e.Å^{-3}$	

Table 4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4296(3)	6930(1)	-12(1)	68(1)
O(2)	4965(4)	7541(2)	882(1)	77(1)
O(3)	9589(3)	5158(1)	911(1)	66(1)
O(4)	9808(3)	4834(1)	2108(1)	62(1)
N(1)	6643(4)	6055(1)	563(1)	44(1)
C(1)	5273(5)	6904(2)	522(1)	56(1)
C(2)	5259(6)	6162(2)	-383(1)	66(1)
C(3)	6456(5)	5441(2)	31(1)	47(1)
C(4)	8138(5)	5797(2)	1015(1)	47(1)
C(5)	7865(4)	6244(2)	1621(1)	47(1)
C(6)	7690(4)	5397(2)	2085(1)	44(1)
C(7)	5682(4)	4701(2)	1941(1)	50(1)
C(8)	5253(6)	3916(2)	2414(1)	65(1)
C(9)	4904(6)	4384(2)	3010(1)	75(1)
C(10)	6968(6)	5037(2)	3159(1)	72(1)
C(11)	7367(6)	5836(2)	2695(1)	64(1)
C(12)	9875(6)	6976(2)	1725(1)	79(1)
C(13)	5087(5)	4496(2)	166(1)	55(1)
C(14)	4892(5)	3801(2)	-348(1)	45(1)
C(15)	2988(5)	3791(2)	-714(1)	62(1)
C(16)	2856(6)	3138(2)	-1181(1)	71(1)
C(17)	4593(6)	2484(2)	-1289(1)	65(1)
C(18)	6497(6)	2472(2)	-932(1)	66(1)
C(19)	6653(5)	3132(2)	-462(1)	56(1)

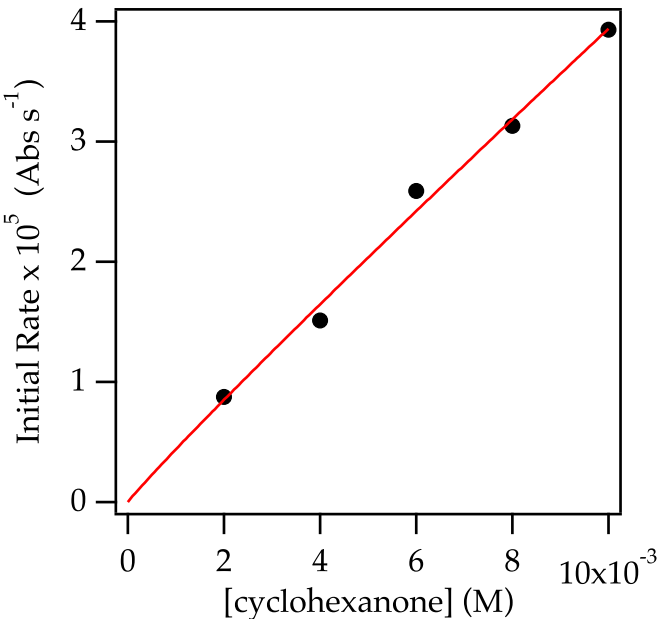


Figure 36. Plot of initial rate vs. [cyclohexanone] in neat THF at -78 °C (0.1 M of oxazolidinone **1**, 0.095 M LDA, THF, -78 °C). The data was fit to $y = ax^b$ such that $b = 0.95 \pm 0.06$ corresponding to a first-order dependence on cyclohexanone.

[cyclohexanone]	Initial Rate x 10^5
0.01	3.93
0.008	3.13
0.006	2.59
0.004	1.51
0.002	0.875

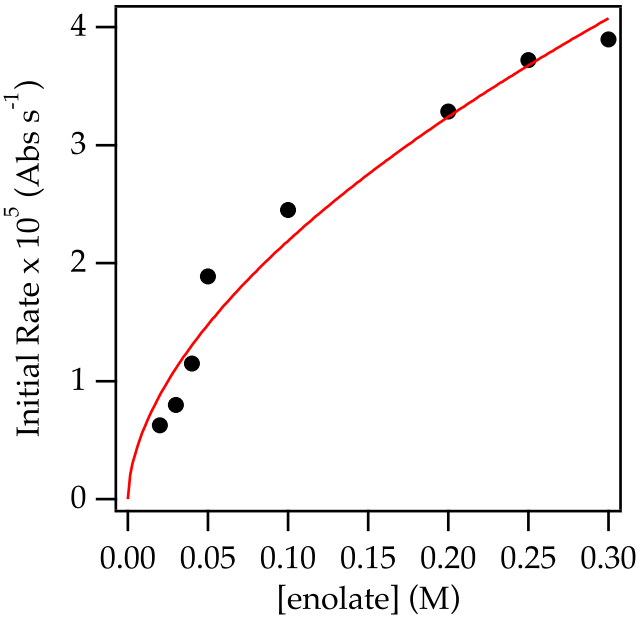


Figure 37. Plot of initial rate vs. [**5**] in neat THF at -78 °C (0.95 equiv LDA, 0.005 M cyclohexanone, THF, -78 °C). The data was fit to $y = ax^b$, such that $b = 0.57 \pm 0.05$ corresponding to a half-order dependence on **5**.

[**5**]	Initial Rate x 10^5
0.02	0.589
0.03	1.059
0.04	1.089
0.05	2.918
0.1	3.115
0.2	3.744
0.25	5.115
0.3	4.647

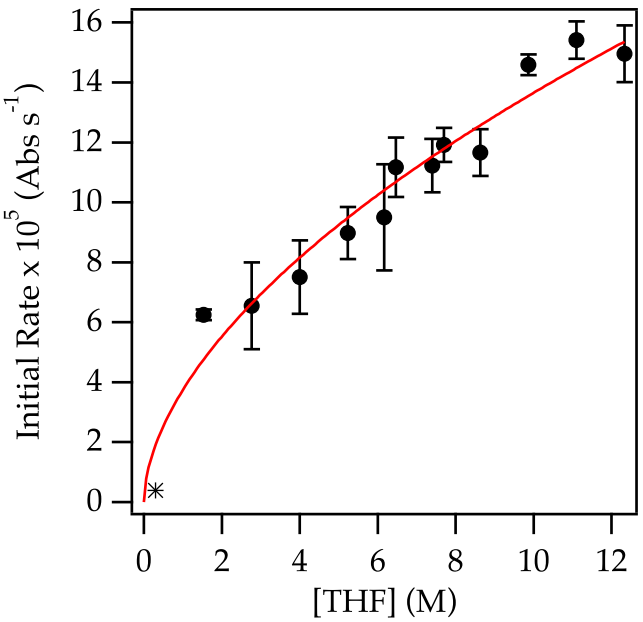


Figure 38. Plot of initial rate vs. [THF] with toluene cosolvent at -78 °C (0.10 M of oxazolidinone **1**, 0.095 M LDA, 0.005 M cyclohexanone, -78 °C). The data was fit to $y = ax^b$, such that $b = 0.56 \pm 0.05$ corresponding to a half-order dependence on THF. The * denotes a measured point that was not included in the fit.

[THF]	Initial Rate x 10^5
12.33	15.62
11.10	15.85
9.86	14.83
8.63	12.21
7.40	11.85
6.17	10.76
7.70	12.32
6.47	11.87
5.24	9.59
4.00	8.37
2.77	7.57
1.54	6.37
12.33	14.28
11.10	14.97
9.86	14.34
8.63	11.11
7.40	10.59
6.17	8.25
7.70	11.52
6.47	10.46
5.24	8.37
4.00	6.64
2.77	5.53
1.54	6.12

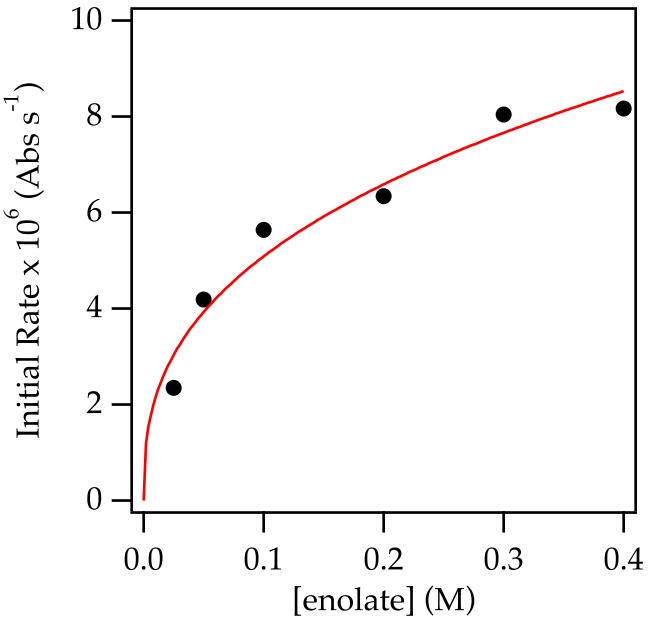


Figure 39. Plot of initial rate vs. [**5**] of a sample containing only tetramer (0.095 equiv LDA, 0.005 M cyclohexanone, 0.8 M THF, toluene, aged 10 minutes at 0 °C, recorded at -40 °C) The data was fit to $y = ax^b$ such that $b = 0.37 \pm 0.05$ corresponding to a fractional order dependence on **5**.

[**5**]	Initial Rate x 10^6
0.025	2.35
0.05	4.19
0.1	5.64
0.2	6.34
0.3	8.04
0.4	8.17

Part 5: Computations Overview of Enolate 5

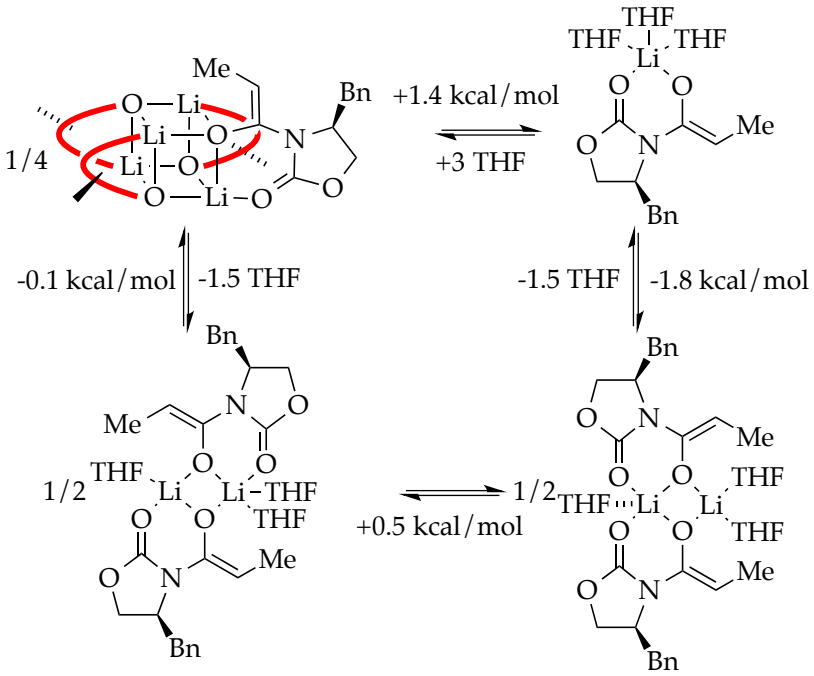


Figure 40. Overview of ground state energies, in kcal/mole of enolate

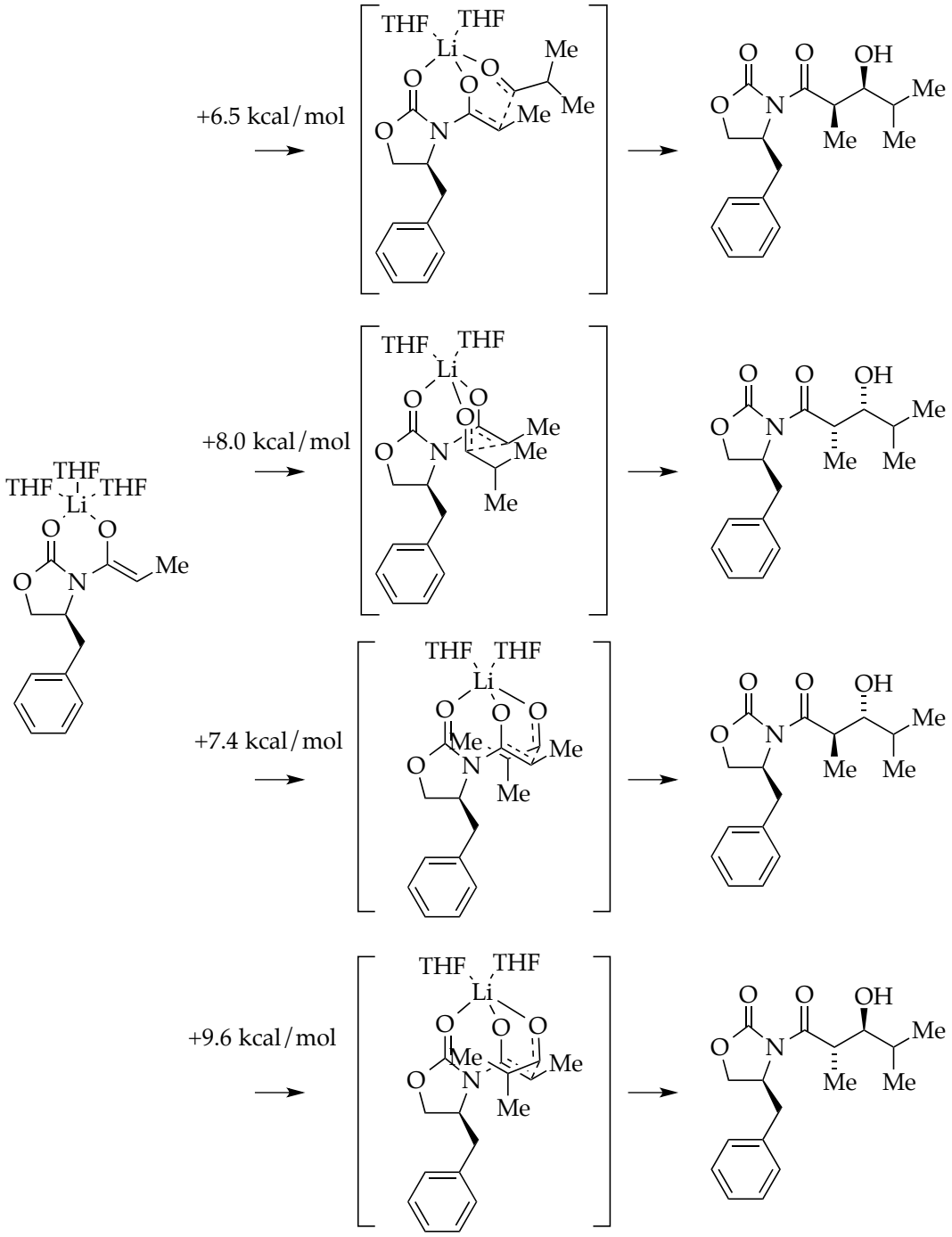


Figure 41. Overview of transition states from a monomer ground state.

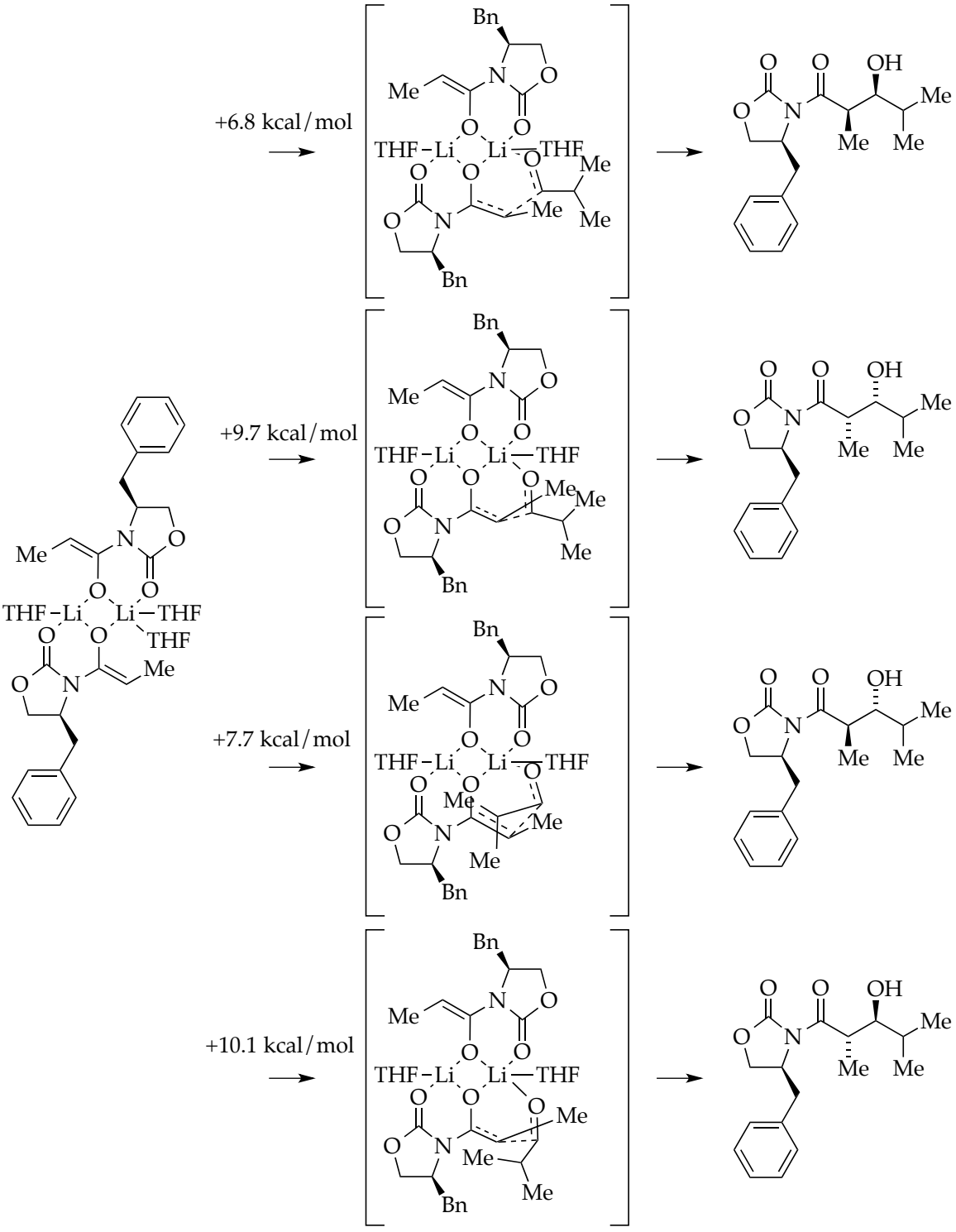


Figure 42. Overview of transition states from a dimer ground state.

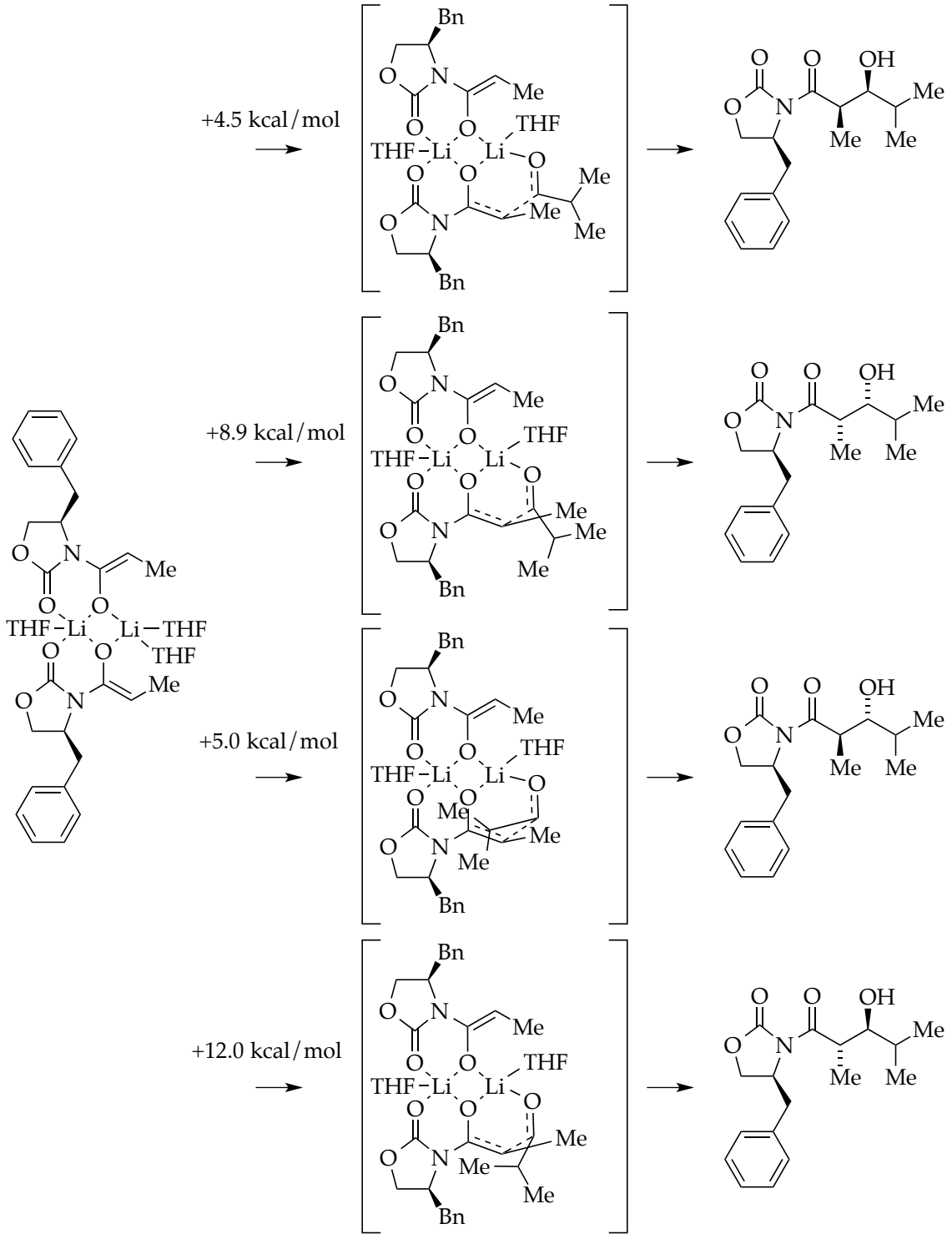


Figure 43. Overview of transition states from a spirocyclic dimer ground state.

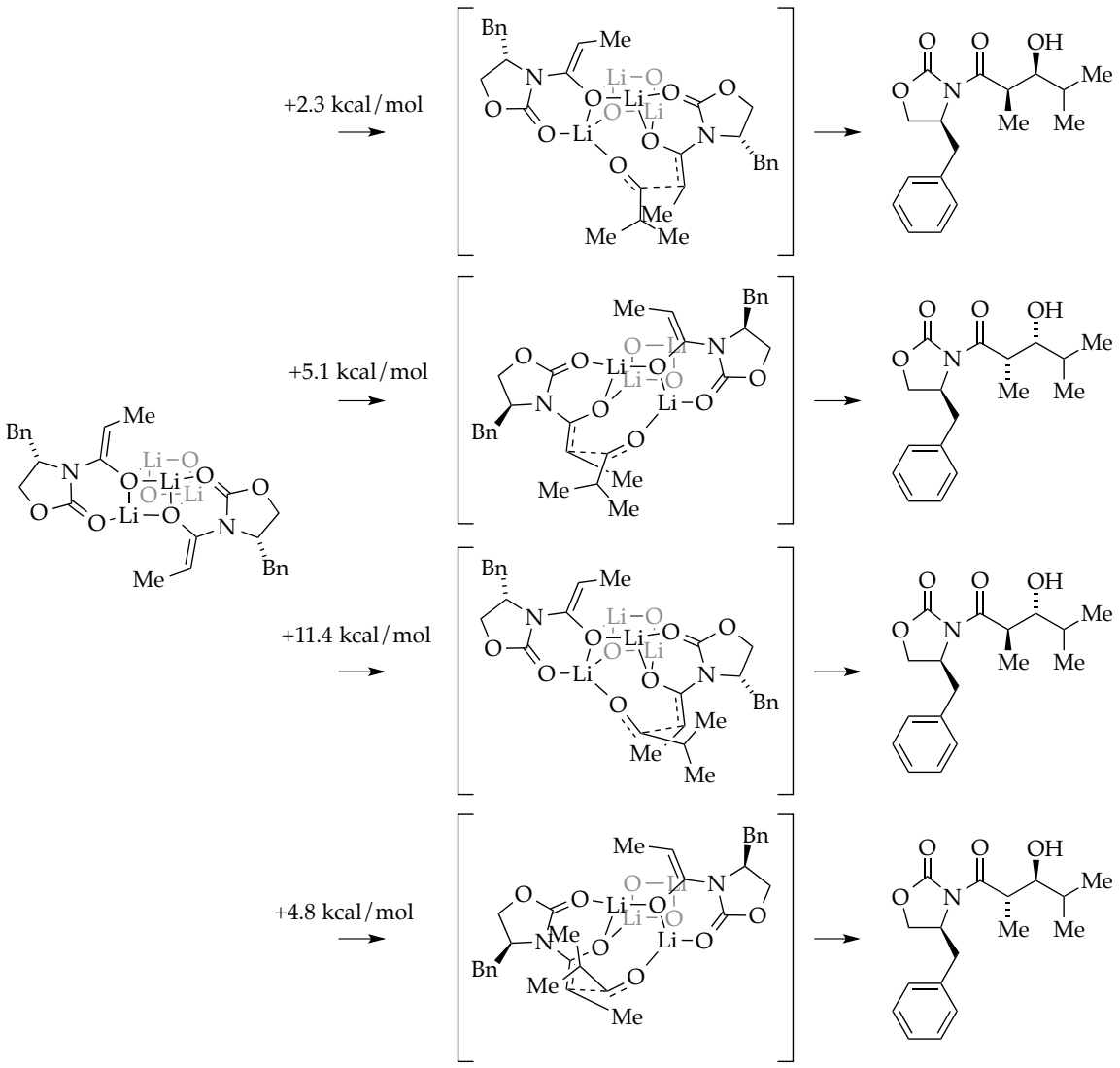


Figure 44. Overview of transition states from a tetramer ground state.

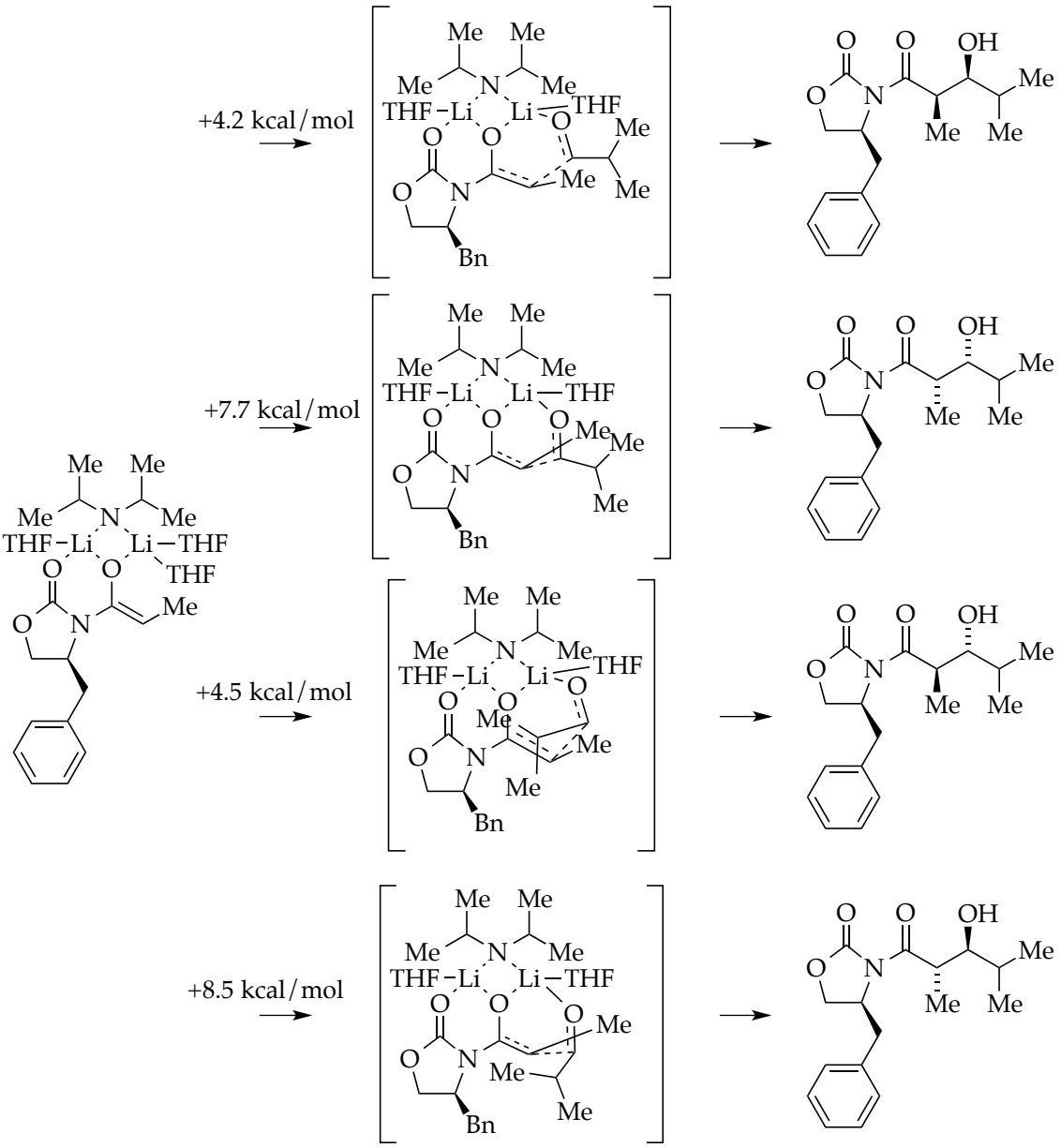


Figure 45. Overview of transition states from a LDA **5** mixed dimer ground state.

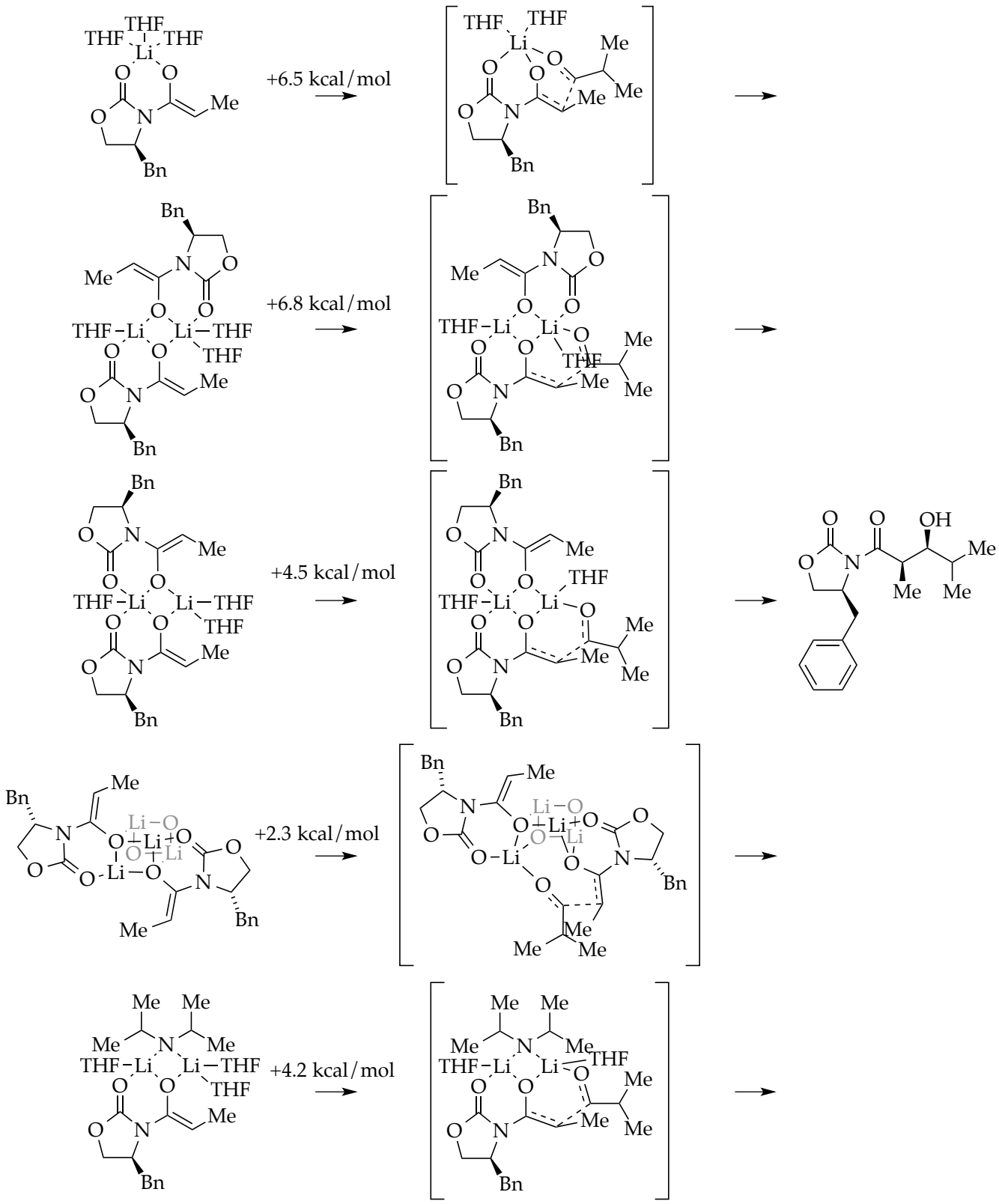


Figure 46. Overview of transition state energies leading to (*R,S*)-**6**

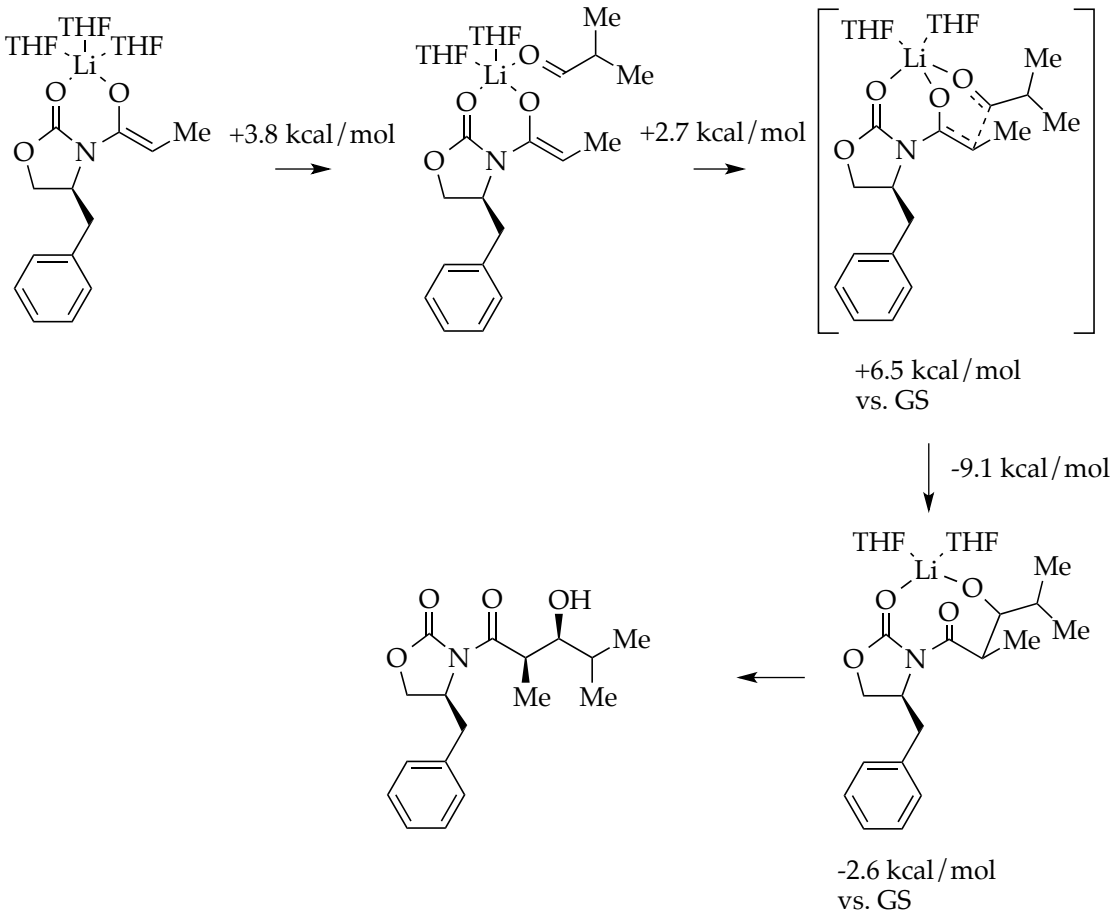


Figure 47. Computational overview of the pathway from monomer to (*R*,*S*)-**6**.

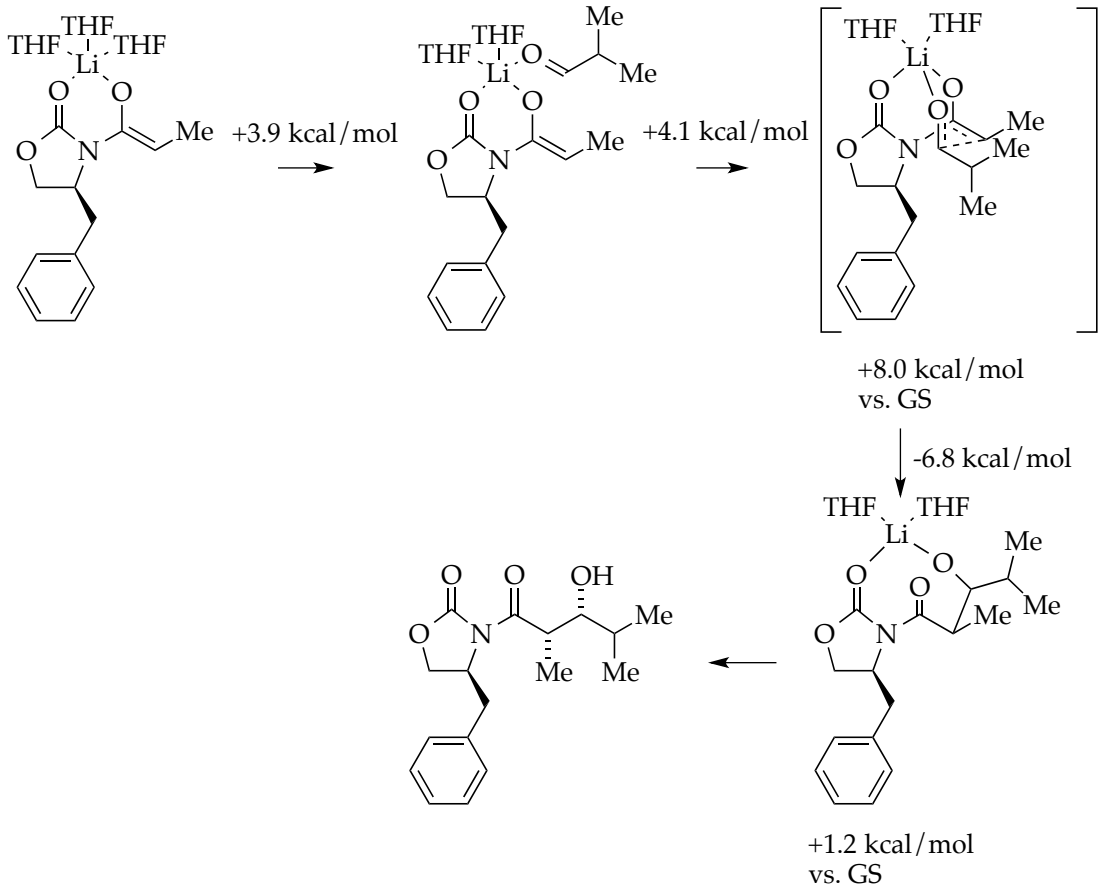


Figure 48. Computational overview of the pathway from monomer to (*S,R*)-**6**.

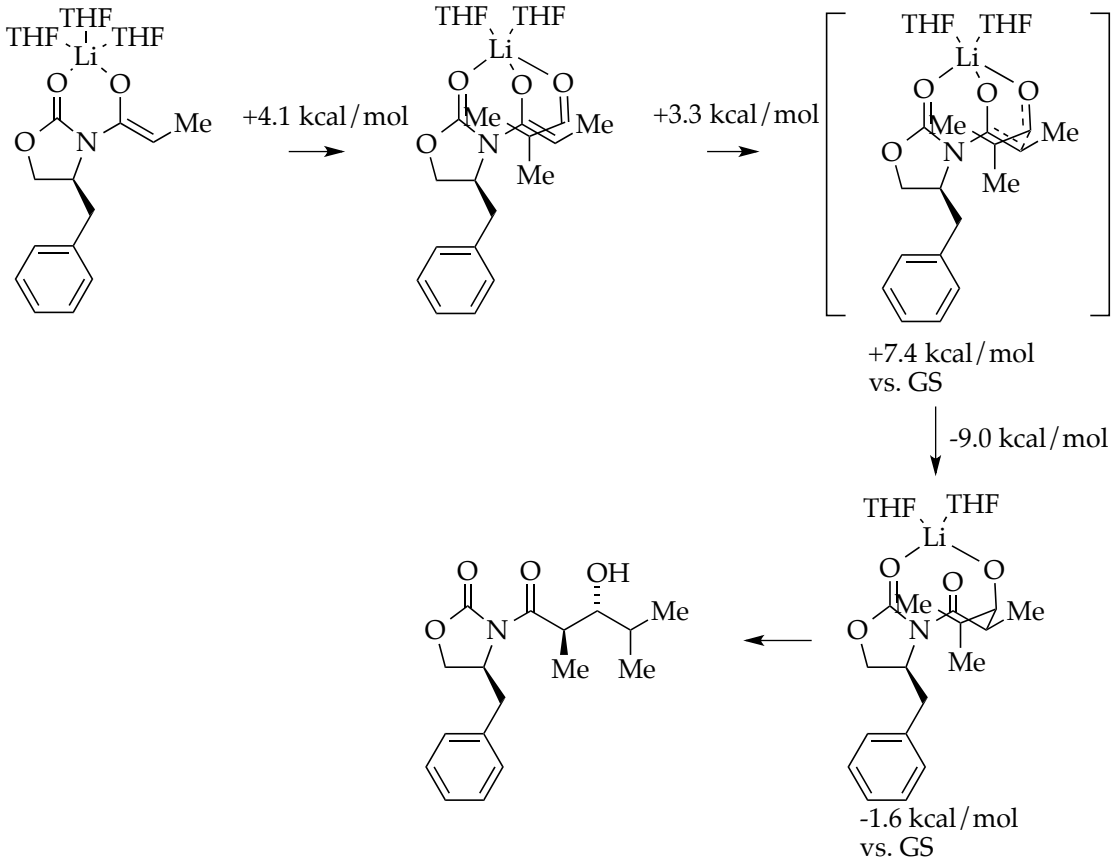


Figure 49. Computational overview of the pathway from monomer to (*R,R*)-**6**.

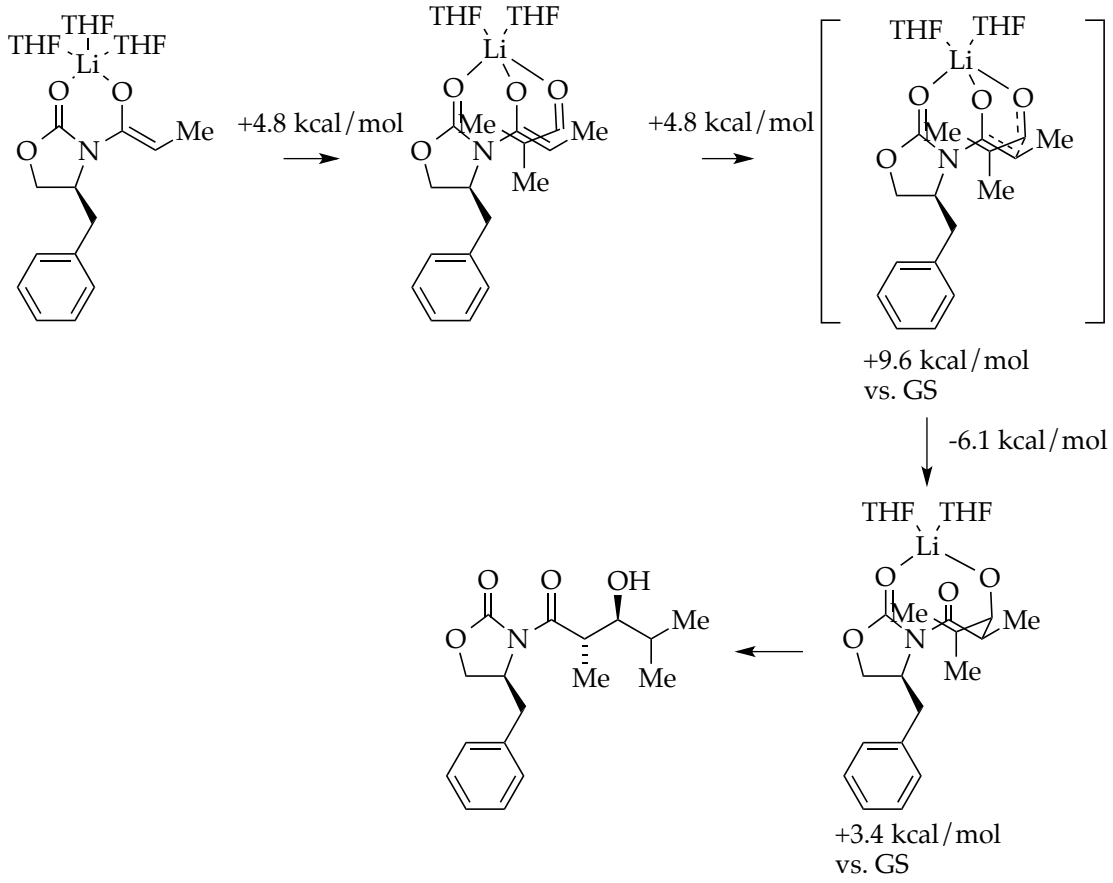


Figure 50. Computational overview of the pathway from monomer to (*S,S*)-**6**.

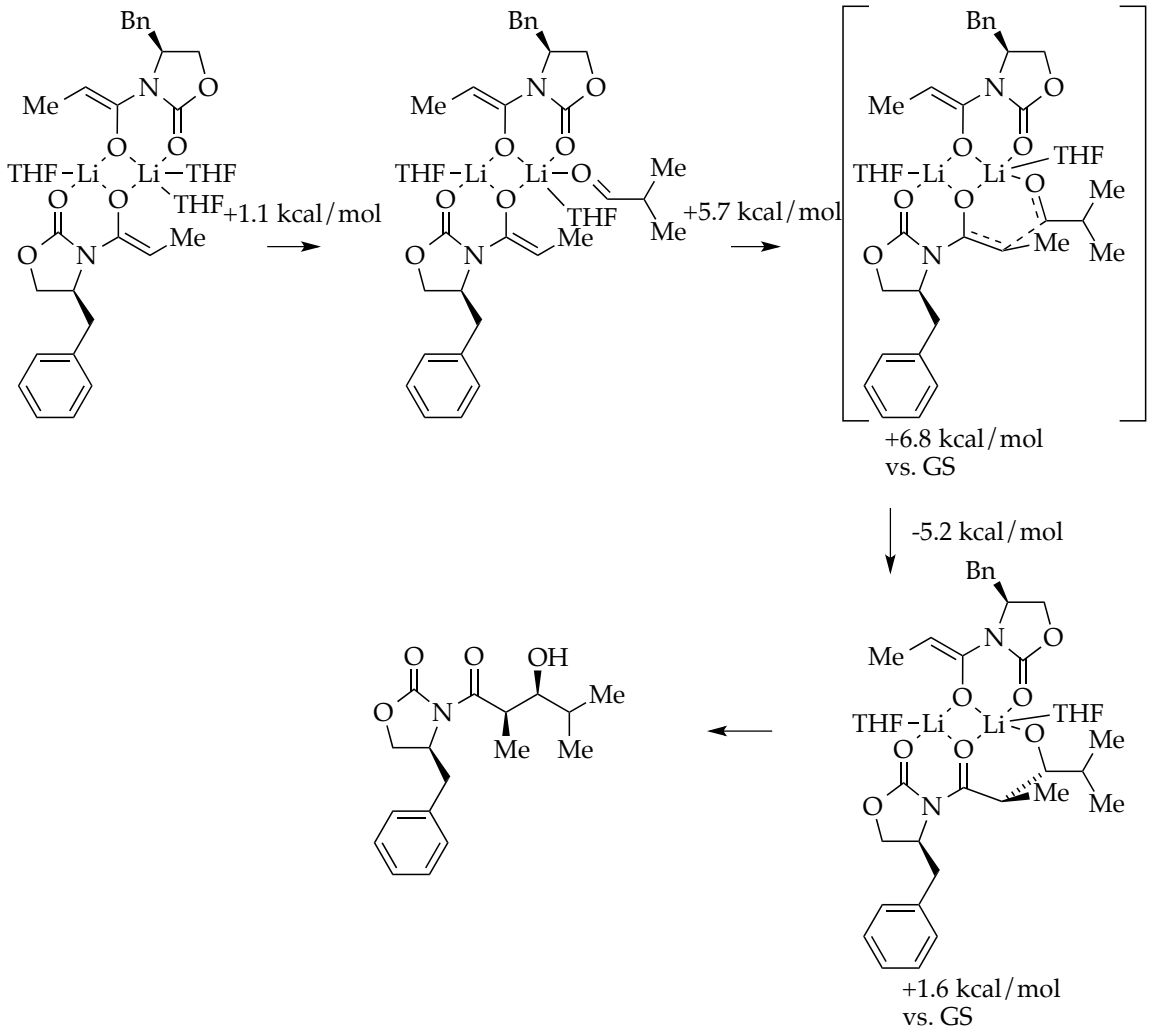


Figure 51. Computational overview of the pathway from dimer to (*R,S*)-**6**.

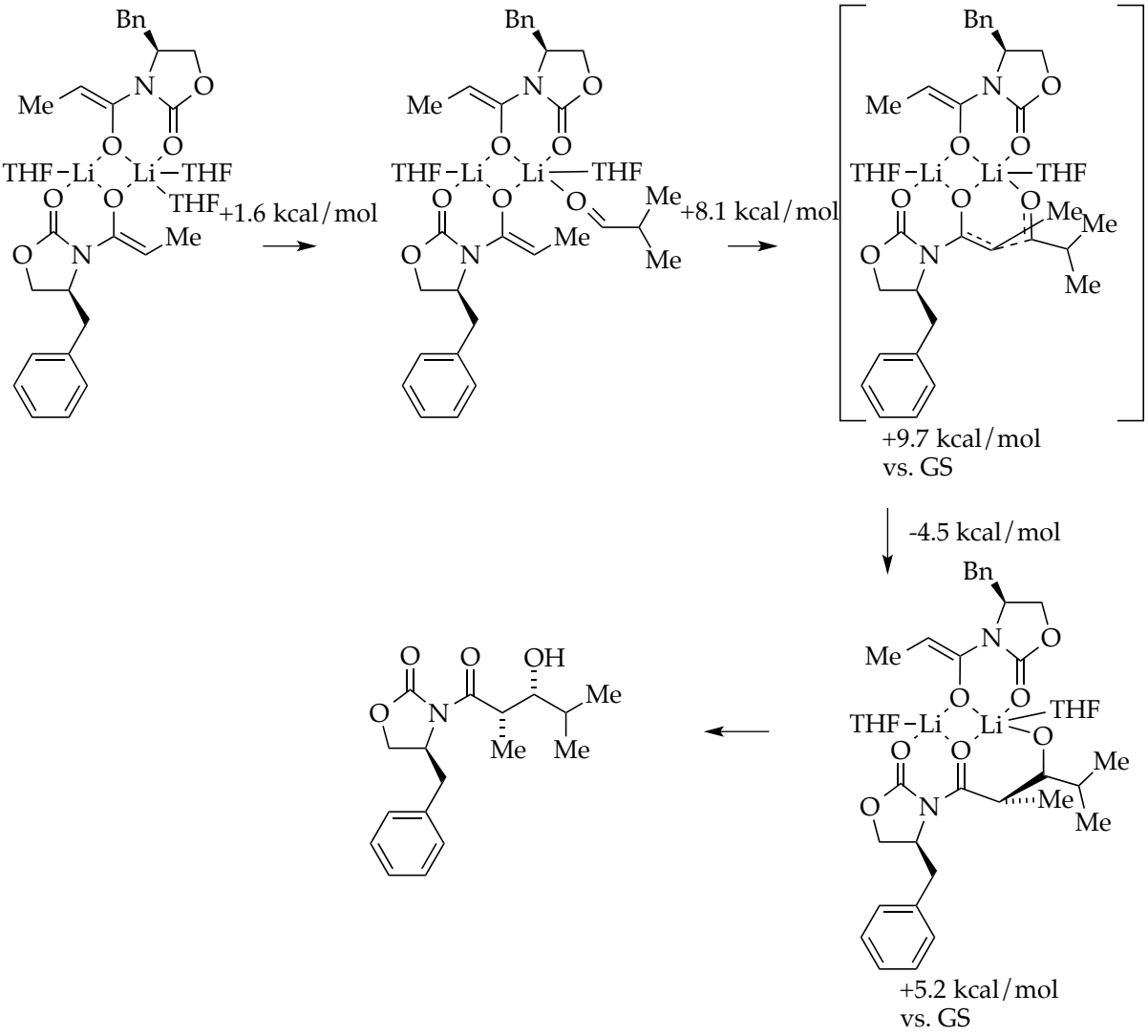


Figure 52. Computational overview of the pathway from dimer to (*S,R*)-**6**.

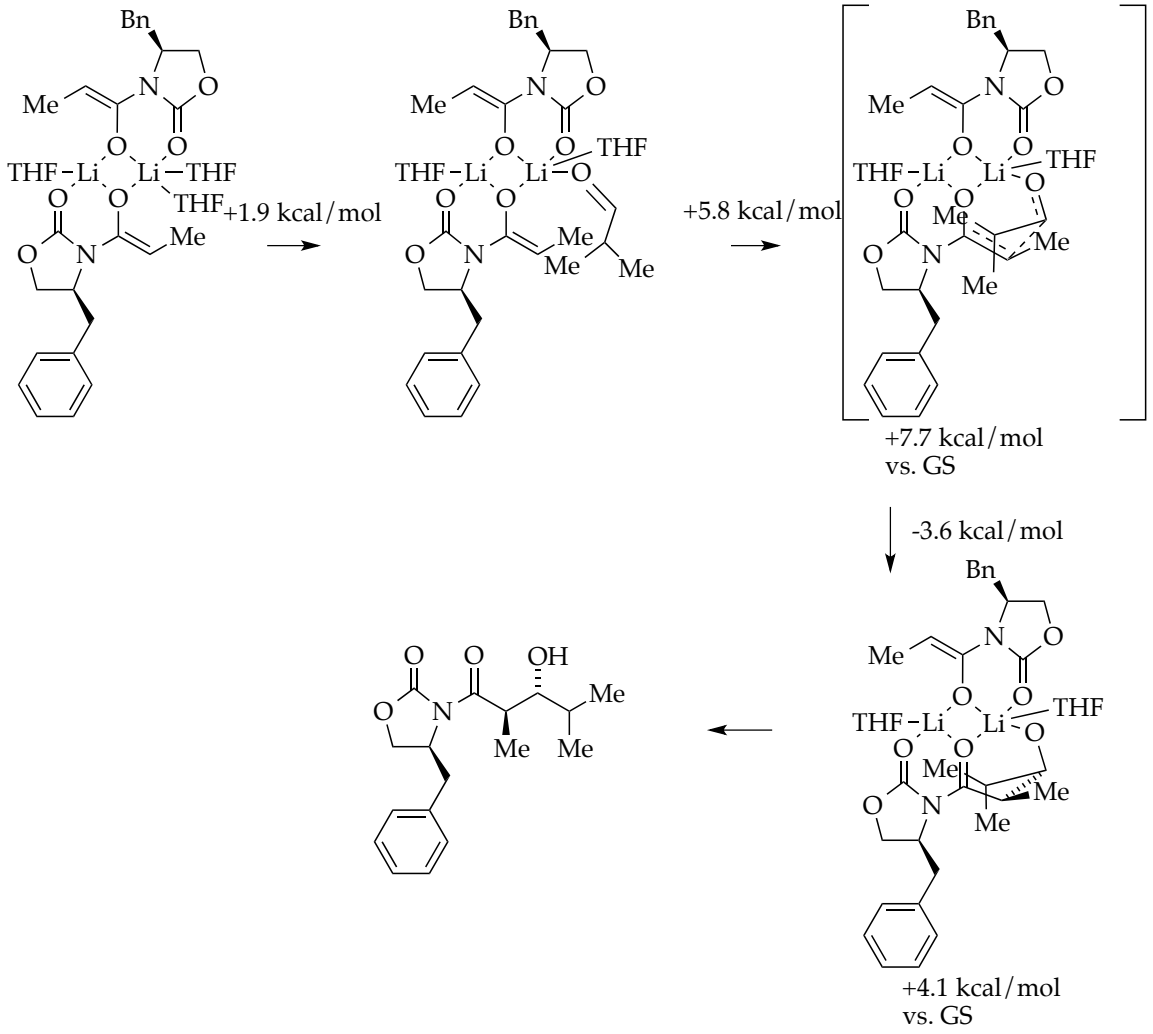


Figure 53. Computational overview of the pathway from dimer to (*R,R*)-**6**.

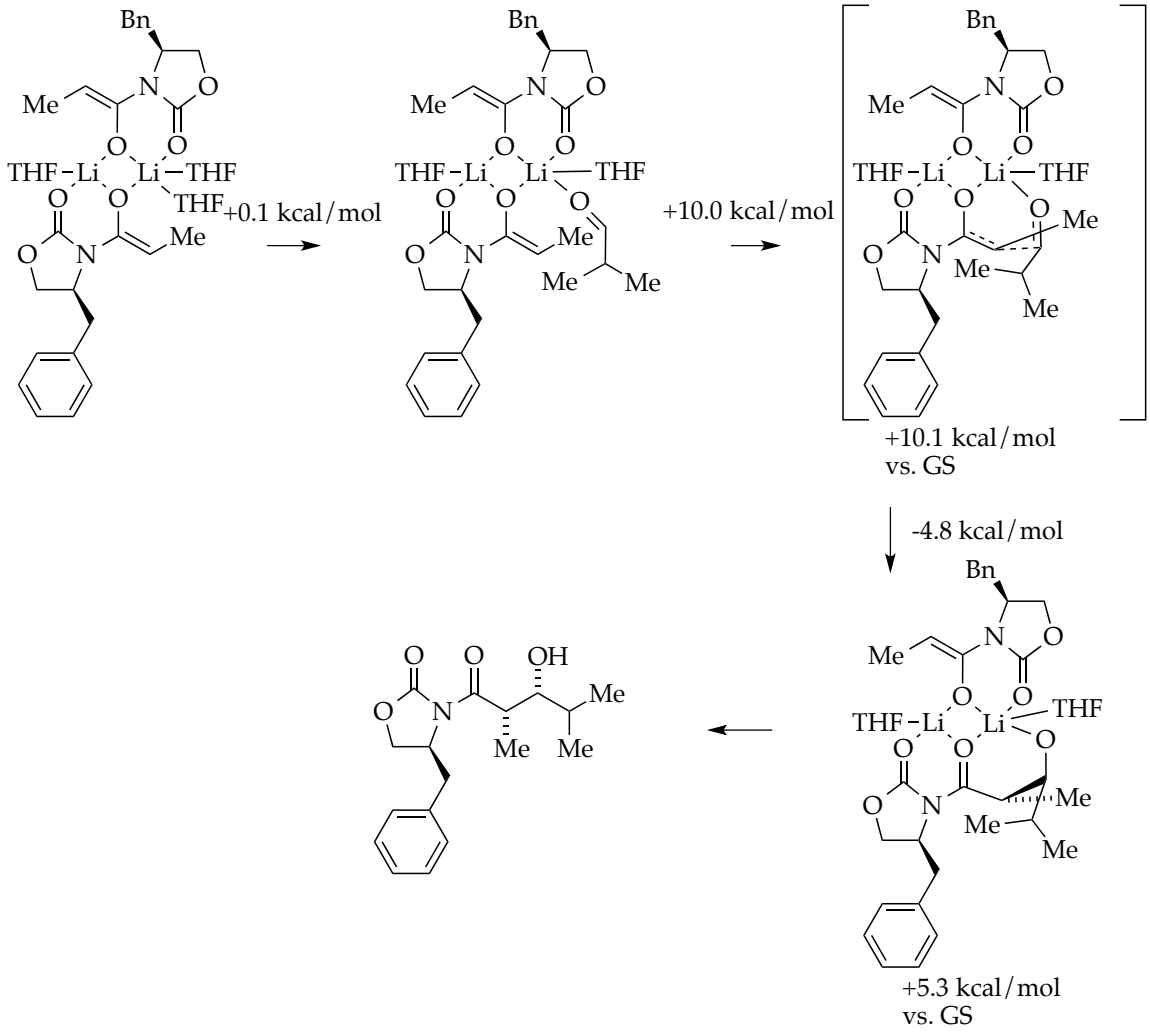


Figure 54. Computational overview of the pathway from dimer to (*S,S*)-**6**.

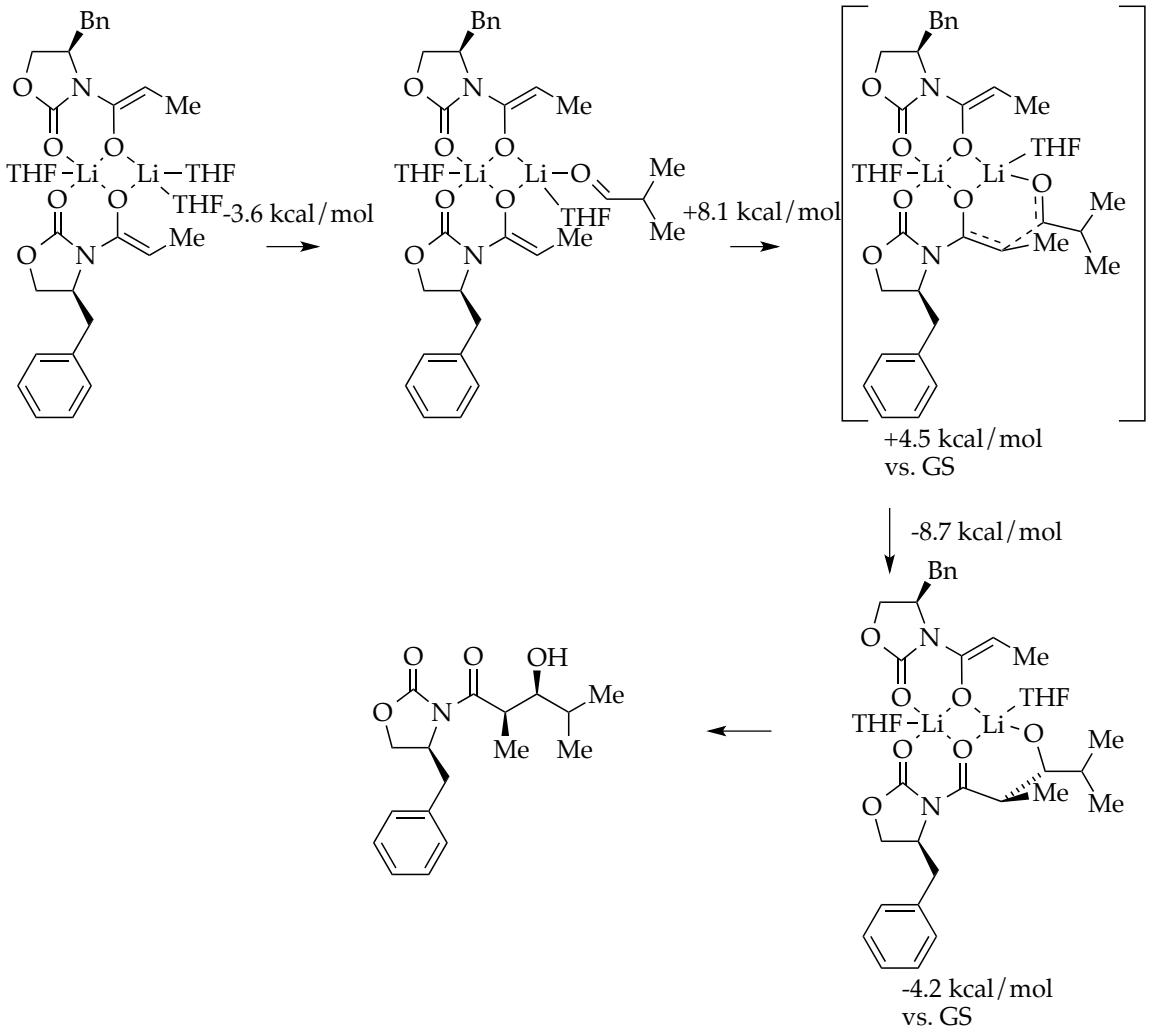


Figure 55. Computational overview of the pathway from spirocyclic dimer to (*R,S*)-**6**.

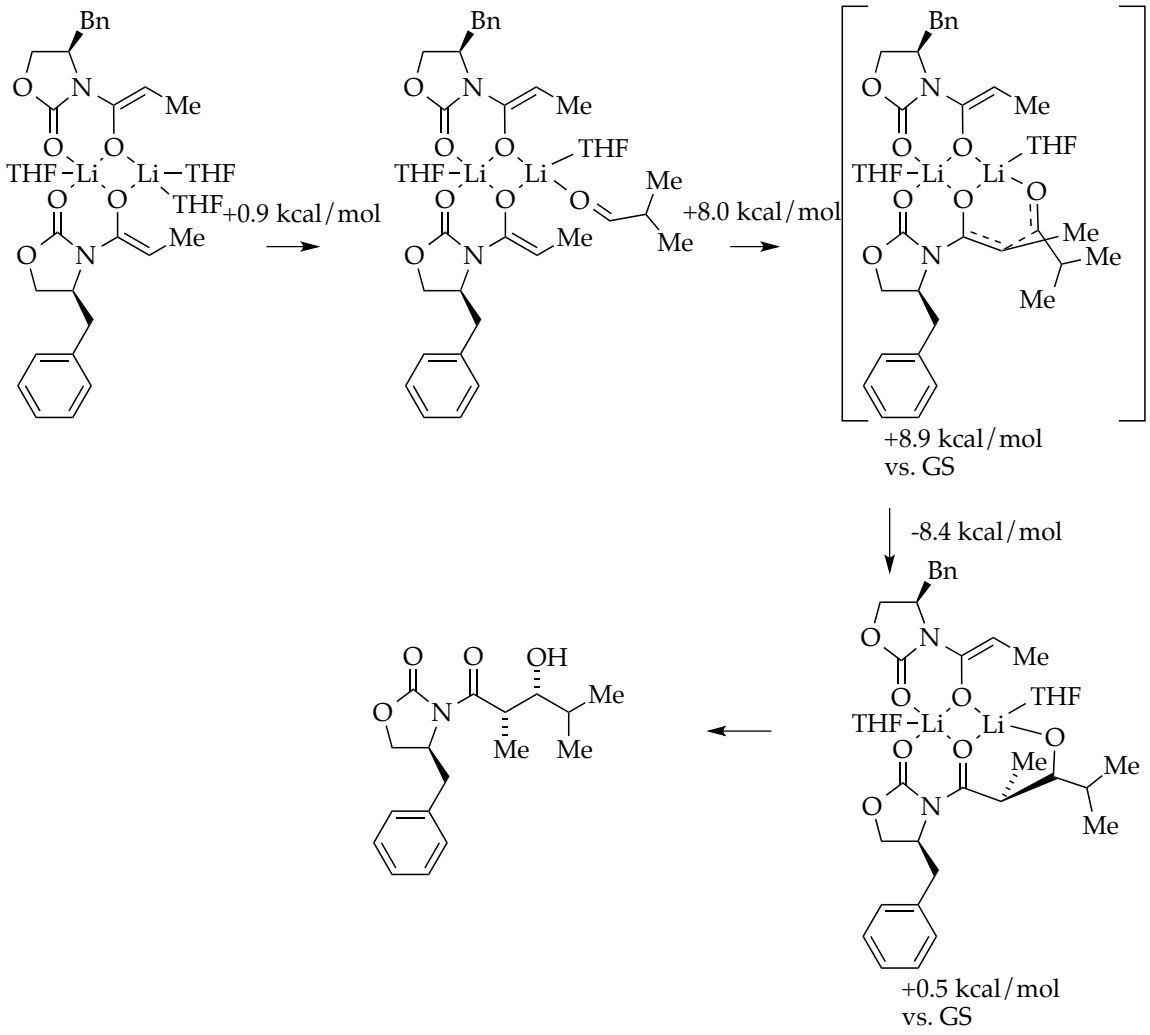


Figure 56. Computational overview of the pathway from spirocyclic dimer to (*S,R*)-**6**.

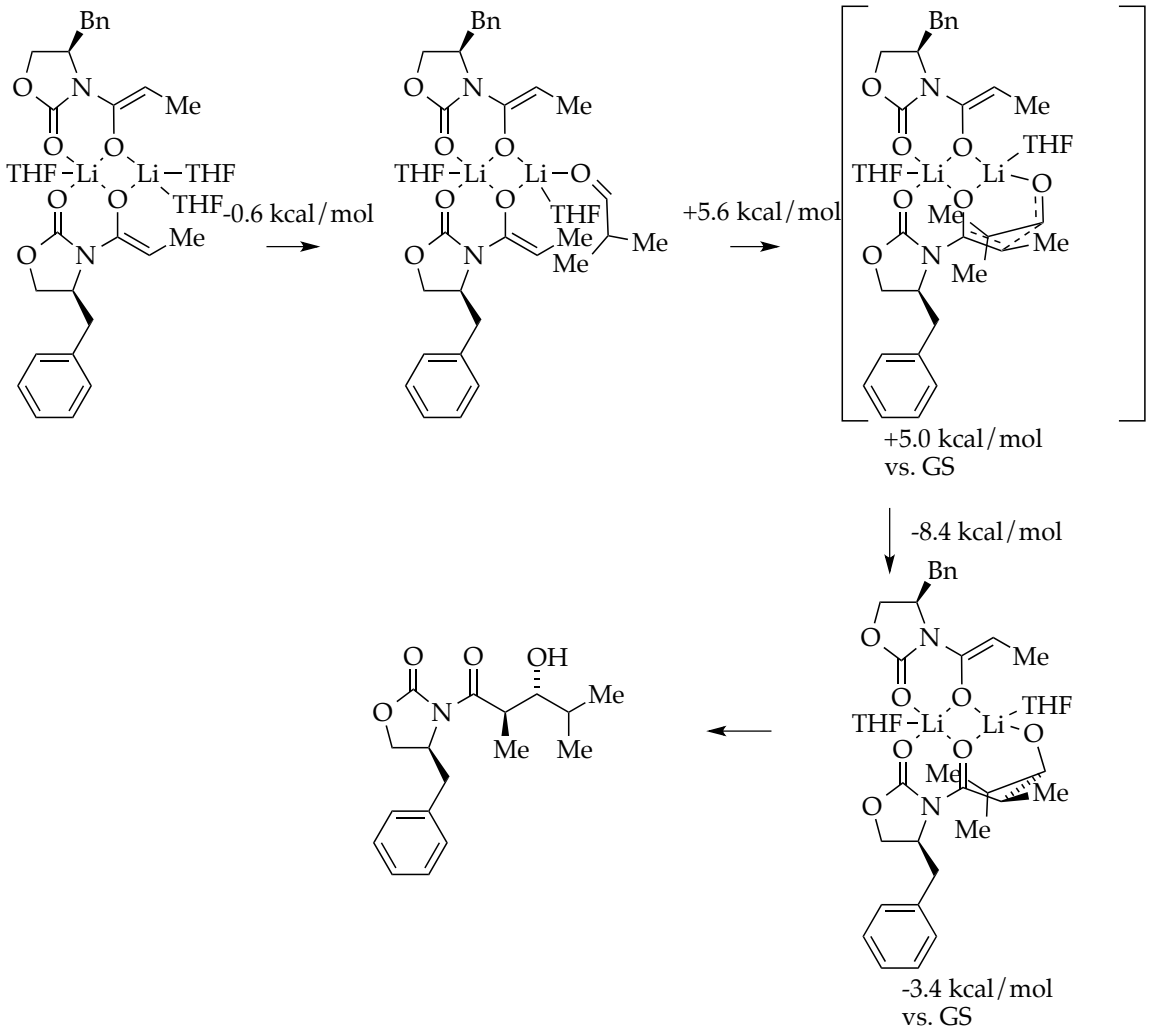


Figure 57. Computational overview of the pathway from spirocyclic dimer to (*R,R*)-**6**.

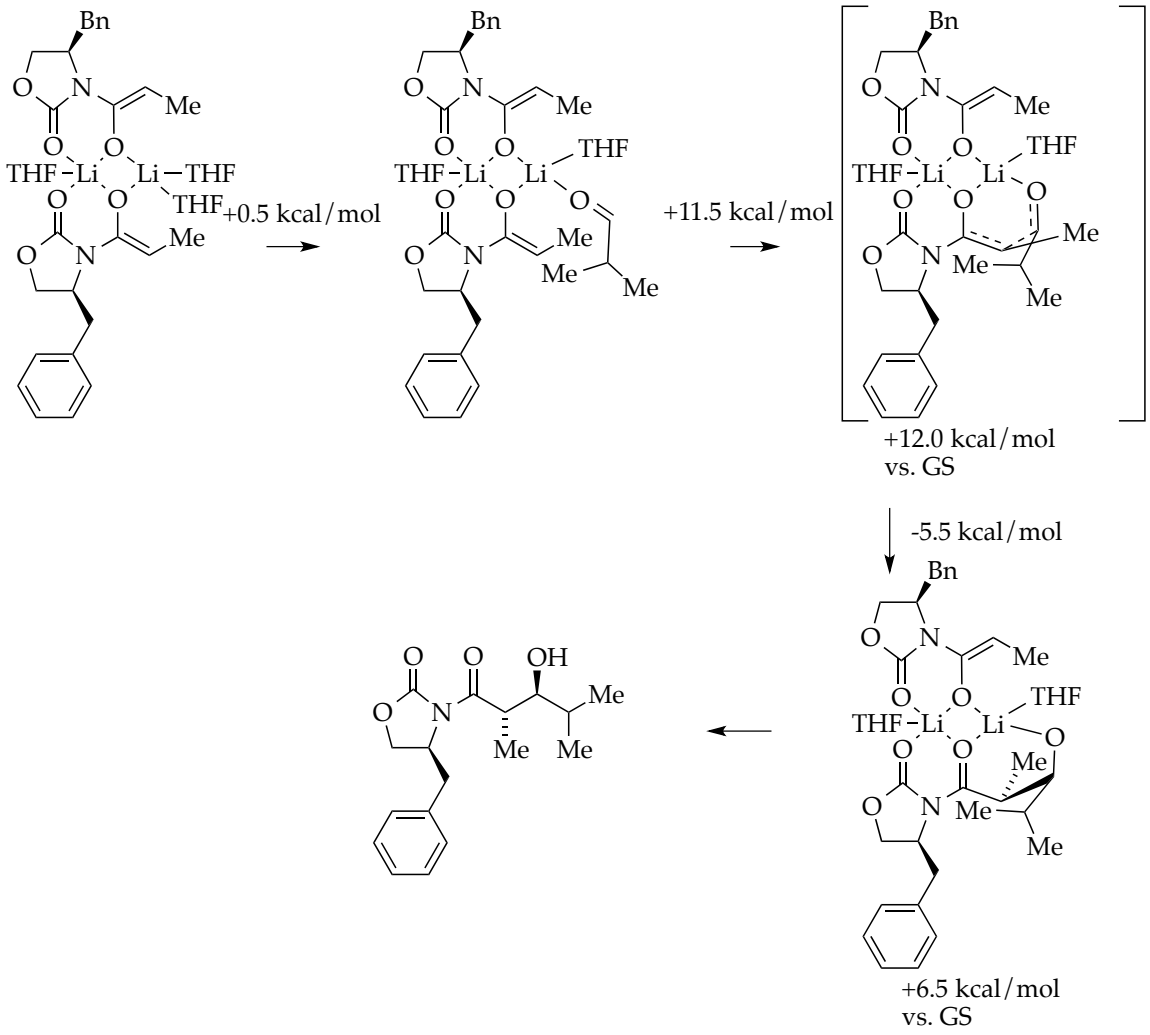


Figure 58. Computational overview of the pathway from spirocyclic dimer to (*S,S*)-**6**.

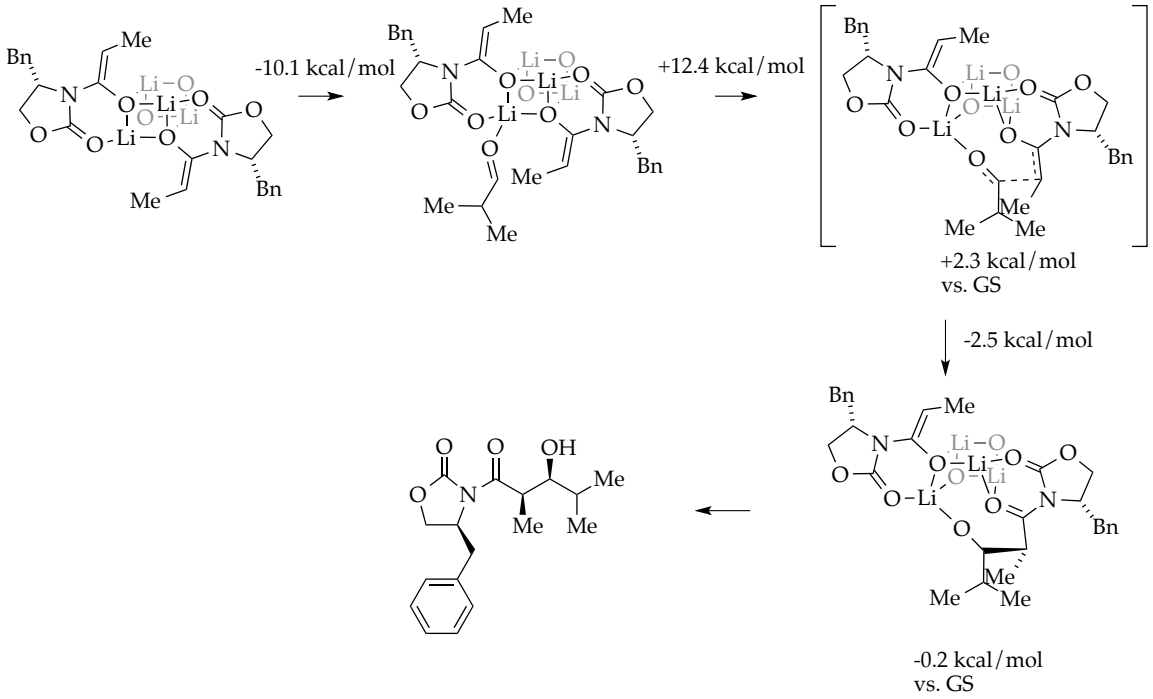


Figure 59. Computational overview of the pathway from tetramer to (*R,S*)-**6**.

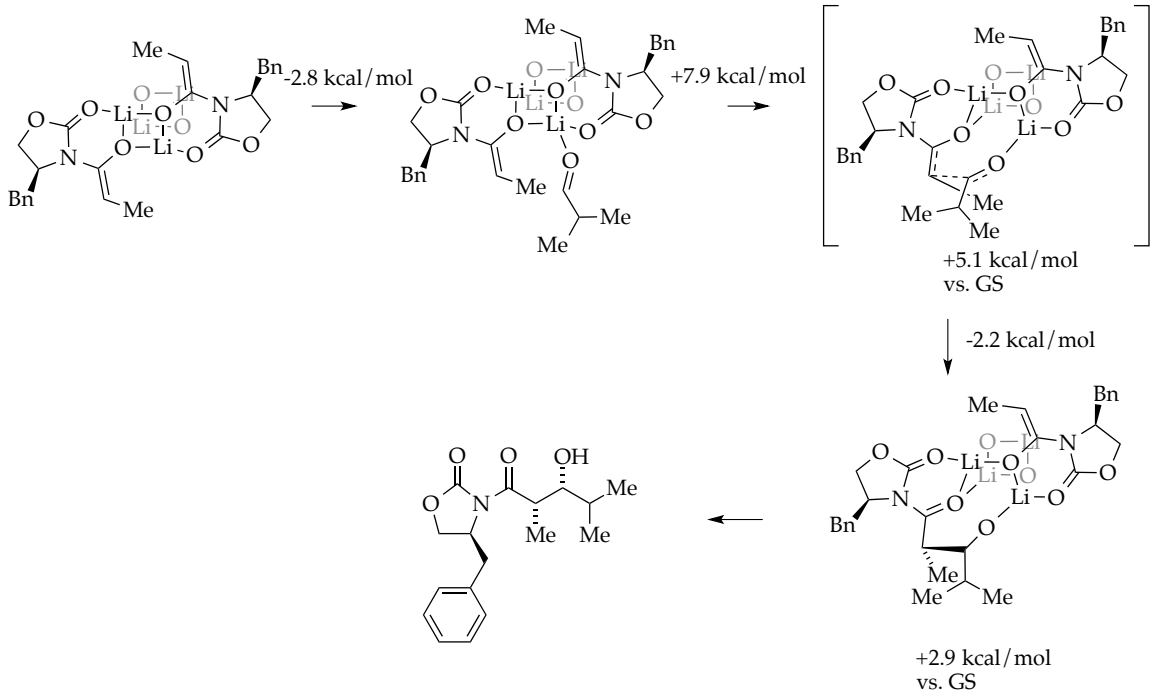


Figure 60. Computational overview of the pathway from tetramer to (*S*,*R*)-**6**.

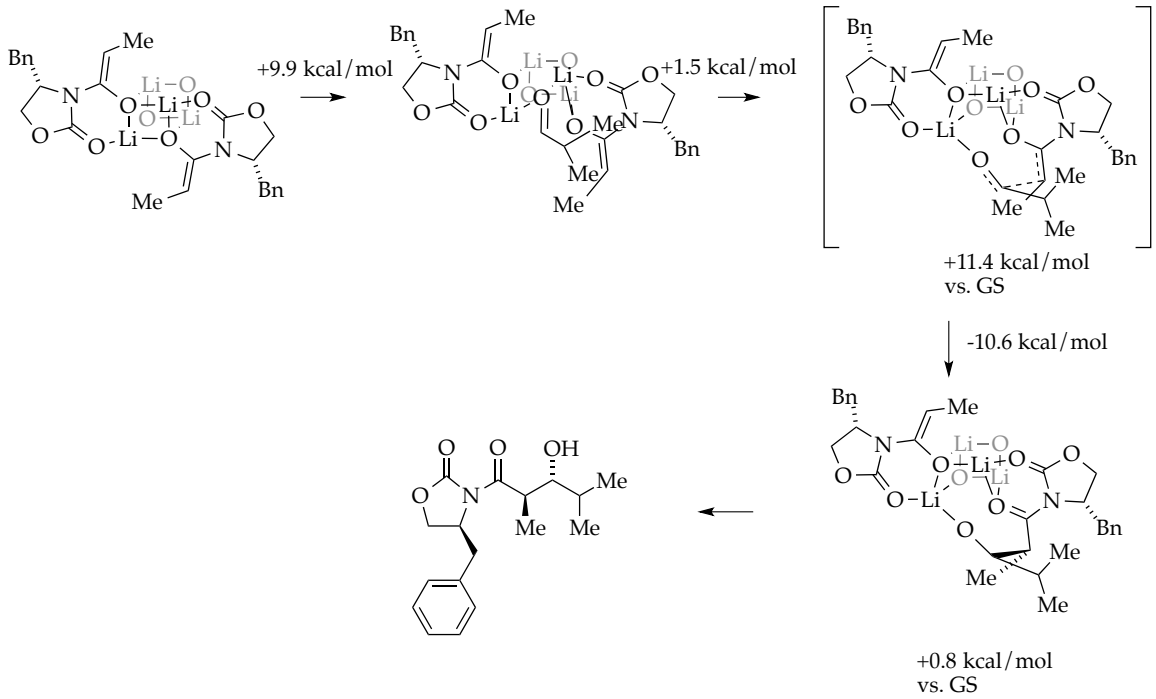


Figure 61. Computational overview of the pathway from tetramer to (*R,R*)-**6**.

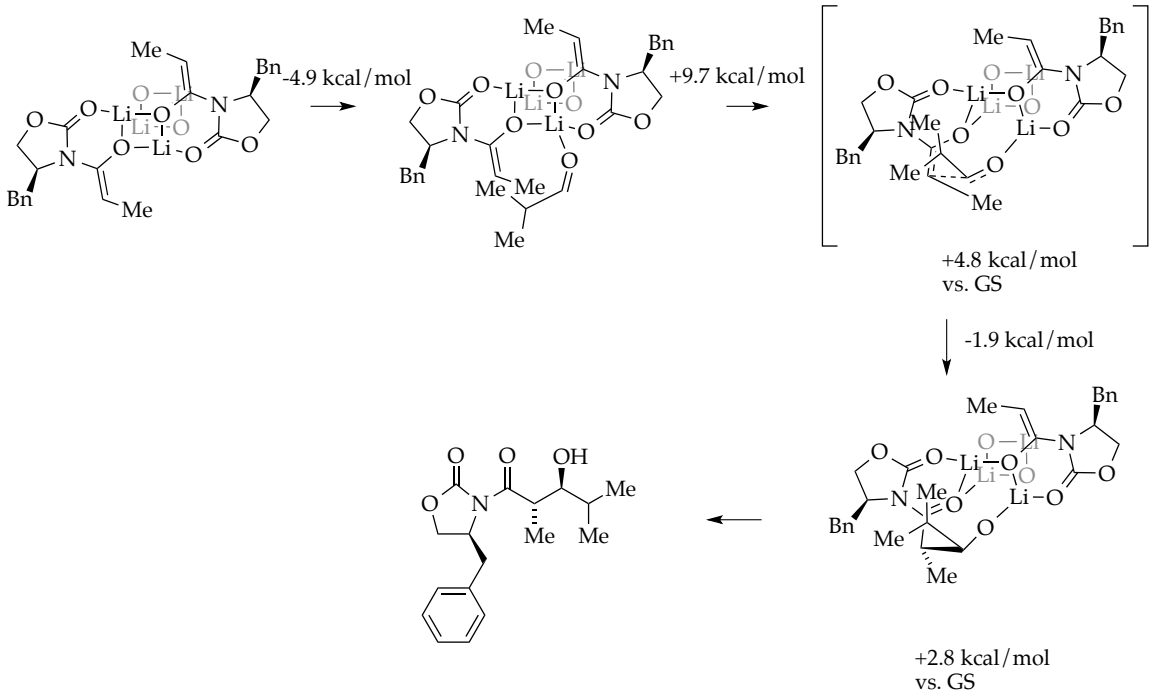


Figure 62. Computational overview of the pathway from tetramer to (*S,S*)-**6**.

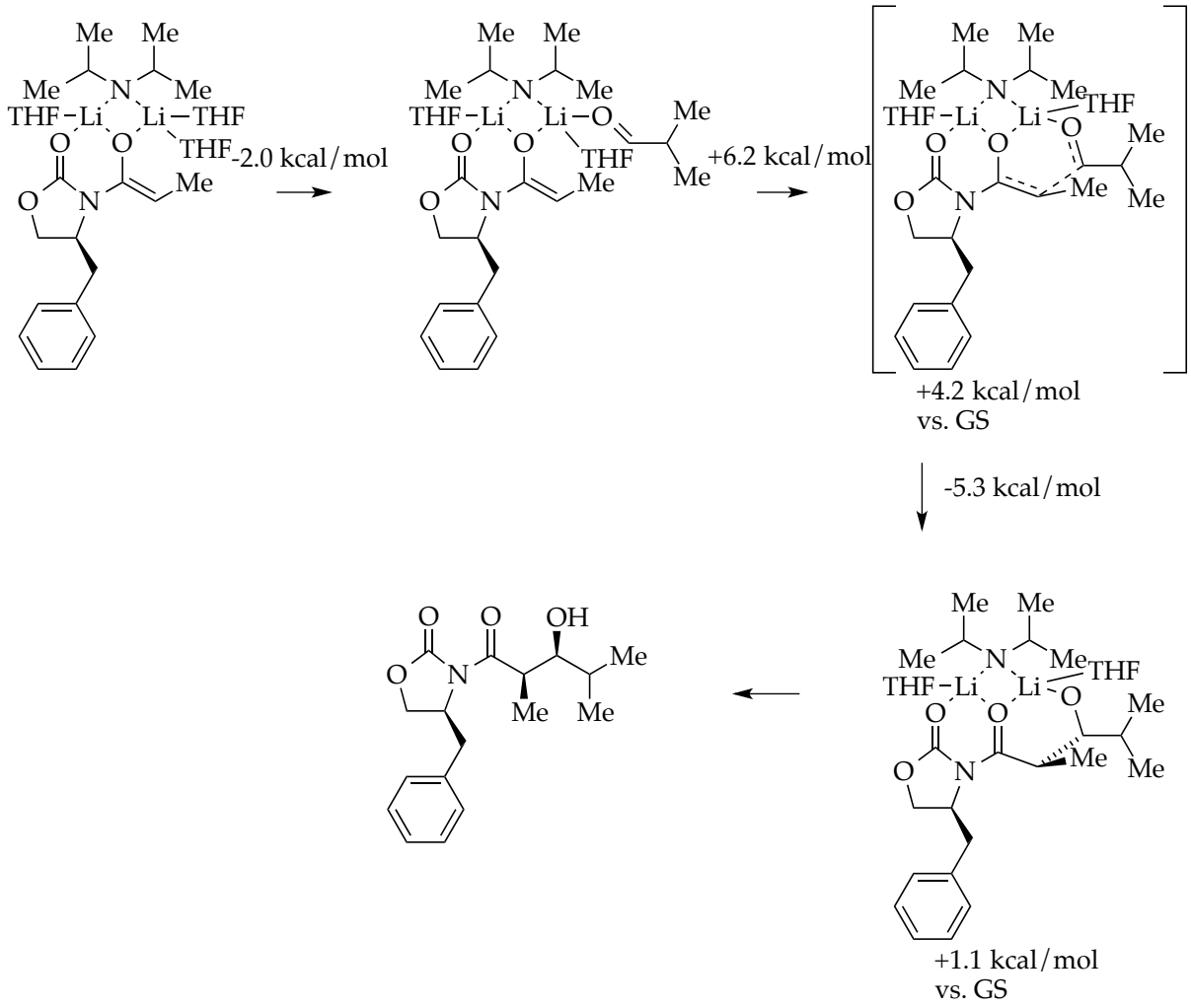


Figure 63. Computational overview of the pathway from LDA **5** mixed dimer to (*R,S*)-**6**.

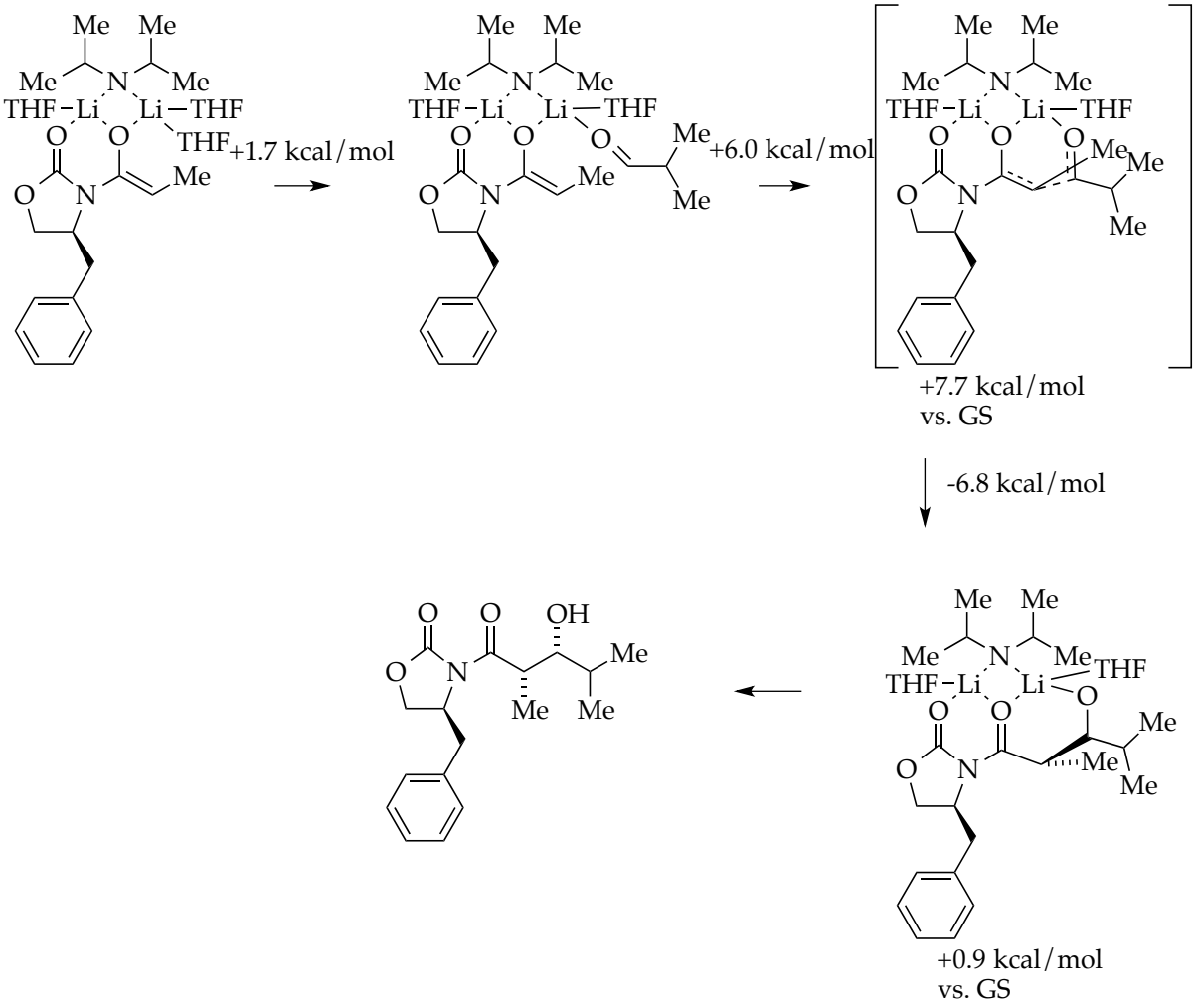


Figure 64. Computational overview of the pathway from LDA **5** mixed dimer to (*S,R*)-**6**.

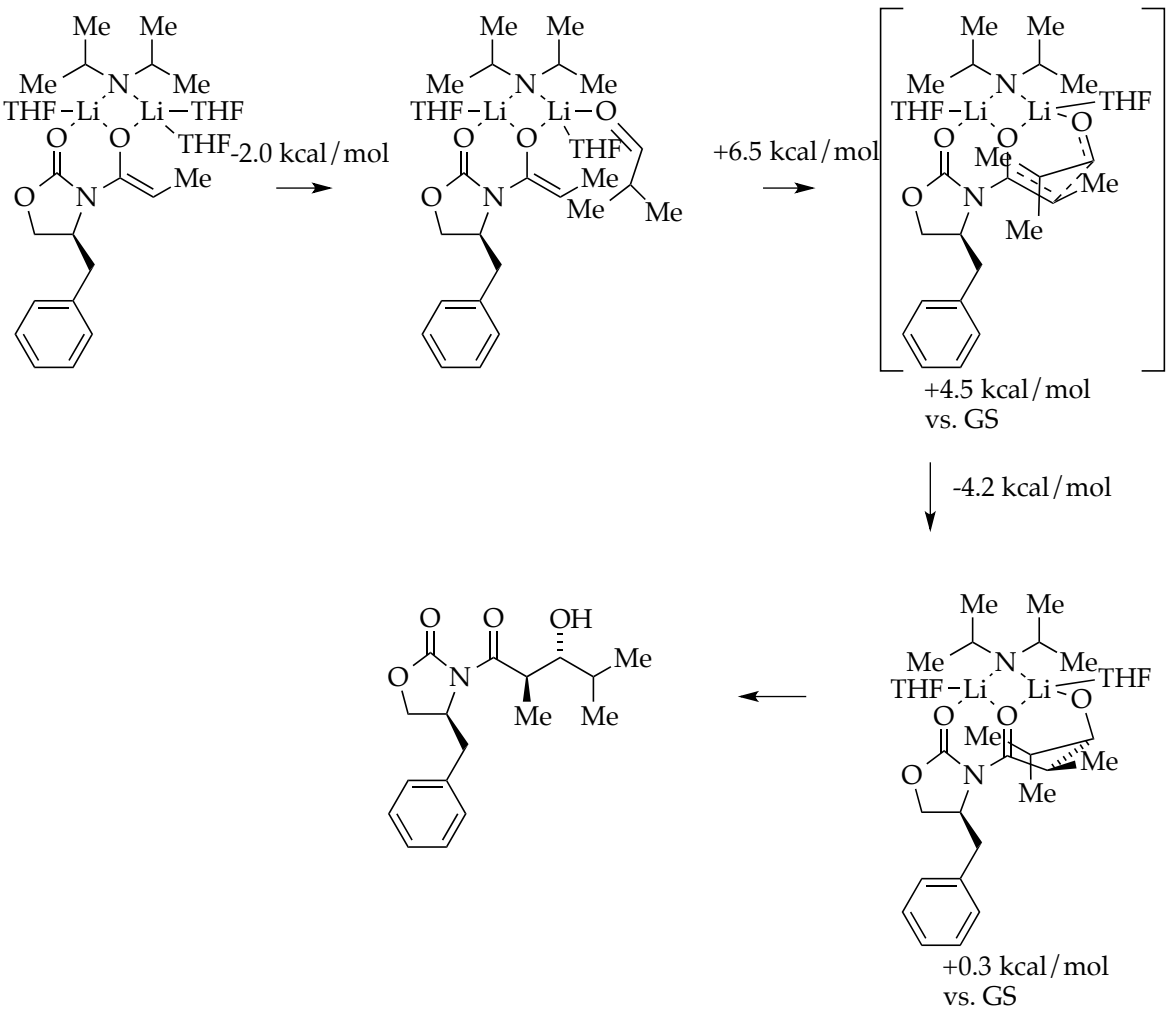


Figure 65. Computational overview of the pathway from LDA **5** mixed dimer to (*R,R*)-**6**.

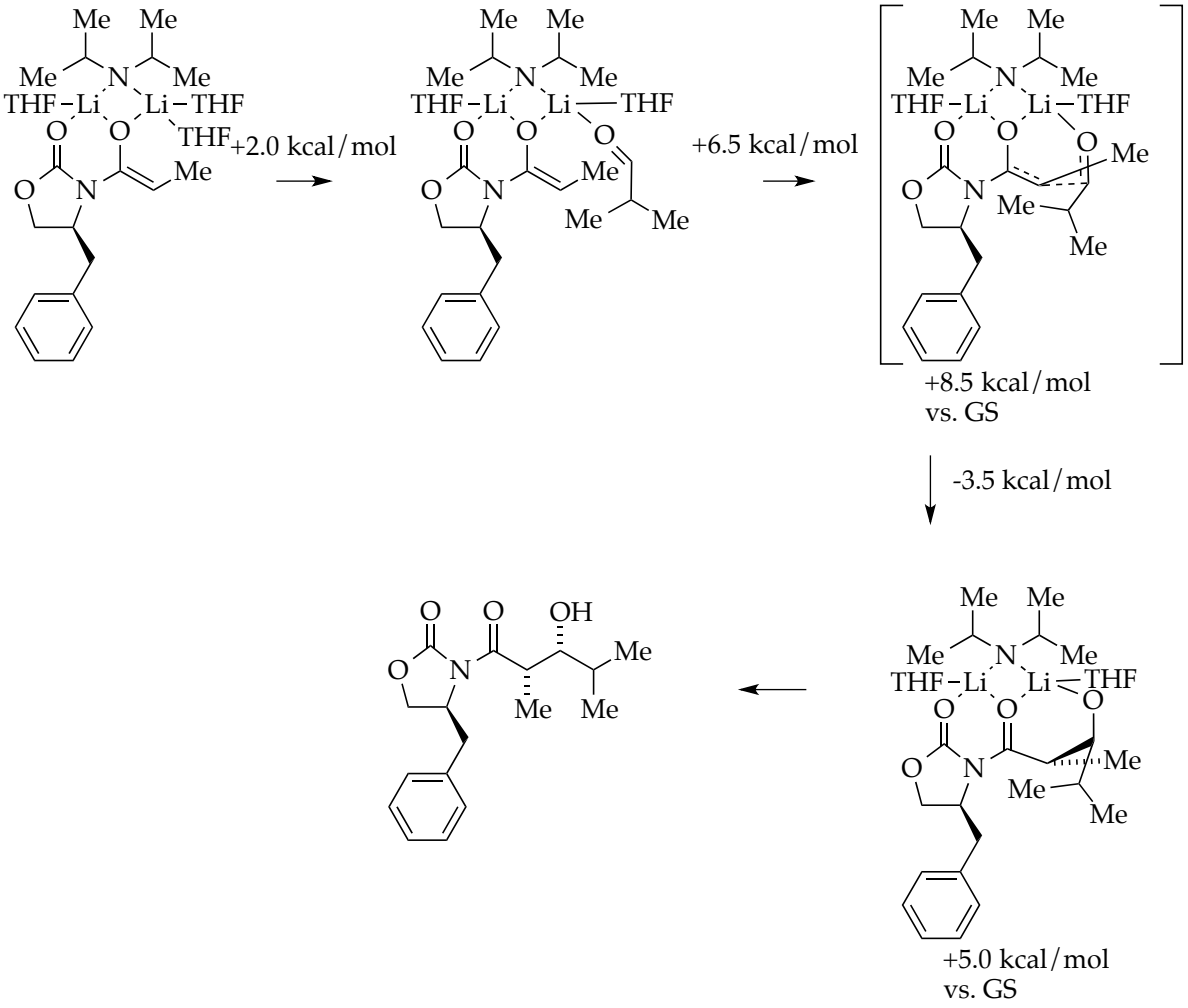
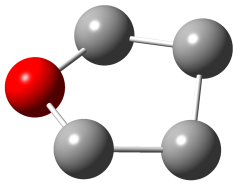


Figure 66. Computational overview of the pathway from LDA **5** mixed dimer to (*S,S*)-**6**.

Part 6: General Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

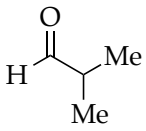
Table 5. Geometric coordinates and thermally corrected MP2 energies for tetrahydrofuran (THF)

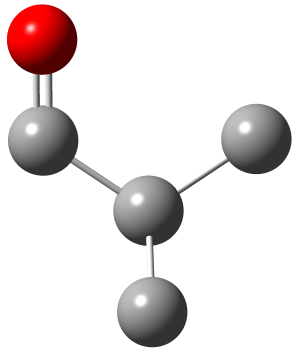


G = -232.349382 Hartree
G_{MP2} = -145312.2903 kcal/mol

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.43133070
C	1.34537191	0.00000000	1.92150203
C	2.24870259	-0.28439627	0.71435321
C	1.43346820	0.33130215	-0.43248249
H	1.58213073	1.41736875	-0.46518645
H	1.68560870	-0.07569023	-1.41670971
H	3.24887201	0.14691464	0.82158362
H	2.35937654	-1.36515207	0.56460786
H	1.57260400	0.98256813	2.36334488
H	1.43285191	-0.75428594	2.71251317
H	-0.30387867	-0.99259206	-0.36803060
H	-0.73798112	0.73090835	-0.35071740

Table 6. Geometric coordinates and thermally corrected MP2 energies for isobutyraldehyde

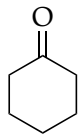


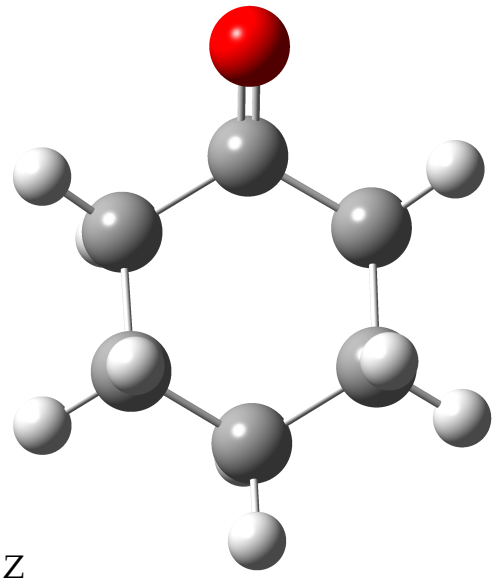


G = -232.363544 Hartree
G_{MP2} = -145322.0041 kcal/mol

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51804360
O	0.98871142	0.00000000	2.21741176
H	-1.01669442	-0.00432437	1.97783460
H	-0.50902248	0.93575331	-0.28845768
C	-0.86800891	-1.16691709	-0.51181954
H	-0.97665751	-1.11346435	-1.60000348
H	-0.40939475	-2.13183567	-0.26580587
H	-1.87266120	-1.14749642	-0.07289657
C	1.41716966	-0.01003020	-0.57458930
H	1.39119220	0.05645201	-1.66758937
H	2.00538647	0.82747058	-0.18828333
H	1.94065329	-0.93189492	-0.29918792

Table 7. Geometric coordinates and thermally corrected MP2 energies for cyclohexanone

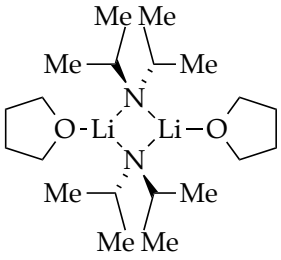


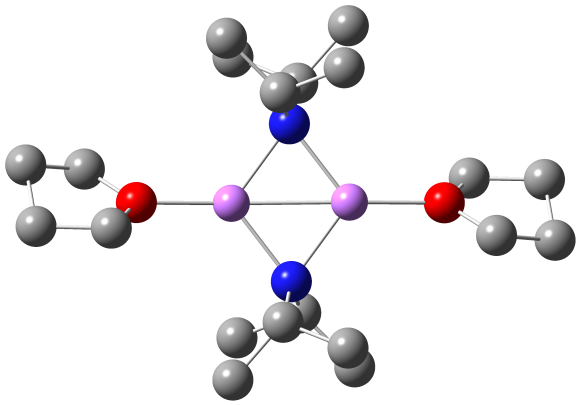


G = -309.757631 Hartree
G_{MP2} = -193725.0256 kcal/mol

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54381400
C	1.41495215	0.00000000	2.11171024
C	2.35410684	1.03938693	1.50983218
C	2.31681547	1.02291955	-0.03344341
C	0.88000532	1.12409962	-0.56472348
H	0.45353190	2.09914072	-0.28575894
H	0.88121541	1.08551480	-1.66105774
H	2.93295106	1.84117007	-0.42520537
H	2.77108858	0.08936311	-0.39372333
H	2.02458134	2.02901051	1.86299877
H	3.36124868	0.86626873	1.90029856
O	1.76860109	-0.77252106	2.98216716
H	-0.50074302	0.91402709	1.89945316
H	-0.54089889	-0.85661114	1.95662514
H	0.37513582	-0.96849679	-0.35913840
H	-1.02895696	0.09191125	-0.36801461

Table 8. Geometric coordinates and thermally corrected MP2 energies for Lithium Diisopropylamide (LDA) with two THF



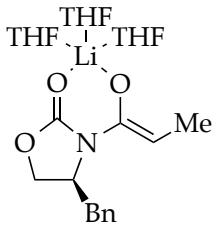


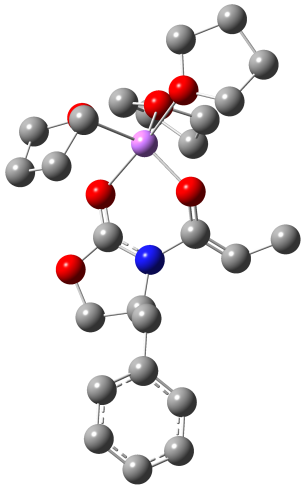
G = -1063.116483 Hartree
G_{MP2} = -664731.8875 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.81410663	1.86918792	0.52758664
Li	0.00000000	0.00000000	2.39346480	C	-0.80797530	3.64048612	-0.06969212
O	0.40731818	0.00000000	4.33666642	H	-1.76144100	4.13531583	-0.30044256
C	-0.31160577	0.75031532	5.34554741	H	-0.12686892	4.41415138	0.30277974
C	0.59705523	0.76867204	6.57773040	H	-0.38833529	3.25131946	-1.00453270
C	1.38039926	-0.54444431	6.42411418	C	-1.67694186	3.10542503	2.23352810
C	1.58550803	-0.61184065	4.91113852	H	-1.90764523	2.30725174	2.94980958
H	1.66334155	-1.62770125	4.51728807	H	-1.02725739	3.83103093	2.73422227
H	2.46883665	-0.03867321	4.59941701	H	-2.61874741	3.61787491	1.98945185
H	0.77815914	-1.39416582	6.76657132	N	-0.10056751	-1.58942643	1.19475018
H	2.32593881	-0.55203312	6.97432432	C	-1.45024064	-2.11026018	0.94660834
H	0.02933285	0.82892055	7.51087129	H	-2.01730929	-1.24034090	0.55530667
H	1.27894121	1.62608966	6.53832804	C	-2.25393575	-2.53615677	2.20621616
H	-0.52831103	1.74382359	4.94463141	H	-1.88302644	-3.47070131	2.63922295
H	-1.25863823	0.23405677	5.54777776	H	-2.18688374	-1.76102302	2.97989617
N	0.10065090	1.58940008	1.19844710	H	-3.31687937	-2.68187367	1.96567937
C	1.45061143	2.11134115	1.44268300	C	-1.61016658	-3.20211490	-0.13915451
H	2.01816461	1.24325327	1.83719553	H	-1.12639271	-2.89814436	-1.07426675
C	2.25270052	2.53174806	0.18014310	H	-1.17230114	-4.15778508	0.17079101
H	1.88051137	3.46383384	-0.25704450	H	-2.67263445	-3.38625648	-0.34991971
H	3.31574980	2.67957908	0.41893210	C	1.01809177	-2.50661996	1.42936074
H	2.18582944	1.75290378	-0.58986241	H	1.81259829	-1.87278768	1.86904874
C	1.61203409	3.20820544	2.52310583	C	0.80533963	-3.64782883	2.45331057
H	2.67477213	3.39277027	2.73208364	H	1.75848838	-4.14330662	2.68391971
H	1.17436550	4.16264437	2.20909523	H	0.38259405	-3.26483646	3.38929575
H	1.12904002	2.90893149	3.46012848	H	0.12597100	-4.41975376	2.07408838
C	-1.01845863	2.50549465	0.96165094	C	1.67956260	-3.09907875	0.15550803

H	1.91199021	-2.29654468	-0.55533363
H	2.62077364	-3.61310777	0.39856207
H	1.03082423	-3.82148659	-0.35101602
O	-0.40911863	0.00065978	-1.94291869
C	0.32168799	-0.73329970	-2.95513878
C	-0.58918940	-0.76559246	-4.18524867
C	-1.39441703	0.53377791	-4.02789288
C	-1.59749716	0.59561021	-2.51430010
H	-2.47134196	0.00877276	-2.20145036
H	-1.68988997	1.60970501	-2.11891500
H	-2.34108731	0.52609058	-4.57613032
H	-0.80739252	1.39406498	-4.37035596
H	-1.25623881	-1.63457594	-4.14535146
H	-0.02267117	-0.81489229	-5.11976866
H	1.25848431	-0.19892221	-3.15816049
H	0.55777425	-1.72358252	-2.55713091

Table 9. Geometric coordinates and thermally corrected MP2 energies for **5** monomer with three THF



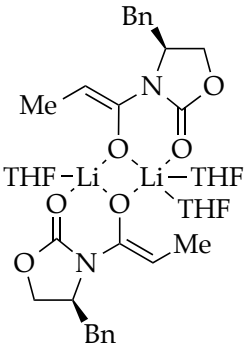


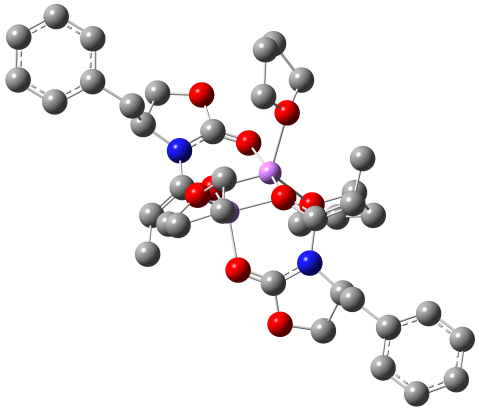
G = -1488.697668 Hartree
G_{MP2} = -931168.1672 kcal/mol
ΔG_{MP2} = 1.777728882 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	-2.85974559	2.47204057	-5.04842001
H	0.00000000	0.00000000	1.09594000	C	-1.34964607	2.25033660	-4.87083115
H	1.03066998	0.00000000	-0.35974383	C	-0.96978914	3.24248220	-3.73607744
C	-0.85316631	-1.14441615	-0.57725508	C	-2.32693566	3.82694767	-3.29082687
H	-0.98029291	-1.93649274	0.16534604	H	-2.50912249	4.80845278	-3.75440419
N	-2.11842155	-0.44096168	-0.80121795	H	-2.43639544	3.90177402	-2.21024045
C	-1.93456686	0.90087743	-0.80409189	H	-0.29145113	4.02946614	-4.08072996
O	-0.64453267	1.20553213	-0.45424963	H	-0.48651079	2.72260351	-2.90494278
O	-2.73602623	1.79426663	-1.06148375	H	-0.79773129	2.43127560	-5.79860894
C	-3.34485027	-1.08936684	-1.31776815	H	-1.15511072	1.21838809	-4.56204428
O	-3.94969478	-0.45044848	-2.25651827	H	-3.43105001	1.58350758	-5.31587396
Li	-4.21593375	1.39759846	-2.49053784	H	-3.05813696	3.26450037	-5.78780773
O	-5.57440760	1.08006719	-4.19391830	O	-5.77654675	2.12760340	-1.31084364
C	-6.63423766	2.00849569	-4.49905687	C	-5.55171938	3.20328131	-0.36813717
C	-7.86470437	1.16241863	-4.89526286	C	-6.20389452	2.76558038	0.95139395
C	-7.48655499	-0.25387141	-4.42289714	C	-6.18305332	1.23294871	0.83754632
C	-5.96920194	-0.24331523	-4.59354319	C	-6.44674952	1.02758075	-0.65219153
H	-5.69196602	-0.41288884	-5.64697535	H	-7.52277834	1.07753907	-0.87734773
H	-5.42006442	-0.93340955	-3.95272046	H	-6.02719185	0.10468583	-1.05784732
H	-7.97754996	-1.04411460	-4.99970343	H	-6.92952530	0.74144810	1.46927937
H	-7.74046493	-0.39221189	-3.36576493	H	-5.19541249	0.83775181	1.09814018
H	-8.00653569	1.17357414	-5.98212222	H	-7.23714986	3.12819324	1.01272392
H	-8.78746392	1.53393194	-4.43899665	H	-5.66267094	3.14306848	1.82431946
H	-6.80171037	2.60700094	-3.59975795	H	-4.47055600	3.33292473	-0.26424186
H	-6.31410918	2.67479076	-5.31025337	H	-5.98776997	4.12185564	-0.77686145
O	-3.32136783	2.90205065	-3.76041224	C	-3.65265587	-2.28855273	-0.75162469

H	-3.05586139	-2.64819289	0.08202871
C	-4.80763651	-3.13596707	-1.20166318
H	-5.28107373	-2.69786790	-2.08585431
H	-4.49742560	-4.15938598	-1.46344715
H	-5.58542299	-3.23902695	-0.42809985
C	-0.29872778	-1.76128376	-1.88291290
H	-1.10608630	-2.36181030	-2.31660968
H	-0.07845946	-0.95007159	-2.58790179
C	0.92905743	-2.61367528	-1.65328589
C	0.80857337	-3.88536082	-1.07149601
C	1.93417077	-4.67054093	-0.82518845
C	3.20612267	-4.19847288	-1.15865892
C	3.34091939	-2.93853995	-1.74203639
C	2.21070224	-2.15475958	-1.98548926
H	2.32357864	-1.17786268	-2.45129386
H	4.32519422	-2.56475485	-2.01236111
H	4.08366141	-4.81104786	-0.96983251
H	1.81846032	-5.65458290	-0.37810616
H	-0.17999370	-4.26448076	-0.82042804

Table 10. Geometric coordinates and thermally corrected MP2 energies for **5** dimer with three THF



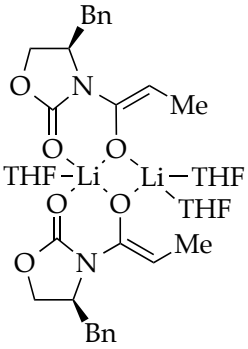


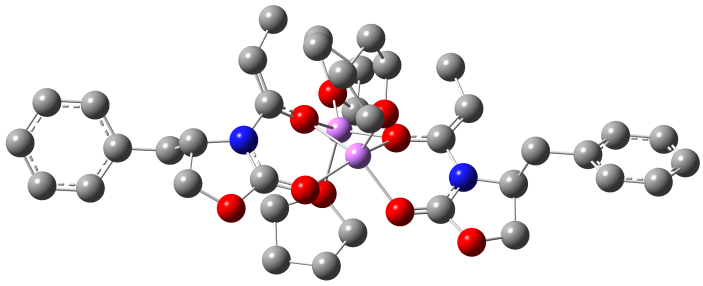
G = -2280.364885 Hartree
G_{MP2} = -1426402.09 kcal/mol
ΔG_{MP2} = 0.464733826 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.01503670	-1.91847151	-3.09335609
O	0.00000000	0.00000000	2.09165270	C	-4.63738511	-0.24444646	-1.86884380
C	0.99342614	0.00000000	2.92031074	H	-4.65688413	-0.80630148	-0.92799016
N	1.35790556	-1.31744840	3.45956960	H	-4.26822896	0.76228810	-1.63740089
C	2.56016196	-1.59371484	4.25589949	C	-6.02304792	-0.17499475	-2.47070542
C	2.69389166	-3.10082569	4.01566581	C	-6.52422398	1.01688896	-3.01127189
H	3.28970852	-3.32774722	3.12388995	C	-7.79327332	1.06592495	-3.59233283
H	3.08959768	-3.65072230	4.87091330	C	-8.58428306	-0.08200330	-3.64294606
O	1.33842747	-3.52980655	3.78567089	C	-8.09927586	-1.27666425	-3.10502875
C	0.61810509	-2.45833344	3.33951555	C	-6.83209370	-1.32052062	-2.52466066
O	-0.53172776	-2.62126051	2.94395121	H	-6.46623006	-2.25219015	-2.09776763
Li	-1.40648311	-1.23455606	1.90689905	H	-8.71140586	-2.17448575	-3.13269963
O	-1.51931076	-1.21005511	0.04284567	H	-9.57282570	-0.04630622	-4.09284627
C	-2.10322095	-1.87011204	-0.91261454	H	-8.16372082	2.00248014	-4.00121262
N	-2.31124588	-1.10492024	-2.14788611	H	-5.91847749	1.91974592	-2.96570610
C	-3.61455113	-0.94601960	-2.79377029	C	-2.57268915	-3.14171282	-0.92038581
C	-3.20408559	-0.12653378	-4.03156278	C	-2.51463799	-4.07748817	0.25310929
H	-3.02663598	-0.76560011	-4.90400252	H	-3.49784619	-4.22365210	0.73022749
H	-3.92124598	0.65268466	-4.29624722	H	-2.17053731	-5.07515484	-0.05321954
O	-1.96007706	0.49962652	-3.66444034	H	-1.82373156	-3.72053407	1.02269769
C	-1.41327035	-0.20250651	-2.61866675	H	-2.99976656	-3.52264780	-1.84452985
O	-0.27332877	0.01906335	-2.23413517	O	-3.05684484	-0.79601339	2.99063715

C	-3.73293446	-1.88287944	3.67130715
C	-3.99883526	-1.39581749	5.10465580
C	-2.93348887	-0.30328514	5.29270751
C	-2.87332658	0.31272248	3.89679561
H	-1.91739946	0.77793082	3.64597446
H	-3.68448258	1.04034412	3.74672057
H	-1.96551540	-0.74898021	5.54843321
H	-3.19328189	0.42576568	6.06651105
H	-3.92101197	-2.20547658	5.83636819
H	-5.00327860	-0.96382360	5.18649221
H	-4.65036860	-2.12158338	3.12323247
H	-3.06775763	-2.75178563	3.64851321
H	3.40864007	-1.04259418	3.84399633
C	2.36379984	-1.24336279	5.75441647
H	2.00086572	-0.21276789	5.81525278
H	1.56911011	-1.88679566	6.15219384
C	3.62684159	-1.41173845	6.57053396
C	4.67443452	-0.48389166	6.46263395
C	5.85297833	-0.64472326	7.19041397
C	6.00683617	-1.73937737	8.04448791
C	4.97270022	-2.66777565	8.16531966
C	3.79460207	-2.50323371	7.43345004
H	2.98877931	-3.22628726	7.54177627
H	5.07891459	-3.51973402	8.83186893
H	6.92375559	-1.86384556	8.61423792
H	6.65006320	0.08813656	7.09520311
H	4.56091358	0.37828175	5.80852951
C	1.74204533	1.06830151	3.31586929
H	2.53273475	0.94198701	4.04598933
C	1.48882385	2.46406972	2.81625263
H	0.88934411	2.44509583	1.90195053
H	0.95726403	3.08984048	3.55268320
H	2.42908239	2.98822003	2.59189110
O	1.95039740	-0.53940289	-0.30104156
C	3.01066083	0.43326776	-0.18837346
C	4.23159562	-0.21769199	-0.84052911
C	3.58024837	-1.06066299	-1.94818025
C	2.30254031	-1.55757141	-1.26565303
H	2.47149455	-2.49894500	-0.72635721
H	1.45970583	-1.67968865	-1.94808768
H	4.21286758	-1.88111916	-2.30110089
H	3.33038284	-0.42837161	-2.80817736
H	4.75128748	-0.86379840	-0.12224776
H	4.94893926	0.51806875	-1.21742955
H	2.71711376	1.34649492	-0.72500813
H	3.13145610	0.67037836	0.87190492
O	-0.43464958	2.06821086	-0.12169904
C	-1.68392735	2.44700904	0.50030975
C	-2.13374394	3.73997457	-0.19545659
C	-1.43959934	3.64357360	-1.56382563
C	-0.11539018	2.97785463	-1.19151905
H	0.61523850	3.71715369	-0.83065384
H	0.32366584	2.39097183	-1.99983444
H	-1.30279422	4.61487808	-2.04978348
H	-2.00155405	2.99444720	-2.24494312
H	-1.77084626	4.61814051	0.35196101
H	-3.22355182	3.81623910	-0.26445268
H	-2.39499499	1.62595679	0.35177415
H	-1.51338682	2.56604152	1.57390323

Table 11. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer with three THF



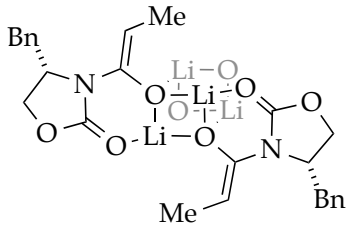


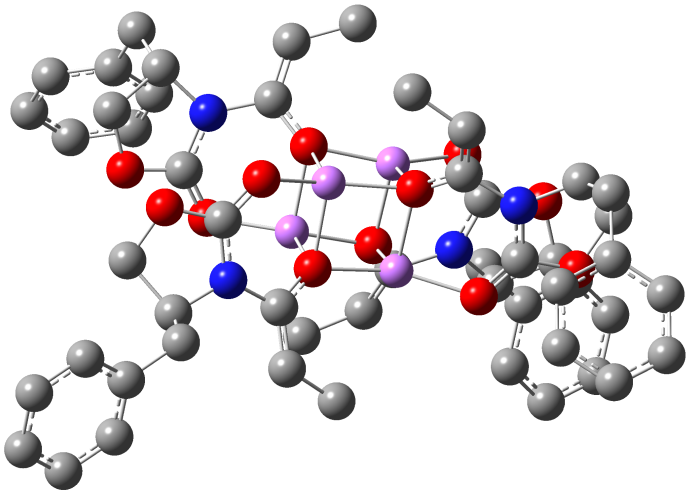
G = -2280.364091 Hartree
G_{MP2} = -1426403.019 kcal/mol
ΔG_{MP2} = 0 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.72451744	0.37921376	0.95129433
Li	0.00000000	0.00000000	2.64675340	C	3.40445209	1.47805017	-0.44200456
O	1.42158727	0.00000000	1.22252404	H	3.75304414	2.50246430	-0.23523650
C	2.70017616	-0.07916138	1.40962945	H	3.90707471	1.16684569	-1.37206797
N	3.10345919	-0.95148272	2.51077992	H	2.33134404	1.53059606	-0.64603361
C	2.24401552	-1.59208037	3.36604910	O	-1.25466153	0.77082323	1.15133164
O	1.02776929	-1.53558835	3.45652268	C	-2.33903443	1.40665717	1.45839205
O	2.95882065	-2.39081439	4.21870318	N	-3.27833763	0.65456561	2.29930224
C	4.32759506	-2.42201987	3.78251697	C	-4.73077112	0.64653867	2.11514336
H	4.48391403	-3.32016850	3.17279330	C	-5.15945031	-0.19230477	3.33455295
H	4.97166502	-2.46372992	4.66237868	H	-5.46704343	0.43695706	4.17750621
C	4.48596158	-1.13545883	2.96439887	H	-5.95582010	-0.90507751	3.11186467
H	5.14564339	-1.29616799	2.10814527	O	-3.98265630	-0.92407155	3.71747341
C	4.98459092	0.06752915	3.80594591	C	-2.88523435	-0.30024934	3.18921826
H	4.81620975	0.97388572	3.21573878	O	-1.75637968	-0.61489450	3.53628732
H	4.35267569	0.14276369	4.69925115	H	-5.13504286	1.65956339	2.19261179
C	6.43976478	-0.04987625	4.20176893	C	-5.14236853	0.04544446	0.75033303
C	7.45608840	0.16992794	3.25907166	H	-4.57047773	0.57672072	-0.01918190
C	8.79973480	0.03606866	3.60749060	H	-4.83084267	-1.00595533	0.72401781
C	9.15487827	-0.31987133	4.91080470	C	-6.62556416	0.16297190	0.47851334
C	8.15613350	-0.53668423	5.86036806	C	-7.47800246	-0.94331326	0.59278459
C	6.81188336	-0.40240949	5.50642505	C	-8.85096762	-0.81906738	0.36880409
H	6.03960493	-0.56195990	6.25609898	C	-9.39471475	0.41901075	0.02600697
H	8.42103710	-0.80659621	6.87943467	C	-8.55630339	1.52988565	-0.09550580
H	10.20173676	-0.42171454	5.18406992	C	-7.18599739	1.40099612	0.12789485
H	9.57085847	0.21525196	2.86257466	H	-6.53770853	2.26833267	0.02029446
H	7.19038623	0.45962248	2.24437674	H	-8.96986830	2.49680664	-0.37034986
C	3.68347372	0.54005379	0.69736431	H	-10.46236076	0.51786082	-0.15067490

H	-9.49325448	-1.69130201	0.45869457
H	-7.06051600	-1.91499147	0.84860301
C	-2.72074104	2.66317182	1.10517845
C	-1.91011929	3.55844301	0.21332943
H	-1.68514161	4.52274127	0.69339912
H	-0.95638209	3.08635815	-0.04003593
H	-2.42612375	3.79961309	-0.73005537
H	-3.64979027	3.06163447	1.50268644
O	0.56543717	1.56534458	3.82778622
C	0.81848338	2.80623787	3.12105374
C	0.19293384	3.92431721	3.97287657
C	-0.83394886	3.16523622	4.83023380
C	-0.11190468	1.84035697	5.06675306
H	-0.76883216	0.99278082	5.27297151
H	0.62610727	1.92902097	5.87845697
H	-1.75134312	2.99488354	4.25567237
H	-1.09103855	3.68309251	5.75993680
H	-0.25934893	4.70673045	3.35625016
H	0.94884927	4.39480471	4.61322193
H	1.89953055	2.92034042	2.98818019
H	0.35016021	2.71692712	2.13801124
O	-0.47667988	-1.98146162	-0.35773118
C	-1.88852367	-2.30284384	-0.34434523
C	-2.03521251	-3.60983883	0.45533688
C	-0.73445918	-3.66009543	1.27479345
C	0.26292025	-3.02676331	0.30947420
H	0.61977938	-3.75107342	-0.43864421
H	1.11486739	-2.55160894	0.79620809
H	-0.45154159	-4.67669763	1.56574388
H	-0.81418570	-3.04994509	2.17958617
H	-2.09680523	-4.47023546	-0.22172596
H	-2.93235790	-3.61166843	1.08185553
H	-2.40341643	-1.46224768	0.12998612
H	-2.24101976	-2.39757185	-1.37842868
O	0.21839509	0.51320090	-1.92850377
C	-0.06066991	1.75496831	-2.60661915
C	0.27203018	1.49708002	-4.07594739
C	1.45504793	0.52320790	-3.96030531
C	1.05687665	-0.33279684	-2.75343972
H	1.90973550	-0.66075765	-2.15252042
H	0.47144132	-1.21172592	-3.04508163
H	2.37968865	1.07287969	-3.75018783
H	1.61358423	-0.07716333	-4.86120721
H	0.51685549	2.41594037	-4.61724649
H	-0.57435396	1.01711052	-4.58180258
H	-1.10637647	2.01280937	-2.42293687
H	0.57588163	2.54552465	-2.18653644

Table 12. Geometric coordinates and thermally corrected MP2 energies for **5** D_{2d} tetramer



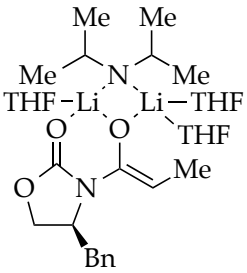


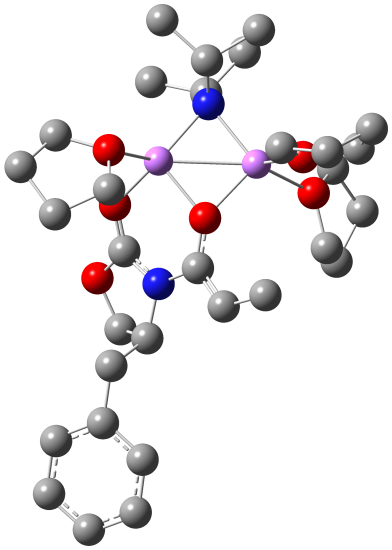
G = -3166.662534 Hartree
G_{MP2} = -1980930.794 kcal/mol
ΔG_{MP2} = 0.375561044 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.92064642	2.98500716	-4.25853369
O	0.00000000	0.00000000	1.89861070	H	-2.82262435	2.37091814	-4.30870624
C	1.05585130	0.00000000	2.52402978	N	-0.95399263	2.35428375	-3.34779468
O	1.12651741	-0.59231240	3.74489124	C	-1.30389776	1.62759451	-2.14149057
C	2.50137875	-0.59782195	4.18227305	C	-2.51844401	1.82556346	-1.57783798
H	2.91749791	-1.59017164	3.98345487	H	-3.18305215	2.57926802	-1.98217944
H	2.50872415	-0.39220160	5.25391674	C	-2.99438943	1.06416526	-0.37019718
C	3.17781310	0.49877718	3.34189588	H	-2.59131260	0.04451436	-0.34260460
H	4.16626791	0.18314087	2.99581318	H	-2.71374752	1.54719054	0.57873746
N	2.26657711	0.53607049	2.19012104	H	-4.08745118	0.97571288	-0.36893686
C	2.64016857	0.95192206	0.85098338	O	-0.38806896	0.77865933	-1.73170696
C	3.69779669	1.77859681	0.67780146	Li	-0.01973221	-1.03106286	-2.49492021
H	4.21004590	2.18878057	1.53828089	O	-0.29270694	-1.07497797	-4.37329619
C	4.20137889	2.17854646	-0.68327539	C	0.60921506	-0.76095601	-5.14394454
H	3.67767766	3.05574343	-1.09407348	O	0.31566577	-0.20466281	-6.34840040
H	5.26669231	2.43481941	-0.64615718	C	1.54258265	0.21819224	-6.97883753
H	4.09136604	1.36805456	-1.41464629	H	1.65326183	1.29511017	-6.81933748
O	1.91456735	0.42211923	-0.10906251	H	1.45933624	0.00014348	-8.04479982
Li	1.55502468	0.97865032	-1.93350744	C	2.64015445	-0.59357477	-6.26983272
O	1.39380755	2.30442534	-3.29685634	H	3.52025717	0.02194645	-6.06248136
C	0.30965783	2.50810502	-3.83698836	N	1.96141851	-0.88569767	-5.00006409
O	0.25857136	2.98092212	-5.11391698	C	2.63442461	-1.13326491	-3.73847330
C	-1.11762441	2.92962831	-5.56274456	C	3.91025443	-1.58519171	-3.73829876
H	-1.26428982	1.99018207	-6.10391756	H	4.39538785	-1.83534211	-4.67272286
H	-1.29118253	3.78066966	-6.22229477	C	4.70369053	-1.77659578	-2.47342918

H	4.54491543	-2.76383502	-2.01229470
H	5.77877359	-1.68808094	-2.66917762
H	4.45237947	-1.02447135	-1.71511423
O	1.92589375	-0.83362023	-2.67215027
Li	2.02399625	-1.43203668	-0.82819381
O	2.48122320	-2.71027372	0.51335988
C	1.60387382	-3.22923745	1.19859453
O	1.88658772	-3.66540840	2.45817005
C	0.64238730	-4.03523705	3.10095144
H	0.28979213	-3.17627251	3.67956500
H	0.83916284	-4.88287767	3.75835927
C	-0.28210093	-4.36744056	1.92457225
H	-1.31338985	-4.06383030	2.11811287
N	0.29868188	-3.48779868	0.89960133
C	-0.42951179	-2.93396175	-0.22670589
C	-1.58962902	-3.51306422	-0.61497172
C	-2.44650780	-2.96492025	-1.72406874
H	-2.39445369	-1.87080114	-1.78073969
H	-2.16391030	-3.35247264	-2.71528466
H	-3.50018829	-3.22708096	-1.57058009
H	-1.92146240	-4.42685102	-0.13735196
O	0.10745189	-1.85154012	-0.74380530
C	-0.21934411	-5.86457803	1.52546649
H	-0.67956097	-5.98204870	0.53947201
H	0.83546271	-6.14444563	1.41482335
C	-0.89574915	-6.76737888	2.53527464
C	-0.14783387	-7.58159975	3.39621336
C	-0.77562379	-8.39588797	4.34147672
C	-2.16692970	-8.40718045	4.44117447
C	-2.92556148	-7.60256720	3.58762981
C	-2.29466474	-6.79220938	2.64443602
H	-2.89585652	-6.17648166	1.97840309
H	-4.01039066	-7.60954720	3.65349266
H	-2.65798285	-9.04089709	5.17467872
H	-0.17618863	-9.02312141	4.99610882
H	0.93731670	-7.58697907	3.31700307
C	3.08848239	-1.84352170	-7.07867600
H	3.52522479	-1.46694662	-8.01314308
H	3.90061567	-2.33790231	-6.53813405
C	1.99971230	-2.84876529	-7.38587567
C	1.39296970	-2.89817868	-8.64807137
C	0.38241242	-3.82094751	-8.92323591
C	-0.03606692	-4.71354003	-7.93611004
C	0.56816950	-4.68316579	-6.67737120
C	1.57967297	-3.76167261	-6.40590449
H	2.05355824	-3.75092519	-5.42748951
H	0.25589155	-5.38118221	-5.90519611
H	-0.82240822	-5.43314494	-8.14759130
H	-0.07362597	-3.84413160	-9.90958802
H	1.72300798	-2.21555350	-9.42887887
C	-2.27063653	4.43620771	-3.83881216
H	-2.59797238	4.42768235	-2.79451128
H	-1.35105396	5.03309284	-3.87459170
C	-3.33214590	5.05957908	-4.72022930
C	-4.66965354	4.64507999	-4.62662679
C	-5.65006310	5.19637888	-5.45075399
C	-5.31053114	6.17692870	-6.38600986
C	-3.98574503	6.60169457	-6.48757954
C	-3.00673072	6.04574187	-5.66104625
H	-1.97767295	6.39055064	-5.73850614
H	-3.71196117	7.36883396	-7.20718153
H	-6.07446573	6.60887797	-7.02677761
H	-6.68075303	4.86372387	-5.35985339
H	-4.94703174	3.88859036	-3.89523453
C	3.32644400	1.84430271	4.10679056
H	3.98833360	1.64375929	4.95970592
H	3.85779343	2.55437463	3.46677069
C	2.03507475	2.46758824	4.59071825
C	1.63137114	2.35463825	5.92787246
C	0.43453407	2.92317978	6.36694327
C	-0.37837431	3.61838011	5.47132229
C	0.01754474	3.74871394	4.13839016
C	1.21540686	3.18176551	3.70287015
H	1.52311115	3.29660402	2.66647921
H	-0.60412635	4.29701291	3.43561711
H	-1.31053469	4.06221548	5.81040796
H	0.14086640	2.82589022	7.40890901
H	2.26617602	1.82667188	6.63698233

Table 13. Geometric coordinates and thermally corrected MP2 energies for LDA **5** mixed dimer with three THF





G = -1787.915892 Hartree
G_{MP2} = -1118227.787 kcal/mol

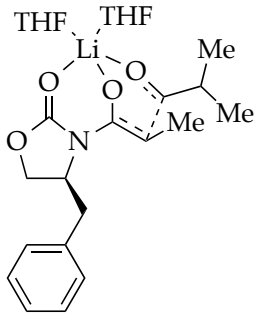
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.60424514	0.17761214	-2.32042560
O	0.00000000	0.00000000	1.95527310	H	-2.59045835	-0.56851309	-3.12149205
C	0.81677532	0.00000000	2.96012211	H	-3.41988556	0.88159084	-2.54563655
N	0.86336440	-1.25049413	3.72021522	H	-1.65758240	0.72808454	-2.35735951
C	1.79873533	-1.52869629	4.81768955	C	-4.15093636	-1.20719898	-0.89977196
C	1.73906511	-3.05949988	4.82987813	H	-4.97307454	-0.52050149	-1.14664786
H	2.47498393	-3.50931433	4.15309160	H	-4.18220751	-2.02305911	-1.63132648
H	1.84234736	-3.49590858	5.82446021	H	-4.35095076	-1.63489513	0.08886877
O	0.41878550	-3.35356258	4.33777452	C	-1.30184465	-2.51169766	-0.81578543
C	-0.01030452	-2.29654314	3.58584778	H	-0.27908561	-2.69076714	-0.43384351
O	-1.05352614	-2.38130518	2.95222075	C	-1.21224699	-2.74465874	-2.34488342
Li	-1.60196420	-1.01790348	1.65312489	H	-0.75201513	-3.71877729	-2.56400519
O	-3.17268196	-0.16877952	2.65474479	H	-2.20243431	-2.74703528	-2.81543969
C	-4.14611398	-1.06788624	3.24103793	H	-0.61428407	-1.96586672	-2.83144184
C	-4.49450081	-0.48672830	4.61974407	C	-2.13643300	-3.66823885	-0.19591145
C	-3.24907053	0.35031306	4.95412108	H	-2.16431602	-3.57777562	0.89509827
C	-2.86645497	0.89408490	3.57906752	H	-3.16684010	-3.68211951	-0.56560736
H	-1.80693666	1.13203475	3.46290128	H	-1.68823204	-4.64366739	-0.43710313
H	-3.46500004	1.78098483	3.32297081	H	2.79615785	-1.16844311	4.55482436
H	-2.44858932	-0.29022317	5.34201444	C	1.33464490	-0.89955373	6.15763737
H	-3.44178883	1.14227780	5.68457171	H	1.13712428	0.16230775	5.98083211
H	-4.70210151	-1.26811167	5.35686772	H	0.37930906	-1.36155505	6.43642879
H	-5.37823608	0.15904441	4.55541500	C	2.34315313	-1.07456927	7.27209315
H	-5.00957212	-1.13231849	2.57142406	C	3.51581682	-0.30401532	7.29926346
H	-3.68121045	-2.05630954	3.31902711	C	4.46504201	-0.47785123	8.30583652
N	-1.62880436	-1.15561486	-0.35706991	C	4.25800259	-1.42742768	9.30920869
C	-2.79402158	-0.45997865	-0.91510556	C	3.09455192	-2.19706269	9.29851281
H	-2.94590531	0.40138762	-0.24044276	C	2.14726157	-2.02041747	8.28760766

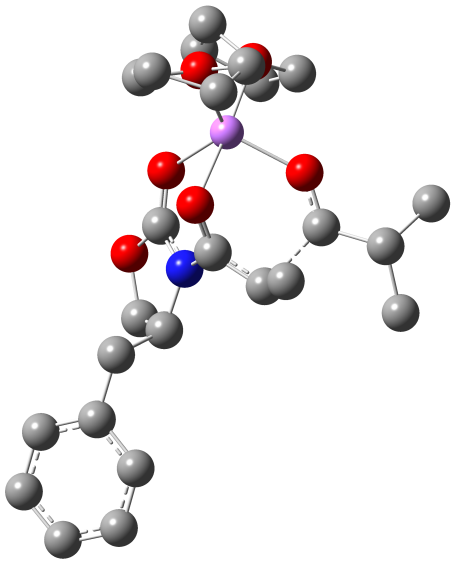
H	1.23707324	-2.61666664	8.29299534
H	2.91980715	-2.93331473	10.07868455
H	4.99570111	-1.56134536	10.09574262
H	5.36451024	0.13235824	8.31064683
H	3.68120297	0.44691548	6.52927166
C	1.64274449	1.01148344	3.35192052
H	2.27420385	0.89551893	4.22458771
C	1.70128412	2.33429163	2.63984709
H	1.21296861	2.27146624	1.66338001
H	1.20945069	3.14221604	3.20615909
H	2.73849715	2.66203795	2.47719136
O	1.88498098	-0.40807203	-0.73275030
C	3.06609920	-0.08405751	0.03289678
C	4.02250377	-1.25102408	-0.20177448
C	3.72754416	-1.60212551	-1.66828398
C	2.21365993	-1.36841124	-1.76585118
H	1.64280187	-2.28135772	-1.57158429
H	1.90271879	-0.96425905	-2.73461539
H	4.00553554	-2.62601657	-1.93533071
H	4.26900447	-0.92134143	-2.33594323
H	3.76381068	-2.09069817	0.45432199
H	5.06815984	-0.98316738	-0.02116547
H	3.49330235	0.85740839	-0.34324412
H	2.76589838	0.05440411	1.07390894
O	-0.04598026	1.98298805	-0.57443947
C	-1.04981245	2.89659415	-0.08657295
C	-0.62465764	4.26987350	-0.60387140
C	-0.02240942	3.91081410	-1.97174993
C	0.66222143	2.56670067	-1.68780703
H	1.71163779	2.69575247	-1.39583512
H	0.61760305	1.87530657	-2.53519427
H	0.67700653	4.66215392	-2.35083385
H	-0.81893016	3.78416484	-2.71383240
H	0.13889366	4.70533971	0.05158547
H	-1.46114362	4.97217859	-0.67056435
H	-2.02872455	2.60073968	-0.48455330
H	-1.06845886	2.81126843	1.00241946

Part 7: 5 Transition State Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table 14. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from **5** monomer with three THF



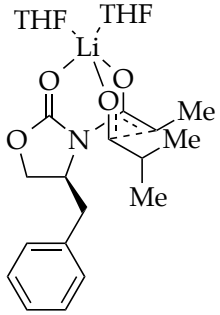


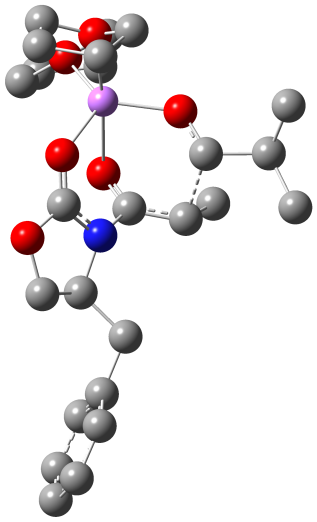
G = -1488.69909 Hartree
G_{MP2} = -931170.4794 kcal/mol
ΔG_{MP2} = 6.531685891 kcal/mol Li vs. **5** monomer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	5.05193591	-3.90326165	7.28607937
O	0.00000000	0.00000000	2.15556350	C	4.16581346	-4.74212579	6.61001325
C	1.20062383	0.00000000	2.47767107	C	3.24895865	-4.20712962	5.70238675
N	1.97103832	-1.20781342	2.19458027	H	2.55228897	-4.86689863	5.18944977
C	2.91332871	-1.83538791	3.12487302	H	4.18280963	-5.81364856	6.79089025
C	3.39473684	-3.02261048	2.26570781	H	5.76454979	-4.31693908	7.99440090
H	4.34717093	-2.81121555	1.76799426	H	5.69261424	-1.86426901	7.58114424
H	3.48136648	-3.95411249	2.82745700	H	4.06256665	-0.92145872	5.98018721
O	2.38430583	-3.19258906	1.25280409	C	1.93624316	1.13447809	2.88014613
C	1.64175263	-2.05449704	1.16783916	H	2.94347803	0.96294765	3.25321074
O	0.84492345	-1.87762509	0.25979921	C	1.17052078	2.28514934	3.49199597
H	3.74685984	-1.16141202	3.34290784	H	0.37923757	2.62165650	2.81386095
C	2.23046005	-2.24554761	4.45088017	H	0.68831756	2.00963020	4.44088752
H	1.74862970	-1.35126303	4.86388087	H	1.82928584	3.13569423	3.69680825
H	1.43236340	-2.96276377	4.22396484	O	-2.02954268	0.27161761	0.01905202
C	3.20064796	-2.82872548	5.45493994	C	-2.84930198	-0.49856166	0.93069781
C	4.09441295	-1.99653035	6.14618464	C	-3.76435425	0.50803037	1.64010979
C	5.01219787	-2.52660747	7.05238657	C	-2.93600264	1.80071258	1.57703249

C	-2.28123078	1.68427402	0.20172996
H	-1.32300433	2.20467757	0.12318397
H	-2.94918912	2.03320270	-0.59875597
H	-2.16317218	1.79208208	2.35171284
H	-3.53879481	2.70834845	1.68284199
H	-4.00457651	0.19847548	2.66180519
H	-4.70678206	0.62958898	1.09218573
H	-3.40179096	-1.24568747	0.34997682
H	-2.18037927	-1.00488010	1.63243841
O	1.22715139	1.48237075	0.17240745
C	2.30382453	1.64579631	0.82786101
C	2.89188560	3.06244442	0.93600396
H	2.14177250	3.70288202	1.41620274
C	3.10514990	3.59528557	-0.49581938
H	3.47114950	4.62910691	-0.47427359
H	3.84826854	2.99126014	-1.03406897
H	2.16902652	3.56452116	-1.05908314
C	4.20300843	3.11866115	1.72868316
H	4.93820175	2.41460509	1.31600851
H	4.64593702	4.12003153	1.67537859
H	4.06279806	2.87469001	2.78609371
H	3.09149910	0.86811514	0.74421368
O	-0.00556598	-0.11678488	-2.09442228
C	1.19653392	0.16940843	-2.82034110
C	1.80293621	-1.20417751	-3.16863974
C	0.58919039	-2.17343267	-3.10212171
C	-0.59134782	-1.25367396	-2.73730822
H	-1.30584452	-1.69273205	-2.03858001
H	-1.13331794	-0.92146235	-3.63642608
H	0.74200968	-2.91887535	-2.31877819
H	0.41478786	-2.69727551	-4.04733109
H	2.55964922	-1.49056634	-2.43274217
H	2.28137023	-1.19345537	-4.15320429
H	0.94065681	0.73102377	-3.73233590
H	1.81125989	0.79588538	-2.17377396

Table 15. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,R*)-**6** from **5** monomer with three THF



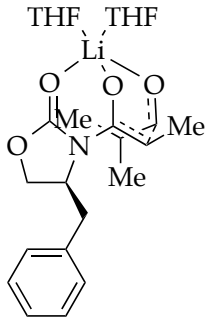


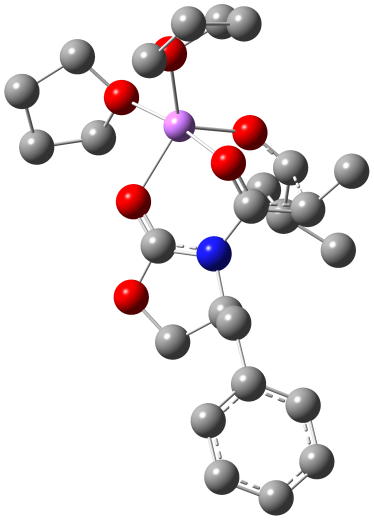
G = -1488.69661 Hartree
G_{MP2} = -931169.8852 kcal/mol
ΔG_{MP2} = 7.995805982 kcal/mol Li vs. **5** monomer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.01150355	0.96856660	-3.13050929
O	0.00000000	0.00000000	-2.25660410	C	1.27555155	2.36057617	-3.33316593
C	1.21404718	0.00000000	-2.52403508	H	0.51573312	2.69578007	-2.61838346
N	1.94433679	-1.27354972	-2.33066760	H	0.76093430	2.16077634	-4.28350353
C	2.37672209	-2.10744518	-3.46781413	H	1.97307187	3.18697655	-3.50611929
C	2.72267043	-3.41222295	-2.72885880	O	-2.04055754	0.16611837	-0.09048972
H	3.78674817	-3.45899452	-2.46848191	C	-2.80922939	-0.61497239	-1.03685287
H	2.44575335	-4.31299263	-3.27750232	C	-3.69916067	0.37879665	-1.79946825
O	1.95872335	-3.36479509	-1.51081338	C	-2.93074981	1.70088305	-1.64291132
C	1.56692481	-2.08394943	-1.28677212	C	-2.36963634	1.56624215	-0.22954198
O	0.98253787	-1.76822780	-0.26146948	H	-1.45452660	2.13917887	-0.05891491
C	3.54641449	-1.54089452	-4.28916699	H	-3.11368613	1.83896258	0.53299486
H	3.23308788	-0.58609508	-4.72362526	H	-2.10478488	1.74592815	-2.35897369
H	4.38109595	-1.32795742	-3.61073005	H	-3.56278792	2.58625940	-1.76575902
C	3.98200760	-2.49142074	-5.38712335	H	-3.84169284	0.08535070	-2.84385860
C	5.14494527	-3.26246193	-5.25954276	H	-4.68837116	0.45292787	-1.33146164
C	5.52679477	-4.15598577	-6.26242629	H	-3.38645936	-1.36386798	-0.48235681
C	4.74841219	-4.29191302	-7.41224199	H	-2.09960991	-1.11765148	-1.69904749
C	3.58923412	-3.52582919	-7.55463254	O	1.16475119	1.50762092	-0.15390427
C	3.21203823	-2.63365672	-6.55128187	C	2.29838605	1.54576492	-0.72711988
H	2.31379456	-2.03232561	-6.67589674	C	3.05596381	2.88493213	-0.75956980
H	2.98131924	-3.61860865	-8.45072965	H	2.40261570	3.62994469	-1.22947016
H	5.04525265	-4.98466937	-8.19494872	C	3.27863501	3.32445551	0.70279644
H	6.43518193	-4.74116186	-6.14594308	H	3.77723779	4.30067188	0.74208631
H	5.76422081	-3.15370335	-4.37178896	H	3.91424381	2.60558841	1.23774482
H	1.51945589	-2.27052061	-4.13820763	H	2.32465508	3.39640435	1.23158260
C	1.99168387	1.14031899	-2.80114491	C	4.39345659	2.82378129	-1.50677955

H	5.01173326	1.99512410	-1.13609099
H	4.96313194	3.74794649	-1.35443420
H	4.26557066	2.69052706	-2.58527706
H	2.98089075	0.67999141	-0.60739333
O	-0.09406539	-0.15476709	2.09014696
C	1.05938239	0.19355024	2.86491347
C	1.78382425	-1.13799939	3.11420243
C	0.63595484	-2.18467803	3.09493195
C	-0.60138955	-1.36877771	2.65837845
H	-1.21190501	-1.85531064	1.89544971
H	-1.24184541	-1.12307382	3.51881876
H	0.85115668	-2.97757297	2.37525447
H	0.47808560	-2.64723940	4.07455094
H	2.48886363	-1.33781086	2.30260627
H	2.34094135	-1.13306260	4.05647359
H	0.73511466	0.65423648	3.81163668
H	1.62296298	0.92268598	2.28239641

Table 16. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,R*)-**6** from **5** monomer with three THF



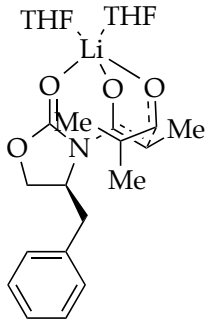


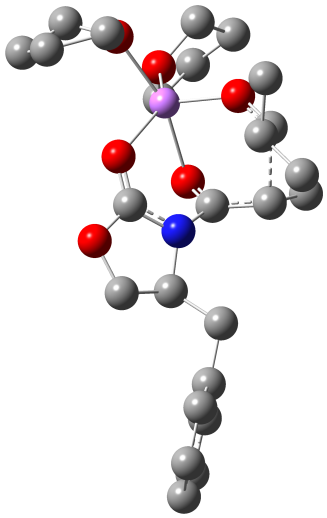
G = -1488.69723 Hartree
G_{MP2} = -931170.4794 kcal/mol
ΔG_{MP2} = 7.40160666 kcal/mol Li vs. **5** monomer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	1.22255389	2.28674449	3.57596117
O	0.00000000	0.00000000	2.21647090	H	0.32886753	2.55832159	3.00594657
C	1.19841668	0.00000000	2.53166518	H	0.90322056	2.04252005	4.59930153
N	1.95768395	-1.21878875	2.26358313	H	1.86706679	3.17134601	3.63659206
C	2.89267814	-1.84583839	3.20222213	O	-2.01370737	0.43824931	0.07915449
C	3.35173700	-3.05484937	2.36173616	C	-2.85598360	-0.37985848	0.92715654
H	4.30424441	-2.86578605	1.85533596	C	-3.72894814	0.59401790	1.72736868
H	3.42790331	-3.97796005	2.93863576	C	-2.83989719	1.84572406	1.79438854
O	2.33337980	-3.22745198	1.35715634	C	-2.18115195	1.83865451	0.41636210
C	1.60874220	-2.07945611	1.25451929	H	-1.19031610	2.29844188	0.39233530
O	0.81249110	-1.90513237	0.34584292	H	-2.82323357	2.30773709	-0.34284970
H	3.73728655	-1.18135973	3.40591535	H	-2.07502690	1.72368240	2.56674818
C	2.20681392	-2.22279671	4.53677101	H	-3.40136550	2.76534416	1.98780690
H	1.74921817	-1.31213331	4.94156364	H	-3.99236368	0.19739286	2.71264569
H	1.38980723	-2.92253353	4.32311329	H	-4.65976207	0.81214066	1.18940937
C	3.16716511	-2.81828219	5.54330493	H	-3.43681939	-1.05386806	0.28755662
C	4.08904676	-2.00194452	6.21625995	H	-2.20416427	-0.96986029	1.57837421
C	4.99763672	-2.54488717	7.12410788	O	1.16943288	1.47429573	0.24490307
C	4.99959036	-3.91854667	7.37785776	C	2.17515865	1.82938848	0.94419559
C	4.08523631	-4.74153112	6.72007257	C	3.58201846	1.34791445	0.52416020
C	3.17780346	-4.19378142	5.81062505	H	3.62148310	0.25645231	0.64761559
H	2.45920782	-4.84071259	5.31179032	C	3.77429997	1.65716553	-0.97345085
H	4.07298556	-5.81035079	6.91662649	H	3.75092503	2.73995720	-1.15413821
H	5.70498036	-4.34208135	8.08757898	H	4.74224840	1.28115690	-1.32811296
H	5.70046725	-1.89472203	7.63843550	H	2.97737976	1.20487565	-1.56813567
H	4.08673946	-0.92896527	6.03480289	C	4.71049727	1.99610269	1.33717297
C	1.94943625	1.14245185	2.90167631	H	4.67030988	1.74171626	2.40111803
H	2.95787300	0.95468083	3.26255061	H	5.69079789	1.68287776	0.95863333

H	4.66499990	3.09025998	1.25772980
H	2.19047682	2.87870641	1.30301667
O	-0.04980516	-0.33450214	-2.07861799
C	1.03563052	-1.03789795	-2.69450917
C	0.47769347	-2.43416890	-3.02332444
C	-1.05434297	-2.19757574	-3.14130400
C	-1.21693364	-0.69699011	-2.82617535
H	-2.08009511	-0.44632132	-2.20950422
H	-1.25010899	-0.10182465	-3.75198372
H	-1.59528664	-2.80928256	-2.41318536
H	-1.44410185	-2.44209100	-4.13457847
H	0.69641926	-3.12247159	-2.20390071
H	0.91482089	-2.84034649	-3.94090681
H	1.34295089	-0.50132977	-3.60557439
H	1.86515626	-1.04578484	-1.98677417

Table 17. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,S*)-**6** from **5** monomer with three THF



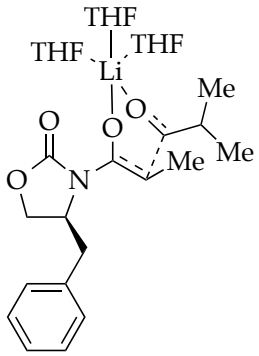


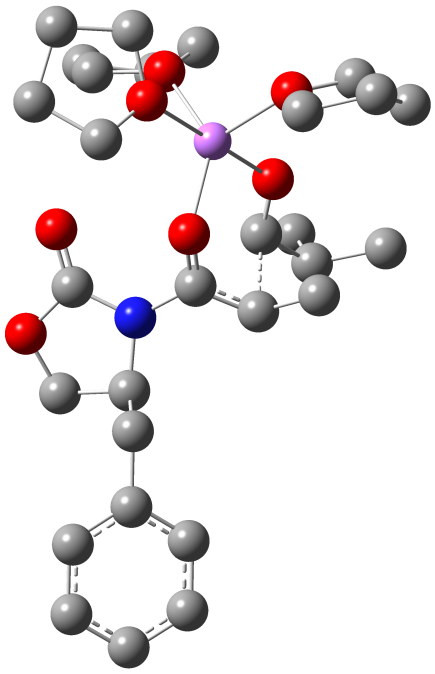
G = -1488.692527 Hartree
G_{MP2} = -931168.3235 kcal/mol
ΔG_{MP2} = 9.557477753 kcal/mol Li vs. **5** monomer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	7.72599063	1.94707408	-5.47477474
O	0.00000000	0.00000000	-2.17940160	H	7.71143124	0.71710313	-7.63785480
C	1.03098976	0.00000000	-2.82972230	H	6.22952858	-1.26193924	-7.91694192
N	2.30134068	-0.31919064	-2.39923015	H	4.77478005	-1.99599598	-6.05681722
C	2.58134067	-0.18688154	-0.95843018	H	3.64316978	1.08955711	-3.21149919
O	1.99453064	0.72388965	-0.35528855	O	-0.29287517	1.29514530	1.60901190
C	3.30816999	-1.23211913	-0.33299990	C	0.60393030	2.39084086	1.91142958
H	3.87761208	-1.88021504	-0.99177897	C	0.69694566	2.44651451	3.43872278
C	3.96006005	-0.91434511	0.99934466	C	0.50119781	0.97161192	3.82067580
H	3.21364931	-0.52933057	1.70058169	C	-0.54399440	0.51322389	2.80337458
H	4.75406778	-0.16055402	0.90747455	H	-0.45716729	-0.54156866	2.53643227
H	4.40746865	-1.81520624	1.43410995	H	-1.56520274	0.72351996	3.15012272
C	3.28153674	0.07327476	-3.42934792	H	1.43292165	0.41298871	3.67622451
C	2.37010233	0.09592224	-4.66877263	H	0.17148051	0.82908035	4.85466219
H	2.38755970	-0.86354875	-5.19922746	H	1.64966149	2.86192111	3.78180246
H	2.60298310	0.89955032	-5.36800918	H	-0.11108819	3.05969594	3.85643076
O	1.04373268	0.30677748	-4.15340441	H	0.18884141	3.30256312	1.46798939
C	4.49206011	-0.86312602	-3.57546167	H	1.57023109	2.17601485	1.44689557
H	5.04515497	-0.86578498	-2.63035001	O	0.80375897	-1.56706342	0.67991972
H	4.12837328	-1.88431342	-3.73965443	C	1.71966308	-2.34417893	0.23544061
C	5.40567150	-0.43728212	-4.70811600	H	2.34028937	-2.86862003	0.99336201
C	5.41239803	-1.12378245	-5.92956786	C	1.36152673	-3.29813862	-0.92651478
C	6.23599599	-0.71222760	-6.97943102	H	0.99343839	-2.69189404	-1.76341080
C	7.06803633	0.39661207	-6.82302032	C	0.20055063	-4.18946529	-0.43992122
C	7.07476072	1.08742544	-5.60912266	H	0.52302840	-4.82834517	0.39346469
C	6.25219569	0.67198335	-4.56232957	H	-0.15155500	-4.84644179	-1.24503945
H	6.27380821	1.20951895	-3.61653087	H	-0.63509969	-3.57962804	-0.08779449

C	2.52504705	-4.17745912	-1.40286595
H	3.28371810	-3.61346381	-1.95420758
H	2.16328459	-4.97254608	-2.06601863
H	3.02201211	-4.66392116	-0.55266642
O	-2.10832771	-0.22024823	-0.08586447
C	-2.64767231	-1.16984506	-1.02142706
C	-3.28640581	-0.34589612	-2.16638574
C	-3.24341748	1.11253925	-1.64452043
C	-2.95604107	0.93344429	-0.15100680
H	-2.41594664	1.75512092	0.32124110
H	-3.88271709	0.74090474	0.41376415
H	-2.41981515	1.65603658	-2.11613271
H	-4.17194218	1.66199612	-1.82955066
H	-2.71686470	-0.44653849	-3.09271389
H	-4.31177177	-0.67844505	-2.35912682
H	-3.39692509	-1.78898306	-0.50734758
H	-1.82303933	-1.80549418	-1.34438808

Table 18. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from **5** monomer with three THF with 3 THF in the transition state



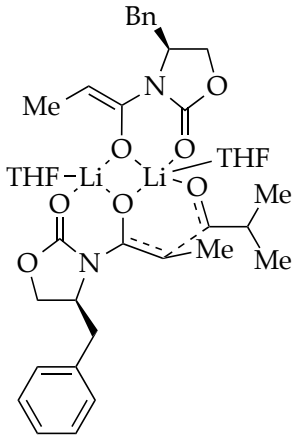


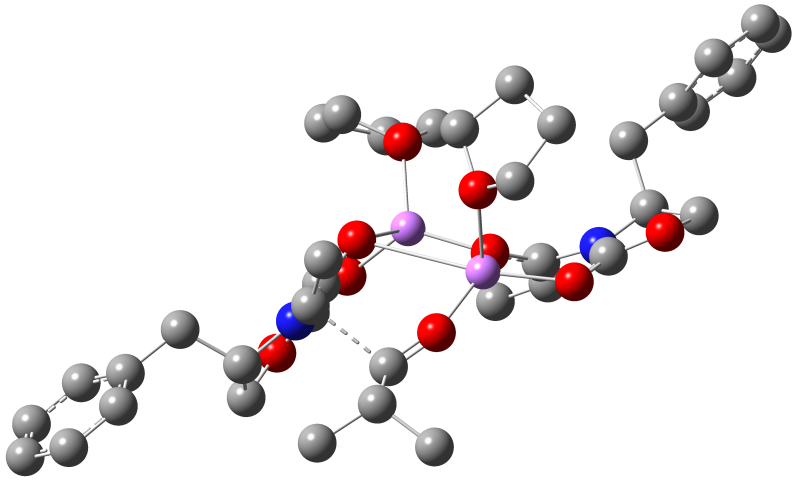
G = -1721.036676 Hartree
G_{MP2} = -1076482.214 kcal/mol
ΔG_{MP2} = 7.95713593 kcal/mol Li vs. **5** monomer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.06813681	-0.69917036	4.59677431
O	0.00000000	0.00000000	1.99497850	O	0.14798793	-2.81692055	2.20089505
C	1.04279733	0.00000000	2.68803939	C	1.95807195	1.07278461	2.72827431
N	1.40616301	-1.21450162	3.38341758	C	1.42118630	2.45048873	2.41886995
C	0.87775129	-2.46726227	3.09844861	H	2.14339141	3.22566283	2.69675190
O	1.33512914	-3.35999010	4.03694077	H	0.48479957	2.66010718	2.95506122
C	2.36377360	-2.74099377	4.82163055	H	1.20692343	2.54749112	1.34680277
H	2.27762366	-3.09175440	5.85172781	H	2.79539959	1.01157338	3.41708783
H	3.34006558	-3.03765402	4.41977499	O	1.94334443	0.69282920	-0.06041257
C	2.11763113	-1.23283999	4.66823050	C	2.81300431	0.40144950	0.80869105
C	1.26405276	-0.61650073	5.80321192	H	2.87750797	-0.64525028	1.16370871
H	0.96081291	0.38561315	5.47879834	C	4.20218633	1.06542647	0.78918968
H	0.34888406	-1.21170412	5.90840013	H	4.60672371	1.03753767	1.80921852
C	2.00123614	-0.53892302	7.12203228	C	4.18728714	2.51078160	0.28487225
C	2.98794019	0.43743205	7.32740143	H	5.20772746	2.90950865	0.23529187
C	3.69496347	0.50099124	8.52765352	H	3.60059237	3.16343556	0.93578856
C	3.42621803	-0.41316748	9.54917805	H	3.75304961	2.56078525	-0.71889786
C	2.44456669	-1.38636456	9.36109657	C	5.11950738	0.19439747	-0.09639873
C	1.73973058	-1.44697199	8.15688098	H	5.15497209	-0.84360230	0.25673084
H	0.96724241	-2.20124934	8.02256161	H	6.14509152	0.58304279	-0.09410474
H	2.22211970	-2.09737511	10.15249360	H	4.76304129	0.18643180	-1.13337214
H	3.97427387	-0.36263604	10.48613800	O	-2.08058874	-0.76248242	0.06619070
H	4.45195955	1.26818622	8.66837984	C	-2.88711758	-1.11449246	-1.06222473
H	3.19497528	1.16110815	6.54141666	C	-3.66068186	-2.40093374	-0.66844405

C	-3.29365776	-2.61130515	0.82142878
C	-2.75419859	-1.24163718	1.23727957
H	-3.57471531	-0.55268242	1.50074950
H	-2.01706176	-1.26178061	2.03708818
H	-4.14716391	-2.93173859	1.42754757
H	-2.50058281	-3.35714044	0.92904278
H	-4.73863433	-2.25875975	-0.79999286
H	-3.36922608	-3.25833513	-1.28291466
H	-2.21136049	-1.24154244	-1.91010798
H	-3.58325947	-0.29273306	-1.29052409
O	0.37917195	-1.50297591	-1.45702329
C	0.21076989	-2.91453101	-1.18491594
C	1.45761169	-3.62857452	-1.75521809
C	2.40790647	-2.47000239	-2.11392770
C	1.42947400	-1.33826763	-2.41953895
H	1.84419808	-0.34020686	-2.27340076
H	1.02099925	-1.42732463	-3.43924942
H	3.02653197	-2.19316406	-1.25360803
H	3.07038864	-2.70230828	-2.95403784
H	1.89560110	-4.32446630	-1.03373118
H	1.19896450	-4.20191706	-2.65264082
H	-0.70924319	-3.26666320	-1.66975090
H	0.10765770	-3.02245543	-0.10464825
O	-0.79727283	1.68413780	-0.94883754
C	-1.82024663	2.40152166	-0.22368273
C	-1.80470486	3.82756193	-0.78092206
C	-0.32896253	4.00204271	-1.17085239
C	0.03025036	2.60792998	-1.69111826
H	-0.20654312	2.50816332	-2.75994204
H	1.07002359	2.32633679	-1.51672608
H	-0.16544136	4.78461944	-1.91848926
H	0.27217340	4.24321656	-0.28677678
H	-2.44545423	3.90169281	-1.66817317
H	-2.15179996	4.56471868	-0.05011810
H	-1.57107724	2.37860251	0.84417703
H	-2.77132572	1.88276870	-0.36883894

Table 19. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from **5** dimer with three THF



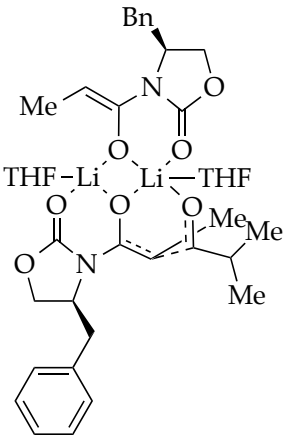


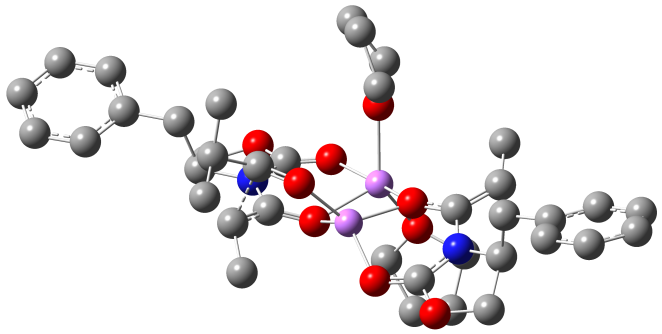
G = -2280.369128 Hartree
G_{MP2} = -1426404.974 kcal/mol
ΔG_{MP2} = 6.829416293 kcal/mol vs. **5** dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	9.17754522	-6.99735482	-1.33089690
O	0.00000000	0.00000000	1.95615030	H	7.60744593	-5.87868162	-2.90399029
Li	1.84171295	0.00000000	2.28282029	H	6.18130865	-4.01910028	-2.12352417
O	2.80646069	-0.15198414	0.65433834	C	3.38503864	-1.36017603	-1.28539027
C	3.30050530	-1.16622317	0.11063726	H	4.02554629	-2.16153763	-1.63481755
N	3.67461626	-2.27569503	0.96349257	C	3.32612094	-0.12631453	-2.15625747
C	4.54169514	-3.39605290	0.56060012	H	2.39588780	0.42025865	-1.97322574
C	4.32352186	-4.34390410	1.74794888	H	4.16085277	0.56168317	-1.95995632
H	3.50638275	-5.05070535	1.56858171	H	3.36730076	-0.39840525	-3.21675506
H	5.22131936	-4.88845741	2.04251772	O	2.42604065	1.56405243	3.38314446
O	3.94126129	-3.47538697	2.83278261	C	1.84956502	1.74363687	4.68782760
C	3.43872796	-2.32397170	2.31898544	C	2.84909751	1.09612348	5.65941509
O	2.88181357	-1.50951401	3.03989990	C	4.20893438	1.19442826	4.91313362
H	4.17270494	-3.84853311	-0.36170238	C	3.83920555	1.78234313	3.53595424
C	6.01369111	-2.94984222	0.38530019	H	4.33002745	1.29843219	2.68965196
H	6.02822253	-2.11624647	-0.32564903	H	4.03764855	2.86311517	3.49456570
H	6.37198733	-2.55824418	1.34537811	H	4.65760679	0.20384257	4.80520694
C	6.91432226	-4.06816316	-0.09366101	H	4.92626181	1.83460668	5.43589436
C	6.85730010	-4.50795154	-1.42486054	H	2.58416274	0.04959895	5.83107230
C	7.66409588	-5.55539468	-1.86797422	H	2.85975084	1.60603998	6.62751663
C	8.54664849	-6.18290962	-0.98556233	H	1.73638886	2.82036790	4.88452903
C	8.61738309	-5.75299700	0.33960099	H	0.86269965	1.27588900	4.67487433
C	7.80652676	-4.70446341	0.77967690	C	-1.08765912	-0.07900740	2.66904122
H	7.87645617	-4.36686102	1.81169055	N	-2.22679636	0.68739212	2.14945442
H	9.30606257	-6.22944094	1.03229085	C	-3.06051487	1.57376022	2.96382551

C	-4.16242387	1.92442350	1.94724626
H	-5.03959465	1.27650688	2.05478571
H	-4.47868238	2.96827931	1.98952754
O	-3.56820187	1.67692581	0.66018242
C	-2.50834724	0.82605103	0.82654320
O	-1.95695787	0.31442151	-0.13795613
H	-3.48490164	1.03191547	3.81286602
C	-2.26656883	2.79253676	3.48984032
H	-1.38224692	2.40163658	4.00585674
H	-1.91031070	3.37494042	2.63119930
C	-3.07604475	3.66487095	4.42341246
C	-3.59716792	4.89541365	4.00182187
C	-4.36805053	5.68196487	4.86070611
C	-4.63177782	5.24742915	6.15981857
C	-4.11632782	4.02405755	6.59491260
C	-3.34595324	3.24269536	5.73439245
H	-2.94005991	2.29551364	6.08439703
H	-4.31070355	3.68032775	7.60761612
H	-5.23016907	5.85817926	6.83043704
H	-4.75872048	6.63519668	4.51411731
H	-3.38750673	5.24679536	2.99359824
C	-1.30868640	-0.74286974	3.83210361
C	-0.29567565	-1.58249577	4.55568679
H	-0.06656883	-1.19594346	5.56209917
H	-0.66264590	-2.60911212	4.70133464
H	0.64684951	-1.65405793	4.00694459
H	-2.31408330	-0.72689066	4.24416492
O	0.50964454	1.87532694	-0.73283493
C	1.22036064	2.92061760	-0.05809843
C	0.30274723	4.16759802	-0.11853179
C	-0.80058968	3.77377283	-1.13711294
C	-0.24452423	2.49665889	-1.77850297
H	0.42107945	2.72823666	-2.62495222
H	-1.00700885	1.78534321	-2.09775532
H	-1.00017031	4.55858711	-1.87351161
H	-1.73954943	3.54439080	-0.62419227
H	0.86355287	5.04983103	-0.44387869
H	-0.12575436	4.39802393	0.86204238
H	1.43444994	2.57110909	0.95305945
H	2.17237779	3.10273015	-0.57676025
O	0.62362293	-1.27445058	-1.19489910
C	1.43758282	-2.19335978	-1.48800102
C	1.44304343	-2.72414225	-2.93584209
H	1.61947946	-1.87161215	-3.60312100
C	0.02427696	-3.25815698	-3.22569084
H	-0.05695029	-3.59416067	-4.26677144
H	-0.21275857	-4.11361630	-2.57896923
H	-0.72227475	-2.48129594	-3.04400707
C	2.48490350	-3.81682883	-3.20328658
H	2.42937701	-4.60620132	-2.44041986
H	2.30423777	-4.29439268	-4.17334826
H	3.50919469	-3.42991084	-3.21796883
H	1.61411585	-3.00185540	-0.74592743

Table 20. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,R*)-**6** from **5** dimer with three THF



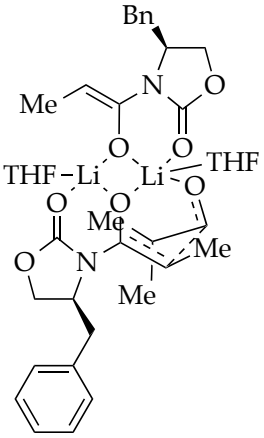


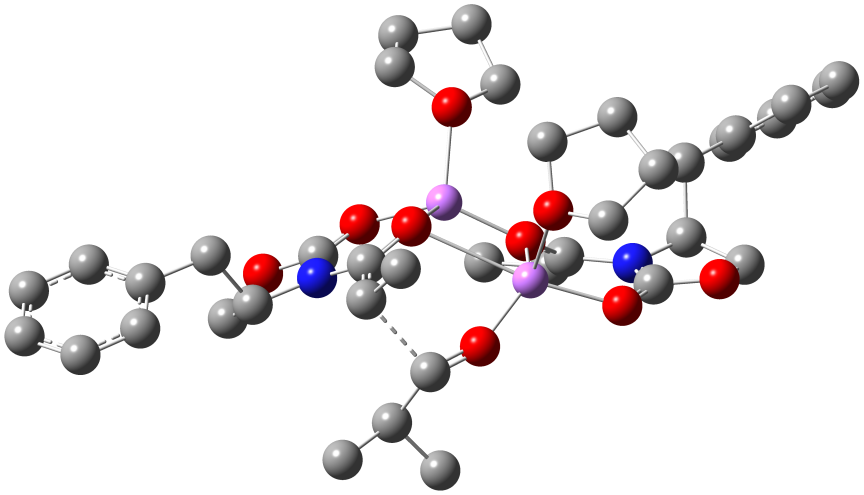
G = -2280.360219 Hartree
G_{MP2} = -1426402.109 kcal/mol
ΔG_{MP2} = 9.694603507 kcal/mol vs. **5** dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-5.55414705	1.59210591	-4.03244176
O	0.00000000	0.00000000	1.98556460	C	-5.38269945	2.35338784	-5.19632977
C	0.78040021	0.00000000	3.01877274	C	-6.40930556	2.46927916	-6.13608214
N	0.26248218	-0.70637054	4.19604943	C	-7.62703854	1.82243376	-5.92473295
C	0.87540069	-0.64283627	5.52968200	C	-7.81347519	1.06395715	-4.76662883
C	0.18877664	-1.83633335	6.20513095	C	-6.78636088	0.95205307	-3.83016536
H	0.77161769	-2.75940072	6.10378181	H	-6.94678851	0.36939194	-2.92517975
H	-0.04337018	-1.66776353	7.25793751	H	-8.76205416	0.56412841	-4.58940704
O	-1.04384806	-1.99045671	5.48359173	H	-8.42804307	1.91276349	-6.65328000
C	-0.91232504	-1.40720694	4.25695037	H	-6.25727183	3.06873794	-7.02969647
O	-1.79444814	-1.55130660	3.42006751	H	-4.44025266	2.87114789	-5.36226139
Li	-1.85911899	-0.33611009	1.94191090	C	-4.21833769	-0.62738246	-0.19464152
O	-1.87925902	-0.81197050	-0.03326498	C	-4.46350698	-1.67585691	0.87688134
C	-2.90486341	-0.56289784	-0.72139400	H	-5.52685704	-1.93000209	0.92803409
N	-2.70931423	-0.11194456	-2.06502903	H	-3.90803194	-2.60121196	0.67953506
C	-3.76513514	0.04726191	-3.07905135	H	-4.15753034	-1.32250344	1.86897360
C	-2.94570032	-0.17369835	-4.35904948	H	-5.03691049	-0.46760471	-0.89068463
H	-2.94384054	-1.22247238	-4.67619414	O	-3.31008218	0.90867502	1.89309979
H	-3.25951672	0.45806314	-5.19060110	C	-4.01632406	1.18343079	0.87434073
O	-1.60311185	0.19479621	-3.99008169	H	-3.52627661	1.72621527	0.03927211
C	-1.46137012	0.08413320	-2.64121083	C	-5.46404146	1.68017155	1.06058320
O	-0.37288844	0.16482801	-2.11171479	H	-5.99345871	1.56635004	0.10379658
H	-4.51663456	-0.73581759	-2.95595169	C	-6.23356076	0.94484216	2.16153755
C	-4.43556028	1.44080013	-3.02299494	H	-7.19588670	1.43563723	2.35024932
H	-4.81613708	1.59827879	-2.00874900	H	-6.43500028	-0.09584807	1.89508873
H	-3.66329384	2.20088884	-3.19362619	H	-5.65595159	0.94655855	3.09099721

C	-5.38557985	3.18981256	1.37423854
H	-4.83892099	3.73728000	0.59592176
H	-6.39035140	3.62331652	1.44536583
H	-4.87218382	3.35560577	2.32789334
H	1.95193925	-0.81427507	5.46106397
C	0.59870788	0.71374550	6.22347522
H	0.92763629	1.50174041	5.53782221
H	-0.48611082	0.82190488	6.34490373
C	1.29223214	0.84595612	7.56124031
C	2.67732423	1.06230577	7.62882064
C	3.32930150	1.15780842	8.85783607
C	2.60583717	1.04050112	10.04711435
C	1.22766374	0.83051591	9.99587958
C	0.57924312	0.73376330	8.76272608
H	-0.49755645	0.58124798	8.73115974
H	0.65386995	0.74544055	10.91509978
H	3.11261354	1.11788788	11.00530616
H	4.40214610	1.33008858	8.88771921
H	3.24729520	1.16834829	6.70794484
C	2.01955546	0.56045578	3.12568451
H	2.58727104	0.44766010	4.04157929
C	2.68451065	1.33086518	2.01971156
H	1.99775950	1.49270832	1.18515516
H	3.02967620	2.31782581	2.36300941
H	3.57451246	0.81709443	1.62179368
O	1.36896445	-1.49209059	-0.44658905
C	2.28321218	-2.04750935	0.51880093
C	1.83296159	-3.49534361	0.68575925
C	1.46584150	-3.86687416	-0.76041972
C	0.90148041	-2.54813855	-1.32166258
H	-0.19134241	-2.52534530	-1.30030644
H	1.23901007	-2.34069552	-2.34252843
H	0.74223109	-4.68511415	-0.82520249
H	2.36342595	-4.16961835	-1.31235188
H	0.94964880	-3.53634360	1.33334252
H	2.60930906	-4.13809708	1.11296444
H	3.30861222	-1.99649373	0.12116380
H	2.21896748	-1.44400515	1.42490369
O	-0.00960766	2.14188337	-0.08315328
C	-0.52313683	2.97389098	0.98039270
C	-0.79197107	4.36314206	0.34650290
C	-0.29726781	4.21761371	-1.11270811
C	0.62918686	3.00312217	-1.02933494
H	1.62720129	3.29152161	-0.66138946
H	0.73833890	2.44336055	-1.95955758
H	0.20881518	5.11350826	-1.48620274
H	-1.13412178	3.99729093	-1.78506069
H	-0.23429761	5.14308852	0.87538129
H	-1.85112199	4.63367741	0.39093709
H	-1.41413230	2.48114301	1.37247400
H	0.22338107	3.03270402	1.78122823

Table 21. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,R*)-**6** from **5** dimer with three THF



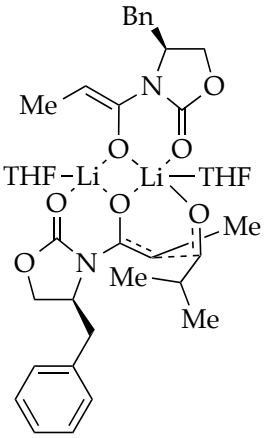


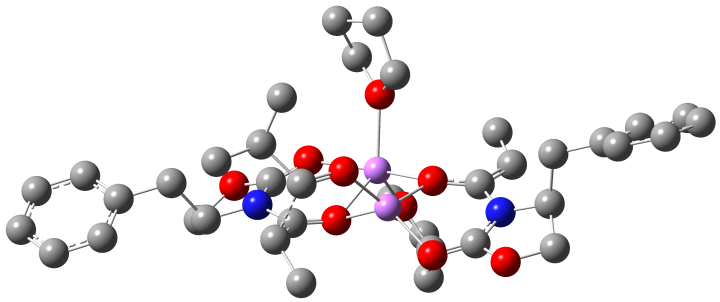
G = -2280.366658 Hartree
G_{MP2} = -1426404.058 kcal/mol
ΔG_{MP2} = 7.744958821 kcal/mol vs. **5** dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	8.43667046	-3.24368511	1.35842241
O	0.00000000	0.00000000	1.97714830	H	10.17411427	-4.79184812	0.51890714
Li	1.85927987	0.00000000	2.20286854	H	10.08654764	-5.61202323	-1.82857703
O	2.65471249	-0.11178775	0.47380784	H	8.24574310	-4.86260844	-3.32544374
C	3.25915389	-1.04237071	-0.09954078	H	6.51243686	-3.31570151	-2.48489613
N	3.86279211	-2.06591706	0.72679062	C	3.26047509	-1.23357844	-1.50509419
C	4.91870637	-2.99370802	0.28310138	H	3.94810011	-1.97794276	-1.89679123
C	4.96057550	-3.94437336	1.48688754	C	3.11905198	0.01002747	-2.36264164
H	4.29063535	-4.80147358	1.36044017	H	2.25718414	0.59978721	-2.04017187
H	5.96350943	-4.29576316	1.73189251	H	4.00926636	0.65322142	-2.30942638
O	4.47601257	-3.14885931	2.58684243	H	2.97648264	-0.26700180	-3.41380204
C	3.73060649	-2.12673075	2.09740284	O	2.39018905	1.58349732	3.30144917
O	3.08001368	-1.41496570	2.84761888	C	1.46045247	2.08713770	4.29422813
H	4.60356811	-3.53024126	-0.61249207	C	2.31783430	2.62222032	5.45019925
C	6.25601155	-2.25947012	0.02140952	C	3.62662106	1.83100105	5.29307601
H	6.06095530	-1.45691118	-0.69873472	C	3.74469526	1.73128804	3.77396224
H	6.57735965	-1.78119330	0.95494230	H	4.30968675	0.86390071	3.42673901
C	7.33987890	-3.18057910	-0.49592957	H	4.18089910	2.64337865	3.34233581
C	7.30712772	-3.64626694	-1.81908236	H	3.52776770	0.82987382	5.72801038
C	8.28679160	-4.51642367	-2.29611895	H	4.48838115	2.32420522	5.75314746
C	9.32126663	-4.93634984	-1.45656103	H	1.83823236	2.47573491	6.42243215
C	9.36921556	-4.47738684	-0.14013804	H	2.50699476	3.69502027	5.32645932
C	8.38526834	-3.60703766	0.33407033	H	0.83784313	2.85727153	3.82802252

H	0.81510610	1.25750677	4.60033727
C	-1.05448197	-0.26052103	2.69444608
N	-2.29220626	0.38045697	2.23174069
C	-3.26307069	1.02672944	3.11781158
C	-4.38467615	1.35382325	2.11406070
H	-5.17538875	0.59523829	2.12202738
H	-4.83141684	2.33816305	2.26644438
O	-3.74742665	1.33372723	0.82554193
C	-2.58140052	0.62284411	0.92443743
O	-1.96224116	0.30031276	-0.07890462
H	-3.62663005	0.32254939	3.87059420
C	-2.66461996	2.25993581	3.83390277
H	-1.74279152	1.92518573	4.32266506
H	-2.38488067	3.00343186	3.07706919
C	-3.60714446	2.86640094	4.84952720
C	-4.28769376	4.06337840	4.58934022
C	-5.17916978	4.60038945	5.52077070
C	-5.40525007	3.94511476	6.73140734
C	-4.73116698	2.75260803	7.00583538
C	-3.84082463	2.22086110	6.07375385
H	-3.31216920	1.29673529	6.29887800
H	-4.89570607	2.23869906	7.94939523
H	-6.09761623	4.36145201	7.45813015
H	-5.69356113	5.53212552	5.30014375
H	-4.10940443	4.58585766	3.65174230
C	-1.16285902	-1.00745711	3.82346628
C	-0.03132960	-1.73657963	4.48922859
H	0.19494994	-1.34388524	5.49413514
H	-0.27110633	-2.80107268	4.62573586
H	0.89043003	-1.69049902	3.90393399
H	-2.15104598	-1.14675007	4.25247551
O	0.44297162	1.90861415	-0.79020332
C	1.05471373	2.97659106	-0.06212146
C	-0.08474843	3.97469786	0.21460016
C	-1.09975639	3.70208089	-0.93136285
C	-0.47097391	2.52577700	-1.70632294
H	0.08736823	2.88144766	-2.58563199
H	-1.18713838	1.76339075	-2.01256227
H	-1.24542756	4.57429455	-1.57655073
H	-2.07573279	3.41695591	-0.52930873
H	0.27418143	5.00886175	0.22755984
H	-0.54001771	3.76836882	1.18872057
H	1.51298677	2.55214642	0.83223675
H	1.84118884	3.43564673	-0.68156764
O	0.55925449	-1.36392956	-1.09333216
C	1.39548530	-2.07059396	-1.73164236
C	1.53101133	-3.56803653	-1.36617256
H	2.01366401	-3.64278796	-0.38181153
C	2.34528124	-4.35248929	-2.40350036
H	3.36354003	-3.96601526	-2.52785590
H	2.42214961	-5.41084818	-2.12689986
H	1.86015256	-4.30664190	-3.38707131
C	0.12120236	-4.17234786	-1.22976900
H	0.17671999	-5.22403077	-0.92158402
H	-0.46235338	-3.61516754	-0.49331215
H	-0.41656024	-4.13068205	-2.18582715
H	1.47264227	-1.90784155	-2.82751044

Table 22. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,S*)-**6** from **5** dimer with three THF



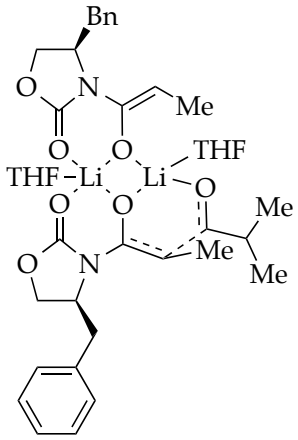


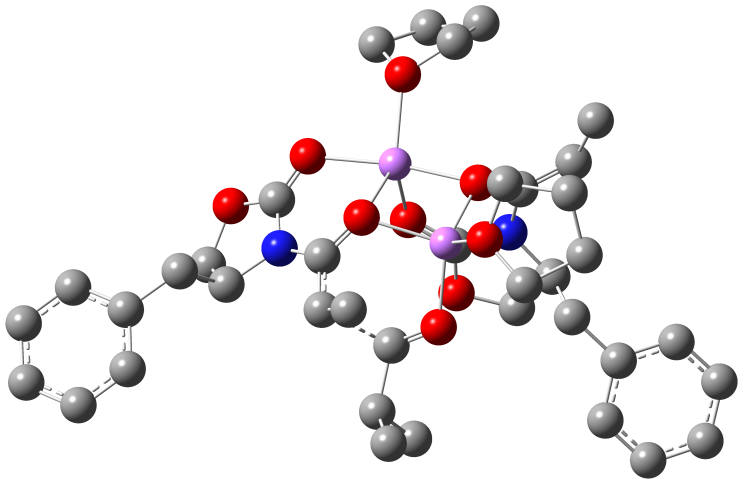
G = -2280.361842 Hartree
G_{MP2} = -1426401.658 kcal/mol
ΔG_{MP2} = 10.1456954 kcal/mol vs. **5** dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-4.52626886	-0.59038891	-3.54602670
O	0.00000000	0.00000000	1.99903120	H	-5.09461871	-0.31091563	-2.65472214
C	0.82408025	0.00000000	2.99620810	H	-4.02808918	0.31976337	-3.90175952
N	0.29703183	-0.55777416	4.25158639	C	-5.45737778	-1.12868172	-4.61263407
C	0.77464784	-0.15891978	5.58244839	C	-5.37254172	-0.68639617	-5.93959497
C	0.08588178	-1.21920109	6.45359535	C	-6.22014033	-1.20022266	-6.92353780
H	0.73109979	-2.08693739	6.63378057	C	-7.16853832	-2.16844289	-6.59352356
H	-0.27450418	-0.83259195	7.40847955	C	-7.26702787	-2.61581812	-5.27389514
O	-1.04492431	-1.64482654	5.67558510	C	-6.41955194	-2.09922319	-4.29434972
C	-0.82071329	-1.33383285	4.36628286	H	-6.51348069	-2.44596178	-3.26714441
O	-1.58770601	-1.74454478	3.50195922	H	-8.00872909	-3.36356490	-5.00588429
Li	-1.76244592	-0.64100413	1.93538902	H	-7.83061856	-2.56820070	-7.35670169
O	-1.67379199	-1.27347226	0.05251977	H	-6.14091020	-0.83953578	-7.94564233
C	-2.69858995	-1.38798783	-0.66094909	H	-4.64405702	0.07778314	-6.20253188
N	-2.55782181	-1.10082336	-2.06342101	C	-3.98663630	-1.69595687	-0.14689708
C	-3.43866856	-1.60867344	-3.13205834	C	-4.07762521	-2.73060649	0.96508816
C	-2.40499750	-1.85094570	-4.24172623	H	-5.10556262	-2.78802757	1.34100704
H	-1.99385485	-2.86630059	-4.21507452	H	-3.79927142	-3.73580481	0.61839791
H	-2.78077573	-1.63444926	-5.24212393	H	-3.43266404	-2.48860546	1.81424598
O	-1.34586156	-0.91991908	-3.94383078	H	-4.77722520	-1.78860006	-0.88810030
C	-1.37959996	-0.62110755	-2.61637532	O	-3.27297006	0.39464970	1.51808692
O	-0.47879922	-0.00638668	-2.08366135	C	-4.35494738	0.04113446	0.94981907
H	-3.90124971	-2.54438806	-2.81087202	C	-5.04167707	1.03018286	-0.01664545

H	-4.42660743	1.10695190	-0.92383260
C	-5.08210202	2.42579216	0.63350393
H	-5.52683891	3.16016272	-0.04969660
H	-5.68568358	2.41277813	1.55010951
H	-4.07595636	2.75604279	0.90258019
C	-6.46183258	0.58326859	-0.38727572
H	-6.48758019	-0.41714609	-0.83320462
H	-7.09998724	0.55599795	0.50532552
H	-6.92326119	1.27894370	-1.09805165
H	-5.08984968	-0.52701204	1.55457296
H	1.85930061	-0.26434872	5.65166102
C	0.37537655	1.29808826	5.91752350
H	0.72993603	1.92211816	5.08992138
H	-0.71949573	1.36378395	5.93249119
C	0.95226075	1.77883045	7.23015805
C	2.31253343	2.11020509	7.32881355
C	2.86360844	2.52488859	8.54077812
C	2.06166443	2.61808732	9.68088918
C	0.70661587	2.29731598	9.59673377
C	0.15915162	1.88121524	8.38104892
H	-0.90111916	1.64439852	8.32101444
H	0.07193607	2.37416638	10.47581617
H	2.48944729	2.94382555	10.62528043
H	3.91858333	2.78136360	8.59449388
H	2.94076072	2.05204268	6.44221340
C	2.10276336	0.46968778	3.03125982
H	2.69615124	0.32926951	3.92816006
C	2.77588666	1.15298405	1.87358886
H	2.04240358	1.51058607	1.14589222
H	3.36470089	2.01726689	2.21316629
H	3.47558266	0.49438093	1.33302998
O	1.61856704	-1.15901008	-0.36214176
C	1.90735762	-2.25941920	0.53230885
C	2.83327849	-3.19017848	-0.25413607
C	3.59066971	-2.20208397	-1.15503326
C	2.49574381	-1.18962837	-1.50276854
H	1.92203653	-1.49668992	-2.38612059
H	2.87530764	-0.17714823	-1.67269079
H	4.02889056	-2.66738755	-2.04351559
H	4.39621806	-1.71609977	-0.59180244
H	2.24975357	-3.89098166	-0.86380493
H	3.49025656	-3.77436602	0.39763051
H	2.38755228	-1.85667144	1.43122356
H	0.95781384	-2.71841465	0.81933811
O	0.00491127	2.08633651	-0.11291516
C	-0.66701746	2.83148148	0.94006150
C	-0.90722279	4.24307081	0.37667867
C	-0.81481853	4.03236171	-1.14347756
C	0.25493382	2.94592898	-1.23416937
H	1.26385581	3.37986867	-1.15125913
H	0.20341027	2.33277074	-2.13552523
H	-0.54804238	4.94091334	-1.69304161
H	-1.76577142	3.65669506	-1.53964308
H	-0.12264216	4.93331014	0.70894167
H	-1.86987196	4.65432183	0.69562749
H	-1.59472901	2.30118271	1.17032134
H	-0.03117147	2.82789518	1.82981514

Table 23. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from **5** spirocyclic dimer with three THF



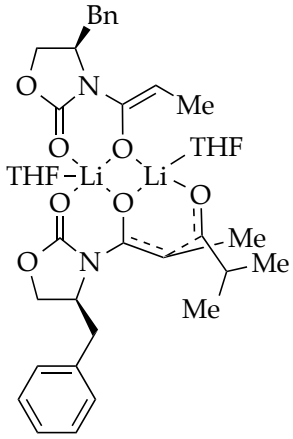


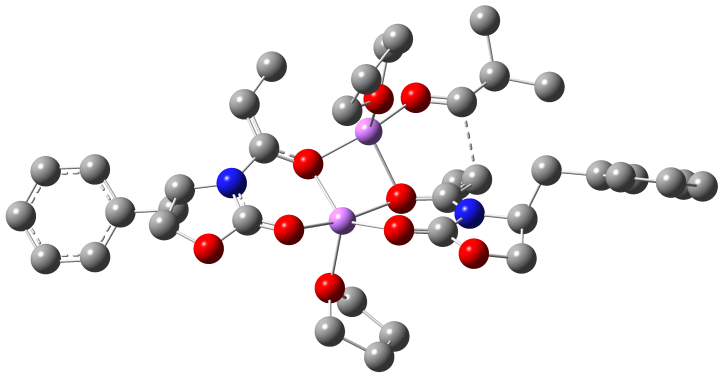
G = -2280.366593 Hartree
G_{MP2} = -1426408.218 kcal/mol
ΔG_{MP2} = 4.514509639 kcal/mol vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.35430851	2.67652496	-0.86288209
Li	0.00000000	0.00000000	2.75606050	H	7.08805689	2.11451341	-1.75564548
O	1.51381912	0.00000000	1.41788634	H	9.05540048	3.61398063	-1.79276054
C	2.43182289	0.86010647	1.53151668	H	9.69331964	4.88767005	0.24730028
N	2.85667370	1.55326002	0.35495484	H	8.34497094	4.63941846	2.32379311
C	2.36618127	1.31054019	-0.92057837	H	6.38203562	3.13931497	2.35846577
O	1.53632929	0.50485539	-1.28436097	C	2.96354359	1.26504968	2.77708131
O	2.99573211	2.12877927	-1.80558241	H	3.79095124	1.96610838	2.76651481
C	3.76438388	3.10460932	-1.07952323	C	2.96721316	0.25444102	3.90396434
H	3.16462024	4.01559226	-0.97861188	H	3.08578847	-0.77053947	3.53201841
H	4.67126203	3.32100188	-1.64541567	H	3.78692081	0.45832742	4.60141843
C	4.03227832	2.43712492	0.27465578	H	2.02710789	0.28339388	4.46826825
H	4.01027871	3.17840436	1.07577536	O	-1.36121043	-0.36752388	1.46521900
C	5.35898718	1.63953077	0.31673258	C	-2.54292088	0.17621473	1.41950485
H	5.35029186	1.02132940	1.22092255	N	-2.55228015	1.63716440	1.28819404
H	5.37398126	0.95397531	-0.53922174	C	-3.41071611	2.52632969	2.07940084
C	6.58219549	2.53061649	0.29749863	C	-2.99313740	3.89694057	1.50879335
C	6.95809437	3.25029195	1.44185216	H	-3.69635885	4.25879121	0.75056976
C	8.06812932	4.09419809	1.42529165	H	-2.86601953	4.66293290	2.27561430
C	8.82638539	4.23274804	0.26037182	O	-1.72140327	3.67148559	0.87337244
C	8.46761033	3.51939190	-0.88353084	C	-1.56349972	2.33283743	0.66451574

O	-0.63523602	1.91214458	-0.01623158
H	-4.46464134	2.33468412	1.85703808
C	-3.17899919	2.36646475	3.59954949
H	-3.33915144	1.30805839	3.83561720
H	-2.12948897	2.58821689	3.82266034
C	-4.11069305	3.22993626	4.42123531
C	-3.65302951	4.38972216	5.06148259
C	-4.52402609	5.19781710	5.79575206
C	-5.87306673	4.85867302	5.90113964
C	-6.34348448	3.70369329	5.27157610
C	-5.46967002	2.89904319	4.54106442
H	-5.84259457	1.99454183	4.06434828
H	-7.39131585	3.42643182	5.35453072
H	-6.55232438	5.48520733	6.47304247
H	-4.14579250	6.09025728	6.28780760
H	-2.60062910	4.65605295	4.99253190
C	-3.75969994	-0.42181010	1.51017276
C	-3.96987196	-1.88610986	1.76964242
H	-4.42732424	-2.40656061	0.91398515
H	-3.01962287	-2.38385006	1.98426201
H	-4.63866826	-2.05878283	2.62638864
H	-4.64727821	0.19294341	1.38834100
O	-0.09770894	-1.38005935	4.19923124
C	-0.53992363	-1.03137109	5.52123546
C	-1.89496169	-1.72284213	5.65490486
C	-1.64892096	-3.06002873	4.92602943
C	-0.54886961	-2.71761382	3.89394628
H	-0.91148890	-2.69496675	2.86392655
H	0.30260735	-3.40618237	3.95813640
H	-2.55382481	-3.44615103	4.44872211
H	-1.29260994	-3.82084112	5.62905648
H	-2.66288757	-1.13749480	5.13759461
H	-2.20532179	-1.85454755	6.69616647
H	0.17833012	-1.41010362	6.26457735
H	-0.56449293	0.05875054	5.57178614
O	0.36469144	1.66477280	3.69881441
C	1.19669825	2.47494059	3.18247234
H	1.05387406	2.75849319	2.12518787
C	1.75931175	3.64295922	4.00502994
C	0.67384589	4.74075946	4.04233280
H	1.06429605	5.65828940	4.49875239
H	0.31390302	4.98583725	3.03584881
H	-0.18375934	4.40388610	4.63642247
H	2.62063417	4.04731538	3.45510095
C	2.19332695	3.25956047	5.42172735
H	3.04920997	2.57847045	5.41155051
H	2.47662715	4.15103491	5.99399991
H	1.37382177	2.76071619	5.94919062
O	-0.66254560	-1.31898227	-1.43741626
C	-1.73749342	-2.24437178	-1.22808179
C	-2.89999341	-1.72698029	-2.09884932
C	-2.19611523	-0.83592905	-3.16127404
C	-0.70092157	-0.99267300	-2.83461809
H	-0.09961671	-0.09584972	-2.97653926
H	-0.25377756	-1.81962012	-3.40771761
H	-2.50125130	0.20914552	-3.05081801
H	-2.42071621	-1.14158560	-4.18808902
H	-3.59251610	-1.13738443	-1.49218349
H	-3.46184126	-2.55154076	-2.54921187
H	-1.41373620	-3.24625319	-1.55024615
H	-1.94536217	-2.25212732	-0.15948421

Table 24. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from **5** spirocyclic dimer with three THF



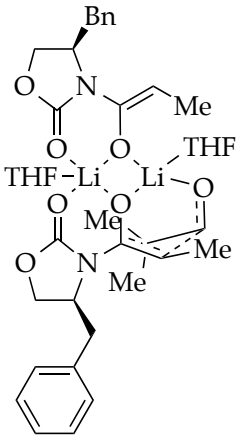


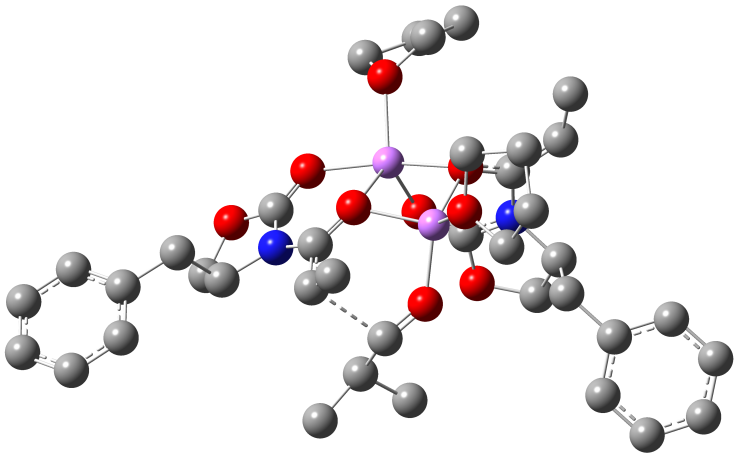
G = -2280.364103 Hartree
G_{MP2} = -1426403.789 kcal/mol
ΔG_{MP2} = 8.943400249 kcal/mol vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.91022233	-1.76059372	-2.76487234
Li	0.00000000	0.00000000	2.69539740	H	8.30090066	-2.15686183	-3.26457510
O	1.36298871	0.00000000	1.39350365	H	10.01888002	-1.81769433	-1.49674347
C	2.56326864	0.49214097	1.38485784	H	9.31702689	-1.08291386	0.77472079
N	3.08363725	0.85149697	0.06651852	H	6.92515471	-0.68799370	1.26939056
C	2.30494990	1.17161837	-1.00571938	C	3.39681123	0.66966629	2.44396796
O	1.09056991	1.31477236	-1.07042116	H	4.35264248	1.16104804	2.29175650
O	3.08487641	1.33705451	-2.11579259	C	3.05513151	0.22851588	3.83978731
C	4.46703747	1.31688369	-1.71684771	H	3.94383284	-0.14252315	4.36788673
H	4.82267759	2.35120639	-1.64432406	H	2.63819370	1.03511134	4.46567232
H	5.04147323	0.79130580	-2.48181663	H	2.31893457	-0.58447817	3.83355830
C	4.46888019	0.61026698	-0.35144658	O	-1.19068823	-1.02187451	1.37311225
H	5.16887088	1.10203984	0.32831012	C	-2.39977044	-1.08747085	1.71231453
C	4.79173134	-0.90126774	-0.41120440	N	-3.30614489	-0.17406669	1.06857062
H	4.51768241	-1.32311431	0.56212500	C	-4.76816489	-0.13676488	1.23109517
H	4.14341599	-1.36706537	-1.16332953	C	-5.17764430	0.47852869	-0.11578149
C	6.24623402	-1.17984250	-0.71713248	H	-5.40668661	-0.28375908	-0.86900679
C	7.22644953	-0.99845050	0.27092065	H	-6.01373875	1.17432567	-0.03866006
C	8.57427074	-1.22416995	-0.00628323	O	-4.01503228	1.20968279	-0.54553105
C	8.96901049	-1.63847143	-1.28077195	C	-2.91083632	0.70110327	0.06785707
C	8.00546043	-1.82731445	-2.27176213	O	-1.79383546	1.02491007	-0.28429957
C	6.65671834	-1.59878351	-1.98994755	H	-5.15674675	-1.15343727	1.32735905

C	-5.20742314	0.71458958	2.44572702
H	-4.71161914	0.31630960	3.33610393
H	-4.83285774	1.73542222	2.30251358
C	-6.70864885	0.72754564	2.64317815
C	-7.47473889	1.85174928	2.30660686
C	-8.86185211	1.85048867	2.46908038
C	-9.50609889	0.72014405	2.97234620
C	-8.75457983	-0.40582185	3.31664704
C	-7.36957841	-0.40003912	3.15390238
H	-6.79226427	-1.27699932	3.43925448
H	-9.24690225	-1.28751111	3.71836720
H	-10.58492992	0.71749551	3.10167349
H	-9.43628001	2.73482866	2.20631857
H	-6.97848991	2.74199217	1.92573234
C	-2.87448465	-1.94981162	2.72570691
C	-2.11121520	-3.24278304	2.93113485
H	-2.59212116	-3.85769731	3.69951274
H	-2.05939554	-3.84755748	2.01474578
H	-1.08385334	-3.03566917	3.24885930
H	-3.95076797	-2.00833896	2.85661756
O	-0.41806528	1.99537841	2.94974445
C	-0.40392738	2.59212415	4.25225080
C	-0.87717954	4.03478210	4.02262935
C	-0.41128738	4.34037895	2.57188503
C	0.12731139	2.98794634	2.05678159
H	1.22302817	2.94328705	2.10740382
H	-0.19127564	2.72978598	1.04694377
H	0.36648050	5.10958587	2.54094788
H	-1.24586443	4.69410530	1.95937051
H	-0.45641351	4.72546609	4.75994883
H	-1.96787562	4.09310635	4.09795825
H	-1.04785008	1.99318197	4.89748252
H	0.61985472	2.56992538	4.65667679
O	-0.84655099	-0.74204283	4.21721782
C	-2.09540963	-0.79989588	4.40690253
H	-2.70897015	0.09392207	4.17355237
C	-2.61271331	-1.57798654	5.62651316
H	-2.16785189	-2.57936883	5.59064945
C	-4.13879313	-1.69230760	5.70810428
H	-4.44139929	-2.12045877	6.67077163
H	-4.61490037	-0.70532122	5.63094283
H	-4.55126123	-2.33077881	4.92076669
C	-2.06024110	-0.87111724	6.88319324
H	-2.35575764	-1.41145068	7.79060624
H	-0.96915408	-0.81713781	6.84673113
H	-2.45162472	0.15230847	6.96485394
O	0.10489835	-1.43771252	-1.45528640
C	-0.31855188	-2.78538065	-1.21267429
C	-1.69985789	-2.90230881	-1.88482541
C	-1.68350732	-1.78326025	-2.96531596
C	-0.29844671	-1.12882255	-2.79776319
H	-0.28881773	-0.04302087	-2.89706211
H	0.43104378	-1.56032611	-3.49960720
H	-2.47698462	-1.05234583	-2.78293978
H	-1.82198591	-2.17516236	-3.97776197
H	-2.49471088	-2.72438471	-1.15421464
H	-1.85896378	-3.89771819	-2.31109260
H	0.40475568	-3.47780910	-1.66932517
H	-0.33035427	-2.92968155	-0.13196141

Table 25. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,R*)-**6** from **5** spirocyclic dimer with three THF



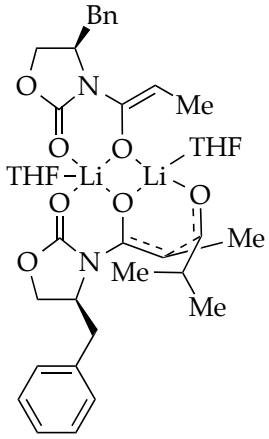


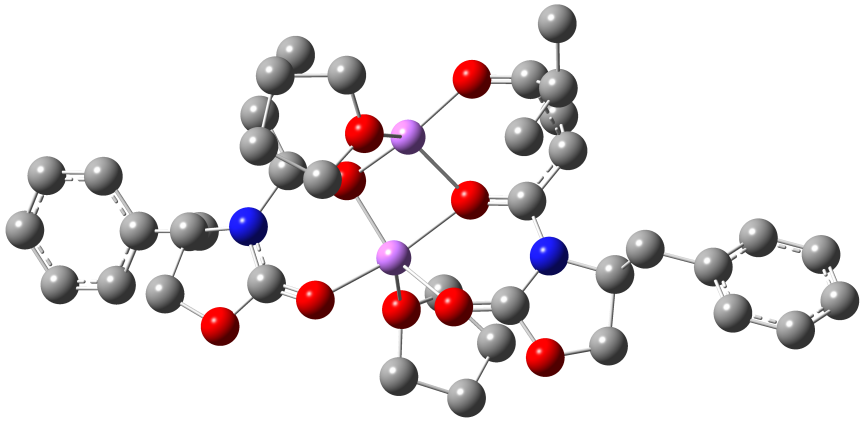
G = -2280.368917 Hartree
G_{MP2} = -1426407.73 kcal/mol
ΔG_{MP2} = 5.003011202 kcal/mol vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.19357781	-2.44653412	-0.42870884
O	0.00000000	0.00000000	2.09913160	H	7.16101480	-1.50158045	-0.96768803
Li	1.95860017	0.00000000	1.88981500	H	9.22763584	-2.85992046	-0.99901998
O	1.97081528	0.52875780	0.06579957	H	9.32766472	-5.01251194	0.24561428
C	2.80569938	0.12044045	-0.84569565	H	7.33820605	-5.78658197	1.52397507
N	2.81504030	-1.32676581	-1.07895275	H	5.27149662	-4.42329137	1.55142121
C	4.02982925	-2.14742012	-1.07580491	C	3.68681134	0.84541341	-1.58222796
C	3.42411232	-3.53186422	-1.38089816	C	3.91924960	2.31933789	-1.41630695
H	3.49381233	-3.78369132	-2.44507359	H	3.62787200	2.89544082	-2.30806551
H	3.86432190	-4.33754462	-0.79107950	H	3.34306290	2.71032176	-0.57232781
O	2.03208975	-3.41973530	-1.03299830	H	4.97995139	2.55201976	-1.23473515
C	1.69876774	-2.09744890	-0.96740101	H	4.26256234	0.33152769	-2.34753379
O	0.53311672	-1.74608892	-0.84309308	O	3.08449519	1.33574629	2.88857710
H	4.69965578	-1.84337932	-1.88558609	C	4.40080947	1.06149454	3.41583691
C	4.78894740	-2.05399819	0.26900845	C	5.04769966	2.43015003	3.65252001
H	5.02071987	-0.99336192	0.42546910	C	4.36644675	3.30121420	2.58442433
H	4.11539699	-2.35810448	1.07803047	C	2.94415524	2.74043295	2.58031402
C	6.06072604	-2.87229711	0.28237939	H	2.43490732	2.81429515	1.61683241
C	6.13465589	-4.08451703	0.98256768	H	2.32198874	3.20951656	3.35452009
C	7.30170976	-4.85167994	0.97051971	H	4.83685409	3.14906584	1.60640205
C	8.41811357	-4.41778755	0.25505240	H	4.39511433	4.37037761	2.81572564
C	8.36059293	-3.20995958	-0.44449573	H	6.13708268	2.39715695	3.55630069

H	4.80669921	2.79984937	4.65628350
H	4.28928940	0.46456469	4.32579271
H	4.95623044	0.47128669	2.67665298
O	2.15747087	-1.73238757	2.64259605
C	1.55672441	-2.33566225	3.57460091
H	1.93226260	-2.20997259	4.60790721
C	0.90425890	-3.70439988	3.31729486
H	0.03589950	-3.55172068	2.66298736
C	1.89239009	-4.60659903	2.55252683
H	1.44758023	-5.59244191	2.37097075
H	2.14909062	-4.16382878	1.58764469
H	2.81539686	-4.75717671	3.12843477
C	0.46042042	-4.37954459	4.62121053
H	-0.23761795	-3.76013410	5.19473051
H	-0.02861660	-5.33933293	4.41898660
H	1.32443042	-4.58215998	5.26742104
C	-0.59197574	-0.74707037	2.92695217
N	-1.75010946	-1.46580321	2.46914385
C	-2.28977004	-1.34779525	1.19547473
O	-1.90749979	-0.68942065	0.25250189
O	-3.41877767	-2.10448723	1.11457170
C	-3.52396294	-2.91794283	2.29527834
H	-3.09374067	-3.90291473	2.08185828
H	-4.57931357	-3.02561137	2.54885969
C	-2.71500985	-2.15182554	3.34755135
H	-2.20361196	-2.84738921	4.01458926
C	-3.56569594	-1.14973853	4.16689883
H	-2.87887879	-0.48899929	4.70673328
H	-4.12784086	-0.52217755	3.46475578
C	-4.50908152	-1.83168957	5.13404422
C	-4.02329130	-2.40254011	6.32024280
C	-4.88071145	-3.05639580	7.20446829
C	-6.24479182	-3.14998488	6.91850162
C	-6.74292166	-2.58252911	5.74553415
C	-5.88038762	-1.92959202	4.86232997
H	-6.27851764	-1.47847977	3.95588925
H	-7.80384622	-2.64266141	5.51761147
H	-6.91410169	-3.65664498	7.60844038
H	-4.48510950	-3.48814770	8.12008090
H	-2.96433558	-2.32399321	6.55860365
C	-0.11840061	-1.02355536	4.22476503
H	-0.74693467	-1.64108702	4.85770810
C	0.67620478	0.02041056	4.97963719
H	0.03287776	0.82720070	5.36219551
H	1.17285155	-0.43166384	5.84763509
H	1.44648872	0.48388093	4.35858008
O	-0.72168074	1.41147948	-1.30749536
C	0.08670708	2.46039459	-1.85571295
C	0.34808199	2.05485187	-3.31992276
C	-0.80655895	1.06353129	-3.64017416
C	-1.64022239	1.04284361	-2.34681471
H	-2.05683902	0.07145362	-2.08296558
H	-2.45311269	1.78453875	-2.38577083
H	-0.41000685	0.06623899	-3.85237146
H	-1.40579751	1.37488370	-4.50176967
H	1.31950921	1.56069514	-3.40505745
H	0.35038909	2.92542043	-3.98370869
H	-0.47014783	3.40864360	-1.79773011
H	0.98428974	2.52341000	-1.24178092

Table 26. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,R*)-**6** from **5** spirocyclic dimer with three THF



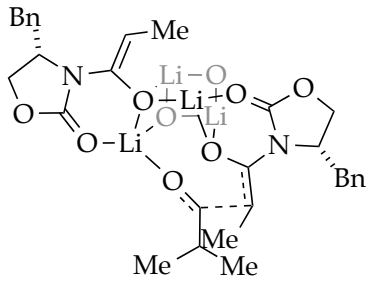


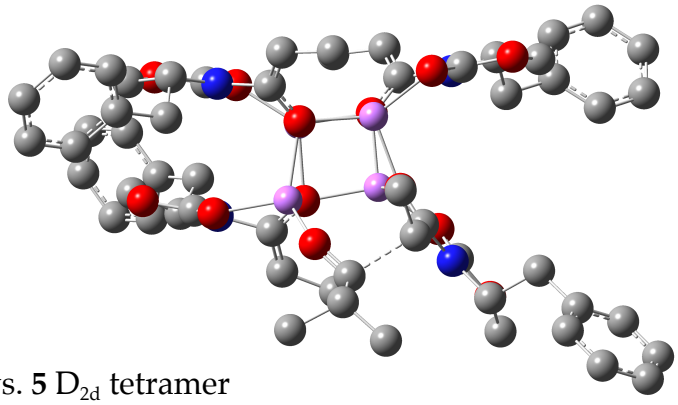
G = -2280.357893 Hartree
G_{MP2} = -1426400.739 kcal/mol
ΔG_{MP2} = 11.99333579 kcal/mol vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	6.79714943	-0.33202144	-2.40917665
Li	0.00000000	0.00000000	2.72130500	H	6.05132255	-0.39944751	-3.19861001
O	1.35644957	0.00000000	1.39292478	H	8.45500942	-0.35812423	-3.78396351
C	2.58159160	0.41850213	1.39619005	H	10.17493231	-0.22980780	-1.99058101
N	3.01506950	1.09548095	0.17225666	H	9.46245690	-0.14942534	0.39248873
C	2.17820559	1.54015870	-0.81161490	H	7.05827049	-0.19211634	0.97264677
O	0.95427465	1.53721240	-0.86667237	C	3.50010544	0.27012715	2.39023878
O	2.90827619	2.04813237	-1.84946445	H	4.48388780	0.71606528	2.29013539
C	4.28667166	2.13026650	-1.44897829	C	3.22049342	-0.51192603	3.64370724
H	4.49662506	3.15865584	-1.13252509	H	4.06911016	-1.15756126	3.91030713
H	4.91419236	1.88105657	-2.30632686	H	3.02819423	0.12223953	4.52461895
C	4.40909219	1.13300765	-0.28782697	H	2.34520847	-1.15861821	3.51570055
H	5.05999530	1.53830515	0.49026717	O	-1.08908123	-1.11687166	1.33864283
C	4.91265737	-0.26943043	-0.70578588	C	-2.28023603	-1.45317022	1.54783965
H	4.72030500	-0.94136190	0.13747811	N	-3.28038298	-0.87798824	0.68377296
H	4.30379747	-0.61987272	-1.54823410	C	-4.65629443	-1.37445532	0.51217439
C	6.37983479	-0.28134781	-1.07223861	C	-4.90411260	-1.00124398	-0.95938268
C	7.36214313	-0.21574839	-0.07192192	H	-4.67888628	-1.82762457	-1.64285665
C	8.71780943	-0.19557595	-0.39801545	H	-5.91537353	-0.64049128	-1.14997025
C	9.11868360	-0.24255470	-1.73544626	O	-3.98159540	0.07254021	-1.22348325
C	8.15380831	-0.31327145	-2.74050401	C	-2.95982779	0.02210585	-0.32235538

O	-1.95911996	0.69516486	-0.46372387
H	-4.66919292	-2.45868212	0.64915430
C	-5.66770694	-0.71474380	1.47787204
H	-5.31856207	-0.87182240	2.50264869
H	-5.65909073	0.36769906	1.30349790
C	-7.07033002	-1.26284464	1.31592225
C	-8.07432814	-0.51371378	0.68786338
C	-9.36129650	-1.03123647	0.52486439
C	-9.66454473	-2.31118669	0.98914397
C	-8.67473716	-3.06777604	1.62088750
C	-7.39152508	-2.54654983	1.78290130
H	-6.63226674	-3.13954646	2.28913867
H	-8.90415474	-4.06242243	1.99401551
H	-10.66564647	-2.71513170	0.86578668
H	-10.12623594	-0.43085743	0.03960811
H	-7.84983212	0.49065252	0.33483797
C	-2.66534074	-2.32353817	2.59610933
C	-1.72606863	-3.48205865	2.89315098
H	-2.08351609	-4.05205648	3.75839165
H	-1.64689243	-4.18355384	2.05006548
H	-0.72105987	-3.11542428	3.12060649
H	-3.72390718	-2.56509543	2.67184231
O	-0.00838657	2.01311500	3.23010546
C	0.28500981	3.11523710	2.35545595
C	1.56347111	3.77306583	2.92052966
C	1.67325466	3.20471792	4.36190856
C	0.35365327	2.44207234	4.54814425
H	-0.43442723	3.10002534	4.94773683
H	0.42010715	1.55146769	5.17592591
H	1.80706830	3.98325550	5.11962220
H	2.51827332	2.51425557	4.42818756
H	1.48317167	4.86473116	2.90826856
H	2.43935546	3.49252257	2.33048330
H	0.39383439	2.71353909	1.34760015
H	-0.56286998	3.81576273	2.37320031
O	-1.01529063	-0.68570970	4.13775119
C	-2.17059551	-1.17168032	4.31919062
C	-3.35980934	-0.24627043	4.62369744
H	-4.28321767	-0.81175577	4.43364143
C	-3.31895904	0.07017059	6.13437618
H	-4.18526116	0.67469744	6.42887164
H	-3.32649760	-0.84506286	6.73861769
H	-2.41017103	0.62985380	6.38269478
C	-3.36027537	1.04623830	3.80370280
H	-3.43893984	0.84907031	2.73072339
H	-4.20282633	1.68664424	4.09231777
H	-2.43131511	1.60011316	3.96037025
H	-2.24418982	-2.11507403	4.89330630
O	0.36263381	-1.30339832	-1.53677949
C	0.13167473	-2.71269777	-1.42068952
C	-1.12513076	-2.99512497	-2.27147040
C	-1.21132656	-1.77297618	-3.23045831
C	0.04713925	-0.95489450	-2.89218450
H	-0.08669595	0.12682945	-2.92558981
H	0.89039716	-1.23551449	-3.54160525
H	-2.10944407	-1.18208741	-3.02911774
H	-1.23352311	-2.06572417	-4.28467261
H	-2.01532534	-3.05738463	-1.63750778
H	-1.03874940	-3.94479685	-2.80841885
H	1.00465134	-3.25506157	-1.81323106
H	0.02005768	-2.93424313	-0.35828271

Table 27. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from **5** D_{2d} tetramer



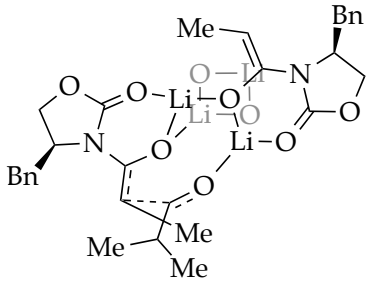


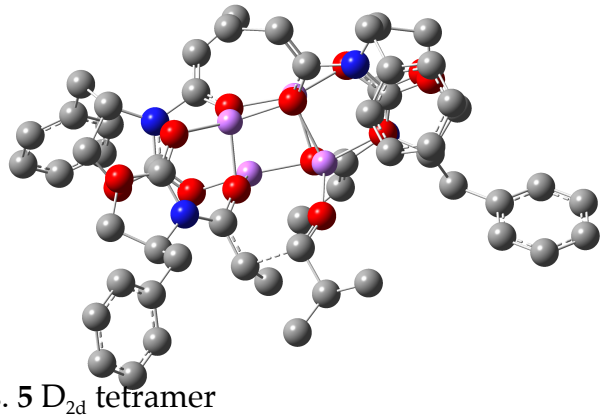
G = -3399.0162 Hartree
G_{MP2} = -2126250.456 kcal/mol
ΔG_{MP2} = 2.342089648 kcal/mol vs. **5** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-3.91005259	-1.49524299	0.01801640
Li	0.00000000	0.00000000	2.74643830	C	-4.44804242	-0.74449802	-0.79022094
O	1.96466194	0.00000000	2.98174704	O	-5.79235645	-0.76474698	-0.97126550
C	2.70087849	0.59894095	2.20599733	C	-6.16406942	0.29481829	-1.87345650
O	4.00280488	0.23666354	2.04948724	H	-6.61639472	1.10213445	-1.28666721
C	4.57478956	0.99087859	0.95787020	H	-6.90204314	-0.09390506	-2.57631069
H	4.65481990	0.32142673	0.09700574	C	-4.85007627	0.74392009	-2.54322515
H	5.56799421	1.32708161	1.25884417	N	-3.86931837	0.17861695	-1.60868045
C	3.58740280	2.14820906	0.69699296	C	-2.42797469	0.34206244	-1.71906807
N	2.40064933	1.65209076	1.40258542	C	-1.88290216	0.45395410	-2.94955689
C	1.10813828	2.32623240	1.44621903	H	-2.52139955	0.31492272	-3.81699121
C	1.12929034	3.66671868	1.61445159	C	-0.42485333	0.73147934	-3.19147586
H	2.09394733	4.13181615	1.79967421	H	0.17790200	-0.18508213	-3.25986817
C	-0.06507022	4.57526463	1.60579325	H	-0.28096986	1.28503690	-4.12742456
H	-0.37663598	4.86108274	2.62285811	H	0.00596975	1.33522621	-2.38346354
H	0.15383623	5.51015607	1.07281847	O	-1.80075674	0.40329466	-0.56243924
H	-0.93240283	4.12028440	1.12119057	C	-4.73327965	2.26918662	-2.71209670
O	0.07545380	1.52090435	1.28530019	H	-4.82079481	2.73673899	-1.72409949
Li	-1.81381840	1.71191339	0.84583371	H	-3.72604715	2.48970736	-3.08079569
O	-3.12459318	3.11090058	1.14891338	C	-5.77996430	2.82028030	-3.65808270
C	-3.72926338	3.21605576	2.20437251	C	-5.67518340	2.60801645	-5.04132249
O	-4.35527408	4.36874211	2.53419318	C	-6.65031529	3.08617337	-5.91611750
C	-4.78780831	4.29440852	3.90890936	C	-7.75068458	3.79098087	-5.42261816
H	-5.73688398	4.82302286	3.99949214	C	-7.86421356	4.01597642	-4.05051679
H	-4.03115544	4.78106805	4.53293584	C	-6.88641854	3.53363723	-3.17800959
C	-4.89389768	2.79045371	4.18771152	H	-6.97596232	3.72473670	-2.11073715
N	-3.91128336	2.28268259	3.20908917	H	-8.71163283	4.57136445	-3.65702817
C	-3.42844597	0.93306173	3.16298492	H	-8.50929452	4.16717169	-6.10359834
O	-2.80572707	0.57415906	2.13368606	H	-6.54785460	2.91413196	-6.98438762
Li	-2.30461121	-0.89857340	0.88539781	H	-4.81485465	2.07211638	-5.43694295

H	-4.74480090	0.26439357	-3.52624153
O	-0.49004294	-1.39891543	1.32062391
C	0.04149509	-2.59253666	1.13516720
N	1.47475816	-2.58362442	0.87167206
C	2.05521897	-1.77179605	-0.04240222
O	1.53112411	-0.89516539	-0.73242293
O	3.38361358	-2.02560169	-0.14033038
C	3.76459151	-2.96206225	0.89363109
H	4.31606036	-2.40685517	1.65648246
H	4.41165830	-3.71774522	0.44604622
C	2.43887002	-3.53441526	1.44203299
H	2.25800415	-4.53590891	1.02976511
C	2.38355714	-3.59805758	2.97967119
C	3.42342786	-4.54001004	3.54891217
C	4.56665316	-4.04642630	4.19250587
C	5.53706565	-4.91444541	4.69767074
C	5.38029325	-6.29447323	4.56528655
C	4.24417809	-6.80055839	3.92933256
C	3.27620031	-5.93050969	3.42833343
H	2.38740100	-6.33477943	2.94786491
H	4.10848165	-7.87449930	3.82965975
H	6.13328387	-6.97157355	4.95977875
H	6.41315160	-4.51043848	5.19849870
H	4.68932770	-2.97199577	4.30933151
H	1.37588096	-3.92090801	3.26358248
H	2.51992091	-2.58352940	3.36899712
C	-0.56723758	-3.79748005	1.18366416
C	-2.01215318	-4.01672813	1.53087468
H	-2.65374684	-4.10473015	0.64244592
H	-2.14040951	-4.93942403	2.11144738
H	-2.41048006	-3.19666063	2.13653879
H	0.02252520	-4.67551283	0.93500502
C	-3.54064560	0.14127398	4.33539074
H	-4.25973903	0.48696573	5.06894695
C	-3.47459306	-1.36183753	4.15899150
H	-4.16826527	-1.72191001	3.38830174
H	-2.45968630	-1.65976617	3.87540252
H	-3.72702919	-1.86902581	5.09585902
C	-6.30792668	2.21555904	3.93113037
H	-6.61709710	2.50458199	2.91912732
H	-6.23741440	1.12237811	3.94145361
C	-7.32720509	2.69013889	4.94498832
C	-8.28362565	3.65762659	4.60907739
C	-9.20824033	4.11053396	5.55255664
C	-9.18878775	3.60105613	6.85097675
C	-8.24286663	2.63373815	7.19852697
C	-7.32230668	2.18299765	6.25309512
H	-6.59797646	1.42021938	6.53185471
H	-8.22537938	2.22541498	8.20540820
H	-9.90840216	3.95017936	7.58630242
H	-9.94520247	4.85749257	5.26992345
H	-8.31350001	4.05074368	3.59492471
H	-4.56776975	2.56559500	5.20443345
C	3.33282247	2.41660931	-0.79716598
H	2.96064832	1.49142775	-1.25121467
H	2.53364801	3.16306973	-0.86897079
C	4.57679577	2.90217972	-1.51142895
C	5.04449598	4.21198086	-1.32450075
C	6.20712278	4.65514269	-1.95456133
C	6.92423955	3.79408212	-2.78844957
C	6.46705088	2.49124872	-2.98884197
C	5.30333135	2.05072595	-2.35488722
H	4.94699257	1.03713511	-2.52447358
H	7.01293005	1.81617969	-3.64289787
H	7.82844036	4.13908691	-3.28284499
H	6.55009332	5.67494417	-1.79971867
H	4.48492010	4.89353331	-0.68692154
H	3.94752967	3.07048797	1.17319391
O	-0.86585242	0.07762788	4.36626791
C	-1.74691847	0.60883395	5.11625976
H	-1.86050626	1.71565736	5.07806782
C	-1.83981912	0.09879664	6.57401275
C	-0.45065206	0.29535943	7.21388585
H	-0.43629815	-0.10250171	8.23603775
H	0.31742337	-0.21019282	6.62419483
H	-0.19063085	1.36125642	7.26585347
H	-2.04143744	-0.97911787	6.54075002
C	-2.91239805	0.79956515	7.41737108
H	-3.93188523	0.52080959	7.12835937
H	-2.79830545	0.54469698	8.47731346
H	-2.82151235	1.89193079	7.33702239

Table 28. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,R*)-**6** from **5** D_{2d} tetramer



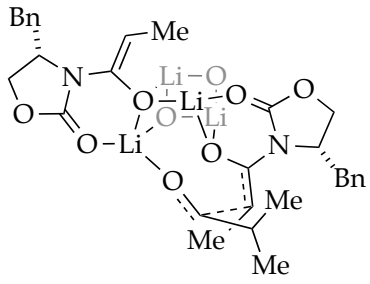


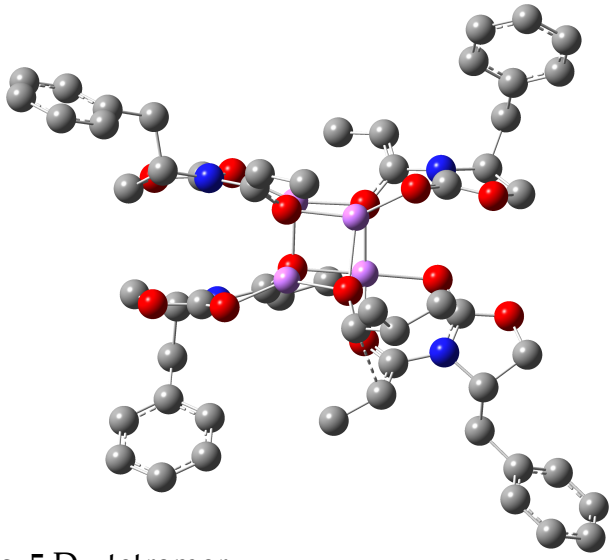
G = -3399.002753 Hartree
G_{MP2} = -2126247.659 kcal/mol
ΔG_{MP2} = 5.138767072 kcal/mol vs. **5** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.28735600	1.05278643	-3.26392100
O	0.00000000	0.00000000	1.94078310	O	0.55115753	0.00866551	-2.61449572
C	0.99820635	0.00000000	2.64833180	Li	-0.07021416	-1.86447698	-2.43333278
O	0.87078559	0.09646201	3.99798408	O	-0.02615338	-2.43790495	-4.29349832
C	2.15155842	-0.12353632	4.61133496	C	1.09738687	-2.54184713	-4.77775908
H	2.18303701	-1.15367197	4.98117537	O	1.40170176	-1.98921741	-5.97913800
H	2.24958425	0.57549087	5.44353866	C	2.81929959	-2.11852570	-6.21571751
C	3.17102919	0.11745077	3.48561183	H	3.28098710	-1.13559663	-6.07907606
H	3.94133010	-0.65866411	3.49992547	H	2.95275513	-2.45140251	-7.24649357
N	2.32093658	-0.07633151	2.30424952	C	3.32172544	-3.14655874	-5.17647303
C	2.84571784	-0.40511294	0.99341546	H	4.19820802	-2.76581388	-4.64242929
C	4.18793730	-0.52346093	0.83098999	N	2.18141658	-3.17408198	-4.25122387
H	4.85928321	-0.34638329	1.66033528	C	2.25790972	-3.49387944	-2.83266925
C	4.81687465	-0.90816248	-0.48322988	C	2.82126233	-4.65770915	-2.44418583
H	4.85109438	-0.08066603	-1.20801311	H	3.09549123	-5.38368968	-3.20010000
H	5.85155740	-1.23470600	-0.33018065	C	3.05191838	-5.02818814	-1.00463728
H	4.29265543	-1.74315034	-0.96844982	H	2.18153568	-5.52394776	-0.55112624
O	1.94719295	-0.59674139	0.04971762	H	3.90018871	-5.71649828	-0.90985041
Li	2.24996992	-0.65637470	-1.86248177	H	3.27293034	-4.15020777	-0.38620407
O	3.18269751	0.33962967	-3.25137189	O	1.77987417	-2.54822014	-2.04662474
C	2.65355009	1.14162706	-4.00427032	Li	1.22242357	-2.43308944	-0.20462152
O	3.33406409	1.65352482	-5.05725858	O	0.83418019	-3.46112032	1.37414649
C	2.42228603	2.39830416	-5.89422270	C	-0.19613245	-3.10807803	1.94983074
H	2.10825986	1.75092032	-6.71943716	O	-0.22197167	-2.92348005	3.28883878
H	2.95166907	3.26677090	-6.28641427	C	-1.54718165	-2.50498217	3.68385972
C	1.25987245	2.75817352	-4.95834515	H	-1.44256141	-1.64787208	4.34861272
H	0.30503626	2.67783200	-5.48109847	H	-2.01808845	-3.33694148	4.21925746
N	1.37725048	1.67192069	-3.96558548	C	-2.28343141	-2.16907356	2.37000910

H	-2.24075465	-1.09044886	2.18266568
N	-1.40851882	-2.85027298	1.39477675
C	-1.53113296	-2.68981189	-0.05030961
C	-2.50409687	-3.39180016	-0.67036746
C	-2.81408020	-3.28930255	-2.13813250
H	-2.22366995	-3.98971767	-2.74779427
H	-3.86997656	-3.51228571	-2.33324547
H	-2.62042474	-2.28204137	-2.52656357
H	-3.07279125	-4.09953359	-0.07663718
O	-0.66050501	-1.86117119	-0.60297727
C	-3.74611686	-2.63841947	2.34805801
H	-4.14038237	-2.46418924	1.34110626
H	-3.77656105	-3.72105925	2.52273777
C	-4.59250061	-1.91562605	3.37680777
C	-5.03673045	-2.56590345	4.53550578
C	-5.80089190	-1.89155645	5.49040563
C	-6.13290880	-0.55023685	5.30023178
C	-5.69904982	0.10992550	4.14810423
C	-4.93812049	-0.56755631	3.19608425
H	-4.61216243	-0.04672567	2.29827073
H	-5.95662423	1.15371491	3.98841147
H	-6.72839609	-0.02325202	6.04099479
H	-6.13867667	-2.41693914	6.38005016
H	-4.79041920	-3.61479456	4.68683841
C	3.70030523	-4.51198731	-5.80493869
H	4.57258073	-4.32626797	-6.44581974
H	4.04892030	-5.16814183	-5.00133730
C	2.61218220	-5.18614598	-6.61364485
C	2.66751316	-5.19550796	-8.01459116
C	1.66513022	-5.80442152	-8.77183528
C	0.58626342	-6.41809526	-8.13546853
C	0.52161755	-6.42352643	-6.74051342
C	1.52574554	-5.81641936	-5.98600968
H	1.46606111	-5.83387645	-4.90144696
H	-0.31175891	-6.90451952	-6.23549350
H	-0.19603091	-6.89369064	-8.72090629
H	1.73116034	-5.80225354	-9.85676945
H	3.51334568	-4.73190542	-8.51903843
C	-0.98225090	1.67666331	-3.26148935
H	-1.11058902	2.49333733	-3.96471572
C	-2.18576358	0.76630663	-3.10424746
H	-2.20807491	-0.02116717	-3.86931470
H	-2.17785533	0.28576142	-2.12034060
H	-3.11410698	1.33931596	-3.19580599
C	1.40507564	4.15539450	-4.31323619
H	0.64931822	4.24673369	-3.52650528
H	2.38315221	4.20704369	-3.81933028
C	1.26383013	5.28141866	-5.31614401
C	0.00634301	5.61456847	-5.84192669
C	-0.12754177	6.63406209	-6.78401379
C	0.99652647	7.34152645	-7.21656913
C	2.25205963	7.02479068	-6.69766846
C	2.38235039	6.00254954	-5.75518087
H	3.36302963	5.77092902	-5.34469606
H	3.13141499	7.57537519	-7.02100624
H	0.89241165	8.13801841	-7.94817864
H	-1.11067837	6.88052295	-7.17594109
H	-0.87772425	5.07992870	-5.50082191
C	3.86764880	1.50413412	3.53483853
H	4.56580320	1.47935105	4.38176260
H	4.47314340	1.60176925	2.62816882
C	2.94549504	2.69623980	3.67186025
C	2.78868365	3.34257126	4.90608660
C	1.92796004	4.43288285	5.04369493
C	1.20776012	4.89620195	3.94243637
C	1.36223986	4.26900674	2.70440680
C	2.22751639	3.18322616	2.56870904
H	2.34731413	2.71009154	1.59780028
H	0.80830351	4.62391105	1.83971540
H	0.53495249	5.74334194	4.04597452
H	1.82350531	4.92006329	6.00978193
H	3.35624885	2.99475937	5.76732142
O	-0.69707615	1.62601802	-0.55841550
C	-0.85388587	2.56047566	-1.40033797
H	0.02363542	3.20042605	-1.63762146
C	-2.15144357	3.39173267	-1.30561792
C	-2.13396025	4.09433984	0.06799376
H	-3.06849815	4.64468621	0.23204479
H	-2.00593415	3.36565077	0.87216266
H	-1.30916839	4.81821189	0.12759375
H	-2.99080662	2.68614810	-1.30403180
C	-2.34540123	4.42193609	-2.42430329
H	-2.56724019	3.95740087	-3.39065394
H	-3.17921040	5.09349075	-2.18837041
H	-1.45227707	5.05046262	-2.54378509

Table 29. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,R*)-**6** from **5** D_{2d} tetramer



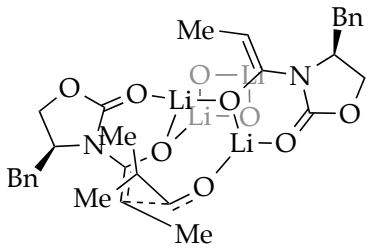


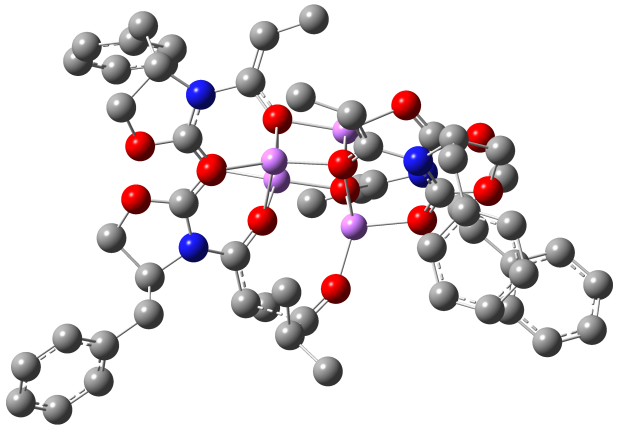
G = -3398.996634 Hartree
G_{MP2} = -2126241.392 kcal/mol
ΔG_{MP2} = 11.40634332 kcal/mol vs. **5** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.68246105	-0.93932651	2.24292417
Li	0.00000000	0.00000000	2.67081310	C	-3.48483833	-2.20828707	2.78870539
O	0.68594493	0.00000000	4.43212981	H	-4.05830519	-3.03801819	2.38465025
C	0.69055304	1.03317225	5.09641099	C	-3.00687680	-2.35494736	4.21202671
O	1.63306325	1.21449818	6.05998950	H	-2.33498424	-1.53510270	4.48353787
C	1.52632050	2.55940828	6.56993717	H	-3.84055334	-2.34931132	4.93210900
H	2.29774862	3.16918779	6.08963325	H	-2.46940428	-3.30070043	4.36407956
H	1.69115943	2.52021860	7.64781496	O	-3.11011334	0.11424819	2.60911318
C	0.10873702	3.00829357	6.18018320	C	-6.82599932	-1.41298991	1.97556863
H	0.10555489	4.03934937	5.81533159	H	-6.34377806	-1.58426733	2.94449925
N	-0.14392644	2.11102326	5.04431094	H	-7.11743098	-0.35597370	1.94442055
C	-1.04476264	2.41787881	3.94502361	C	-8.04259040	-2.30053853	1.82800715
C	-2.00112045	3.36015760	4.12428130	C	-7.97696621	-3.65998707	2.16938681
H	-2.13864592	3.81614097	5.09563973	C	-9.08466531	-4.49233543	2.01250862
C	-2.92871124	3.80291310	3.02504389	C	-10.28296587	-3.97828783	1.51124053
H	-3.83449069	3.18086762	2.95297025	C	-10.36421428	-2.62759031	1.17216146
H	-3.26491616	4.83398482	3.18772801	C	-9.25195902	-1.79774666	1.32974453
H	-2.44031584	3.78418245	2.04180647	H	-9.32797034	-0.74226367	1.07659667
O	-0.79895529	1.77411045	2.82891478	H	-11.29429538	-2.21574300	0.78942680
Li	-2.24693460	1.39552908	1.47642674	H	-11.14768164	-4.62534144	1.39203287
O	-3.82454110	1.20752922	0.19764040	H	-9.01465711	-5.54149408	2.28745856
C	-4.57569308	0.24479376	0.24248844	H	-7.05165503	-4.06663149	2.57286850
O	-5.60428516	0.12774662	-0.64839926	O	-0.85236286	1.78343918	0.06890000
C	-6.18797412	-1.18470372	-0.52097817	C	-0.99516654	2.45171181	-1.06014448
H	-5.78216118	-1.82159890	-1.31410484	N	-1.60151522	1.69585561	-2.14276326
H	-7.26846396	-1.09505966	-0.64170787	C	-1.36191299	0.36819001	-2.30646871
C	-5.76511358	-1.66213657	0.87709016	O	-0.43963901	-0.29960612	-1.83696607
H	-5.50443777	-2.72259633	0.85055843	O	-2.30182493	-0.20052082	-3.09351954
N	-4.56240800	-0.84008878	1.07968695	C	-3.34664031	0.76050545	-3.35812331

H	-4.22795859	0.47698201	-2.77756195
H	-3.56891787	0.71577543	-4.42578930
C	-2.77646092	2.12689594	-2.91498662
H	-3.46698156	2.63262243	-2.23448985
C	-2.48458066	3.06903185	-4.11108678
H	-3.45754966	3.29007298	-4.57009970
H	-2.11520771	4.02061690	-3.71717586
C	-1.54271138	2.52355262	-5.16372273
C	-2.03361796	2.08766808	-6.40248373
C	-1.17719440	1.57392451	-7.37800940
C	0.19246255	1.48930510	-7.12871812
C	0.69729496	1.92683783	-5.90235771
C	-0.16052506	2.44153870	-4.92997702
H	0.24638035	2.78409312	-3.98265836
H	1.76370851	1.87039858	-5.70073788
H	0.86291715	1.09032205	-7.88523547
H	-1.58096078	1.24463447	-8.33198769
H	-3.09923874	2.16310714	-6.61093372
C	-0.65861320	3.74474886	-1.26918352
H	-0.74043420	4.15460078	-2.26770909
C	-0.12973270	4.65274919	-0.19165977
H	0.96591641	4.61215289	-0.09507190
H	-0.38901761	5.69783985	-0.39900363
H	-0.54883319	4.41109035	0.79324251
Li	0.46826932	2.22682598	1.44466884
O	1.99467233	3.09009381	2.23133929
C	2.91559179	2.40300728	2.66139224
O	3.66563101	2.83345964	3.71658862
C	4.54232101	1.75268460	4.12047883
H	4.05627317	1.20321004	4.93227849
H	5.48137290	2.18849123	4.46375911
C	4.68025527	0.91204613	2.84691822
H	4.75092800	-0.15570843	3.06601660
N	3.37832424	1.19622864	2.22675441
C	2.67403316	0.30991872	1.31770044
C	3.37787260	-0.63745602	0.65526712
C	2.74531825	-1.65452856	-0.25128988
H	1.70038652	-1.83547944	0.02030865
H	2.75753890	-1.35094432	-1.30917690
H	3.26678246	-2.61836349	-0.19021626
H	4.45667268	-0.66527190	0.74900383
O	1.37368210	0.50110670	1.27147476
C	5.87113460	1.37175571	1.96541406
H	5.76299113	0.92760876	0.97134265
H	5.79606668	2.45799882	1.83233362
C	7.21543697	1.01113223	2.56080399
C	8.04151747	1.98875262	3.13134041
C	9.27186111	1.64902599	3.69825235
C	9.69580877	0.32013240	3.70455746
C	8.88403401	-0.66482520	3.13683427
C	7.65723276	-0.32090023	2.57030888
H	7.03768220	-1.09488128	2.12173308
H	9.20917685	-1.70190728	3.13068973
H	10.65324221	0.05302618	4.14360933
H	9.89886440	2.42432370	4.13079035
H	7.72289734	3.02902329	3.12049375
C	-0.91165812	2.89287623	7.34704962
H	-0.57786580	3.59817762	8.11973349
H	-1.88310784	3.25403512	6.99770598
C	-1.07200250	1.51239083	7.94588940
C	-0.44718041	1.17033384	9.15287990
C	-0.59087426	-0.10600332	9.69941792
C	-1.36820415	-1.06192347	9.04498300
C	-2.00533706	-0.73084567	7.84707378
C	-1.86162770	0.54597092	7.30352205
H	-2.36855027	0.79954541	6.37583404
H	-2.62015385	-1.46543058	7.33405578
H	-1.48285123	-2.05615260	9.46859561
H	-0.09947353	-0.35028396	10.63769676
H	0.14823922	1.91506701	9.67786302
O	-0.86271547	-1.27667707	1.39793096
C	-1.30008154	-2.40932432	1.74133680
C	-1.58351177	-3.53247140	0.75314164
H	-2.27104033	-4.22291862	1.25667272
C	-0.26328643	-4.30331669	0.51610304
H	-0.45734556	-5.19511909	-0.09095959
H	0.46527090	-3.68422581	-0.01616429
H	0.19109850	-4.63129468	1.45870155
C	-2.19939176	-3.07167132	-0.56973632
H	-2.39712042	-3.93653977	-1.21383438
H	-3.14515668	-2.54701082	-0.40234776
H	-1.53262430	-2.39437131	-1.11031646
H	-1.06515255	-2.75578068	2.75704468

Table 30. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,S*)-**6** from **5** D_{2d} tetramer



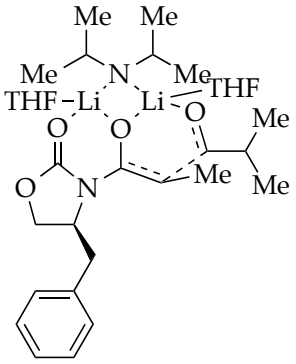


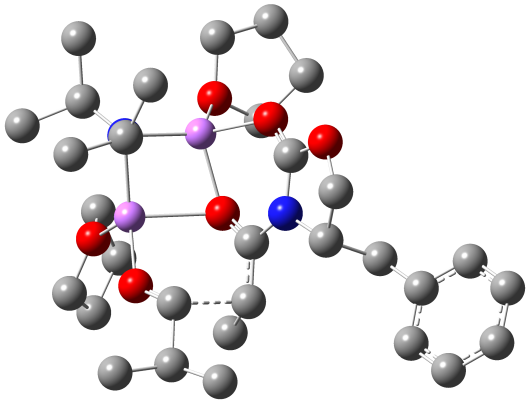
G = -3398.99907 Hartree
G_{MP2} = -2126248.026 kcal/mol
ΔG_{MP2} = 4.772167067 kcal/mol vs. **5** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.36327381	2.22699369	-3.96601355
O	0.00000000	0.00000000	1.95469910	C	-2.29755834	0.47278482	-3.02041830
C	0.98221044	0.00000000	2.68334283	H	-2.15630591	-0.08858569	-2.09286173
O	0.82811889	-0.04776095	4.03345096	H	-3.24806024	1.01273622	-2.94531709
C	2.10902824	-0.28100146	4.64279552	H	-2.38235399	-0.23931844	-3.85182362
H	2.19120406	-1.34931275	4.86773685	O	0.53718292	-0.02097289	-2.51384640
H	2.15315883	0.30208803	5.56390430	Li	0.20347696	-1.97146649	-2.36623312
C	3.12776029	0.16700089	3.58251405	O	0.38134071	-2.47682548	-4.23053096
H	3.95646232	-0.54423680	3.51990518	C	1.51141812	-2.59299733	-4.69490621
N	2.31392866	0.04896051	2.36543203	O	1.79528843	-2.15497523	-5.95120657
C	2.87866997	-0.12764564	1.04347842	C	3.21428631	-2.28669120	-6.18721111
C	4.22215618	-0.03439916	0.87753561	H	3.66618938	-1.29334018	-6.11091091
H	4.86409772	0.20539640	1.71408390	H	3.34503422	-2.68126259	-7.19640437
C	4.88549723	-0.24848423	-0.45844497	C	3.71698423	-3.24542908	-5.08887446
H	4.71803923	0.58042280	-1.16323619	H	4.63695224	-2.87369048	-4.62783955
H	5.97032631	-0.34145565	-0.33765038	N	2.62317042	-3.12729817	-4.11609107
H	4.54679033	-1.16973361	-0.95427739	C	2.75283686	-3.30266035	-2.67794822
O	2.01733922	-0.41400399	0.08937010	C	3.55428827	-4.27627755	-2.19351480
Li	2.34121496	-0.45852827	-1.81313503	H	3.99846429	-4.98620843	-2.87984460
O	3.09592809	0.50032357	-3.35305094	C	3.84339684	-4.44996020	-0.72656356
C	2.42604226	0.98279462	-4.25183050	H	3.06585601	-5.02599368	-0.20480663
O	2.95050542	1.19705283	-5.48116020	H	4.79178491	-4.97928007	-0.57817264
C	1.87706872	1.52686861	-6.39550500	H	3.92455821	-3.48701778	-0.20720645
H	1.56726179	0.60598117	-6.89861752	O	2.08535079	-2.41523631	-1.96827391
H	2.25896348	2.24505122	-7.12088645	Li	1.49863267	-2.31631179	-0.12652777
C	0.77603094	2.09231172	-5.48748817	O	1.22206772	-3.40302658	1.43770627
H	-0.21125374	1.77224465	-5.82614398	C	0.15097829	-3.18030729	2.00469867
N	1.10791530	1.40138589	-4.22374178	O	0.09057359	-3.01769614	3.34595801
C	0.15040940	0.88894901	-3.28734447	C	-1.27998549	-2.76684150	3.73013465
C	-1.15250063	1.45793974	-3.22387497	H	-1.28453056	-1.92189517	4.41791372

H	-1.65822569	-3.66259228	4.23539473
C	-2.03047091	-2.48401696	2.41265738
H	-2.09495829	-1.40335860	2.24260268
N	-1.07676745	-3.05547983	1.43963225
C	-1.20490576	-2.90685458	-0.00666393
C	-2.08664406	-3.71539395	-0.63413099
C	-2.39210601	-3.64914278	-2.10495461
H	-2.28870102	-2.63011008	-2.49730979
H	-1.73526092	-4.29625343	-2.70612203
H	-3.42132186	-3.96908152	-2.30823381
H	-2.57900544	-4.48193857	-0.04517074
O	-0.43037100	-1.98551768	-0.55216836
C	-3.43599713	-3.10020221	2.36211481
H	-3.83704634	-2.94390114	1.35485333
H	-3.35602746	-4.18407980	2.51175341
C	-4.36187230	-2.49410792	3.39835716
C	-4.75755595	-3.22128175	4.52853023
C	-5.59431117	-2.65343740	5.49179857
C	-6.04811977	-1.34332578	5.33892055
C	-5.66296016	-0.60738062	4.21572555
C	-4.82978140	-1.17882756	3.25472004
H	-4.54165982	-0.59991412	2.37988973
H	-6.01448436	0.41278651	4.08563911
H	-6.69977120	-0.89907098	6.08660564
H	-5.89247776	-3.23705394	6.35903306
H	-4.41413764	-4.24639316	4.65086406
C	3.98322988	-4.68013747	-5.62097512
H	4.78170016	-4.58764244	-6.36927057
H	4.39937599	-5.28163325	-4.80746329
C	2.78796010	-5.38154041	-6.22876703
C	2.64013219	-5.48141632	-7.61886295
C	1.53083431	-6.11680570	-8.17989278
C	0.55008826	-6.66668041	-7.35430550
C	0.68997163	-6.58373317	-5.96719017
C	1.80029558	-5.95010923	-5.40894032
H	1.90482230	-5.89696883	-4.32823990
H	-0.06466292	-7.01676424	-5.31613328
H	-0.31419229	-7.16275941	-7.78765461
H	1.43729140	-6.18582314	-9.26058091
H	3.40850076	-5.06943036	-8.27046853
C	0.82553412	3.63108777	-5.35504716
H	0.13995957	3.92971737	-4.55554672
H	1.83211984	3.92028905	-5.02983977
C	0.46748434	4.33782188	-6.64610004
C	-0.86008513	4.36565841	-7.09925255
C	-1.19374613	4.99452339	-8.29834885
C	-0.20299961	5.61057458	-9.06652417
C	1.12016511	5.59550178	-8.62517626
C	1.45048651	4.96319476	-7.42450978
H	2.48271963	4.96690283	-7.08055908
H	1.89689460	6.07946599	-9.21119014
H	-0.46287249	6.10353301	-9.99923218
H	-2.22840596	5.00872829	-8.63028848
H	-1.64205531	3.89994134	-6.50260767
C	3.71439143	1.58438235	3.82749024
H	4.38588533	1.49989118	4.69210657
H	4.33935409	1.84448862	2.96778722
C	2.70376710	2.68314303	4.07534837
C	2.43168405	3.13012799	5.37595168
C	1.49291964	4.13638066	5.60942599
C	0.81145797	4.71662318	4.53936118
C	1.08132533	4.28991743	3.23748835
C	2.02152608	3.28532437	3.00756305
H	2.23285950	2.96858314	1.98954622
H	0.56275030	4.74152042	2.39643577
H	0.08007796	5.50052033	4.71708038
H	1.29890557	4.46869699	6.62604053
H	2.97037704	2.69407822	6.21528168
O	-0.85087205	1.53978469	-0.56531339
C	-1.18347887	2.36597810	-1.47957975
C	-0.41367101	3.70347131	-1.57404184
H	-0.59987569	4.14232943	-2.56522101
C	1.09346318	3.55246047	-1.34901590
H	1.57200446	2.95524364	-2.13116677
H	1.58516247	4.53268144	-1.33013770
H	1.28105995	3.05116528	-0.39466425
C	-1.02075700	4.65917493	-0.52753099
H	-0.88969170	4.24863874	0.48013934
H	-0.53878881	5.64376896	-0.56771274
H	-2.09556103	4.80394775	-0.69161056
H	-2.27053251	2.55531384	-1.61049620

Table 31. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,S*)-**6** from LDA **5** mixed dimer with three THF



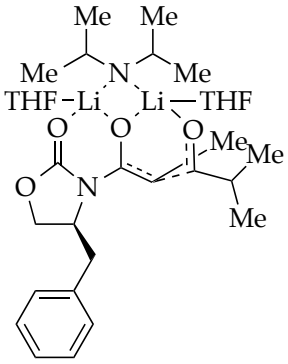


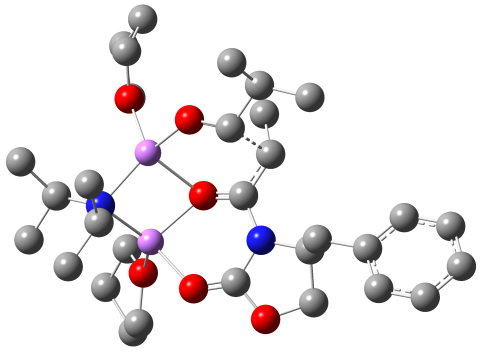
G = -1787.920851 Hartree
G_{MP2} = -1118233.28 kcal/mol
ΔG_{MP2} = 4.221059292 kcal/mol vs. **5** LDA mixed dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.66610284	-1.27702979	3.83968753
Li	0.00000000	0.00000000	2.61238600	C	-1.16965419	-2.42092498	3.62827604
N	1.51225768	0.00000000	1.26976654	C	-1.80196980	-3.17317594	4.81347162
C	2.34589095	1.20864602	1.24529876	H	-2.59094114	-2.53601098	5.23282317
H	1.65042150	2.00898199	0.93507602	C	-0.70980976	-3.33512510	5.89195787
C	2.90276616	1.69527612	2.61219566	H	-1.11959613	-3.82081929	6.78589641
H	3.71053434	1.05815741	2.98628151	H	0.11746681	-3.95548927	5.52302821
H	3.30556949	2.71537369	2.52466791	H	-0.30046661	-2.36220277	6.17461282
H	2.10668055	1.70900187	3.36452444	C	-2.38442650	-4.54183335	4.44238601
C	3.49424506	1.25358233	0.20753087	H	-2.67279177	-5.09635292	5.34277186
H	3.88920582	2.27481408	0.11043304	H	-3.27475051	-4.46353021	3.80979063
H	4.33440108	0.61141386	0.49655539	H	-1.64184724	-5.15254805	3.91075734
H	3.14682378	0.92506717	-0.77885930	H	-0.65191653	-3.10128919	2.92137035
C	2.13799080	-1.32421250	1.40613649	O	-0.53438301	1.74774296	3.42880632
H	1.28552701	-2.00764068	1.58289765	C	-0.79695267	2.98404009	2.75663502
C	3.07291924	-1.54690466	2.62045015	C	-2.21661124	3.36597546	3.19900634
H	3.29852312	-2.61564654	2.74231379	C	-2.33232856	2.74902107	4.62041700
H	4.03097154	-1.02836224	2.49830452	C	-1.05983345	1.88160369	4.75834790
H	2.60705819	-1.19024853	3.54583548	H	-1.23263742	0.87030157	5.12846877
C	2.83175904	-1.90150651	0.14023526	H	-0.30940749	2.37694262	5.39118945
H	2.19733593	-1.77003744	-0.74325244	H	-3.23785437	2.14236507	4.71035431
H	3.79577753	-1.42414228	-0.06320235	H	-2.37045989	3.51599465	5.40019054
H	3.02430715	-2.97774923	0.26335386	H	-2.95208414	2.91527001	2.52576316

H	-2.37283712	4.44912644	3.19165893
H	-0.06001990	3.73734019	3.07428385
H	-0.68447205	2.80778756	1.68489605
O	-1.54859792	-0.55108223	1.08561684
C	-2.06545227	-1.68985046	1.22544250
N	-1.73120288	-2.70311759	0.26023242
C	-2.34011926	-4.04491328	0.19106033
C	-1.34771234	-4.73123729	-0.75460518
H	-0.51646110	-5.19947243	-0.21707318
H	-1.81123709	-5.45747491	-1.42284360
O	-0.82315863	-3.65078139	-1.55242880
C	-0.94958217	-2.49055212	-0.86307753
O	-0.43185174	-1.46237477	-1.26437780
H	-2.32760455	-4.51795409	1.17460963
C	-3.78312463	-4.00111768	-0.37039996
H	-4.36672170	-3.30737083	0.24426280
H	-3.74494044	-3.57690782	-1.38128512
C	-4.44211373	-5.36391661	-0.40127250
C	-4.87878644	-5.97321394	0.78479756
C	-5.46177974	-7.23983907	0.76662180
C	-5.62133609	-7.92119615	-0.44229358
C	-5.19686203	-7.32524077	-1.62996666
C	-4.61195607	-6.05730239	-1.60712390
H	-4.29310849	-5.59512421	-2.53906464
H	-5.32307911	-7.84376754	-2.57663601
H	-6.07769292	-8.90710369	-0.45758923
H	-5.79608209	-7.69303077	1.69604788
H	-4.76973451	-5.44733189	1.73127839
C	-2.83974880	-2.06524978	2.34752009
H	-3.36032205	-3.01347522	2.28891715
C	-3.56652052	-0.96711007	3.09069552
H	-2.84818500	-0.28991361	3.56382030
H	-4.20552066	-0.36651421	2.42901507
H	-4.20581359	-1.39062176	3.87294087
O	-0.52178209	1.65830598	-1.00018327
C	0.31737039	1.97290827	-2.14273584
C	-0.63471223	2.24616743	-3.31861729
C	-1.92592418	1.53077043	-2.88608995
C	-1.91100938	1.76133340	-1.37769891
H	-2.45907707	1.01961927	-0.79315878
H	-2.28196505	2.76505796	-1.12294268
H	-1.86143098	0.45821383	-3.09951422
H	-2.82294329	1.93157453	-3.36826965
H	-0.23430082	1.87602501	-4.26681485
H	-0.81503053	3.32205717	-3.42684120
H	0.94660053	2.83167975	-1.88942698
H	0.96345423	1.10816051	-2.32656674

Table 32. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,R*)-**6** from LDA **5** mixed dimer with three THF



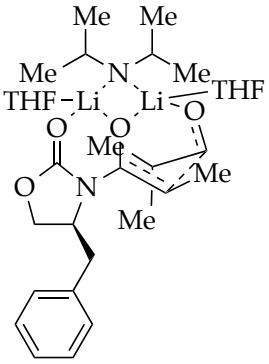


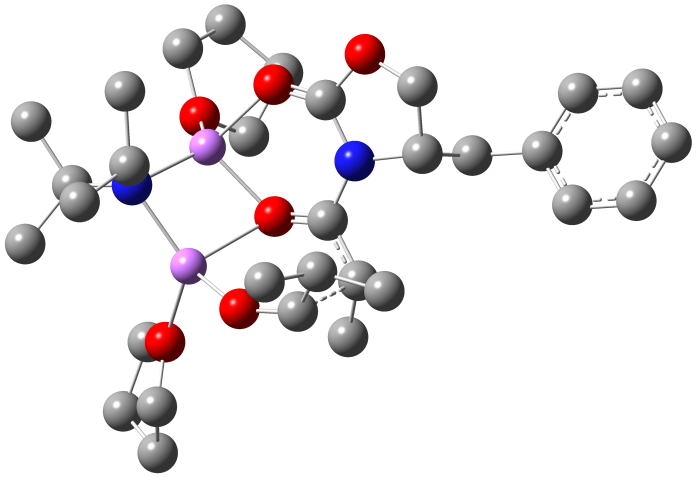
G = -1787.918608 Hartree
G_{MP2} = -1118229.796 kcal/mol
ΔG_{MP2} = 7.705352619 kcal/mol vs. **5** LDA mixed dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.57571582	-0.85537765	3.05084482
O	0.00000000	0.00000000	2.13893550	N	-1.17203781	1.62591670	-0.21431003
C	1.09260373	0.00000000	2.76294633	C	-0.35105552	2.81376806	-0.49996286
N	1.34869072	1.10317427	3.65419765	H	0.32809433	2.88787276	0.36881757
C	2.42948393	1.17060803	4.65530532	C	0.60574884	2.71187603	-1.71976657
C	1.76946588	2.07736765	5.70250138	H	0.07282427	2.75234668	-2.67547668
H	1.21861669	1.50886720	6.46012356	H	1.32786785	3.54177579	-1.71349553
H	2.46707674	2.75833349	6.19063771	H	1.17235364	1.77445648	-1.68342168
O	0.82723676	2.86022369	4.94412426	C	-1.07619377	4.17981629	-0.54886858
C	0.50376812	2.18933584	3.80889329	H	-0.34893540	5.00361352	-0.54645997
O	-0.40220537	2.57528951	3.09349360	H	-1.68453304	4.29100843	-1.45446520
Li	-1.29967818	1.44954228	1.75737504	H	-1.73320827	4.30579458	0.31949654
O	-3.01125876	1.11624870	2.77621831	C	-2.36944612	1.34879159	-1.01293566
C	-3.92610927	0.03181908	2.50820730	H	-2.65185656	0.31828369	-0.72885310
C	-5.29648366	0.50196417	3.00893208	C	-2.20423696	1.29691689	-2.55156796
C	-4.91474527	1.48538490	4.12715459	H	-3.10259875	0.87464226	-3.02430248
C	-3.66581353	2.14804537	3.54637464	H	-2.05242015	2.29362867	-2.98216344
H	-2.95636977	2.50888826	4.29425623	H	-1.34688365	0.67419333	-2.83028075
H	-3.92593608	2.98065056	2.87913847	C	-3.63158007	2.19608396	-0.68471732
H	-4.66849651	0.94378396	5.04838179	H	-3.78092011	2.24920453	0.39986907
H	-5.70403068	2.20766727	4.35628256	H	-3.55903992	3.22152848	-1.06072988
H	-5.92169834	-0.32733690	3.35336823	H	-4.53108065	1.74771809	-1.13327728
H	-5.83511261	1.02569652	2.21104588	H	2.61795304	0.17496552	5.06258991
H	-3.90613625	-0.17928691	1.43481425	C	3.73326766	1.77086928	4.07825766

H	4.03393870	1.16963924	3.21536087
H	3.51065946	2.77666559	3.70177883
C	4.85279188	1.82916831	5.09656956
C	5.51401351	0.65922336	5.50034508
C	6.52868945	0.70384102	6.45605973
C	6.90300427	1.92317795	7.02553364
C	6.25844852	3.09510723	6.62930197
C	5.24186485	3.04588889	5.67307945
H	4.75225481	3.96572234	5.36030514
H	6.54802271	4.05004771	7.05969859
H	7.69568662	1.95892446	7.76781549
H	7.03199008	-0.21286323	6.75182796
H	5.24048132	-0.29421047	5.05310943
C	2.09976392	-0.97662858	2.58405099
H	2.94032209	-0.93849140	3.26881997
C	1.64793896	-2.36486667	2.18291697
H	1.17386733	-2.34260954	1.19608774
H	2.50156836	-3.05008766	2.13751489
H	0.92287031	-2.78853880	2.89218823
O	-0.74444934	-1.74188709	-0.77686341
C	-1.73955221	-2.61949424	-0.21552139
C	-1.68011024	-3.91256873	-1.03970066
C	-0.22489523	-3.91711347	-1.53536201
C	0.02375587	-2.43041047	-1.78774720
H	-0.33835384	-2.12636180	-2.77963434
H	1.06242310	-2.11700019	-1.66836819
H	-0.07494235	-4.52769955	-2.43108356
H	0.44642989	-4.28726680	-0.75133726
H	-2.37001415	-3.85745456	-1.88996421
H	-1.94197058	-4.79573653	-0.44894069
H	-1.48893618	-2.79437052	0.83821049
H	-2.71338506	-2.12112710	-0.26661687
O	1.86346214	-0.35577081	-0.10204662
C	2.83520616	-0.23579606	0.69956651
H	3.07682759	0.77123440	1.09325271
C	4.08671699	-1.09482073	0.44311096
C	4.64783712	-0.67637869	-0.93321327
H	4.97797644	0.37063336	-0.92045337
H	5.51264216	-1.29551334	-1.20130837
H	3.88623036	-0.77897267	-1.71022628
C	5.17870524	-0.98081464	1.51193665
H	5.45564297	0.06782548	1.68382817
H	4.87490090	-1.41435713	2.46995118
H	6.08720883	-1.50300314	1.18987491
H	3.75636069	-2.13813153	0.36420124

Table 33. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R,R*)-**6** from LDA **5** mixed dimer with three THF



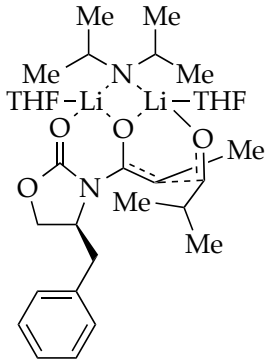


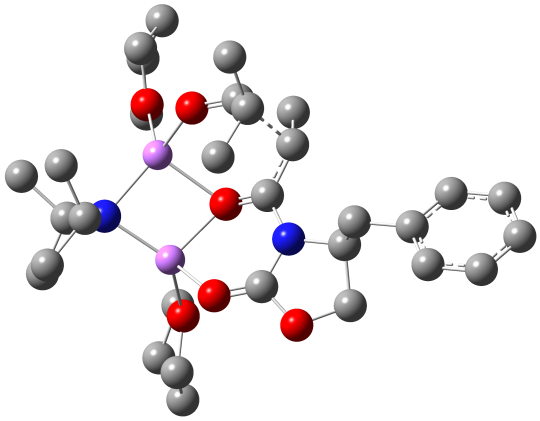
G = -1787.921424 Hartree
G_{MP2} = -1118232.972 kcal/mol
ΔG_{MP2} = 4.529442357 kcal/mol vs. **5** LDA mixed dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.24316615	-2.95795888	3.14160359
O	0.00000000	0.00000000	2.17324780	N	-1.12823821	-1.66928111	-0.18890581
C	1.09212466	0.00000000	2.79511352	C	-2.40777195	-1.53762934	-0.89585269
N	1.39521715	-1.13901433	3.61995352	H	-2.97805903	-0.81087986	-0.28928500
C	2.45562201	-1.17757273	4.64476528	C	-2.35215182	-0.90081595	-2.31287690
C	2.46213636	-2.67795532	4.96169457	H	-1.94210608	-1.58405723	-3.06333089
H	3.16412139	-3.23205487	4.32954523	H	-3.35883909	-0.61159127	-2.65061341
H	2.65766378	-2.90110974	6.01098565	H	-1.72481657	-0.00270970	-2.29954689
O	1.12526579	-3.11136824	4.64569338	C	-3.31270920	-2.79258826	-0.96279536
C	0.57648398	-2.24892031	3.75444642	H	-4.32297689	-2.52590639	-1.30489834
O	-0.48781372	-2.49829476	3.21749379	H	-2.92414206	-3.54218526	-1.66225500
Li	-1.30145774	-1.42758815	1.76492677	H	-3.39967643	-3.26736075	0.02151420
O	-3.07833541	-0.97226495	2.59846539	C	-0.19149265	-2.74468399	-0.54991164
C	-3.89607246	-2.08427752	3.04334648	H	0.74273079	-2.47335326	-0.02656401
C	-4.50075157	-1.66193024	4.39200519	C	0.21222225	-2.86112459	-2.03960330
C	-3.52209816	-0.57985854	4.87777585	H	1.07073435	-3.53742284	-2.15610358
C	-3.13816740	0.09571424	3.56320389	H	-0.60025647	-3.26561340	-2.65510536
H	-2.16129850	0.58472965	3.56797854	H	0.49298877	-1.88312401	-2.44706507
H	-3.90079571	0.82498605	3.25275499	C	-0.52895412	-4.16473272	-0.01631171
H	-2.63920495	-1.03977878	5.33647042	H	-0.79233820	-4.12407453	1.04684131
H	-3.96649856	0.11391292	5.59817458	H	-1.36240802	-4.62888191	-0.55371016
H	-4.59202619	-2.50349399	5.08483416	H	0.33824182	-4.83336070	-0.12199199
H	-5.49947348	-1.23265250	4.25043665	H	3.41161113	-0.87625895	4.21588646
H	-4.65095731	-2.29040211	2.27854295	C	2.11227611	-0.28992478	5.86561825

H	1.91133021	0.72308126	5.49948965
H	1.18117612	-0.66050487	6.31188293
C	3.21610130	-0.26703316	6.90137629
C	4.39689837	0.45403244	6.66840331
C	5.43048005	0.45670846	7.60442256
C	5.30024198	-0.26197480	8.79512772
C	4.12941707	-0.97875789	9.04259993
C	3.09721355	-0.97994297	8.10190654
H	2.18246498	-1.53214734	8.30755360
H	4.01509222	-1.53488552	9.96921982
H	6.10410953	-0.25827118	9.52606328
H	6.33593099	1.02417305	7.40667146
H	4.50394837	1.02715771	5.74952858
C	2.08802893	0.99258051	2.61733336
H	2.93503719	0.96603279	3.29599029
C	1.61481462	2.38773796	2.25438112
H	0.97104539	2.35704224	1.37130250
H	1.04894444	2.86069753	3.06959377
H	2.47238435	3.03345937	2.03226198
O	1.85444072	0.28530807	-0.01835068
C	2.84184419	0.39506542	0.77045453
C	3.74809479	-0.82880454	1.02491698
H	3.18279847	-1.56631532	1.61101083
C	4.08593936	-1.48268231	-0.32854851
H	4.64898208	-0.79040922	-0.96802354
H	4.70174165	-2.37851011	-0.18178068
H	3.17295917	-1.76342635	-0.85827690
C	5.03767052	-0.45364822	1.76679787
H	4.84942828	0.02178770	2.73624215
H	5.66091802	-1.33786883	1.94421678
H	5.63268758	0.25100516	1.17163806
H	3.42525960	1.33918143	0.73044289
O	-0.68317644	1.79400243	-0.68033881
C	-1.95676818	2.43909140	-0.47035905
C	-1.99000822	3.63658253	-1.43055969
C	-0.49628400	3.94167776	-1.63116869
C	0.10645402	2.53819430	-1.63152374
H	1.14565907	2.47715054	-1.30448010
H	0.01777248	2.06665605	-2.62046411
H	-0.10547023	4.52493691	-0.78865202
H	-0.28720315	4.49075527	-2.55441072
H	-2.55638435	4.48038294	-1.02472768
H	-2.44820171	3.34936258	-2.38399424
H	-2.75367757	1.71293540	-0.65723992
H	-2.00776951	2.75529693	0.57901283

Table 34. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S,S*)-**6** from LDA **5** mixed dimer with three THF



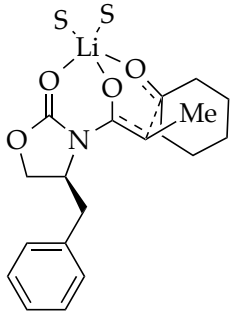


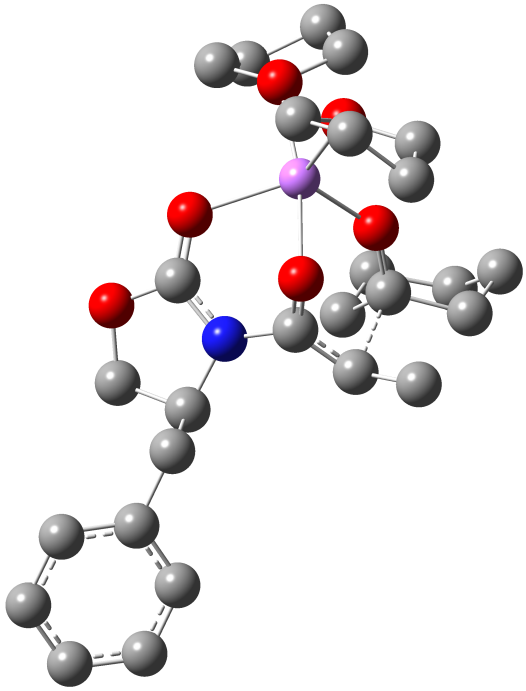
G = -1787.915442 Hartree
G_{MP2} = -1118229.026 kcal/mol
ΔG_{MP2} = 8.475350098 kcal/mol vs. **5** LDA mixed dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.15759342	2.60915063	-1.92455062
O	0.00000000	0.00000000	2.11375040	H	-0.44526068	2.49547315	-2.83160386
C	1.05391460	0.00000000	2.79457845	H	0.77537299	3.51007301	-2.05429319
N	1.17998089	1.00309641	3.81916230	H	0.83338624	1.74919929	-1.85332084
C	2.04391571	0.91066798	5.01143557	C	-1.58550127	3.99744023	-0.74886572
C	1.18119996	1.68232810	6.02153602	H	-0.95291312	4.88922765	-0.85736435
H	0.49342889	1.02899430	6.56960377	H	-2.25364063	3.96970606	-1.61826349
H	1.76252459	2.27683496	6.72653632	H	-2.20224705	4.12658095	0.14832565
O	0.40282009	2.58222034	5.20542792	C	-2.59065743	1.01949925	-0.87620386
C	0.31092991	2.07282235	3.95031028	H	-2.75376532	0.00441718	-0.46731351
O	-0.43527159	2.56050148	3.12167372	C	-2.52015284	0.81822512	-2.41042522
Li	-1.34989083	1.41025331	1.77816483	H	-3.39816534	0.26270462	-2.77089435
O	-2.97460238	1.02410203	2.94006317	H	-2.50275367	1.77356093	-2.94754039
C	-3.82405225	-0.12961728	2.75461817	H	-1.62087321	0.25744931	-2.68751871
C	-5.23124211	0.31464590	3.16569191	C	-3.90971840	1.77564294	-0.54647249
C	-4.93485922	1.40030353	4.21228583	H	-3.99289547	1.94040901	0.53380343
C	-3.69558990	2.07504438	3.62228679	H	-3.96764038	2.75255946	-1.03661918
H	-3.02622830	2.51548866	4.36485033	H	-4.78541262	1.19473195	-0.87386148
H	-3.96823350	2.84861381	2.89239028	H	2.15344927	-0.13686576	5.30180070
H	-4.69971907	0.94543292	5.18217036	C	3.43537094	1.55468918	4.80588285
H	-5.76302727	2.10063120	4.35645684	H	3.91223731	1.08302649	3.94168955
H	-5.83334989	-0.51219160	3.55448962	H	3.29312901	2.61063122	4.54731540
H	-5.75851636	0.74770071	2.30825935	C	4.32231264	1.42644623	6.02694005
H	-3.75471475	-0.44303074	1.70906773	C	4.88647322	0.18856764	6.37063019
H	-3.44999299	-0.94073642	3.39278278	C	5.68636078	0.05635935	7.50519787
N	-1.37826984	1.48637207	-0.19919115	C	5.93948457	1.16412922	8.31768936
C	-0.71380387	2.72291585	-0.64368683	C	5.38985034	2.40231080	7.98496366
H	0.01188803	2.94259801	0.15892008	C	4.58785308	2.52993252	6.84873543

H	4.17347693	3.50175770	6.58870395
H	5.58780232	3.27220064	8.60552009
H	6.56580491	1.06284665	9.19974522
H	6.11796579	-0.91012605	7.75169095
H	4.70678919	-0.67773000	5.73680971
C	2.13160162	-0.89491874	2.56361067
H	2.96826768	-0.82765516	3.25604681
C	1.75359492	-2.31681698	2.17684398
H	1.13273992	-2.31850907	1.27644149
H	2.65465773	-2.90596055	1.97099218
H	1.19761420	-2.83175424	2.97300398
O	-0.47023559	-1.82602765	-0.85712701
C	-1.56111778	-2.74742786	-0.65779770
C	-1.23711477	-3.99632742	-1.49907840
C	0.28024423	-3.87587000	-1.72177953
C	0.45562981	-2.36306495	-1.82267683
H	0.19232319	-1.99824601	-2.82650748
H	1.44220506	-1.98525014	-1.55131542
H	0.62684564	-4.40443932	-2.61520818
H	0.83149495	-4.26307354	-0.85672440
H	-1.76336198	-3.95766765	-2.45970798
H	-1.52889092	-4.92318933	-0.99590387
H	-1.61438690	-2.97275377	0.41401419
H	-2.49772031	-2.26693072	-0.96003075
O	1.88021883	-0.08608408	-0.05045950
C	2.85975086	-0.25875127	0.74265269
C	3.84730797	0.89880887	0.97852197
C	4.87635935	0.87197829	-0.17142017
H	5.63721289	1.64909745	-0.03038626
H	5.39110466	-0.09497614	-0.22991353
H	4.38046571	1.05044033	-1.13211223
C	3.16861103	2.26871334	1.05479891
H	2.44518909	2.32441857	1.87306880
H	3.91238827	3.06077975	1.20444604
H	2.62696010	2.47582672	0.12772830
H	4.39606794	0.69801264	1.90966763
H	3.40565755	-1.22276248	0.67403868

Table 35. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*R*)-**7** from **5** monomer with three THF



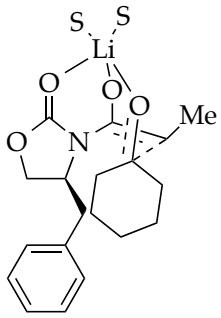


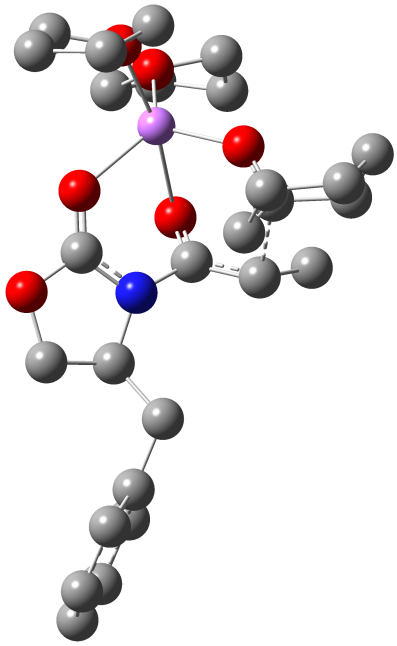
G = -1566.085972 Hartree
G_{MP2} = -979574.4836 kcal/mol
ΔG_{MP2} = 6.418902434 kcal/mol vs. **5** monomer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.53810572	-4.76645494	5.36128284
O	0.00000000	0.00000000	2.19833890	H	4.20399388	-5.71216760	6.92638182
C	1.20354930	0.00000000	2.49321960	H	5.90072955	-4.23350477	7.98744913
N	1.95048797	-1.22185806	2.23807992	H	5.90787849	-1.80003956	7.46841953
C	2.92025224	-1.82318067	3.15707186	H	4.24187105	-0.85801470	5.90517831
C	3.35380295	-3.05228118	2.33088104	C	1.94831622	1.15685573	2.85220079
H	4.29455023	-2.87907259	1.79788897	H	2.96551642	0.98722797	3.20357548
H	3.44025547	-3.96266562	2.92629976	C	1.18408254	2.23481650	3.59747890
O	2.31157678	-3.24322928	1.35432413	H	0.28995007	2.53095615	3.04106149
C	1.58085049	-2.10017563	1.25019742	H	0.85036139	1.89014244	4.58690788
O	0.76543373	-1.93745865	0.35788765	H	1.80076917	3.12462079	3.75495721
H	3.76903713	-1.15131136	3.31401612	O	-1.96274204	0.63110139	0.04812905
C	2.28354721	-2.16984310	4.52382687	C	-2.88685299	-0.28317419	0.68170167
H	1.84204011	-1.25020083	4.92644165	C	-3.78615035	0.57277826	1.58310764
H	1.45802529	-2.87199919	4.35559349	C	-2.87540149	1.76678240	1.91214264
C	3.27858807	-2.74778314	5.50678799	C	-2.12756115	1.95913363	0.59428106
C	4.23768951	-1.92537619	6.11735908	H	-1.12859521	2.38814904	0.69834102
C	5.17627798	-2.45486559	7.00236303	H	-2.71291562	2.56229233	-0.11561503
C	5.17183406	-3.82073097	7.29536545	H	-2.16537349	1.49770532	2.69960756
C	4.22118956	-4.64949161	6.69929437	H	-3.42866560	2.66047719	2.21862505
C	3.28390055	-4.11533998	5.81242520	H	-4.12169299	0.02684406	2.47021921

H	-4.67534624	0.90865438	1.03555759
H	-3.43825740	-0.81577488	-0.10050351
H	-2.30396222	-1.00529076	1.26404207
O	-0.07035577	-0.34862271	-2.05677666
C	0.02257864	0.86120797	-2.84321581
C	0.96329255	0.54664885	-4.02739666
C	1.62745699	-0.77901112	-3.61141505
C	0.52168188	-1.43290481	-2.78555114
H	0.86446839	-2.16319970	-2.05172027
H	-0.23354056	-1.90116598	-3.43672592
H	2.50199704	-0.59135875	-2.97807310
H	1.94312848	-1.38825038	-4.46446400
H	1.68727015	1.34799757	-4.20328347
H	0.38975199	0.40956784	-4.95131701
H	-0.98102250	1.15080936	-3.17668603
H	0.41680766	1.63581979	-2.18033019
O	1.18766196	1.49012029	0.19234099
C	2.23069327	1.79398688	0.88078581
C	2.48013659	3.29697734	1.09408512
C	3.01228005	3.90706431	-0.21942735
C	4.29261636	3.19947476	-0.68835417
C	4.08343298	1.68233060	-0.81204945
C	3.54387369	1.07960647	0.50217233
H	4.29906677	1.20665858	1.28974567
H	3.36273015	0.00771982	0.37579432
H	3.36100175	1.47593216	-1.61269091
H	5.02349626	1.18885382	-1.09333872
H	5.09810622	3.39364219	0.03666777
H	4.63018300	3.61661753	-1.64647253
H	3.19794535	4.98091163	-0.08437112
H	2.23495306	3.81045977	-0.98841586
H	3.21503745	3.46483000	1.89250966
H	1.54590896	3.78696355	1.38342040

Table 36. Geometric coordinates and thermally corrected MP2 energies for the transition state leading to (*S*)-**7** from **5** monomer with three THF





G = -1566.08112 Hartree
G_{MP2} = -979571.1681 kcal/mol
ΔG_{MP2} = 9.734378081 kcal/mol vs. **5** monomer with three THF

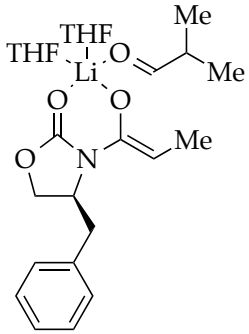
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	5.29427834	1.30668095	5.92216250
O	0.00000000	0.00000000	2.06946300	C	6.04340586	1.00149039	7.06047788
C	1.00575259	0.00000000	2.76030870	C	6.80731831	-0.16505170	7.10363428
N	2.31037179	0.18354881	2.35785722	C	6.82144580	-1.02117829	6.00011926
C	2.65199174	-0.12078741	0.95609848	C	6.07381456	-0.71168717	4.86430987
O	2.02705647	-1.04110522	0.41554487	H	6.10229908	-1.37773607	4.00437538
C	3.52053524	0.77247802	0.26935529	H	7.42074268	-1.92757005	6.02113012
H	4.11122931	1.44029422	0.89137809	H	7.39286366	-0.40309070	7.98743595
C	4.24945912	0.17301714	-0.92147285	H	6.03252330	1.67856227	7.91052117
H	3.53787490	-0.18355573	-1.67250752	H	4.71093395	2.22443816	5.89220974
H	4.86846336	-0.68661431	-0.62896542	H	3.54401695	-1.17443405	3.39499237
H	4.90927199	0.90594080	-1.39436022	O	-0.40852530	-1.66836743	-1.14210967
C	3.22163561	-0.12558846	3.47653310	C	-0.21726757	-3.00266412	-0.61964150
C	2.25516665	0.03652722	4.66311096	C	0.48552880	-3.79973121	-1.72618046
H	2.30663852	1.04515947	5.08958057	C	1.23974928	-2.69879729	-2.48821714
H	2.40803545	-0.69792953	5.45447390	C	0.24536849	-1.54086979	-2.42640886
O	0.94219342	-0.15447101	4.10789619	H	0.70936303	-0.55196165	-2.45965837
C	4.46721811	0.77040291	3.57982444	H	-0.51336495	-1.61587969	-3.21882883
H	5.07211935	0.63038703	2.67823313	H	2.15277115	-2.42549945	-1.95085639
H	4.14501541	1.81825784	3.59169684	H	1.49792108	-2.98026046	-3.51419892
C	5.29594535	0.45475783	4.80984059	H	1.14333462	-4.57578448	-1.32263163

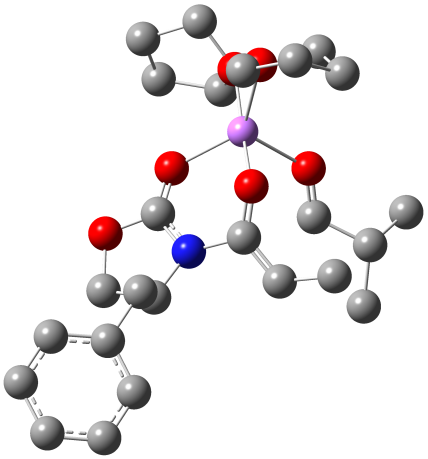
H	-0.24877957	-4.28504186	-2.38087410
H	-1.19718029	-3.41253449	-0.35069360
H	0.40314737	-2.92649335	0.27870888
O	-1.96014626	0.67057913	-0.12669750
C	-2.26967097	2.02139715	-0.48126823
C	-2.69861711	2.68497575	0.83645676
C	-3.28086971	1.50639749	1.66472067
C	-2.96156164	0.25864850	0.81120067
H	-2.54881199	-0.57291426	1.38457256
H	-3.84960237	-0.08760560	0.26172506
H	-2.79719325	1.44149924	2.64269810
H	-4.35835212	1.60758613	1.82930341
H	-1.82719519	3.11221482	1.34125187
H	-3.42211329	3.49037413	0.67524356
H	-3.08995763	2.02806800	-1.21662676
H	-1.37167634	2.44134403	-0.93661009
O	1.05324844	1.34702807	-0.81125117
C	2.08223259	2.03811031	-0.45433243
C	1.89024688	3.01650517	0.72578193
C	1.12428305	4.26945456	0.25303674
C	1.82735459	4.95078870	-0.92949607
C	2.06667204	3.96083078	-2.07824474
C	2.85317367	2.72353946	-1.59943015
H	2.97947191	2.01808206	-2.42543341
H	3.85018851	3.04166705	-1.26592869
H	1.10292861	3.62836046	-2.48569236
H	2.60823801	4.45093189	-2.89831585
H	1.23773811	5.80827986	-1.28031983
H	2.79432585	5.35498670	-0.59225612
H	0.11165524	3.97373231	-0.04900699
H	1.01214010	4.97341535	1.08883782
H	2.86234625	3.33008331	1.12982878
H	1.33721006	2.52215749	1.52926679

Part 8: 5 IRC Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table 37. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,S*)-**6** from **5** monomer with three THF



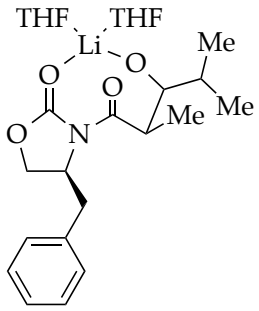


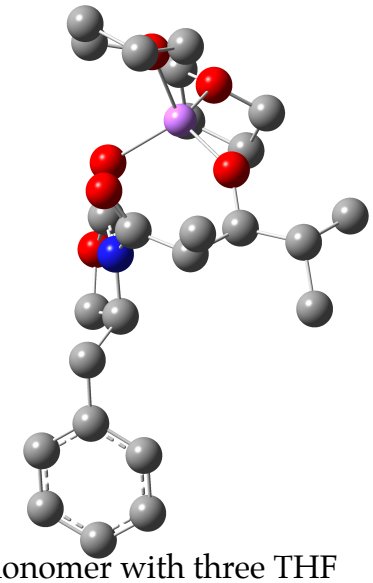
G = -1488.708185 Hartree
G_{MP2} = -931174.079 kcal/mol
ΔG_{MP2} = -2.729626092 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = 3.802059799 kcal/mol Li vs. **5** monomer (*R,S*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	3.10546634	-5.50577838	6.27929520
O	0.00000000	0.00000000	1.94046660	C	2.44652435	-4.79680075	5.27240585
C	1.11965626	0.00000000	2.54616987	H	1.95575344	-5.33791637	4.46600952
N	2.02793843	-1.12522156	2.21269764	H	3.13032250	-6.59194527	6.24640118
C	2.70707254	-1.94795170	3.21932031	H	4.23564122	-5.37153733	8.11210525
C	3.45983553	-2.93044676	2.30345226	H	4.14764020	-2.88559838	8.17752994
H	4.48626919	-2.60188723	2.10389502	H	2.97125339	-1.63637878	6.39617534
H	3.47681020	-3.95429622	2.68131314	C	1.61310163	0.90129786	3.45289671
O	2.72788360	-2.91255980	1.06344721	H	2.60852731	0.74837980	3.86189622
C	1.97963185	-1.77171667	1.01727398	C	0.77581201	2.01086755	4.02129066
O	1.39955032	-1.44676067	-0.01415889	H	-0.14801327	2.11786096	3.44475206
H	3.41411216	-1.34430218	3.79511413	H	0.49155241	1.83383609	5.07111722
C	1.70746433	-2.62063874	4.18975503	H	1.29864221	2.97917064	4.00659070
H	1.08461540	-1.82426557	4.61223667	O	-2.09160435	-0.02932085	-0.11031578
H	1.04633240	-3.27757909	3.61153517	C	-2.79882247	-0.73068698	0.94611718
C	2.39276726	-3.39653988	5.29246188	C	-3.80136196	0.27273529	1.53850954
C	3.01553321	-2.72285291	6.35454510	C	-3.18568013	1.62804820	1.15500125
C	3.67584937	-3.42651231	7.36120722	C	-2.59297113	1.31853024	-0.21712196
C	3.72431046	-4.82224654	7.32615499	H	-1.75640429	1.96217419	-0.49941282

H	-3.35860681	1.36245961	-1.00648191
H	-2.38274477	1.89022328	1.85123974
H	-3.91503543	2.44403322	1.12848168
H	-3.91840003	0.14611286	2.61882083
H	-4.78932811	0.15809038	1.07607709
H	-3.28698579	-1.61088929	0.51153568
H	-2.04880253	-1.04259060	1.67608343
O	0.94960517	1.84733917	0.03534704
C	2.00280123	2.15877624	0.57591087
C	2.29589684	3.56434729	1.07213089
H	1.50376352	3.79918389	1.79655547
C	2.17655163	4.56272624	-0.09721176
H	2.30338396	5.58903825	0.26476095
H	2.94759068	4.37722730	-0.85534372
H	1.19769447	4.48090907	-0.57814154
C	3.65912103	3.63861859	1.76720535
H	4.47322460	3.42132175	1.06356336
H	3.83486474	4.63920235	2.17635256
H	3.71824970	2.91646085	2.58835531
H	2.82040620	1.41809469	0.66065339
O	-0.03395421	0.03220315	-2.18705180
C	1.24278942	0.06653460	-2.84094499
C	1.52491792	-1.37550604	-3.32411744
C	0.15508747	-2.08942181	-3.18047001
C	-0.81422410	-0.93369955	-2.90222574
H	-1.66732292	-1.18553961	-2.27153543
H	-1.17965129	-0.48620133	-3.84110148
H	0.17606987	-2.77194712	-2.32654685
H	-0.12557707	-2.66050694	-4.07127386
H	2.27828862	-1.85836974	-2.69835806
H	1.88525259	-1.37861781	-4.35810275
H	1.19238373	0.76761800	-3.68771689
H	1.96577640	0.44115334	-2.11565395

Table 38. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,S*)-**6** from **5** monomer with three THF



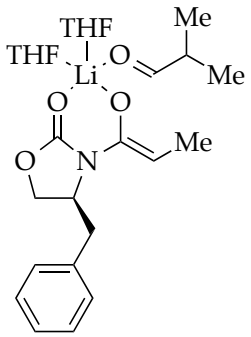


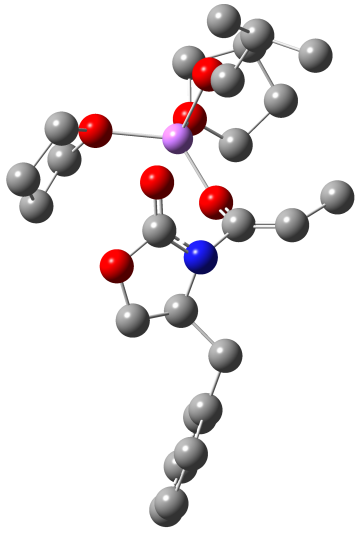
G = -1488.706172 Hartree
G_{MP2} = -931180.4326 kcal/mol
ΔG_{MP2} = -2.551572784 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -9.083258675 kcal/mol Li vs. **5** monomer (*R,S*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	2.05778743	1.22570675	2.76694081
O	0.00000000	0.00000000	3.07164130	H	3.01026645	1.04680905	3.28185620
C	1.19140990	0.00000000	2.85139587	C	1.34179093	2.42880033	3.38392549
N	1.82686287	-1.25777009	2.51834637	H	0.50625545	2.73041041	2.74718691
C	3.18419450	-1.67430876	2.89648277	H	0.94132552	2.19326375	4.37577081
C	3.21158930	-3.08893875	2.27842095	H	2.02444899	3.27757857	3.48589612
H	4.15028477	-3.32537538	1.77665993	O	-1.90118902	0.52353298	0.25810530
H	2.99527422	-3.86196118	3.02397284	C	-2.78977987	-0.24173909	1.10850178
O	2.15851470	-3.09907552	1.29629057	C	-3.61069903	0.78572135	1.89727718
C	1.32197259	-2.05152605	1.51195603	C	-2.66290515	1.99498631	1.94361452
O	0.32182583	-1.87961886	0.83960007	C	-2.00936592	1.93568794	0.56423734
H	3.92443999	-1.02865355	2.40766353	H	-0.99693707	2.34643095	0.52866437
C	3.42174456	-1.67730572	4.41830839	H	-2.63413171	2.41537108	-0.20256203
H	3.27767605	-0.65968854	4.79999494	H	-1.90406608	1.84861387	2.71816866
H	2.65474906	-2.30424935	4.88793701	H	-3.17975404	2.94294242	2.12463937
C	4.80775061	-2.17391243	4.77934478	H	-3.88837058	0.41681036	2.88932259
C	5.93581330	-1.37524007	4.53796383	H	-4.53197751	1.04071353	1.35922686
C	7.21618248	-1.83542969	4.84371859	H	-3.40439140	-0.88750216	0.47189197
C	7.39094973	-3.10477982	5.39988332	H	-2.17468592	-0.86411786	1.76560677
C	6.27734867	-3.90679791	5.65001992	O	1.23119509	1.23836923	0.45892659
C	4.99672044	-3.44328267	5.34113171	C	2.36073084	1.38355707	1.18693362
H	4.13278462	-4.07021154	5.55084914	C	3.12016284	2.71742548	0.90586889
H	6.40223760	-4.89263286	6.08995314	H	2.45859342	3.54098039	1.20816968
H	8.38793980	-3.46274765	5.64157951	C	3.36410661	2.85875775	-0.60198852
H	8.07718270	-1.20035397	4.65325866	H	3.84978913	3.81451840	-0.83693306
H	5.80994584	-0.38018561	4.11608403	H	4.01841480	2.05552154	-0.97076093

H	2.41651725	2.80211771	-1.14216045
C	4.44372292	2.83614936	1.67622905
H	5.10281058	1.98432231	1.45524208
H	4.98576847	3.74587559	1.39004975
H	4.29963443	2.87414190	2.76249180
H	3.11630686	0.57846741	0.97873233
O	0.15475630	-0.56183666	-1.93304428
C	1.36543087	-0.17601407	-2.60266281
C	2.21162350	-1.46061731	-2.68194432
C	1.16934647	-2.60780797	-2.55722436
C	-0.17554648	-1.86986327	-2.41496683
H	-0.85555915	-2.32404325	-1.69202688
H	-0.68836260	-1.77809700	-3.38425824
H	1.36702738	-3.21097626	-1.66756787
H	1.17154309	-3.27385133	-3.42579161
H	2.92640935	-1.50041773	-1.85451159
H	2.78197345	-1.50882709	-3.61483458
H	1.11603842	0.19986156	-3.60636497
H	1.80619535	0.62347572	-2.00624698

Table 39. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,R*)-**6** from **5** monomer with three THF



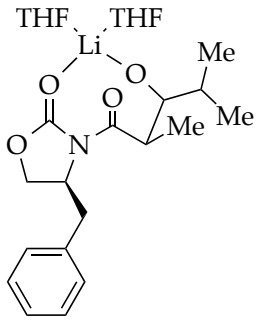


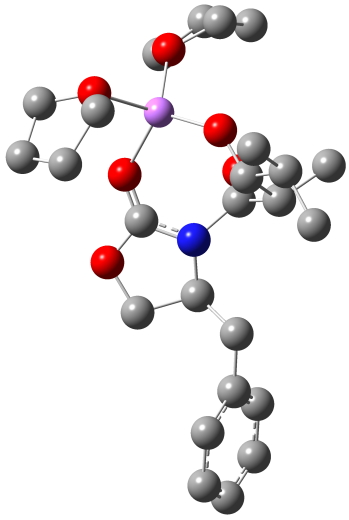
G = -1488.710578 Hartree
G_{MP2} = -931174.003 kcal/mol
ΔG_{MP2} = 3.877975016 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -5.700287545 kcal/mol Li vs. **5** monomer (*S,R*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.31423857	-2.32516828	-3.38313541
O	0.00000000	0.00000000	-1.82773040	C	1.46386462	1.02751223	-3.43098980
C	0.94572960	0.00000000	-2.71141391	H	2.25987159	0.80386101	-4.13481910
N	1.50520793	-1.33684513	-3.01778527	C	0.98173510	2.44533988	-3.31870984
C	0.70023544	-2.27654550	-3.80748597	H	0.19311371	2.52064292	-2.56298907
C	1.45982641	-3.58437888	-3.53548307	H	0.56907349	2.82132402	-4.26775767
H	2.22140312	-3.77496927	-4.30222099	H	1.78579582	3.14314978	-3.03746158
H	0.81584968	-4.46077848	-3.44382534	O	-1.74225097	0.87289286	0.51765191
O	2.12198638	-3.36651193	-2.27652905	C	-2.39931790	1.64765015	-0.50424303
C	2.17438431	-2.01407606	-2.03751283	C	-2.12934700	3.12399652	-0.14383204
O	2.75760191	-1.56523132	-1.06520238	C	-1.68479620	3.07897910	1.34507851
C	0.60604076	-1.88821777	-5.29059001	C	-1.88614080	1.60824489	1.73967238
H	0.22727756	-0.86062576	-5.33777573	H	-1.14384610	1.22526367	2.44304460
H	1.61831907	-1.87087659	-5.71274346	H	-2.89290215	1.43572048	2.15026286
C	-0.28321517	-2.82314655	-6.08309581	H	-0.62904282	3.34760072	1.43913702
C	0.26025179	-3.80777582	-6.91908472	H	-2.26389114	3.75473827	1.98198199
C	-0.56360206	-4.68588558	-7.62639791	H	-1.33694625	3.53958103	-0.77250571
C	-1.95067505	-4.59344738	-7.50784293	H	-3.02416689	3.73653191	-0.29145185
C	-2.50679493	-3.61505822	-6.68038547	H	-3.47557719	1.42259515	-0.47995608
C	-1.67995377	-2.73941508	-5.97704133	H	-1.97163364	1.32486836	-1.45421085
H	-2.12093123	-1.97369061	-5.34218575	O	1.40620074	1.20244407	0.79530299
H	-3.58652157	-3.52981552	-6.58731325	C	2.52044705	1.29023230	0.28978964
H	-2.59390723	-5.27389669	-8.05949986	C	3.56346217	2.28063668	0.74122796
H	-0.12030592	-5.43890706	-8.27304386	H	3.12178337	2.88806953	1.54028591
H	1.34067003	-3.88109763	-7.02432780	C	4.77984852	1.50615873	1.28878876

H	5.56507988	2.20748995	1.59203294
H	5.19800954	0.83815952	0.52683803
H	4.50977556	0.89969965	2.16005668
C	3.95990589	3.18085067	-0.44510236
H	4.34664894	2.58474764	-1.27977273
H	4.74304993	3.88313587	-0.13847465
H	3.10628835	3.76020207	-0.81269580
H	2.80160594	0.60811995	-0.53023827
O	-0.14538950	-1.61914757	1.18380807
C	0.93224129	-2.53301749	1.49234359
C	0.51110932	-3.91201572	0.92726647
C	-0.92616591	-3.68037292	0.39965987
C	-1.34934964	-2.39742304	1.11534293
H	-2.09460907	-1.79722311	0.59034205
H	-1.71036093	-2.60610802	2.13482576
H	-0.91404703	-3.50946438	-0.68175361
H	-1.59898050	-4.51882322	0.60530831
H	1.18323839	-4.23315795	0.12831749
H	0.52853396	-4.67399725	1.71327044
H	1.06238397	-2.56577044	2.58246214
H	1.83304521	-2.13729638	1.02350167

Table 40. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,R*)-**6** from **5** monomer with three THF



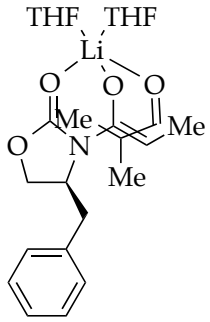


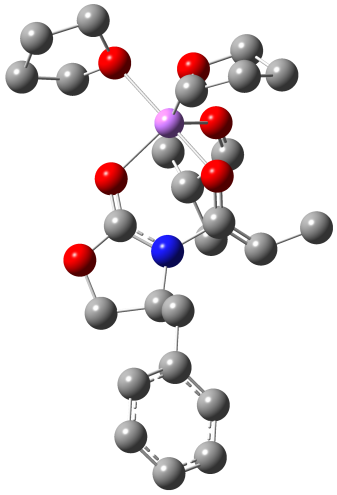
G = -1488.701899 Hartree
G_{MP2} = -931176.7029 kcal/mol
ΔG_{MP2} = 1.178118224 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -8.400144337 kcal/mol Li vs. **5** monomer (*S,R*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.00561674	0.99532081	-3.26707343
O	0.00000000	0.00000000	-3.28022010	C	1.37592035	2.43577348	-3.40576019
C	1.16475918	0.00000000	-2.95165513	H	0.51981917	2.73521444	-2.79544128
N	1.78861946	-1.29586321	-2.60654334	H	1.01562258	2.23999890	-4.42149864
C	2.45612189	-2.11698047	-3.63570719	H	2.07953999	3.27225588	-3.44936273
C	2.59310576	-3.44111563	-2.86397239	O	-1.91155639	0.48942006	-0.29578276
H	3.56126484	-3.51285469	-2.35529873	C	-2.78635017	-0.28241741	-1.15180453
H	2.44286261	-4.32477673	-3.48462501	C	-3.63746143	0.73697873	-1.91722764
O	1.55771032	-3.39936720	-1.86577506	C	-2.71143960	1.96321651	-1.96277182
C	1.14490290	-2.11600796	-1.70727302	C	-2.04224632	1.90314411	-0.59066844
O	0.33946806	-1.80730337	-0.84598911	H	-1.03520552	2.32723099	-0.56222279
C	3.79618245	-1.56147888	-4.14610845	H	-2.66722620	2.36685951	0.18558504
H	3.61355923	-0.60909924	-4.65627498	H	-1.95970354	1.83908053	-2.74884345
H	4.43649209	-1.34512026	-3.28334338	H	-3.24658776	2.90358668	-2.12941825
C	4.48390118	-2.52475891	-5.09438781	H	-3.92377194	0.37370328	-2.90897446
C	5.59021188	-3.27842991	-4.68095005	H	-4.55456261	0.96978206	-1.36230638
C	6.20497553	-4.18362242	-5.54841330	H	-3.37933863	-0.95533389	-0.52282408
C	5.72022923	-4.34894292	-6.84608292	H	-2.16357090	-0.87964308	-1.82592693
C	4.62096511	-3.60022103	-7.27253583	O	1.14837431	1.28787995	-0.51233998
C	4.01064756	-2.69577229	-6.40397250	C	2.30937069	1.33449848	-1.20247342
H	3.16269367	-2.10797054	-6.74965330	C	3.15916165	2.60941344	-0.90446950
H	4.24222669	-3.71573402	-8.28456112	H	2.56090261	3.47996154	-1.20718601
H	6.19893209	-5.05086824	-7.52333097	C	3.38926289	2.72080665	0.60834649
H	7.06550658	-4.75467657	-5.21022806	H	3.94320647	3.63442746	0.85934635
H	5.98239883	-3.14631024	-3.67498838	H	3.97347412	1.86649934	0.98014032
H	1.77246729	-2.24745560	-4.48796372	H	2.43105072	2.73402141	1.13265986
C	2.03825479	1.20152310	-2.79246959	C	4.49927472	2.64097061	-1.65428517

H	5.08488616	1.73416394	-1.44721460
H	5.10720172	3.49812786	-1.33919650
H	4.37476104	2.71604132	-2.74106949
H	2.98742328	0.47128202	-0.98178298
O	0.12894207	-0.57018372	1.94125894
C	1.35124309	-0.21579931	2.60558810
C	2.21557393	-1.48294423	2.53099894
C	1.17536885	-2.63632794	2.48975583
C	-0.18076184	-1.90891153	2.35435767
H	-0.83879402	-2.33935386	1.59773227
H	-0.71312602	-1.87248584	3.31595200
H	1.35165380	-3.29149082	1.63285213
H	1.20376664	-3.25185832	3.39446785
H	2.81222499	-1.47168592	1.61378289
H	2.90435952	-1.56148592	3.37790058
H	1.13007901	0.05924169	3.64834966
H	1.76045117	0.64469480	2.07548830

Table 41. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,R*)-**6** from **5** monomer with three THF



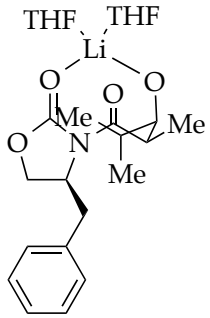


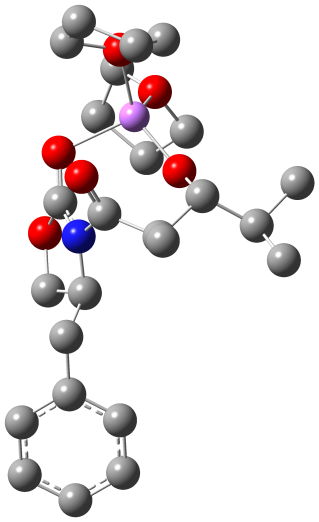
G = -1488.706809 Hartree
G_{MP2} = -931173.8147 kcal/mol
ΔG_{MP2} = 4.066321104 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -3.335285556 kcal/mol Li vs. **5** monomer (*R,R*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.55424912	0.72424636	3.94280329
O	0.00000000	0.00000000	1.93822720	C	0.74299448	2.02720952	4.02378575
C	1.10541915	0.00000000	2.57427812	H	-0.13510869	2.17569186	3.38800096
N	2.01401928	-1.13423316	2.26177287	H	0.38190679	1.85437311	5.05088350
C	2.62400349	-1.99214830	3.28218749	H	1.30385802	2.97272269	4.05021105
C	3.39647542	-2.97434680	2.38267567	O	-2.11347432	-0.08924079	-0.00794979
H	4.43742126	-2.66471201	2.23487781	C	-2.64725059	-1.13964546	0.83658460
H	3.37484610	-4.00499943	2.74130994	C	-3.76441236	-0.49264110	1.66001407
O	2.72050417	-2.91793708	1.11160659	C	-3.26678878	0.95550744	1.78279486
C	1.99960647	-1.75925713	1.05700708	C	-2.64606277	1.19247640	0.40677670
O	1.46662583	-1.40364226	0.00835504	H	-1.82335884	1.91139682	0.41562816
H	3.31504056	-1.41675948	3.90461739	H	-3.39710426	1.51258894	-0.32958336
C	1.56195701	-2.65984521	4.18819290	H	-2.48873004	1.02180176	2.54869652
H	0.93647840	-1.85704092	4.59420356	H	-4.06257574	1.67080626	2.01412512
H	0.91680463	-3.29058959	3.56444773	H	-3.90223140	-0.98540735	2.62733173
C	2.17347450	-3.47124164	5.30849674	H	-4.71858342	-0.52940019	1.11956403
C	2.74637170	-2.83127766	6.41842969	H	-2.99625452	-1.95167096	0.18923673
C	3.34163790	-3.56741875	7.44229323	H	-1.83536301	-1.49671709	1.47727812
C	3.37362923	-4.96252254	7.37663335	O	0.78939080	1.93355542	0.09607463
C	2.80326498	-5.61274774	6.28208456	C	1.81816572	2.44153912	0.51158984
C	2.20943107	-4.87132639	5.25825086	C	3.21252573	1.97069449	0.15034001
H	1.75633004	-5.38665365	4.41378010	H	3.15614623	0.88645757	0.00035136
H	2.81541635	-6.69814426	6.22487888	C	3.59319578	2.63332116	-1.19402371
H	3.83431097	-5.53719724	8.17565079	H	3.61059401	3.72703989	-1.10686018
H	3.77544283	-3.05226128	8.29550752	H	4.59359403	2.30877328	-1.50187531
H	2.71432888	-1.74550958	6.48308670	H	2.88308085	2.36432627	-1.98219779
C	1.57566423	0.89042673	3.49950275	C	4.23029472	2.30324555	1.24764014

H	3.95495127	1.82179008	2.19036638
H	5.23143032	1.96523206	0.95751822
H	4.28411608	3.38595233	1.42041965
H	1.76243824	3.36788421	1.12004543
O	-0.03152973	-0.03191927	-2.18215582
C	1.17329247	-0.36540902	-2.88227669
C	0.96416926	-1.80039263	-3.40594612
C	-0.58137825	-1.96457790	-3.41998003
C	-1.09397417	-0.58577063	-2.96763622
H	-1.98013260	-0.60858461	-2.33399818
H	-1.28211158	0.06803776	-3.83428424
H	-0.89043958	-2.73897076	-2.71130512
H	-0.97120776	-2.23961987	-4.40521622
H	1.42321356	-2.51972150	-2.72379689
H	1.40998349	-1.93578531	-4.39647660
H	1.31638557	0.34574836	-3.71121919
H	1.99858408	-0.27327911	-2.17679919

Table 42. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,R*)-**6** from **5** monomer with three THF



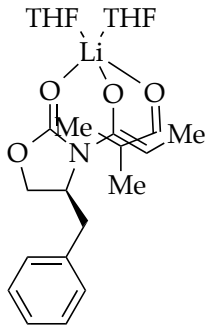


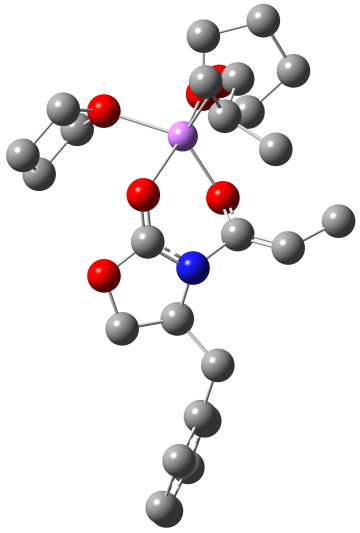
G = -1488.704554 Hartree
G_{MP2} = -931179.4901 kcal/mol
ΔG_{MP2} = -1.609076654 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -9.010683315 kcal/mol Li vs. **5** monomer (*R,R*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	1.66745213	2.11891971	4.08741039
O	0.00000000	0.00000000	3.12084270	H	0.59300832	2.32194606	4.07484048
C	1.18272987	0.00000000	2.85120697	H	1.90056244	1.62702118	5.04075697
N	1.80125526	-1.23921260	2.45640965	H	2.19666935	3.07370067	4.06479412
C	3.21234587	-1.60147435	2.65631032	O	-1.89612145	0.54468016	0.21383455
C	3.21832834	-3.00695725	2.02571448	C	-2.75481284	-0.15409594	1.15464733
H	4.11589544	-3.21968568	1.44480595	C	-3.52434883	0.93330318	1.91565362
H	3.07938743	-3.79082845	2.77870585	C	-2.57806232	2.14020609	1.81423187
O	2.08759031	-3.02354900	1.13678174	C	-2.01303193	1.97278317	0.40555891
C	1.23562516	-2.01735637	1.46563836	H	-1.01736474	2.40310421	0.26833572
O	0.17526016	-1.86859247	0.88882551	H	-2.69220022	2.38188163	-0.35608509
H	3.85693065	-0.92600049	2.08002652	H	-1.77297180	2.04873256	2.54995294
C	3.64179977	-1.60744362	4.13533347	H	-3.08273931	3.10124727	1.95505790
H	3.53021716	-0.59620810	4.54290526	H	-3.73584108	0.63951012	2.94797934
H	2.95070007	-2.25191257	4.69116064	H	-4.47902150	1.15258452	1.42201968
C	5.07026452	-2.08241537	4.31538678	H	-3.40759855	-0.82683612	0.58815445
C	6.14715613	-1.25603011	3.96040173	H	-2.11232771	-0.74216294	1.81473619
C	7.46264833	-1.69848620	4.09606082	O	1.40617596	0.96361477	0.55329947
C	7.72493160	-2.97735557	4.59285027	C	1.79901399	1.91295682	1.45702201
C	6.66360485	-3.80680126	4.95563657	C	3.05213312	2.68481818	0.94022135
C	5.34764687	-3.36088231	4.81694405	H	3.79999413	1.90713828	0.71589200
H	4.52614388	-4.00970187	5.11291329	C	2.69901029	3.39265523	-0.37588104
H	6.85743646	-4.80018618	5.35140216	H	1.99886637	4.22034661	-0.19317941
H	8.74981853	-3.32129801	4.70186455	H	3.59123207	3.81662009	-0.85415274
H	8.28346746	-1.04233919	3.81915436	H	2.22227025	2.69480573	-1.06790768
H	5.95405150	-0.25391861	3.58314065	C	3.67975185	3.68830552	1.91962298
C	2.05095605	1.24501997	2.88555071	H	4.07429976	3.20940414	2.82314595
H	3.10895166	0.96658544	2.94641365	H	4.51515848	4.21715824	1.44344002

H	2.95248020	4.44921661	2.23244083
H	1.00827652	2.68052636	1.64603295
O	0.25954274	-0.47478045	-1.93088976
C	1.62775329	-0.38006868	-2.36939241
C	2.13763215	-1.83473251	-2.44788168
C	0.84252152	-2.69340215	-2.48442768
C	-0.28302822	-1.64864713	-2.54684760
H	-1.18338834	-1.92450189	-1.99348085
H	-0.56029212	-1.41578895	-3.58637229
H	0.75441878	-3.28253985	-1.56862035
H	0.81013059	-3.37750392	-3.33822542
H	2.73414122	-2.08689667	-1.56669169
H	2.76599910	-1.98768479	-3.33102005
H	1.65096023	0.10444235	-3.35655883
H	2.13819607	0.24479374	-1.63461603

Table 43. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,S*)-**6** from **5** monomer with three THF



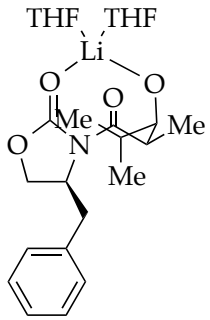


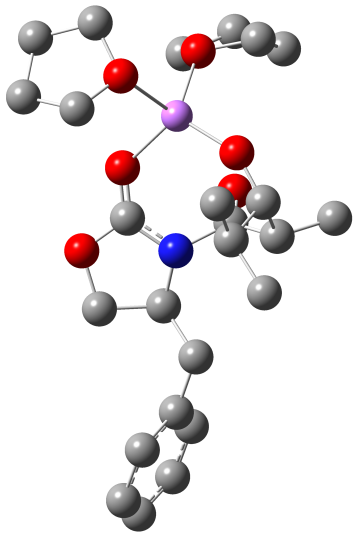
G = -1488.707506 Hartree
G_{MP2} = -931173.1143 kcal/mol
ΔG_{MP2} = 4.766672814 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -4.790804939 kcal/mol Li vs. **5** monomer (*S,S*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	8.55080771	0.81697420	-2.27832127
O	0.00000000	0.00000000	-2.50027400	H	9.21600903	0.99018867	-4.67033737
C	1.16825151	0.00000000	-2.86199160	H	7.71882556	0.06921811	-6.43157101
N	2.16909691	-0.84612132	-2.48620158	H	5.57993544	-1.00437385	-5.80641911
C	2.03061901	-1.54956058	-1.18403321	H	3.86718186	0.32330888	-2.06232570
O	1.66717839	-0.79680308	-0.20217354	O	0.21315426	0.40455097	2.06367028
C	2.33658380	-2.87460679	-1.19677915	C	1.23574750	-0.28216443	2.80524353
H	2.59579231	-3.33393548	-2.14605969	C	0.49652644	-1.35903837	3.62687105
C	2.34435310	-3.72628337	0.04152697	C	-0.97986471	-0.87278139	3.64435523
H	2.01101877	-3.14064250	0.90404452	C	-0.91961431	0.48872333	2.93258680
H	3.34551615	-4.12163476	0.27431510	H	-1.79087232	0.71517512	2.31546197
H	1.68150346	-4.60072419	-0.04585305	H	-0.76777237	1.30838688	3.65303721
C	3.46443954	-0.27764226	-2.89243690	H	-1.61511829	-1.55872260	3.07791864
C	3.01177315	0.63801627	-4.04065957	H	-1.38827396	-0.78748837	4.65636346
H	3.05848347	0.12231303	-5.00800127	H	0.57654384	-2.33753854	3.14464468
H	3.56533125	1.57595190	-4.10481154	H	0.91718064	-1.45084264	4.63330175
O	1.63440933	0.93678020	-3.74700831	H	1.74115105	0.43959803	3.46542263
C	4.51075622	-1.32475622	-3.30032661	H	1.93766848	-0.67107775	2.06812003
H	4.64082201	-2.00707178	-2.45327530	O	-1.59930379	-1.29526677	0.21704712
H	4.10894430	-1.91855967	-4.13051132	C	-2.15793651	-2.20267372	-0.37653910
C	5.83370921	-0.69712441	-3.68878305	H	-2.77924606	-2.91813404	0.20692561
C	6.22462744	-0.59660575	-5.03065269	C	-2.09938510	-2.47549139	-1.85482080
C	7.43347428	0.00656502	-5.38453379	H	-1.53821929	-1.66186737	-2.32220605
C	8.27382371	0.52230801	-4.39758116	C	-3.53473108	-2.53659442	-2.41179800
C	7.89903100	0.42591813	-3.05541394	H	-4.12381420	-3.32256193	-1.92170798
C	6.69189185	-0.17910422	-2.70662666	H	-3.50669255	-2.76162976	-3.48318391
H	6.41321489	-0.25996708	-1.65807677	H	-4.06203552	-1.58468149	-2.28181649

C	-1.34595005	-3.80410778	-2.07894821
H	-0.29607187	-3.70816977	-1.78298646
H	-1.37900222	-4.06731135	-3.14217322
H	-1.80351408	-4.62938548	-1.51757875
O	-0.78102546	1.90275411	-0.20796325
C	-1.58836065	2.34877006	-1.31359678
C	-0.70739820	3.31913254	-2.13398654
C	0.52633518	3.56314520	-1.22653865
C	0.08560507	2.99694216	0.12660166
H	0.88911139	2.59663710	0.74633472
H	-0.47695805	3.74337514	0.70974642
H	1.38539900	3.00089486	-1.60426594
H	0.81044788	4.61826814	-1.16271244
H	-0.40713640	2.86864501	-3.08216975
H	-1.24560577	4.24792575	-2.34944676
H	-2.48001076	2.85470999	-0.91579891
H	-1.88635101	1.46160791	-1.87064723

Table 44. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,S*)-**6** from **5** monomer with three THF



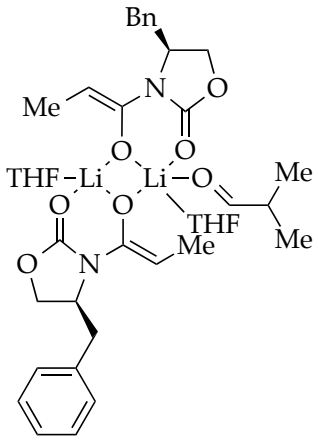


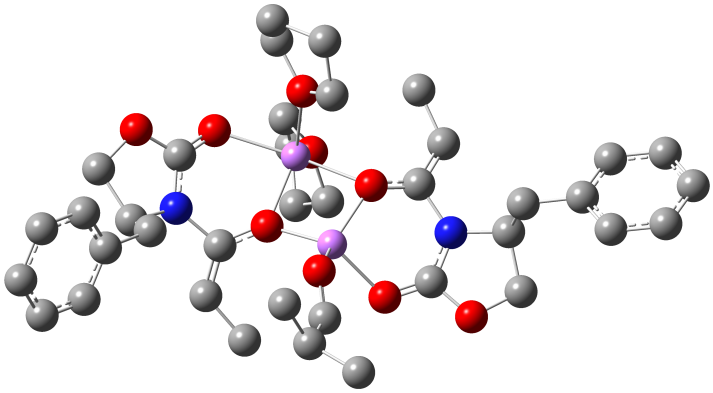
G = -1488.697621 Hartree
G_{MP2} = -931174.44 kcal/mol
ΔG_{MP2} = 3.440967193 kcal/mol Li vs. **5** monomer with three THF
ΔG_{MP2} = -6.11651056 kcal/mol Li vs. **5** monomer (*S,S*)-**6** transition state

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.20164762	2.32780443	-7.48693840
O	0.00000000	0.00000000	-2.02475640	H	6.65811512	0.21714067	-8.72290424
C	0.95232866	0.00000000	-2.78494820	H	6.13014066	-1.96951687	-7.66023630
N	2.26239126	0.34320297	-2.52284753	H	5.15014556	-2.04279757	-5.39062523
C	2.54651683	1.27801325	-1.41133135	H	2.92368558	1.52600488	-4.13872275
O	1.91110732	2.30560544	-1.36130431	O	-1.01277107	1.63276559	0.65204632
C	3.60648069	0.84959690	-0.44224426	C	-1.37130491	2.67702543	-0.28571870
H	4.45153710	0.43715575	-1.00380887	C	-1.10601274	3.99972445	0.43818089
C	4.06797328	2.03234047	0.41324504	C	0.05752304	3.62461856	1.36934823
H	3.25520858	2.35117345	1.07234805	C	-0.31354821	2.20380351	1.79256165
H	4.37260799	2.89430427	-0.19137934	H	0.54677570	1.55908345	1.99011578
H	4.91624551	1.73030266	1.03617774	H	-0.99754572	2.20094816	2.65248283
C	2.99215130	0.48053229	-3.80220638	H	0.99724151	3.61232526	0.80833437
C	2.12040103	-0.41467945	-4.69690720	H	0.16393768	4.30144507	2.22315553
H	2.49115083	-1.44596139	-4.71929849	H	-0.86038445	4.80819904	-0.25720973
H	2.01733356	-0.04346656	-5.71681997	H	-1.98374828	4.30559559	1.02095897
O	0.82480510	-0.40918418	-4.07304077	H	-2.42031676	2.53726021	-0.56878081
C	4.47065593	0.05970848	-3.76832541	H	-0.74258526	2.57111317	-1.17555450
H	5.01587395	0.73170040	-3.09646518	O	1.63677677	-0.07850151	0.66346058
H	4.54031701	-0.94702489	-3.34169229	C	2.95896589	-0.30393087	0.48916712
C	5.09978119	0.09863439	-5.14795819	H	3.53586728	-0.20566721	1.44198976
C	5.36765377	-1.08228277	-5.85269758	C	3.29457610	-1.74065589	-0.02714027
C	5.92477612	-1.04198067	-7.13249917	H	2.87778721	-1.83971061	-1.04110422
C	6.22231008	0.18400407	-7.72816278	C	2.59924286	-2.77061669	0.87484990
C	5.96463006	1.36857884	-7.03448621	H	3.00780460	-2.72663013	1.89403507
C	5.41011539	1.32442935	-5.75560891	H	2.74964601	-3.79200282	0.50105896
H	5.22543437	2.25220804	-5.21794637	H	1.52876857	-2.56459638	0.94082204

C	4.80204685	-2.03709372	-0.07911118
H	5.34229230	-1.41344309	-0.80180434
H	4.98767051	-3.08293402	-0.35463840
H	5.26345658	-1.87281489	0.90399082
O	-1.40055039	-1.45353733	0.31800574
C	-1.38171067	-2.62110412	-0.51444581
C	-2.50200009	-2.40080274	-1.54679039
C	-3.46726812	-1.41009008	-0.83603086
C	-2.78597915	-1.14077778	0.52005309
H	-2.83284001	-0.10441022	0.85658275
H	-3.19046416	-1.79689562	1.30540938
H	-3.55908682	-0.48533493	-1.41297486
H	-4.47281296	-1.82180801	-0.70446761
H	-2.09258152	-1.94983325	-2.45372246
H	-2.98930682	-3.34162141	-1.82089293
H	-1.57358020	-3.50888580	0.10671187
H	-0.38204971	-2.69969144	-0.94513671

Table 45. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,S*)-**6** from **5** dimer with three THF



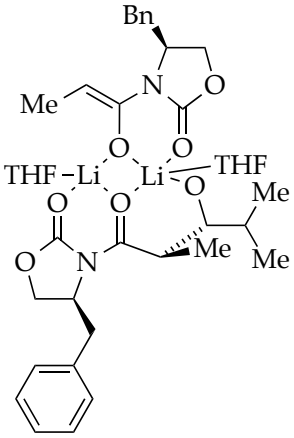


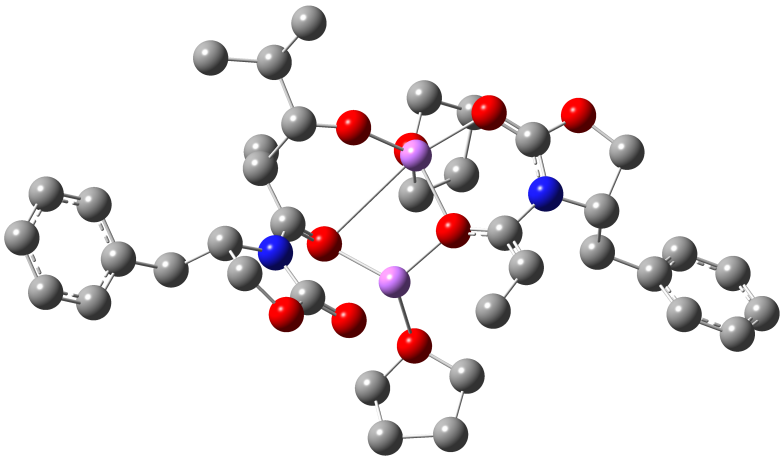
G = -2280.378242 Hartree
G_{MP2} = -1426410.726 kcal/mol
ΔG_{MP2} = 2.007089482 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -5.751794463 kcal/mol vs. **5** dimer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	8.72014195	-0.54059104	0.60966039
O	0.00000000	0.00000000	1.96313560	H	10.88362927	-1.16599348	-0.41468817
Li	1.86056166	0.00000000	1.96440864	H	10.95722290	-2.03399772	-2.74521698
O	2.19047654	-0.23176880	0.14317016	H	8.84433406	-2.26237340	-4.03971546
C	3.01252308	-1.03021680	-0.45146984	H	6.68323972	-1.63567816	-3.01152596
N	4.06244493	-1.62079737	0.40509651	C	3.04816421	-1.37759953	-1.76889049
C	5.40444243	-1.97255328	-0.07995664	H	3.76943231	-2.11498084	-2.10635044
C	5.96114166	-2.70755592	1.14877558	C	2.13862863	-0.77721445	-2.80345061
H	5.81220940	-3.79145221	1.08461346	H	1.65572467	0.12555629	-2.41979347
H	7.01464730	-2.49890424	1.34270426	H	2.69529470	-0.50780507	-3.71264653
O	5.18415735	-2.20616290	2.25145036	H	1.33550127	-1.46230218	-3.11592161
C	4.01793620	-1.68940730	1.76369254	O	2.53715619	1.65853205	2.92270441
O	3.12624999	-1.35911111	2.54162033	C	2.05379538	1.85280358	4.26257551
H	5.33970857	-2.65540069	-0.92964483	C	3.14594768	1.26378230	5.16996608
C	6.21151382	-0.71842198	-0.49110853	C	4.44214937	1.39262096	4.32211050
H	5.58721184	-0.15466410	-1.19283240	C	3.94482999	1.93688065	2.96705800
H	6.35753584	-0.09151637	0.39759978	H	4.39689943	1.45924316	2.09498533
C	7.54390838	-1.05933469	-1.12025595	H	4.09591334	3.02381337	2.89158711
C	7.60219015	-1.54370627	-2.43617461	H	4.91716921	0.41655866	4.19823023
C	8.82033732	-1.89373301	-3.01748898	H	5.17212677	2.07048442	4.77543547
C	10.00719034	-1.76398773	-2.29205167	H	2.93357067	0.21243062	5.38059166
C	9.96517897	-1.27843367	-0.98496959	H	3.20945480	1.79510997	6.12452403
C	8.74269531	-0.93007904	-0.40617877	H	1.91785057	2.93014210	4.44218279

H	1.08606041	1.35268176	4.33517318
C	-1.00654432	-0.09889331	2.77811148
N	-2.21438938	0.61502345	2.35662294
C	-3.03736795	1.43646079	3.24721895
C	-4.19912997	1.78617148	2.30022129
H	-5.04289512	1.09638521	2.41631352
H	-4.55613626	2.81209545	2.40765889
O	-3.65682602	1.62520091	0.97796475
C	-2.55792427	0.80893829	1.05324774
O	-2.03519325	0.36797227	0.04117483
H	-3.40215778	0.84587304	4.09169619
C	-2.26106357	2.66190786	3.78445346
H	-1.33827564	2.28167594	4.23678197
H	-1.97173291	3.29233066	2.93470584
C	-3.04953797	3.46356354	4.79580528
C	-3.62784729	4.69489099	4.45935605
C	-4.37664700	5.41611811	5.39202713
C	-4.56068720	4.91397469	6.68047665
C	-3.98774031	3.68895138	7.03086370
C	-3.23945336	2.97313792	6.09705624
H	-2.78678051	2.02521464	6.38119715
H	-4.11952113	3.29330190	8.03465886
H	-5.14171739	5.47394715	7.40828287
H	-4.81243726	6.37144581	5.11117122
H	-3.48013082	5.09863798	3.45979254
C	-1.07684743	-0.74802268	3.96963243
C	0.05490960	-1.51988128	4.58635671
H	0.36995348	-1.10592844	5.55784378
H	-0.22978332	-2.56479539	4.78020527
H	0.93404311	-1.54253556	3.93604345
H	-2.02924068	-0.76659685	4.49202958
O	0.23992893	1.74579689	-1.13200516
C	1.10937684	2.80451316	-0.70935534
C	0.18769420	4.01780153	-0.45246980
C	-1.11836027	3.66490044	-1.21832182
C	-0.76445370	2.36007151	-1.94858204
H	-0.34451452	2.56152938	-2.94643391
H	-1.59220561	1.65655851	-2.03136020
H	-1.42926424	4.45216346	-1.91237125
H	-1.94251420	3.48588898	-0.52178805
H	0.64472279	4.94525729	-0.81228352
H	-0.00729170	4.14138116	0.61730728
H	1.65206488	2.45210509	0.16815166
H	1.83170309	3.01824325	-1.51142096
O	-0.27402224	-1.85749787	-0.82443682
C	0.28426704	-2.81308858	-0.31217191
C	0.11193971	-4.24060134	-0.77412866
H	-0.41361695	-4.20775653	-1.73548775
C	-0.76290212	-4.98208054	0.25866797
H	-0.89081189	-6.02853784	-0.04024561
H	-0.29814946	-4.97148865	1.25225839
H	-1.75427456	-4.52476393	0.34210310
C	1.48190165	-4.91870589	-0.94250525
H	2.02913535	-4.93896597	0.00837244
H	1.35369830	-5.95445162	-1.27656316
H	2.09978475	-4.38950774	-1.67476329
H	0.93390033	-2.66356209	0.57162331

Table 46. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,S*)-**6** from **5** dimer with three THF



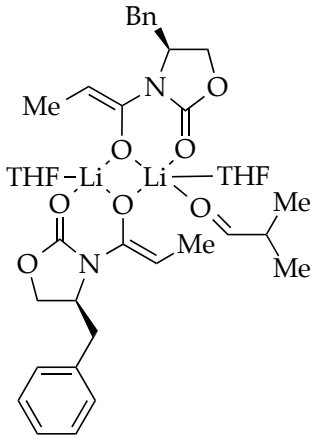


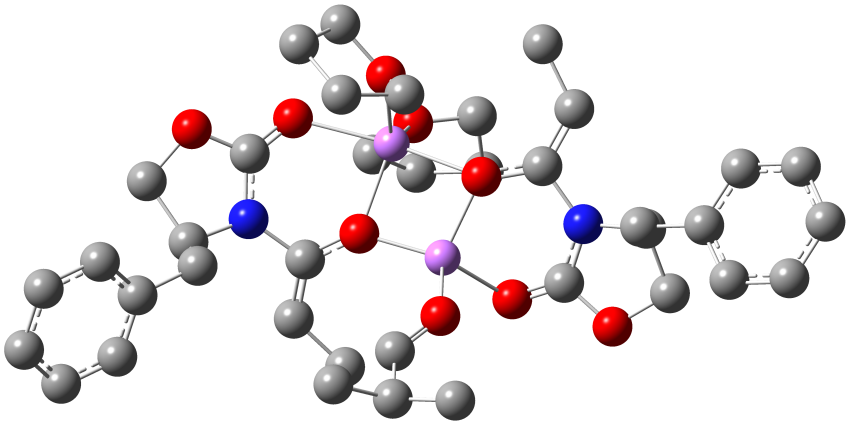
G = -2280.370915 Hartree
G_{MP2} = -1426410.187 kcal/mol
ΔG_{MP2} = 2.546300776 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -5.21258317 kcal/mol vs. **5** dimer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.56059455	-4.88408228	0.32987049
O	0.00000000	0.00000000	2.01264840	H	7.67246811	-4.66342630	1.38945854
Li	1.81434575	0.00000000	2.41230253	H	8.93492058	-6.54113761	0.38832749
O	2.91093690	0.00694140	0.80303784	H	8.70934308	-7.04375480	-2.03766332
C	3.29871924	-0.96693513	0.15807046	H	7.21052907	-5.64716160	-3.44987762
N	3.64483486	-2.16106188	0.84634573	H	5.94995030	-3.77444658	-2.44977172
C	4.40828346	-3.29614818	0.29185562	C	3.27878923	-1.01490310	-1.32284915
C	4.10831484	-4.36125370	1.35578283	H	4.08279836	-1.64791994	-1.70819450
H	3.23260201	-4.96621200	1.10149677	C	3.34702432	0.38744941	-1.92844440
H	4.95707343	-5.00975831	1.57374301	H	2.44486996	0.94552941	-1.66818446
O	3.80005236	-3.60442030	2.54791354	H	4.21729501	0.94489286	-1.56169037
C	3.39612430	-2.36540596	2.19684505	H	3.42294280	0.32566061	-3.01824676
O	2.89810454	-1.59974706	3.00280611	O	2.33960876	1.41449909	3.70687927
H	3.99431932	-3.59110287	-0.67256195	C	1.56878212	1.58303924	4.91333197
C	5.91245542	-2.96055048	0.15977585	C	2.43724200	1.01430960	6.05978222
H	6.00680682	-2.05513757	-0.45146930	C	3.83824442	0.82672872	5.41772195
H	6.30296235	-2.71405029	1.15493188	C	3.71761800	1.56689060	4.08140540
C	6.71071730	-4.09200608	-0.45317089	H	4.32184237	1.14984406	3.27336104
C	6.59671022	-4.38316305	-1.82102602	H	3.94730080	2.63787626	4.18714069
C	7.30964080	-5.43890234	-2.38800063	H	4.03210698	-0.23335553	5.23379292
C	8.15190901	-6.22257440	-1.59558956	H	4.64718251	1.22301955	6.03894082
C	8.27718694	-5.94141099	-0.23510674	H	2.04221752	0.06114375	6.42084321

H	2.46355858	1.70614756	6.90731321
H	1.36885151	2.65408699	5.05645939
H	0.62174563	1.06030548	4.76534522
C	-1.10337928	-0.16386177	2.68525210
N	-2.25620396	0.59542808	2.18449447
C	-3.11469432	1.43367625	3.02257629
C	-4.21494467	1.80089326	2.00920047
H	-5.08318457	1.13725545	2.09009746
H	-4.54707683	2.83806211	2.08393992
O	-3.60966329	1.60490556	0.71919940
C	-2.53281116	0.76938091	0.86382086
O	-1.96764011	0.29822993	-0.11099301
H	-3.53598468	0.85202440	3.84680997
C	-2.35132829	2.64715462	3.60338783
H	-1.46503426	2.25371201	4.11373028
H	-1.99773709	3.26898223	2.77187060
C	-3.18586881	3.46870914	4.56073013
C	-3.70552058	4.71542338	4.18744386
C	-4.49688051	5.45723981	5.06720383
C	-4.78305240	4.96077794	6.33908575
C	-4.26992206	3.72027254	6.72588664
C	-3.47904142	2.98371046	5.84471157
H	-3.07529853	2.02272792	6.15741875
H	-4.48241657	3.32821154	7.71717785
H	-5.39750644	5.53650410	7.02597108
H	-4.88613712	6.42388343	4.75822530
H	-3.47890297	5.11428123	3.20082981
C	-1.33540362	-0.90797488	3.79716661
C	-0.31987037	-1.76357287	4.49830876
H	-0.13072252	-1.43641519	5.53400578
H	-0.66039660	-2.80697303	4.56757278
H	0.64008250	-1.77658372	3.97545718
H	-2.35342741	-0.95147625	4.17488935
O	0.42228794	2.01224402	-0.54798447
C	0.99752685	3.06845007	0.22939297
C	0.03630254	4.27857472	0.09956948
C	-0.98734011	3.82989315	-0.97492017
C	-0.30120370	2.62204006	-1.62163622
H	0.39933343	2.93244950	-2.41333718
H	-0.98874638	1.87349902	-2.01738191
H	-1.21928590	4.61867863	-1.69756483
H	-1.92426082	3.50851779	-0.51007346
H	0.58156235	5.17598549	-0.21079833
H	-0.45499929	4.51014378	1.05000877
H	1.10949598	2.69481822	1.24926298
H	1.99445288	3.31068253	-0.16604890
O	0.82098088	-1.15518493	-1.07808446
C	1.83612947	-1.76916000	-1.66494278
C	1.67820396	-1.91828545	-3.21386717
H	1.57159342	-0.90569544	-3.62596042
C	0.37049357	-2.67433250	-3.49002947
H	0.16163217	-2.72413816	-4.56650861
H	0.43095366	-3.70559602	-3.11408380
H	-0.46197876	-2.18047168	-2.98423471
C	2.85871118	-2.61878640	-3.90170807
H	3.07604100	-3.58400184	-3.42044626
H	2.62979652	-2.83175414	-4.95323906
H	3.77691142	-2.01870541	-3.88758421
H	2.00953366	-2.81637265	-1.29010782

Table 47. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,R*)-**6** from **5** dimer with three THF



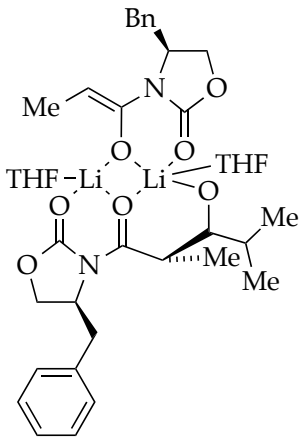


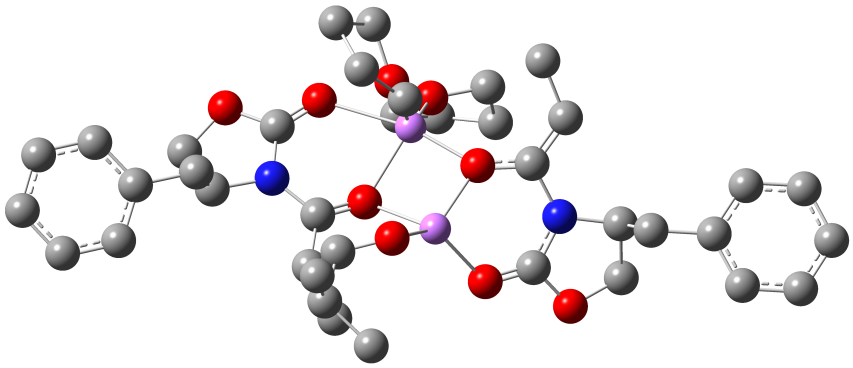
G = -2280.377656 Hartree
G_{MP2} = -1426410.255 kcal/mol
ΔG_{MP2} = 2.477608632 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -8.146462528 kcal/mol vs. **5** dimer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.39070276	0.16998598	-2.11008714
O	0.00000000	0.00000000	2.11681690	H	-4.17683318	-1.55330075	-3.15969502
C	0.79926558	0.00000000	3.13669465	C	-4.81030452	0.17867725	-2.02503074
N	0.39315558	-0.86287656	4.26288126	H	-4.92889625	-0.35978294	-1.07781650
C	0.57705805	-0.50022151	5.67312033	H	-4.41206198	1.17288069	-1.78790326
C	0.19891777	-1.82662718	6.35225220	C	-6.14181553	0.29451848	-2.73275345
H	1.07782412	-2.44663715	6.56238672	C	-6.54613656	1.49492915	-3.33218043
H	-0.37957258	-1.69867543	7.26897930	C	-7.76326995	1.58462868	-4.01112188
O	-0.61988638	-2.51044392	5.38666325	C	-8.59835250	0.47070344	-4.10111091
C	-0.38313932	-1.97538873	4.15425079	C	-8.21024275	-0.73150323	-3.50485244
O	-0.86061530	-2.49792899	3.14990883	C	-6.99429833	-0.81648711	-2.82729448
Li	-1.47252285	-1.13296836	1.91298044	H	-6.70230644	-1.75461774	-2.35919710
O	-1.70153021	-1.04063319	0.07252047	H	-8.85736191	-1.60278591	-3.56405835
C	-2.40758053	-1.58845264	-0.86725292	H	-9.54652055	0.53878308	-4.62748974
N	-2.51445860	-0.79692456	-2.09569710	H	-8.05903436	2.52649059	-4.46580054
C	-3.75309381	-0.59471096	-2.84775395	H	-5.90616665	2.37162961	-3.25696922
C	-3.21290913	0.17188377	-4.07015686	C	-3.07048432	-2.77614684	-0.85609393
H	-3.02507741	-0.49392375	-4.92006514	C	-3.07703944	-3.73719175	0.29955769
H	-3.86128343	0.98896518	-4.39192976	H	-2.75740994	-4.74055296	-0.01610113
O	-1.95780405	0.72467071	-3.63743770	H	-2.39761445	-3.42382513	1.09777069
C	-1.52189567	0.02123296	-2.54380555	H	-4.07713117	-3.86523701	0.74603993

H	-3.57335529	-3.09461449	-1.76502539
O	-3.24977684	-0.65909426	2.82819198
C	-4.32997628	-0.89603116	2.31296190
H	-4.36689705	-1.30244220	1.28322198
C	-5.66482486	-0.66678205	2.98187537
H	-6.15063143	-1.65743372	2.98629462
C	-5.52939786	-0.15445095	4.41628346
H	-6.51653348	-0.05518806	4.88010976
H	-4.92758048	-0.83595527	5.02483124
H	-5.04205062	0.82614122	4.43564224
C	-6.52418808	0.25552691	2.09009231
H	-6.60069787	-0.12274585	1.06422629
H	-7.53823666	0.33246796	2.49523406
H	-6.09913837	1.26505102	2.05017352
H	1.62181702	-0.25758940	5.87798013
C	-0.31166565	0.70212785	6.06960018
H	-0.10400362	1.50032447	5.34812760
H	-1.36304523	0.41528888	5.94608051
C	-0.05267828	1.18455904	7.47928842
C	1.10885916	1.91449702	7.77606365
C	1.37538706	2.34003879	9.07684714
C	0.48169054	2.04406926	10.10910697
C	-0.67931390	1.32344947	9.82828778
C	-0.94173222	0.89823097	8.52397978
H	-1.85551910	0.34715618	8.31107177
H	-1.38493017	1.09420455	10.62270630
H	0.68717219	2.37763965	11.12273593
H	2.27849196	2.90819660	9.28458877
H	1.80372735	2.15893585	6.97510697
C	1.95174572	0.70006339	3.32174496
H	2.53579625	0.51573814	4.21828023
C	2.50954128	1.69389723	2.34332956
H	1.83713953	1.83617926	1.49403184
H	2.67508005	2.67692972	2.81100923
H	3.48601730	1.37756201	1.94361958
O	1.59350826	-1.24035042	-0.41108033
C	2.61200853	-1.62500271	0.53161395
C	2.44220770	-3.13283568	0.69160287
C	2.11560173	-3.55432094	-0.75062514
C	1.29594450	-2.36308528	-1.27960192
H	0.22006048	-2.54580728	-1.22098466
H	1.55133414	-2.09209438	-2.30919812
H	1.55877543	-4.49443560	-0.80992564
H	3.04041633	-3.67540359	-1.32743175
H	1.59904632	-3.34328953	1.35958149
H	3.33590666	-3.62215255	1.09243533
H	3.60305979	-1.38097328	0.11826203
H	2.45352730	-1.05241123	1.44626919
O	0.02788598	2.14126599	-0.01988689
C	-0.79758518	2.86928793	0.89767273
C	-1.85814439	3.54534106	0.01241633
C	-1.13810402	3.71283194	-1.35608337
C	0.22069935	3.01221558	-1.14267560
H	1.00807406	3.74127288	-0.89778505
H	0.53820149	2.39347295	-1.98054368
H	-1.00670640	4.76374038	-1.63295335
H	-1.69816215	3.22478048	-2.15881162
H	-2.19640168	4.49712825	0.43445872
H	-2.73449523	2.89661706	-0.08973514
H	-1.17786416	2.15329493	1.62628477
H	-0.18385960	3.61894192	1.42142668

Table 48. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,R*)-**6** from **5** dimer with three THF



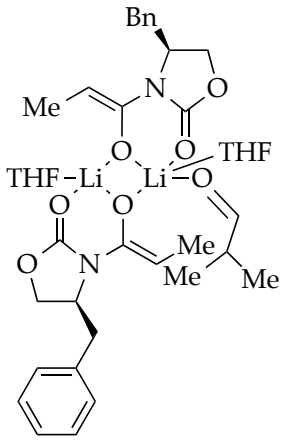


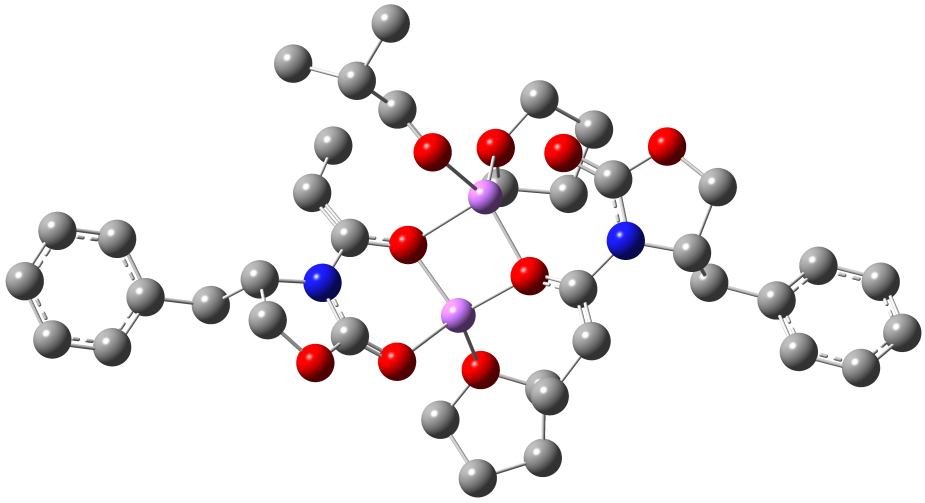
G = -2280.364449 Hartree
G_{MP2} = -1426406.566 kcal/mol
ΔG_{MP2} = 6.166755249 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -4.457315911 kcal/mol vs. **5** dimer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.71990760	-1.08390114	-2.76732026
O	0.00000000	0.00000000	1.94385910	C	-4.56743869	1.07331416	-3.04319823
C	0.78515689	0.00000000	2.97479469	H	-4.86261461	1.34638430	-2.02421445
N	0.47094327	-1.01064529	3.98660964	H	-3.78406897	1.78024889	-3.34348874
C	1.25481379	-1.24478785	5.20576890	C	-5.75151857	1.16797502	-3.98225983
C	0.78988807	-2.66452919	5.54871560	C	-5.63169406	1.76662464	-5.24364784
H	1.41519781	-3.43076532	5.07495550	C	-6.72089083	1.82639369	-6.11567515
H	0.72499690	-2.85875337	6.62036286	C	-7.95020013	1.28658808	-5.73690437
O	-0.53381760	-2.73904786	4.99094204	C	-8.08533844	0.69260104	-4.47990509
C	-0.64079340	-1.81084025	3.99473466	C	-6.99576174	0.63587445	-3.61147334
O	-1.64333371	-1.78088740	3.29406871	H	-7.11602363	0.18572870	-2.62802710
Li	-1.87200008	-0.35446463	2.00758908	H	-9.04227414	0.27970437	-4.17219349
O	-1.85826583	-0.94813976	-0.04869141	H	-8.79978883	1.33446203	-6.41247757
C	-2.90216023	-0.75811885	-0.68185568	H	-6.60846637	2.29995335	-7.08729972
N	-2.82841445	-0.45136030	-2.05589450	H	-4.68049237	2.20367301	-5.54069069
C	-3.95314183	-0.34554616	-3.00776129	C	-4.23178212	-0.77987193	-0.01028456
C	-3.22789588	-0.72069379	-4.30771678	C	-4.39414901	-2.04996008	0.84120857
H	-3.25173201	-1.79856470	-4.50216792	H	-5.42803914	-2.13503418	1.18512998
H	-3.59714787	-0.18261408	-5.18083365	H	-4.16107356	-2.95291979	0.26325995
O	-1.86022696	-0.32770159	-4.07776006	H	-3.74247762	-2.03423253	1.71741606
C	-1.61380852	-0.30304805	-2.74330424	H	-5.04356217	-0.72752108	-0.74109724
O	-0.50204509	-0.16134657	-2.29323389	O	-3.29685184	0.72857472	1.74466976

C	-4.29233939	0.61733228	0.86319567
H	-4.23738427	1.39125979	0.05106183
C	-5.73287998	0.79193915	1.47999587
H	-6.46624280	0.28705684	0.82930421
C	-5.84120054	0.21821694	2.89923138
H	-6.84075744	0.40587999	3.31219985
H	-5.65918904	-0.85887535	2.93779323
H	-5.09856904	0.69495969	3.54471994
C	-6.08129065	2.28948560	1.50462304
H	-6.10484557	2.71699370	0.49405589
H	-7.06137892	2.46544579	1.96549460
H	-5.32997160	2.83876283	2.08436638
H	2.32203985	-1.22527374	4.97222043
C	0.92847390	-0.21229241	6.31546301
H	1.05412292	0.78746055	5.88808864
H	-0.13157723	-0.31714117	6.57703089
C	1.79098590	-0.37883121	7.54732128
C	3.13309399	0.03152240	7.53959520
C	3.94349406	-0.14378567	8.66082838
C	3.42488812	-0.73334998	9.81616555
C	2.09123653	-1.14192775	9.84061333
C	1.28384505	-0.96566070	8.71479974
H	0.24152197	-1.27604859	8.74566548
H	1.67527889	-1.59450027	10.73704092
H	4.05463229	-0.86735406	10.69160190
H	4.97906645	0.18560405	8.63517289
H	3.54317311	0.50357504	6.64899636
C	1.87002240	0.79613557	3.19188771
H	2.45434904	0.68488654	4.09752463
C	2.30287796	1.87392758	2.23835043
H	1.63493552	1.91885769	1.37416620
H	2.29870185	2.86711479	2.71297402
H	3.32667988	1.71723492	1.86301906
O	1.61418748	-1.14121235	-0.53289529
C	2.75755210	-1.34256107	0.32513461
C	2.88007427	-2.85721742	0.46368322
C	2.49696191	-3.32493171	-0.94913282
C	1.41073585	-2.31666790	-1.35643674
H	0.40311389	-2.69370043	-1.15138703
H	1.46531051	-2.02425539	-2.40848517
H	2.13501934	-4.35709599	-0.98156903
H	3.36209544	-3.25162949	-1.61868647
H	2.15831033	-3.22568276	1.20207376
H	3.88156660	-3.17633119	0.76903582
H	3.65007442	-0.91737092	-0.15751927
H	2.56965216	-0.81718237	1.26303874
O	-0.30352791	2.00210841	-0.33221649
C	-1.03757195	2.87103617	0.56202581
C	-1.56329260	4.01940323	-0.32962091
C	-0.74112838	3.89921553	-1.64220386
C	0.32310216	2.84768125	-1.29951763
H	1.21594308	3.31748877	-0.85723357
H	0.62719298	2.22030626	-2.13970623
H	-0.29653580	4.84807179	-1.95856646
H	-1.37250450	3.53979997	-2.46212569
H	-1.41867747	4.98957483	0.15597982
H	-2.63388096	3.90912333	-0.52445555
H	-1.81676552	2.26939981	1.03903322
H	-0.34767218	3.24875710	1.32820711

Table 49. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,R*)-**6** from **5** dimer with three THF



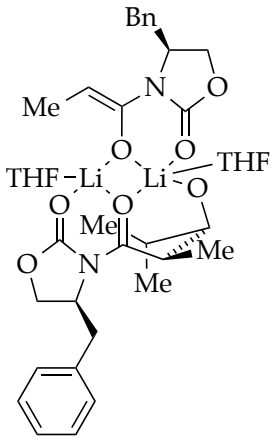


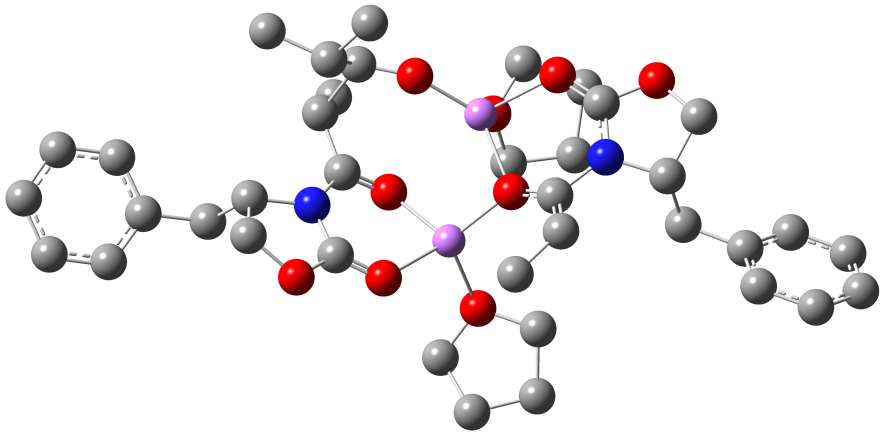
G = -2280.37782 Hartree
G_{MP2} = -1426409.915 kcal/mol
ΔG_{MP2} = -5.856926396 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = 2.817500077 kcal/mol vs. **5** dimer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.76064247	-3.96785530	-1.07163805
O	0.00000000	0.00000000	1.96705330	H	7.86408259	-3.94440843	0.01115784
Li	1.87777764	0.00000000	1.90962824	H	9.28140427	-5.47218852	-1.32136481
O	2.09252290	-0.00162736	0.03900514	H	9.07657527	-5.52163471	-3.80081751
C	2.96694253	-0.59716264	-0.69850087	H	7.44188414	-4.02257061	-4.92911571
N	3.59865857	-1.77352982	-0.08711238	H	6.02728309	-2.49796599	-3.59465319
C	4.47758188	-2.72196334	-0.78420201	C	3.33091113	-0.28604638	-1.97770548
C	4.33999006	-3.93259150	0.14432126	H	4.11400768	-0.85202517	-2.46848186
H	3.49075706	-4.57003092	-0.12712944	C	2.81152071	0.92294949	-2.70555421
H	5.24525265	-4.53667167	0.21983550	H	1.90304354	1.30545764	-2.23378732
O	4.07865335	-3.34200758	1.43233794	H	3.54444248	1.74611575	-2.72440974
C	3.52838379	-2.10946865	1.23447134	H	2.57916095	0.69711754	-3.75683195
O	3.09806065	-1.47309312	2.19130751	O	2.57973742	1.47643275	3.07938007
H	4.08098401	-2.93159173	-1.78034590	C	1.72482243	2.05871658	4.09364024
C	5.93839799	-2.20785385	-0.88102877	C	2.59293313	2.22107322	5.35750212
H	5.91666647	-1.20467620	-1.31768245	C	3.79771874	1.30501672	5.07712288
H	6.32970223	-2.10387938	0.13853143	C	3.93465840	1.42959250	3.56209172
C	6.83171463	-3.12123686	-1.69171736	H	4.41886849	0.57717679	3.08205435
C	6.73216907	-3.15676779	-3.09125811	H	4.45946681	2.35461943	3.27970961
C	7.53188840	-4.01435997	-3.84592439	H	3.56725025	0.26768846	5.34390733
C	8.45093681	-4.85502000	-3.21342495	H	4.70228178	1.60842540	5.61332940
C	8.56451757	-4.82763778	-1.82335678	H	2.05105509	1.94622013	6.26715677

H	2.92379004	3.26017969	5.46768614
H	1.33978659	3.01670276	3.72532695
H	0.88308677	1.37663080	4.23844647
C	-0.95837235	-0.35158530	2.76984597
N	-2.29389737	0.10370303	2.36644857
C	-3.29564636	0.64127325	3.28938411
C	-4.49774357	0.79584942	2.33833275
H	-5.18289207	-0.05694916	2.40223876
H	-5.05890498	1.71912775	2.49477558
O	-3.92707982	0.82400503	1.01867654
C	-2.67227724	0.27449790	1.07139944
O	-2.06278090	0.01415021	0.04393702
H	-3.52767902	-0.08516184	4.07277646
C	-2.82719695	1.95904427	3.95022871
H	-1.84987756	1.75650821	4.40293320
H	-2.67571855	2.71082127	3.16595999
C	-3.79440863	2.47100347	4.99396885
C	-4.63030900	3.56632334	4.73867240
C	-5.54108347	4.01472823	5.69792502
C	-5.63065790	3.37146212	6.93254357
C	-4.80089224	2.28047274	7.20250615
C	-3.89214646	1.83701272	6.24237670
H	-3.24171882	0.99337635	6.46467095
H	-4.85798101	1.77758782	8.16444752
H	-6.33738543	3.71944439	7.68106816
H	-6.17703980	4.86888042	5.48011238
H	-4.55911269	4.08099758	3.78258528
C	-0.89132066	-1.04773160	3.93464715
C	0.37083797	-1.60109892	4.53404960
H	0.68826625	-1.06158938	5.44222466
H	0.23416591	-2.64891321	4.83581352
H	1.20588153	-1.58166947	3.82840427
H	-1.81943760	-1.27951299	4.44912055
O	-0.04979693	1.96769024	-0.92886147
C	0.69104919	2.96396435	-0.20954541
C	-0.37357765	3.69017726	0.62014155
C	-1.62714313	3.64110043	-0.29432207
C	-1.23911727	2.62342297	-1.39503075
H	-1.01623675	3.13452959	-2.34349481
H	-1.98862299	1.85032783	-1.56158232
H	-1.85585987	4.61997913	-0.72818452
H	-2.51264793	3.30737795	0.25415706
H	-0.07632263	4.71031612	0.88405702
H	-0.55063159	3.13329728	1.54579848
H	1.45998213	2.44698754	0.36450602
H	1.17544694	3.64734190	-0.92553226
O	-0.01314799	-1.56469439	-1.31521813
C	0.23350063	-1.50757020	-2.50775038
C	0.28670756	-2.71786092	-3.41369930
H	0.44983893	-3.59140878	-2.77124642
C	1.41650143	-2.59442155	-4.44615528
H	2.38975318	-2.48097379	-3.95805696
H	1.44742758	-3.48243561	-5.08727442
H	1.26434518	-1.72167848	-5.09327636
C	-1.09189881	-2.85774131	-4.09700521
H	-1.09318645	-3.72725080	-4.76389480
H	-1.88859995	-2.98752754	-3.35770044
H	-1.32611842	-1.97287528	-4.70179013
H	0.36529778	-0.52467307	-3.00117587

Table 50. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,R*)-**6** from **5** dimer with three THF



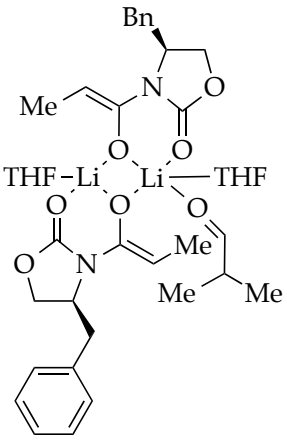


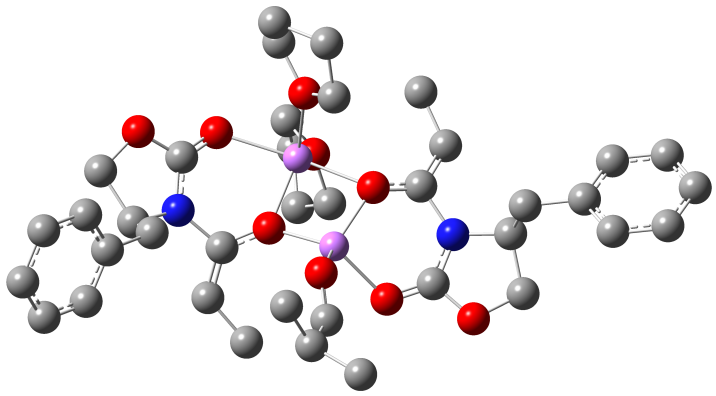
G = -2280.368139 Hartree
G_{MP2} = -1426407.684 kcal/mol
ΔG_{MP2} = 5.048707634 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -3.625718839 kcal/mol vs. **5** dimer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	9.10679348	-4.89726373	-0.18437012
O	0.00000000	0.00000000	2.01276920	C	8.19132601	-3.96351049	0.30609583
Li	1.84125504	0.00000000	2.31398683	H	8.27340052	-3.61885706	1.33490257
O	2.72958483	-0.08715780	0.59533792	H	9.88879180	-5.27899722	0.46655769
C	3.24017276	-1.03894350	0.00307938	H	9.73206560	-6.05845931	-1.89099375
N	3.80822575	-2.09972845	0.77001428	H	7.94585460	-5.15564364	-3.36931499
C	4.78090272	-3.09700179	0.28254084	H	6.33443088	-3.49774669	-2.50103928
C	4.76501952	-4.07860936	1.46192129	C	3.15067203	-1.19282409	-1.45973822
H	4.02772353	-4.87614519	1.32657422	H	3.90152015	-1.88095275	-1.85294929
H	5.74114140	-4.51087798	1.68300834	C	3.22474694	0.15983044	-2.17533515
O	4.35815153	-3.27705896	2.59227279	H	2.38790995	0.78898796	-1.86390215
C	3.68731043	-2.19142067	2.14912555	H	4.16134005	0.69070904	-1.96163820
O	3.09298807	-1.45351260	2.91583131	H	3.16327437	0.00301716	-3.25772643
H	4.40986556	-3.58161514	-0.61965115	O	2.36021498	1.51915640	3.48393093
C	6.16634539	-2.45889495	0.02136876	C	1.38826741	2.04742986	4.42369410
H	6.03007142	-1.63499736	-0.68900919	C	2.18835845	2.51810575	5.64858048
H	6.52757493	-2.01542483	0.95753592	C	3.48559972	1.69936750	5.54345473
C	7.17748007	-3.45062965	-0.51395405	C	3.68841638	1.63865622	4.03178214
C	7.10518479	-3.89385616	-1.84305266	H	4.26145709	0.77389820	3.69131694
C	8.01654147	-4.82708900	-2.33594515	H	4.15764293	2.55691069	3.65049490
C	9.02016532	-5.33325035	-1.50660880	H	3.33947597	0.68910950	5.94239456

H	4.33001797	2.15888184	6.06622357
H	1.64699174	2.34987383	6.58407010
H	2.41021544	3.58924620	5.57687845
H	0.83614721	2.85689444	3.93556120
H	0.68658270	1.24243046	4.66269965
C	-1.05576255	-0.27056215	2.72470136
N	-2.29963558	0.35497122	2.25937059
C	-3.29469623	0.96149683	3.14711111
C	-4.42543691	1.25078777	2.14377350
H	-5.17891266	0.45507148	2.13580460
H	-4.91832828	2.21063848	2.30949707
O	-3.78004397	1.28122947	0.86034378
C	-2.58978998	0.60881509	0.95245130
O	-1.95674488	0.32727055	-0.05274296
H	-3.63320619	0.24354405	3.89800561
C	-2.74302049	2.21627345	3.86381385
H	-1.81146610	1.91609287	4.35634780
H	-2.48712933	2.96674259	3.10549004
C	-3.70958984	2.79287227	4.87417697
C	-4.43300037	3.96243717	4.60490071
C	-5.34589306	4.47211817	5.53082765
C	-5.55045003	3.81671542	6.74518951
C	-4.83390468	2.65136001	7.02859879
C	-3.92256035	2.14662125	6.10168952
H	-3.36143663	1.24342790	6.33320705
H	-4.98202322	2.13757915	7.97495289
H	-6.25926753	4.21196530	7.46782014
H	-5.89382462	5.38276612	5.30303175
H	-4.27196580	4.48478786	3.66412814
C	-1.15872691	-1.02016107	3.85359130
C	-0.02167911	-1.74133677	4.51892712
H	0.24679601	-1.31135983	5.49848851
H	-0.27949789	-2.79281885	4.70949073
H	0.88284366	-1.74299494	3.90536723
H	-2.14487253	-1.17258636	4.28196479
O	0.47420345	1.99476021	-0.67021013
C	0.97105108	3.06429229	0.13532588
C	-0.23926512	3.98680688	0.37405889
C	-1.16974621	3.69293759	-0.83658694
C	-0.42111774	2.59251866	-1.61626649
H	0.16341077	3.02002862	-2.44550061
H	-1.06600057	1.80042359	-1.99708478
H	-1.33977901	4.57876839	-1.45684798
H	-2.14343129	3.32741778	-0.49997824
H	0.05720397	5.03892711	0.43639258
H	-0.73608039	3.72566986	1.31405129
H	1.39456337	2.62917823	1.04236674
H	1.76849439	3.59398493	-0.41018103
O	0.67578375	-1.23097578	-1.10056823
C	1.61945027	-1.85043921	-1.77871673
C	1.63799133	-3.40704301	-1.60015099
H	2.01672926	-3.63664309	-0.59107074
C	2.50438505	-4.12604919	-2.64681488
H	3.55848518	-3.81793474	-2.63495479
H	2.48257850	-5.21349559	-2.50192357
H	2.12625269	-3.92415568	-3.65736787
C	0.19809900	-3.93527318	-1.67300781
H	0.16444654	-5.01805088	-1.49409089
H	-0.42685013	-3.42527915	-0.93765113
H	-0.23291056	-3.74535189	-2.66512337
H	1.58351529	-1.66888735	-2.88350581

Table 51. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,S*)-**6** from **5** dimer with three THF



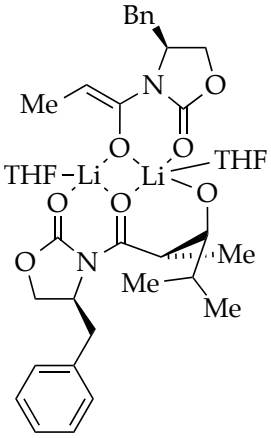


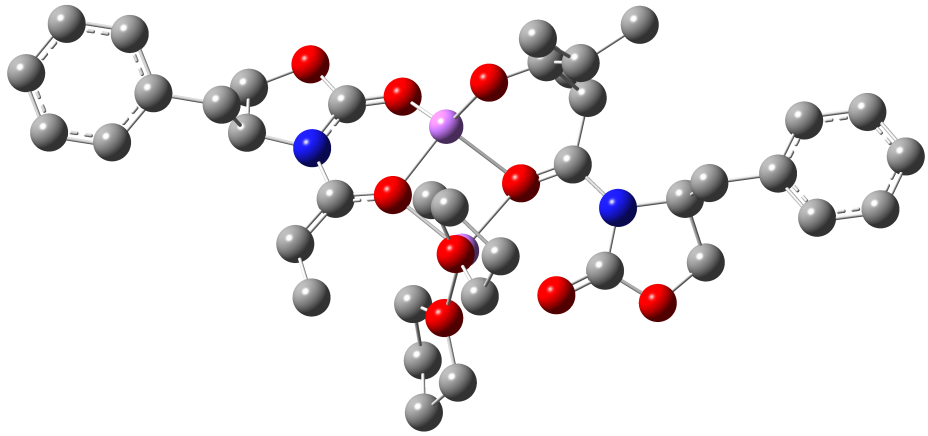
G = -2280.383667 Hartree
G_{MP2} = -1426411.693 kcal/mol
ΔG_{MP2} = 1.039700804 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -10.03546225 kcal/mol vs. **5** dimer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.40337201	0.18031379	-1.50268407
O	0.00000000	0.00000000	2.13946330	C	-6.02464858	-0.99320089	-2.31034631
C	0.92510137	0.00000000	3.04210300	C	-6.71179761	0.12088612	-2.81111342
N	0.63692804	-0.80850326	4.24695856	C	-7.98844439	-0.00932693	-3.36237140
C	1.08660616	-0.43820342	5.59575706	C	-8.60022017	-1.26162735	-3.42289738
C	0.68548474	-1.69708294	6.37918819	C	-7.92843056	-2.38100541	-2.92539891
H	1.51110450	-2.41347748	6.45911233	C	-6.65454407	-2.24600766	-2.37460667
H	0.29293531	-1.48624020	7.37562388	H	-6.14165286	-3.12123961	-1.98058617
O	-0.36022416	-2.29376755	5.59152608	H	-8.39976096	-3.35985253	-2.96233881
C	-0.26304365	-1.82463048	4.31237738	H	-9.59406311	-1.36539822	-3.85001427
O	-0.95284009	-2.32834977	3.42742449	H	-8.50479019	0.86912962	-3.74082463
Li	-1.43759517	-1.17265159	1.94522497	H	-6.24573125	1.10265176	-2.75812130
O	-1.36242006	-1.40229802	0.10939320	C	-2.20169429	-3.43973334	-0.83335316
C	-1.88719120	-2.11973197	-0.83609942	C	-2.00477931	-4.35227259	0.34325850
N	-2.21272150	-1.38335478	-2.06154996	H	-2.95063691	-4.79596199	0.69324746
C	-3.53534807	-1.40698895	-2.68877435	H	-1.34433856	-5.19762896	0.09848317
C	-3.26517407	-0.52196341	-3.91899966	H	-1.55374197	-3.82347641	1.18844827
H	-3.00002580	-1.11704598	-4.80050429	H	-2.58547762	-3.87926071	-1.75046407
H	-4.09444742	0.14249064	-4.16941790	O	-3.41298614	-0.88712857	2.47264682
O	-2.12925386	0.28145742	-3.55096162	C	-4.00738847	-1.76272869	3.08120088
C	-1.47585021	-0.33453445	-2.51607538	C	-5.49100224	-1.75325860	3.36271827
O	-0.38763892	0.06765013	-2.12877990	H	-5.87196241	-2.67733728	2.89513165
H	-3.79802654	-2.42281746	-2.99646888	C	-6.20475634	-0.54129454	2.76252454
C	-4.63037856	-0.86633806	-1.73847545	H	-7.28190725	-0.60138973	2.95115351
H	-4.54761976	-1.43313733	-0.80401445	H	-5.83114778	0.38884897	3.20371969

H	-6.04709115	-0.48132836	1.68156414
C	-5.71137231	-1.89269415	4.88465329
H	-5.17724807	-2.75750056	5.29429985
H	-5.36375887	-0.99665814	5.41180469
H	-6.77692189	-2.01970914	5.10109150
H	-3.44199324	-2.62906093	3.47441707
H	2.17066029	-0.31063377	5.61886111
C	0.40771449	0.86254648	6.08528865
H	0.57037250	1.61472309	5.30567219
H	-0.67326428	0.68809557	6.15422934
C	0.95127104	1.34641870	7.41090715
C	2.22032876	1.94187034	7.48151697
C	2.74582844	2.36655312	8.70124062
C	2.00928722	2.20528031	9.87743035
C	0.74456301	1.61928043	9.82198248
C	0.22277499	1.19382394	8.59819481
H	-0.76922315	0.74802644	8.56199547
H	0.16006536	1.49547203	10.73003494
H	2.41689513	2.53883877	10.82795441
H	3.72875691	2.82954081	8.73341530
H	2.79444366	2.08255081	6.56796353
C	2.10979075	0.66964288	3.04927821
H	2.81068870	0.49751419	3.86002574
C	2.54525781	1.60983699	1.96145407
H	1.71423374	1.84320454	1.29076837
H	2.92529190	2.55560949	2.37660073
H	3.35353223	1.19131878	1.34236935
O	1.85225297	-0.79071082	-0.28819937
C	2.06580910	-2.08662392	0.31264036
C	2.75519684	-2.92240540	-0.76610005
C	3.59673890	-1.86429521	-1.49674939
C	2.67433117	-0.63938765	-1.46397552
H	2.01571794	-0.59360105	-2.33739499
H	3.22092262	0.30694318	-1.38423088
H	3.86889957	-2.15284936	-2.51687957
H	4.52229220	-1.66661376	-0.94257550
H	2.00973261	-3.35396889	-1.44417483
H	3.35220113	-3.73921078	-0.34817908
H	2.69773802	-1.96259696	1.20192316
H	1.09166396	-2.47492827	0.61706350
O	-0.41278405	2.07053265	0.00059677
C	-1.15704695	2.70365590	1.06735154
C	-1.32077974	4.17513964	0.65748756
C	-1.19081549	4.11513469	-0.87296630
C	-0.13943198	3.02037003	-1.04569873
H	0.87586701	3.42492503	-0.91416854
H	-0.19046997	2.48373543	-1.99384608
H	-0.89045153	5.06711052	-1.32221424
H	-2.13816637	3.80400579	-1.32971799
H	-0.51241924	4.78402724	1.07985346
H	-2.27123709	4.59816656	0.99770073
H	-2.12193628	2.19000795	1.15340891
H	-0.61156484	2.56424972	2.00291730

Table 52. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,S*)-**6** from **5** dimer with three THF



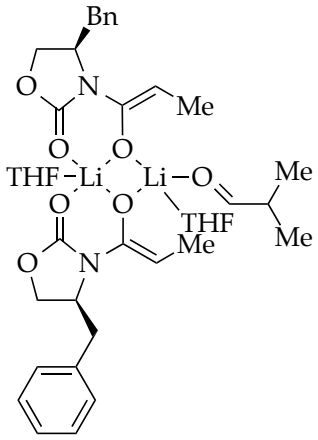


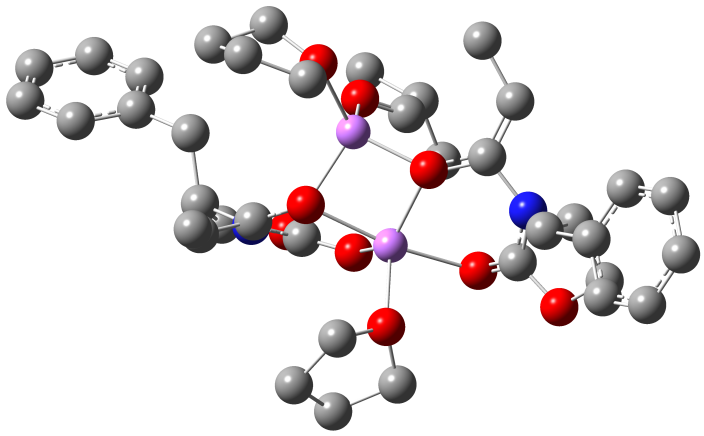
G = -2280.364375 Hartree
G_{MP2} = -1426406.503 kcal/mol
ΔG_{MP2} = 6.229692127 kcal/mol vs. **5** dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -4.845470928 kcal/mol vs. **5** dimer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.08013346	0.26372079	-2.54413854
O	0.00000000	0.00000000	1.96146220	H	-3.94989132	0.64118088	-3.83610281
C	0.86855414	0.00000000	2.92126141	C	-5.66224299	-0.49937227	-4.47575505
N	0.47500657	-0.74397814	4.12317981	C	-5.52680272	-0.10204067	-5.81276563
C	1.07553561	-0.53576543	5.44700466	C	-6.48624370	-0.45023026	-6.76595907
C	0.52535316	-1.75727005	6.19658481	C	-7.59893791	-1.20505214	-6.39443460
H	1.21833790	-2.60638522	6.16600371	C	-7.74861686	-1.60465430	-5.06439793
H	0.25733003	-1.54776691	7.23361250	C	-6.78908674	-1.25356597	-4.11523537
O	-0.66640606	-2.11291700	5.47822508	H	-6.92407093	-1.55788313	-3.07944774
C	-0.59989697	-1.58543977	4.22075045	H	-8.61707594	-2.18468529	-4.76398807
O	-1.44448420	-1.88888194	3.38762037	H	-8.34801598	-1.47541474	-7.13354826
Li	-1.81341910	-0.56594334	2.01495854	H	-6.36473270	-0.12705955	-7.79637406
O	-1.75776666	-1.13829034	0.02983703	H	-4.66809590	0.49750470	-6.10789007
C	-2.80179121	-1.17494575	-0.62763618	C	-4.12429755	-1.37098698	0.02266520
N	-2.71857309	-1.00112559	-2.02988912	C	-4.11623137	-2.64394662	0.89122078
C	-3.74046618	-1.35200008	-3.03863557	H	-5.11935033	-2.80342112	1.30020694
C	-2.82603822	-1.82861796	-4.17574179	H	-3.83713398	-3.53793048	0.31913767
H	-2.59158561	-2.89640286	-4.10492357	H	-3.42349010	-2.54544543	1.73083446
H	-3.21341243	-1.60107564	-5.16884739	H	-4.92173901	-1.44866035	-0.71959442
O	-1.60912833	-1.07811995	-3.98224900	C	-4.44043108	-0.07266596	1.02539155
C	-1.50630627	-0.71999088	-2.67757926	O	-3.36482525	0.31878867	1.70671723
O	-0.50386037	-0.22143563	-2.22127370	C	-5.14848701	1.07766851	0.23321210
H	-4.36581883	-2.16700957	-2.67005163	H	-4.52189489	1.33118912	-0.63849828
C	-4.61135597	-0.14155763	-3.44481131	C	-5.23748797	2.32898044	1.11850076

H	-5.68281362	3.17006812	0.57078479
H	-5.86516338	2.13303543	1.99802293
H	-4.24870531	2.61462661	1.48142515
C	-6.55975818	0.69837343	-0.24423279
H	-6.58028537	-0.18081029	-0.89949234
H	-7.20102525	0.46974378	0.61675790
H	-7.03052828	1.52362107	-0.79299372
H	-5.23548423	-0.52450433	1.67047721
H	2.16454693	-0.59284679	5.38779505
C	0.65645306	0.82369513	6.05719492
H	0.89036935	1.59369916	5.31426393
H	-0.43204942	0.82116285	6.19270536
C	1.35078808	1.12027938	7.36765336
C	2.70023452	1.50579213	7.38593958
C	3.35912326	1.75457741	8.58949166
C	2.67816360	1.62386698	9.80227835
C	1.33514883	1.24645748	9.79959669
C	0.67966428	0.99699133	8.59178542
H	-0.37125596	0.71545330	8.59781183
H	0.79356527	1.14962560	10.73704666
H	3.18969585	1.82053878	10.74070400
H	4.40321927	2.05697947	8.58088880
H	3.23403480	1.62323080	6.44497947
C	2.08812173	0.60840807	2.94015616
H	2.74341371	0.47734698	3.79387577
C	2.60967456	1.45418823	1.81205270
H	1.80681939	1.73370087	1.12394140
H	3.06903805	2.38058029	2.18648798
H	3.38563508	0.94362868	1.21739495
O	1.64285857	-1.07836721	-0.41272658
C	2.06020015	-2.13324920	0.48527232
C	3.07708450	-2.95615035	-0.30643516
C	3.73742404	-1.88170988	-1.18458937
C	2.55164729	-0.97382071	-1.52683820
H	2.03118636	-1.30018783	-2.43465849
H	2.83343908	0.07726415	-1.64735056
H	4.22543352	-2.28575591	-2.07693359
H	4.48781912	-1.32980810	-0.60635494
H	2.56907055	-3.70123782	-0.93087681
H	3.78556850	-3.48142734	0.34141442
H	2.50073897	-1.67658655	1.37884830
H	1.16928340	-2.69330808	0.78147044
O	-0.28025222	2.00986100	-0.24087294
C	-1.02947042	2.72057479	0.79030000
C	-1.44148786	4.06659715	0.16410642
C	-1.25670247	3.83190348	-1.34562685
C	-0.06687566	2.87466922	-1.36262758
H	0.88061721	3.42280547	-1.23867983
H	-0.00043440	2.24727873	-2.25406699
H	-1.07235401	4.75261614	-1.90866735
H	-2.13937109	3.33937369	-1.77079910
H	-0.78038565	4.87315393	0.50230782
H	-2.46642130	4.34195321	0.42926816
H	-1.88096314	2.08942974	1.05996460
H	-0.38537632	2.84049465	1.66611665

Table 53. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,S*)-**6** from **5** spirocyclic dimer with three THF



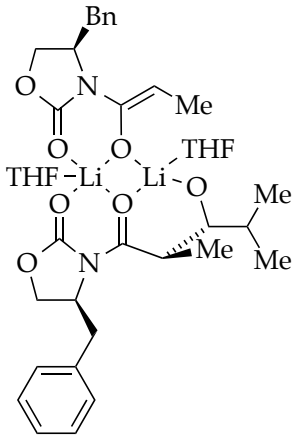


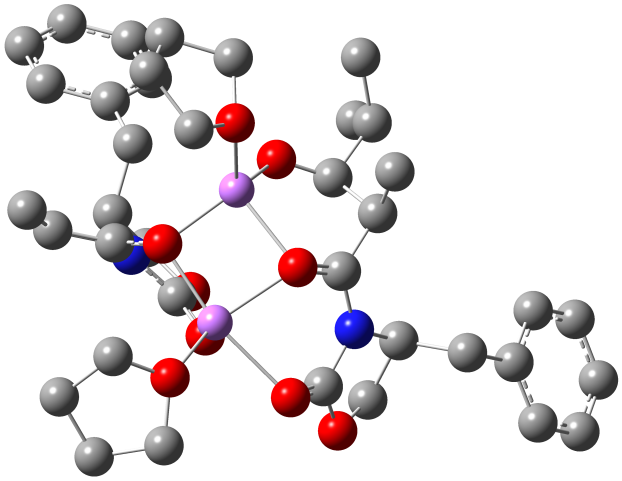
G = -2280.382776 Hartree
G_{MP2} = -1426416.289 kcal/mol
ΔG_{MP2} = -3.556295138 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -8.070804778 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.06392920	-3.89351151	-1.95638144
Li	0.00000000	0.00000000	2.62264960	C	5.84724270	-3.27309218	-1.66432118
O	1.42690130	0.00000000	1.40703456	H	5.00612606	-3.39023371	-2.34450208
C	2.66212282	0.39198929	1.29617112	H	7.16474266	-4.48279716	-2.86420075
N	3.19574647	0.37772305	-0.06685244	H	9.09121825	-4.24516213	-1.30740038
C	2.44727005	0.67978810	-1.16253473	H	8.83134234	-2.90746352	0.77476189
O	1.30484352	1.11430058	-1.21037647	H	6.67122759	-1.81715784	1.28977763
O	3.16328442	0.43054178	-2.30058556	C	3.53198675	0.78509197	2.26246704
C	4.51840492	0.11335890	-1.93308274	H	4.51049121	1.14095474	1.95077855
H	5.13720048	1.00495312	-2.08618805	C	3.24707870	0.77261931	3.73693716
H	4.87588830	-0.68819926	-2.58200935	H	2.29001593	0.29311407	3.96126969
C	4.44377926	-0.28603332	-0.44734151	H	4.02634181	0.23124128	4.29481109
H	5.28914894	0.13487816	0.10397860	H	3.21399633	1.78651932	4.16686903
C	4.38235321	-1.81063534	-0.19184117	O	-1.23473538	-0.84795760	1.47167845
H	4.11421866	-1.94640274	0.86239093	C	-2.52804220	-0.87919076	1.40931252
H	3.56600352	-2.23211481	-0.79046049	N	-3.17024062	0.40395480	1.09733897
C	5.68659085	-2.51225487	-0.49833405	C	-4.38227896	0.90147260	1.75676885
C	6.78066555	-2.39251089	0.37261095	C	-4.61381307	2.19849714	0.96170940
C	7.99775052	-3.00925430	0.08453277	H	-5.31757002	2.05189014	0.13449735
C	8.14408452	-3.76171565	-1.08336730	H	-4.95134096	3.03323634	1.57825772

O	-3.32602082	2.52636233	0.40979074	H	-0.13835031	-3.14112063	6.33319713
C	-2.55507565	1.39364285	0.39380952	H	-2.43637275	-1.87271489	4.75556731
O	-1.48581153	1.38097337	-0.20040270	H	-2.22994678	-1.91128167	6.52239441
H	-5.21606827	0.21124457	1.60278821	H	-0.34781529	-0.33128614	6.39424157
C	-4.16803547	1.10989711	3.27455044	H	-1.42996489	0.32721757	5.13947520
H	-3.82533795	0.15036314	3.67837496	O	-0.47452641	1.98253596	2.94082000
H	-3.35453616	1.83081417	3.41612664	C	0.12214956	2.77739545	2.22266898
C	-5.42025942	1.56460838	3.99010761	H	0.92855493	2.41015097	1.56685638
C	-5.57455219	2.89303344	4.40947565	C	-0.15367157	4.25886747	2.16562867
C	-6.74379990	3.31479236	5.04638122	C	-0.27428048	4.70039736	0.69100720
C	-7.78178411	2.41092882	5.27411375	H	-0.33350518	5.79245197	0.63274448
C	-7.64065840	1.08265931	4.86502542	H	0.58823431	4.37133538	0.10169774
C	-6.47088611	0.66561692	4.23062970	H	-1.17199824	4.27516381	0.23288435
H	-6.36469714	-0.37348222	3.92515222	H	0.76645953	4.71793620	2.56965962
H	-8.44090575	0.36942344	5.04517375	C	-1.35059136	4.68429235	3.01745612
H	-8.69189438	2.73627335	5.77080823	H	-1.24657713	4.34792537	4.05364906
H	-6.84031073	4.34877383	5.36733937	H	-1.45091294	5.77488117	3.01493864
H	-4.76445294	3.60084225	4.24618526	H	-2.27431839	4.25815735	2.61106608
C	-3.36004059	-1.93631020	1.61344770	O	-0.05786001	-1.45345891	-1.45482288
C	-2.88026966	-3.30612355	2.00135381	C	-0.68299082	-2.72392702	-1.21383401
H	-3.07477331	-4.05622882	1.21924568	C	-2.02259974	-2.68892297	-1.98384817
H	-1.80111576	-3.29612395	2.18274011	C	-1.85787189	-1.49563036	-2.96577566
H	-3.37287556	-3.67940372	2.91237094	C	-0.38351249	-1.10044736	-2.80811739
H	-4.42678749	-1.80463642	1.45597970	H	-0.17258899	-0.03747110	-2.92459747
O	0.09457032	-0.84402685	4.42430426	H	0.25940653	-1.67337491	-3.49443228
C	-0.87073989	-0.55723728	5.45339974	H	-2.50004114	-0.66130734	-2.66751625
C	-1.70161614	-1.83244050	5.56720965	H	-2.10492170	-1.75703402	-3.99965511
C	-0.62899323	-2.92012986	5.37843462	H	-2.85597173	-2.52070729	-1.29666196
C	0.36396492	-2.26968905	4.39645262	H	-2.20131982	-3.63352525	-2.50782509
H	0.21745317	-2.60241483	3.36506067	H	-0.02623284	-3.52127854	-1.59338183
H	1.40922108	-2.43527941	4.67814807	H	-0.79215007	-2.82203996	-0.13405136
H	-1.03905061	-3.85544420	4.98742719				

Table 54. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,S*)-**6** from **5** spirocyclic dimer with three THF



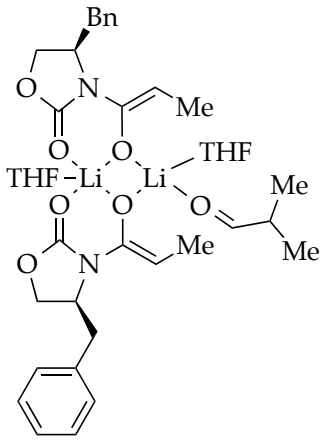


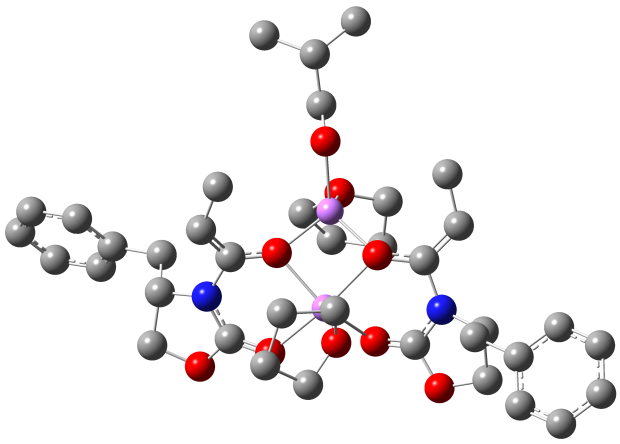
G = -2280.374161 Hartree
G_{MP2} = -1426416.972 kcal/mol
ΔG_{MP2} = -4.239659853 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -8.754169492 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.33112629	5.56653985	-0.49305521
Li	0.00000000	0.00000000	2.84477140	C	6.56533357	4.40137500	-0.57329759
O	1.54430207	0.00000000	1.41373443	H	6.47787089	3.87897819	-1.52365150
C	2.35848558	0.91665144	1.57912537	H	7.82843241	5.94705198	-1.38122853
N	2.73069222	1.71909802	0.49563146	H	8.05674507	7.14182006	0.78911713
C	2.30519301	1.48474073	-0.82467526	H	6.92451875	6.24250119	2.81395717
O	1.78226369	0.49137088	-1.27186470	H	5.57709553	4.17754047	2.67012960
O	2.62733316	2.55633435	-1.58067630	C	2.87744172	1.26284464	2.93932595
C	3.01688779	3.64577221	-0.71622133	H	3.75968523	1.90412413	2.85826327
H	2.12938988	4.24948578	-0.50465781	C	3.25039466	-0.00675973	3.71825446
H	3.76726196	4.24081641	-1.23675921	H	3.93154346	-0.64358152	3.14105632
C	3.55060980	2.94637608	0.54057403	H	3.75657358	0.26382410	4.64902278
H	3.31215757	3.52465400	1.43420647	H	2.36272336	-0.59380938	3.96190320
C	5.06528812	2.63830043	0.46967469	O	-1.33352179	-0.25617434	1.45211927
H	5.31664135	1.94883744	1.28374196	C	-2.42660794	0.45701774	1.40645809
H	5.26648473	2.10555747	-0.46757437	N	-2.21785925	1.90705878	1.36772933
C	5.91849563	3.88653810	0.55785754	C	-2.86498909	2.85688733	2.28229372
C	6.06093431	4.56704923	1.77649629	C	-2.20062346	4.18007305	1.83407249
C	6.82353813	5.73144740	1.86025676	H	-2.87113502	4.79954880	1.22972130
C	7.46039150	6.23591900	0.72394279	H	-1.82186605	4.77102952	2.66975751

O	-1.08255286	3.79657402	1.00736262
C	-1.17896249	2.47531465	0.71128447
O	-0.39623349	1.95127651	-0.08061403
H	-3.94095942	2.89285417	2.08175361
C	-2.63974895	2.49746255	3.76780879
H	-3.01477846	1.47591876	3.90537117
H	-1.56053880	2.47167478	3.96845449
C	-3.37316677	3.43983980	4.69743231
C	-2.69139316	4.43121068	5.41646328
C	-3.37760498	5.31618062	6.25128916
C	-4.76357039	5.22510223	6.38126087
C	-5.45734860	4.23971971	5.67457204
C	-4.76730987	3.35783411	4.84345462
H	-5.31440484	2.58536524	4.30619295
H	-6.53646817	4.15471269	5.77575688
H	-5.29929364	5.91130450	7.03192622
H	-2.82651997	6.07335543	6.80336725
H	-1.60961900	4.49952358	5.33114446
C	-3.71760755	0.04079962	1.42794701
C	-4.14864319	-1.38709536	1.60386975
H	-4.63132556	-1.79871844	0.70403316
H	-3.29221468	-2.02675859	1.83785861
H	-4.87858493	-1.49454538	2.41992640
H	-4.49848015	0.78955815	1.32291987
O	-0.06417969	-1.61150471	4.05153251
C	-0.35849433	-1.35410424	5.43596072
C	-1.80945654	-1.80206356	5.59468066
C	-1.86353497	-3.06051476	4.70238168
C	-0.75828084	-2.81181163	3.64770543
H	-1.14828209	-2.61945738	2.64616691
H	-0.04240536	-3.64219159	3.60222383
H	-2.84556948	-3.20060282	4.24173376
H	-1.64076852	-3.95883302	5.28842905
H	-2.48000656	-1.02631541	5.20889707
H	-2.08197156	-2.00451914	6.63517050
H	0.31557865	-1.94674674	6.07361331
H	-0.17511719	-0.29118086	5.60007221
O	0.54805382	1.47705929	3.77506286
C	1.70731455	2.14897879	3.64692487
H	1.61937003	3.02427221	2.95241784
C	2.26628377	2.76730792	4.98850060
C	1.73605301	4.19987121	5.15650660
H	2.07901873	4.65011944	6.09660316
H	2.05842219	4.85113734	4.33455944
H	0.63912011	4.19565383	5.16713530
H	3.36443961	2.82980889	4.91807767
C	1.90482099	1.93638788	6.22583760
H	2.26090935	0.90494461	6.15812298
H	2.33776823	2.38540440	7.12912533
H	0.81828625	1.90041437	6.34643325
O	-0.59516642	-1.26672011	-1.43722059
C	-1.76108350	-2.08802057	-1.26723147
C	-2.82044825	-1.48867544	-2.21155235
C	-1.98050998	-0.71124312	-3.26494967
C	-0.52495135	-0.97871621	-2.84316906
H	0.15557884	-0.13765058	-2.96916185
H	-0.11323499	-1.85579164	-3.36492148
H	-2.20029802	0.35948587	-3.21759345
H	-2.17119538	-1.04570717	-4.28947829
H	-3.47630533	-0.80944907	-1.66008677
H	-3.44287647	-2.26790900	-2.66249486
H	-1.51092807	-3.12178572	-1.55005169
H	-2.02452144	-2.04862155	-0.21137287

Table 55. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,R*)-**6** from **5** spirocyclic dimer with three THF



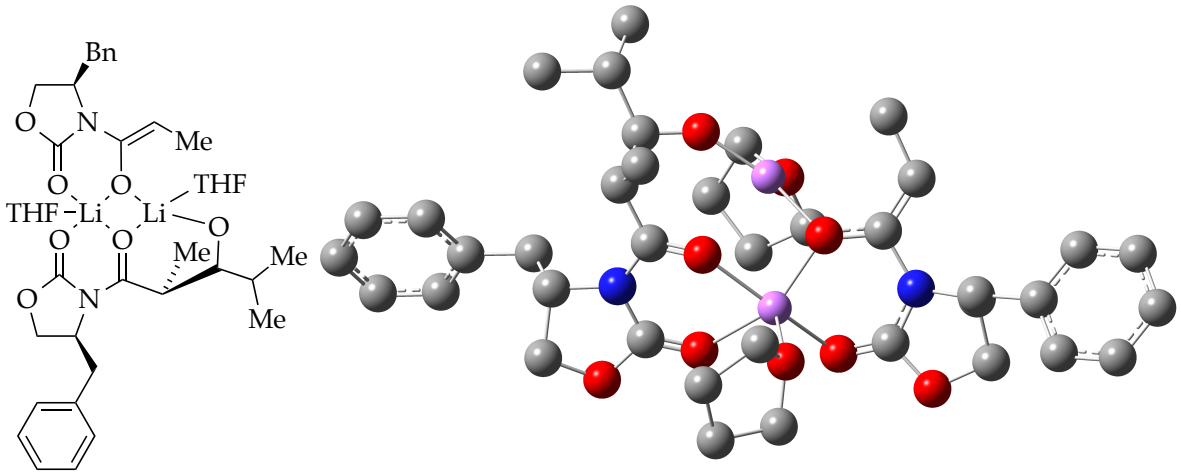


G = -2280.380075 Hartree
G_{MP2} = -1426411.821 kcal/mol
ΔG_{MP2} = -8.031894421 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = 0.911505828kcal/mol vs. **5** spirocyclic dimer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	8.57471154	-1.41607854	-2.39858573
Li	0.00000000	0.00000000	2.67777070	C	7.46748425	-1.44364498	-3.24683352
O	1.43342210	0.00000000	1.48325479	C	6.18668941	-1.22513864	-2.73454407
C	2.64791298	0.44747378	1.41198983	H	5.32714854	-1.25937142	-3.40074660
N	3.04205417	0.99302765	0.11393971	H	7.59784377	-1.63914554	-4.30814257
C	2.16326243	1.48022009	-0.81053694	H	9.57212601	-1.58761095	-2.79451673
O	0.95475157	1.64732066	-0.71851164	H	9.24749018	-1.15759813	-0.36501701
O	2.82716768	1.80095624	-1.96043711	H	6.97545890	-0.78028369	0.53735220
C	4.24108263	1.68668340	-1.72771900	C	3.60228084	0.44146602	2.38319099
H	4.64598941	2.68872823	-1.54366659	H	4.55412977	0.92654428	2.19059545
H	4.70851403	1.26780932	-2.62055526	C	3.41079935	-0.20429668	3.72632644
C	4.36157429	0.78153879	-0.49080137	H	4.32181446	-0.72545019	4.05202006
H	5.15440051	1.14512897	0.16740516	H	3.16546668	0.51616614	4.52599734
C	4.60721987	-0.71210480	-0.81270394	H	2.59928971	-0.93865200	3.69660854
H	4.45940474	-1.26576113	0.12131928	O	-1.31375809	-0.51054153	1.44752633
H	3.83304849	-1.04528101	-1.51354708	C	-2.45963281	-1.08871421	1.24975281
C	5.98769203	-0.97674423	-1.36956363	N	-3.29174638	-0.46321365	0.21751541
C	7.11082096	-0.95664230	-0.52793382	C	-4.73197328	-0.23136833	0.34279117
C	8.39167298	-1.17289281	-1.03513644	C	-5.04943391	0.29024918	-1.07127958

H	-5.41687202	-0.50708066	-1.72753815
H	-5.76084062	1.11819092	-1.08071926
O	-3.79223401	0.76118931	-1.58507089
C	-2.78073447	0.18289660	-0.86922930
O	-1.61859295	0.27546411	-1.23346221
H	-5.26066204	-1.17049086	0.52675954
C	-5.06173796	0.76325078	1.48085599
H	-4.57609118	0.38328143	2.38721336
H	-4.60178427	1.73021395	1.24256013
C	-6.54786887	0.92678913	1.70921712
C	-7.23098325	2.06841101	1.26895404
C	-8.60867121	2.19900158	1.45737997
C	-9.32754809	1.18511281	2.09097858
C	-8.65922344	0.04264339	2.53795008
C	-7.28335118	-0.08295070	2.34894770
H	-6.76811860	-0.97120337	2.70917151
H	-9.20982497	-0.74937093	3.03905521
H	-10.39929755	1.28508749	2.24005564
H	-9.11782155	3.09486496	1.11154819
H	-6.67602407	2.86841942	0.78330870
C	-2.98946471	-2.17524368	1.87029278
C	-2.31799789	-2.92787565	2.98245180
H	-2.87103666	-2.85687796	3.93386986
H	-2.23844997	-4.00115706	2.75496810
H	-1.30743146	-2.55226014	3.16147976
H	-3.94905910	-2.55060534	1.52587678
O	-0.38091108	1.90906192	3.38902528
C	0.71045497	2.85238375	3.27843560
C	0.32335186	3.75771628	2.11378295
C	-1.19542983	3.89522685	2.31451690
C	-1.59638068	2.52020542	2.87751011
H	-1.98842372	1.84490228	2.11289973
H	-2.32319435	2.59547464	3.69563957
H	-1.72530377	4.12805086	1.38629972
H	-1.41753041	4.68873790	3.03801740
H	0.54208054	3.25659472	1.16555931
H	0.84590086	4.71938412	2.13562645
H	0.79478077	3.41821892	4.21904901
H	1.62705697	2.28076283	3.11491639
O	0.06785062	-0.91077068	4.50138221
C	-0.27270152	-0.39974657	5.55538848
H	-0.59581556	0.66049527	5.56213817
C	-0.29732284	-1.11635575	6.88082492
H	0.09328503	-2.12639008	6.71367692
C	-1.75698985	-1.20115106	7.37173888
H	-1.79547439	-1.70309041	8.34452706
H	-2.19419464	-0.20242943	7.49327889
H	-2.38132910	-1.76555805	6.67098302
C	0.59720929	-0.36811488	7.88727638
H	0.56658980	-0.86926438	8.86072210
H	1.63978766	-0.33833688	7.55304029
H	0.25525698	0.66411529	8.03218942
O	0.87981246	-1.55151290	-1.12096626
C	1.17745312	-2.73754610	-0.36776027
C	-0.04979291	-3.64012253	-0.56043661
C	-0.59140851	-3.22290614	-1.95619567
C	0.27345139	-2.00303859	-2.34273855
H	-0.29143559	-1.16440550	-2.74981655
H	1.06690664	-2.28887779	-3.04973059
H	-1.64819959	-2.94837347	-1.89354124
H	-0.49917882	-4.02372309	-2.69705457
H	-0.79435323	-3.42963700	0.21244063
H	0.20989535	-4.70222390	-0.50589915
H	2.08713053	-3.20609776	-0.77633511
H	1.36416824	-2.42210339	0.65943762

Table 56. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,R*)-**6** from **5** spirocyclic dimer with three THF

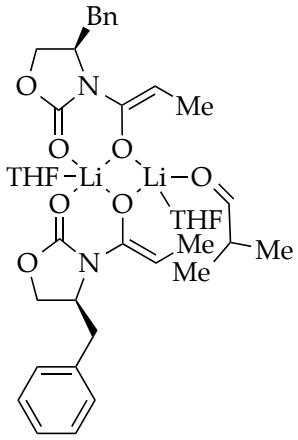


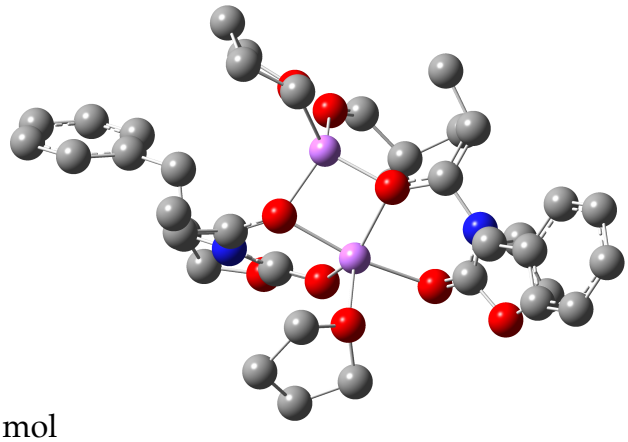
G = -2280.371513 Hartree
G_{MP2} = -1426412.222 kcal/mol
ΔG_{MP2} = 0.510486238 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -8.432914011 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	8.03483529	-1.01023867	-2.28777201
Li	0.00000000	0.00000000	2.96762440	C	6.67187330	-0.89366722	-2.00556545
O	1.20973113	0.00000000	1.49941207	H	5.94688027	-0.96515594	-2.81384211
C	2.42591324	0.45567154	1.56728997	H	8.36242206	-1.16370398	-3.31281378
N	2.95114065	1.03146497	0.33034103	H	10.03258684	-1.02652570	-1.47349051
C	2.18300772	1.48581955	-0.69969144	H	9.25807361	-0.69587774	0.86814772
O	0.96295004	1.57812013	-0.78278577	H	6.84187974	-0.49960145	1.36195972
O	2.97758118	1.86720323	-1.74340134	C	3.25901520	0.41389992	2.63916484
C	4.35005495	1.84629852	-1.31097091	H	4.22726553	0.90058604	2.58701850
H	4.65020003	2.86992607	-1.05923922	C	2.87677443	-0.24460575	3.93632443
H	4.96792095	1.48083652	-2.13306717	H	3.75369690	-0.67793418	4.43468491
C	4.35531506	0.92431033	-0.08156261	H	2.41566116	0.44866699	4.65771734
H	5.01623694	1.32645185	0.68961552	H	2.16258255	-1.06235663	3.77308986
C	4.74934354	-0.54127648	-0.38175175	O	-1.20723707	-1.33690435	1.03812898
H	4.47686041	-1.12863177	0.50200307	C	-2.37199751	-1.42647458	1.41313758
H	4.13614871	-0.90202322	-1.21645584	N	-3.36377003	-0.67268032	0.73143150
C	6.22040936	-0.70135089	-0.69288611	C	-4.83263329	-0.80353756	0.82010011
C	7.17426515	-0.63284720	0.33444032	C	-5.21477623	-0.38473223	-0.60799431
C	8.53607288	-0.74711183	0.05720095	H	-5.25193669	-1.23461777	-1.29823021
C	8.97165246	-0.93461848	-1.25690402	H	-6.15067312	0.17142994	-0.66055583

O	-4.14497466	0.49126296	-1.02069658
C	-3.03028200	0.20819678	-0.30387887
O	-1.95117007	0.68988913	-0.57092919
H	-5.10533914	-1.84415259	1.00661277
C	-5.45324970	0.11195407	1.89980680
H	-4.97129535	-0.11344369	2.85669655
H	-5.20297932	1.15181709	1.65582913
C	-6.95417303	-0.05675616	2.01028935
C	-7.83257585	0.90437105	1.49233410
C	-9.21587571	0.73228657	1.57858063
C	-9.74209779	-0.40816019	2.18561518
C	-8.87777076	-1.37172448	2.71071128
C	-7.49702974	-1.19598501	2.62398811
H	-6.83243304	-1.94433681	3.05093260
H	-9.27914528	-2.25775912	3.19528658
H	-10.81790689	-0.54299214	2.25616562
H	-9.87994491	1.49227435	1.17560536
H	-7.43019002	1.80355468	1.03038940
C	-2.75667148	-2.25762889	2.59096415
C	-1.90746174	-3.53596289	2.62649127
H	-2.28519119	-4.22340596	3.38874466
H	-1.92000699	-4.06211104	1.66469585
H	-0.87313665	-3.28049949	2.86733602
H	-3.82210362	-2.50328019	2.56336192
O	-0.16129050	1.96544110	3.42139786
C	-1.19246989	2.34715024	4.34581257
C	-2.20778241	3.16585440	3.51798852
C	-1.41765676	3.56528233	2.23992897
C	0.00951334	3.07238541	2.52652170
H	0.61080690	3.85013807	3.02166894
H	0.54021936	2.70700218	1.64737377
H	-1.44636547	4.64127002	2.04163182
H	-1.81645710	3.05400927	1.35849249
H	-2.56343914	4.03736537	4.07682906
H	-3.08338533	2.56046070	3.26359285
H	-1.58196003	1.41869794	4.76457391
H	-0.74807400	2.96094187	5.14348897
O	-1.24412064	-0.83913395	3.93517454
C	-2.48384286	-1.33581565	3.92068862
H	-3.27470338	-0.54092854	3.85802550
C	-2.83876306	-2.15012373	5.20887025
H	-2.11819965	-2.97586145	5.27686564
C	-4.26243058	-2.72623044	5.21802099
H	-4.49172027	-3.18599888	6.18716846
H	-5.00818667	-1.93484893	5.05474608
H	-4.41496356	-3.49710965	4.45298301
C	-2.62162332	-1.24931106	6.43303198
H	-2.78731313	-1.80256332	7.36608327
H	-1.60422218	-0.85207352	6.43218203
H	-3.32060872	-0.40041889	6.42285747
O	0.53910034	-1.23857506	-1.55634005
C	0.37346967	-2.66020649	-1.47350483
C	-0.87441010	-2.97751235	-2.32176913
C	-0.99954952	-1.75412491	-3.27415925
C	0.21004324	-0.87598481	-2.90565145
H	0.01656238	0.19714634	-2.91444506
H	1.07100766	-1.09191246	-3.55605717
H	-1.93153522	-1.21169317	-3.09077217
H	-0.98396061	-2.03971915	-4.33045468
H	-1.75925542	-3.06584103	-1.68413718
H	-0.76208167	-3.92202513	-2.86293368
H	1.26772385	-3.15132903	-1.88542710
H	0.27676467	-2.91357128	-0.41716108

Table 57. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,R*)-**6** from **5** spirocyclic dimer with three THF



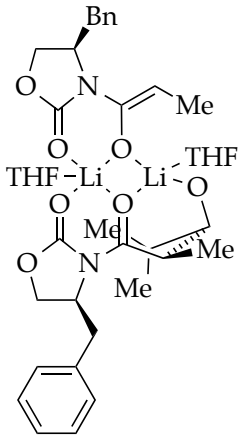


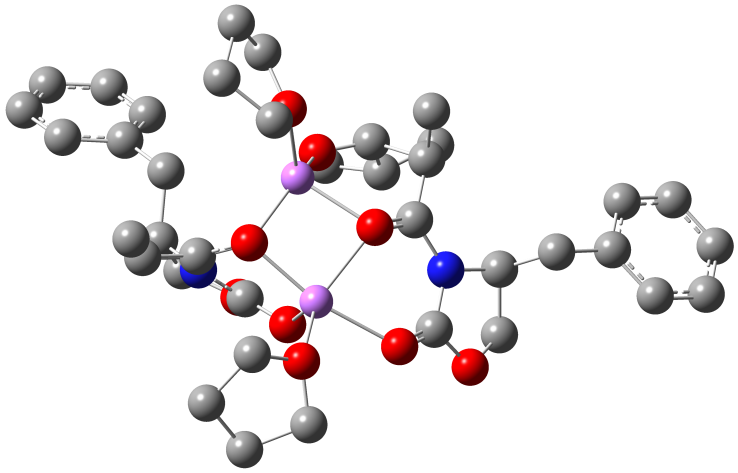
G = -2280.380525 Hartree
G_{MP2} = -1426413.372 kcal/mol
ΔG_{MP2} = -0.639321011 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -5.642332213 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.41153682	-0.91813345	-1.98686886
O	0.00000000	0.00000000	2.01174800	H	7.16578252	0.14186747	-1.97365115
Li	1.86084650	0.00000000	1.87282299	H	9.36224538	-0.59747643	-2.83741000
O	1.93011052	0.70440738	0.13427013	H	9.95056313	-3.01537690	-2.85155079
C	2.79511431	0.77254727	-0.82737329	H	8.31738796	-4.68284440	-1.98953440
N	2.90597569	-0.43471908	-1.65145860	H	6.12022850	-3.93865202	-1.12878895
C	4.17217886	-0.97368755	-2.15596898	C	3.61306254	1.80999716	-1.15167085
C	3.65274258	-2.14983180	-3.00203070	C	3.66191774	3.09159056	-0.37006261
H	3.54190250	-1.87830078	-4.05797822	H	3.33971563	3.95958824	-0.96568313
H	4.27021357	-3.04651515	-2.92442535	H	3.00251962	3.02732370	0.50089296
O	2.34975406	-2.44158342	-2.46789080	H	4.67633475	3.32623873	-0.01100985
C	1.89699308	-1.34110215	-1.78715340	H	4.24458929	1.73213292	-2.03184845
O	0.73778813	-1.28038256	-1.40577723	O	2.99177472	1.00539213	3.18123235
H	4.67516475	-0.24286961	-2.79512131	C	4.43216484	0.93579620	3.13286184
C	5.12441498	-1.38602998	-1.00853119	C	4.91535469	2.07602833	4.02751771
H	5.23340580	-0.51332667	-0.35496813	C	3.85083481	3.15245508	3.75952398
H	4.64068415	-2.17326583	-0.41800795	C	2.56866008	2.32329004	3.60858094
C	6.47742270	-1.84697520	-1.50265108	H	1.87681077	2.72386422	2.86194816
C	6.82529656	-3.20443738	-1.51313803	H	2.03400781	2.21107531	4.55866441
C	8.06680104	-3.62519630	-1.99501432	H	4.07623111	3.68071145	2.82661736
C	8.98336860	-2.69071708	-2.47743264	H	3.77276691	3.89413143	4.56005228
C	8.65164708	-1.33367627	-2.47055892	H	5.93066325	2.40193480	3.78198134

H	4.89824622	1.76809742	5.07972231
H	4.72818288	-0.05958395	3.47304248
H	4.76397854	1.07164184	2.09458208
O	2.65196940	-1.88371427	2.10484877
C	2.21540201	-3.02296519	2.04131448
H	2.85910037	-3.85593685	2.40168291
C	0.87010120	-3.44832282	1.52252570
H	0.35422290	-2.57207716	1.12224465
C	1.06698500	-4.49647952	0.40934280
H	0.08817076	-4.83544109	0.05536551
H	1.60156444	-4.08097321	-0.45021399
H	1.61496389	-5.37406649	0.77743208
C	0.05490419	-4.02592811	2.70021309
H	-0.17567577	-3.24979444	3.43640375
H	-0.89231211	-4.42422605	2.32101668
H	0.58826325	-4.84724001	3.19687128
C	-0.97451728	-0.26976344	2.82435745
N	-2.30882795	-0.24423022	2.22064928
C	-2.55571346	-0.59095491	0.92684116
O	-1.79144910	-1.06672668	0.09927557
O	-3.86292573	-0.33173154	0.61627760
C	-4.55836226	0.03888024	1.81982363
H	-5.11080975	-0.83452504	2.18525975
H	-5.26359266	0.83742463	1.58235875
C	-3.45076031	0.46788478	2.79817635
H	-3.66815321	0.10121432	3.80477245
C	-3.20045787	1.99388776	2.85700402
H	-2.25748117	2.14065316	3.39615941
H	-3.05032233	2.36176369	1.83493276
C	-4.31910255	2.74884628	3.53935130
C	-4.45550935	2.70788131	4.93562946
C	-5.50054761	3.37474238	5.57422285
C	-6.43176721	4.09913230	4.82605379
C	-6.30656801	4.15253303	3.43760609
C	-5.25874601	3.48237267	2.80232764
H	-5.16083718	3.53845948	1.72016665
H	-7.02153789	4.71926227	2.84666759
H	-7.24498821	4.62151315	5.32283341
H	-5.58556244	3.33385849	6.65716680
H	-3.72779045	2.15434699	5.52573492
C	-0.93857102	-0.54116212	4.15672810
H	-1.87127342	-0.79886030	4.65109291
C	0.30003752	-0.52849787	5.00609064
H	0.20886690	0.16608925	5.85611573
H	0.51480921	-1.51632708	5.44394381
H	1.18203492	-0.23124243	4.43211844
O	-0.98452108	1.56327495	-0.93496688
C	-0.30283257	2.80856424	-1.15569883
C	0.08236845	2.82699627	-2.65340650
C	-0.75373192	1.67282774	-3.26983989
C	-1.71476214	1.28374611	-2.13987291
H	-1.99227850	0.22991611	-2.11131699
H	-2.62781158	1.89927216	-2.16073364
H	-0.11179074	0.82151780	-3.51510149
H	-1.28461430	1.96948605	-4.18005483
H	1.15361457	2.64945494	-2.77914926
H	-0.15494628	3.79450304	-3.10795625
H	-0.98389098	3.63681809	-0.90900735
H	0.55161358	2.82429716	-0.47889121

Table 58. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,R*)-**6** from **5** spirocyclic dimer with three THF



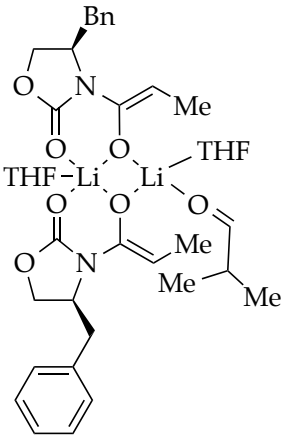


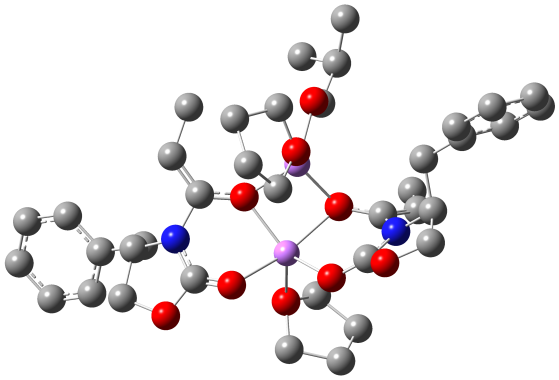
G = -2280.373456 Hartree
G_{MP2} = -1426416.164 kcal/mol
ΔG_{MP2} = -3.430739718 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -8.43375092 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	8.30462489	-4.49805993	0.79706434
O	0.00000000	0.00000000	2.12543790	C	8.23185188	-3.43527426	-0.10671542
Li	2.04916736	0.00000000	1.95416917	C	7.08012183	-2.65176509	-0.17413266
O	1.93739436	0.47147093	0.07311467	H	7.03698831	-1.81821735	-0.87273325
C	2.73677792	-0.07505910	-0.80157827	H	9.07534168	-3.21330547	-0.75578698
N	2.71034875	-1.53844209	-0.83383772	H	9.20232062	-5.10827772	0.85270085
C	3.90860545	-2.37856997	-0.72540648	H	7.26869084	-5.58456916	2.34489370
C	3.26780313	-3.78303269	-0.77488994	H	5.22994717	-4.18371214	2.22297533
H	3.35620267	-4.24250304	-1.76520058	C	3.61083254	0.52481362	-1.64939093
H	3.66941030	-4.46577435	-0.02445862	C	3.88988116	2.00019573	-1.67801056
O	1.86822071	-3.57937205	-0.49949701	H	3.56347065	2.47576954	-2.61595605
C	1.57789243	-2.25719013	-0.61729536	H	3.37629230	2.50950449	-0.85696016
O	0.41872433	-1.85621195	-0.55084236	H	4.96506984	2.21536033	-1.58389109
H	4.55238472	-2.23222337	-1.59846329	H	4.15721608	-0.10170485	-2.34965125
C	4.72134161	-2.07434229	0.55520701	O	2.97610434	1.55778127	2.84400869
H	4.98662750	-1.01061076	0.51055421	C	4.23505609	1.37006537	3.53217122
H	4.07600886	-2.20838276	1.43219042	C	4.93493389	2.73466568	3.50653736
C	5.97763196	-2.91190271	0.65530155	C	4.34630212	3.38499071	2.24356885
C	6.06728177	-3.97859022	1.56063511	C	2.90325690	2.88368123	2.28039468
C	7.21939555	-4.76513782	1.63215223	H	2.43113135	2.79084455	1.30017259

H	2.27684002	3.51393571	2.92777268
H	4.85271565	3.01230821	1.34583365
H	4.41381548	4.47731626	2.24717435
H	6.02476587	2.64117614	3.47894567
H	4.66889289	3.32107835	4.39417630
H	4.02667700	1.00251683	4.54120196
H	4.80733507	0.60353716	2.99760599
O	2.24516378	-1.55450362	2.88133053
C	1.50553416	-2.06327369	3.87802306
H	2.02408192	-2.02705485	4.86965276
C	1.09075138	-3.56341502	3.68198741
H	0.29514253	-3.60735540	2.92076821
C	2.27661815	-4.36834857	3.13721512
H	2.00575204	-5.42297589	2.99876294
H	2.59735164	-3.95808657	2.17966305
H	3.12535947	-4.32618689	3.83347711
C	0.58934687	-4.22079442	4.97952156
H	-0.28527050	-3.72339974	5.41793070
H	0.31354410	-5.26909533	4.81069869
H	1.37841149	-4.20889813	5.74274263
C	-0.49355754	-0.81702567	2.90949540
N	-1.65462504	-1.51549992	2.53336384
C	-2.29531710	-1.33437344	1.29650191
O	-2.02165618	-0.55892178	0.41145994
O	-3.35045934	-2.17822798	1.22297959
C	-3.30107575	-3.10764674	2.32419269
H	-2.80792792	-4.02290658	1.98161394
H	-4.32335327	-3.32904200	2.63144024
C	-2.48483693	-2.37782282	3.39780855
H	-1.86176546	-3.08273977	3.94721560
C	-3.35390156	-1.54263528	4.36935923
H	-2.68757742	-0.90155622	4.95809694
H	-3.99134752	-0.87613390	3.77571338
C	-4.20157349	-2.39893580	5.28653783
C	-3.62005939	-3.07802871	6.36764982
C	-4.39024270	-3.88866612	7.20082828
C	-5.76000163	-4.03258695	6.96830082
C	-6.35247407	-3.35832430	5.90040699
C	-5.57753635	-2.54858800	5.06730719
H	-6.04928666	-2.01621147	4.24398420
H	-7.41884601	-3.45718441	5.71607299
H	-6.36115273	-4.66181733	7.61882723
H	-3.92162070	-4.40408277	8.03485447
H	-2.55622716	-2.96364913	6.56562315
C	0.17245388	-1.15038074	4.20359120
H	-0.48930293	-1.72834891	4.85077631
C	0.59705122	0.12453838	4.95041563
H	-0.25976761	0.77197342	5.17692348
H	1.06682453	-0.15789134	5.89914028
H	1.31820272	0.70235251	4.36854169
O	-0.71934975	1.26001359	-1.42847220
C	0.12650176	2.19992570	-2.10785578
C	0.32806150	1.62467026	-3.52410531
C	-0.86646115	0.64489453	-3.70024175
C	-1.67629215	0.82055794	-2.40481260
H	-2.13720689	-0.08974270	-2.02292344
H	-2.45047839	1.59469551	-2.51980636
H	-0.50925339	-0.38567862	-3.78586231
H	-1.46889170	0.86484426	-4.58727410
H	1.28079164	1.09199671	-3.58280782
H	0.33483182	2.41648236	-4.27992069
H	-0.38162424	3.17580179	-2.14103448
H	1.04154869	2.28171686	-1.52299185

Table 59. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,S*)-**6** from **5** spirocyclic dimer with three THF



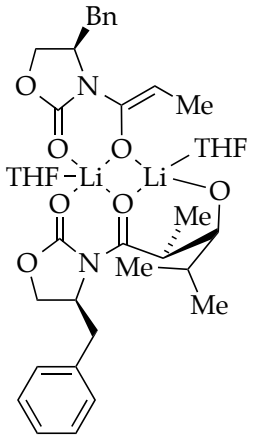


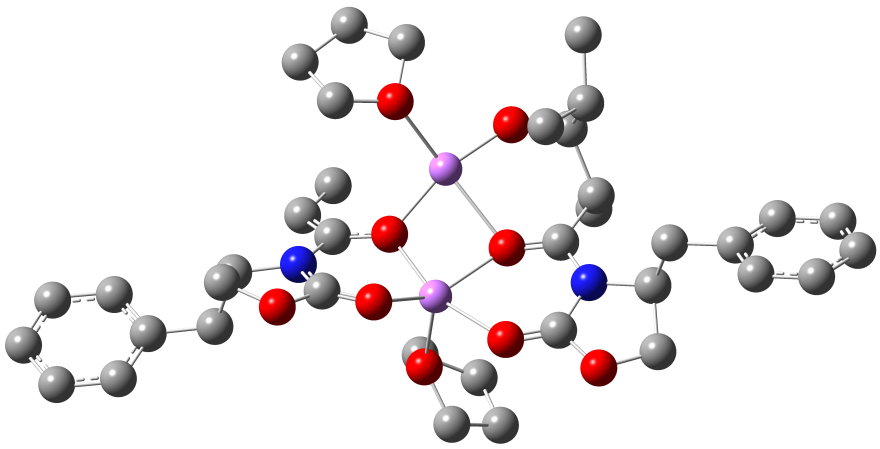
G = -2280.378761 Hartree
G_{MP2} = -1426412.247 kcal/mol
ΔG_{MP2} = 0.485882721kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -11.50745307 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.49005228	-2.53653890	-2.65036249
Li	0.00000000	0.00000000	2.60954310	C	6.20917028	-2.13897652	-2.26053025
O	1.45537568	0.00000000	1.42937248	H	5.38203964	-2.22387242	-2.96232018
C	2.66906501	0.45379665	1.36482268	H	7.65356497	-2.92087982	-3.65391026
N	3.14800567	0.76754215	0.01717431	H	9.55177964	-2.75550413	-2.05351468
C	2.33358053	1.15916615	-1.00311621	H	9.14985943	-1.89097677	0.24501075
O	1.14145759	1.42998191	-0.97681488	H	6.87654014	-1.19658676	0.93169019
O	3.04539115	1.22653210	-2.16900711	C	3.57305204	0.63447170	2.36616484
C	4.44038843	1.04497124	-1.86946410	H	4.52933759	1.08795744	2.12198743
H	4.92097623	2.02972183	-1.83962620	C	3.35553471	0.23021869	3.79551826
H	4.89169277	0.44757380	-2.66379941	H	4.17861002	-0.39787516	4.16966220
C	4.45877439	0.35515929	-0.49468979	H	3.29309953	1.08992426	4.48202348
H	5.26285693	0.76185717	0.12364363	H	2.42985775	-0.34077225	3.90782730
C	4.58949926	-1.18542163	-0.55143685	O	-1.12710122	-0.97971025	1.43883156
H	4.34994845	-1.56123532	0.44978792	C	-2.41396201	-1.14356814	1.37144551
H	3.82669625	-1.57531494	-1.23602042	N	-3.18480806	0.07480076	1.10715401
C	5.96756473	-1.64544342	-0.97128929	C	-4.32473702	0.51983960	1.91273258
C	7.04733338	-1.56391429	-0.07831598	C	-4.71185160	1.79998468	1.14694074
C	8.32820361	-1.95817493	-0.46355172	H	-5.51592418	1.61693921	0.42528739
C	8.55451175	-2.44522596	-1.75325031	H	-4.99594970	2.62781456	1.79900126

O	-3.52651918	2.17462942	0.42103735	H	2.03852771	3.04677352	3.72140760
C	-2.70604676	1.08346409	0.32888856	H	-0.41374675	4.82858982	3.25797602
O	-1.70758930	1.10121043	-0.37649414	H	1.01519742	4.69477661	2.22028647
H	-5.13830029	-0.20998284	1.86546650	H	0.33012893	2.54180537	1.37428184
C	-3.93318944	0.74450863	3.39275753	H	-1.28676627	3.15762460	1.77871135
H	-3.51242093	-0.20014877	3.75668043	O	0.01109994	-1.08693099	4.34451246
H	-3.12878378	1.48763747	3.43587433	C	0.12061393	-2.29071519	4.16286438
C	-5.10338199	1.16442069	4.25368569	C	0.06585612	-3.33082964	5.25349969
C	-5.25461399	2.49250859	4.67551573	H	-0.77696465	-3.98447257	4.97105747
C	-6.35185455	2.88237245	5.44654639	C	1.34808253	-4.18938918	5.18779111
C	-7.32041322	1.94603908	5.80909753	H	1.27362851	-5.02935442	5.88566771
C	-7.18151584	0.61779099	5.39932441	H	1.51202851	-4.59778766	4.18414052
C	-6.08337857	0.23306691	4.63055319	H	2.22824928	-3.59701938	5.46256647
H	-5.97719020	-0.80606856	4.32521155	C	-0.18504337	-2.73409127	6.63888879
H	-7.92706713	-0.12048070	5.68345622	H	-1.10261884	-2.13845100	6.65551238
H	-8.17433205	2.24653947	6.41029697	H	-0.27593531	-3.53075126	7.38482342
H	-6.44648633	3.91698270	5.76621338	H	0.64099223	-2.07980930	6.93737815
H	-4.49788400	3.22631940	4.40592745	H	0.27359327	-2.66868532	3.13571275
C	-3.13785065	-2.28267854	1.52792739	O	0.20306530	-1.32174446	-1.55466914
C	-2.54398697	-3.61758088	1.87541393	C	-0.33402652	-2.64759281	-1.41687450
H	-2.82952691	-3.96302407	2.88312433	C	-1.67718596	-2.64847602	-2.18299175
H	-2.86923691	-4.40456836	1.17992478	C	-1.62758890	-1.34654106	-3.02798257
H	-1.45111463	-3.57653842	1.83516282	C	-0.18113480	-0.86596263	-2.86304913
H	-4.21388529	-2.23477330	1.38407009	H	-0.05189442	0.21630755	-2.87714564
O	-0.42583441	1.89319656	3.19218118	H	0.48384949	-1.32300569	-3.61258854
C	-0.29348631	2.93797959	2.17908861	H	-2.30828892	-0.59635529	-2.61652088
C	0.35177782	4.13635845	2.88692196	H	-1.89155989	-1.50962390	-4.07774710
C	1.09007926	3.47676513	4.06192831	H	-2.51953226	-2.63392439	-1.48649439
C	0.11981146	2.36164472	4.44394005	H	-1.77101886	-3.54244463	-2.80826208
H	-0.69717329	2.73849699	5.07673792	H	0.37543791	-3.36641447	-1.85325461
H	0.58635792	1.51021959	4.94488452	H	-0.43383873	-2.83855203	-0.34795568
H	1.29141282	4.16330149	4.89039793				

Table 60. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,S*)-**6** from **5** spirocyclic dimer with three THF



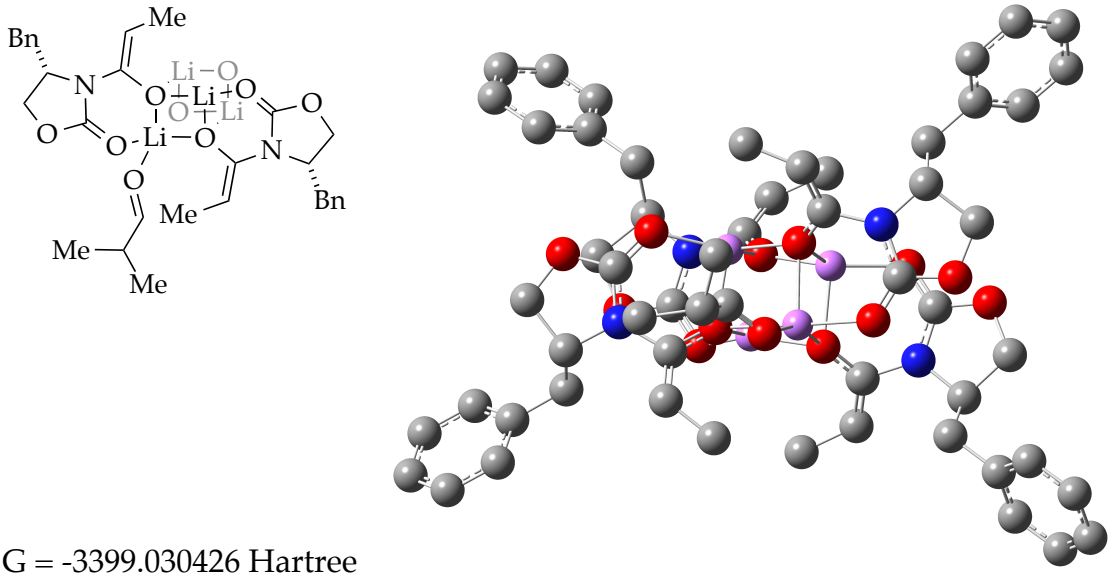


G = -2280.362701 Hartree
G_{MP2} = -1426406.197 kcal/mol
ΔG_{MP2} = 6.535766459 kcal/mol vs. **5** spirocyclic dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -5.45756933 kcal/mol vs. **5** spirocyclic dimer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	6.68537602	2.15266926	-2.24043963
Li	0.00000000	0.00000000	2.96561520	H	5.93943843	2.25555128	-3.02579189
O	1.26203026	0.00000000	1.49991689	H	8.23547178	3.09774374	-3.39890771
C	2.51250755	0.33479227	1.40466470	H	9.96039343	2.84998366	-1.62234087
N	2.78775689	1.42031407	0.46463906	H	9.36196642	1.74630647	0.52617949
C	1.86313844	2.01509641	-0.35585789	H	7.06799923	0.90509554	0.89461201
O	0.69655114	1.72374661	-0.57781443	C	3.55970929	-0.20497761	2.08822361
O	2.43625980	3.07539561	-0.99913286	H	4.56733579	0.15869360	1.92375619
C	3.73957365	3.30760483	-0.43754081	C	3.39429724	-1.31953041	3.08357651
H	3.66167537	4.09948033	0.31693538	H	4.00862479	-2.19623296	2.82749848
H	4.40827488	3.63095630	-1.23679279	H	3.69044953	-1.02352974	4.10175418
C	4.12348556	1.95741681	0.17918341	H	2.35194026	-1.64969133	3.13139916
H	4.67819270	2.09481086	1.11060465	O	-1.28395383	-0.83397377	1.30898904
C	4.92012612	1.04609730	-0.78900116	C	-2.46799626	-1.12361295	1.47266621
H	4.92797690	0.03739791	-0.36356699	N	-3.37954724	-0.86048318	0.42368382
H	4.36819764	0.99178101	-1.73547437	C	-4.82260960	-1.17142517	0.38190127
C	6.33125414	1.53338858	-1.03400383	C	-5.02623017	-1.27733618	-1.13753978
C	7.31681145	1.39572930	-0.04433345	H	-4.89961360	-2.30143606	-1.50541717
C	8.61283384	1.86681223	-0.25211974	H	-5.98659931	-0.88516276	-1.47224687
C	8.94999251	2.48512760	-1.45857542	O	-3.98161335	-0.45962038	-1.70110070
C	7.98234249	2.62470454	-2.45361572	C	-2.96391057	-0.34374478	-0.81353253

O	-1.89316465	0.13088624	-1.11572001
H	-5.01313503	-2.13182765	0.86449300
C	-5.68452222	-0.06663718	1.03419702
H	-5.34116634	0.07601246	2.06341259
H	-5.49775746	0.87527421	0.50446030
C	-7.16218120	-0.39824651	1.01514356
C	-8.03708607	0.24301224	0.12812404
C	-9.39513645	-0.08169253	0.09986446
C	-9.89921615	-1.05623294	0.96123869
C	-9.03909835	-1.69955232	1.85438507
C	-7.68398432	-1.37155013	1.88061523
H	-7.02573796	-1.86741605	2.59141544
H	-9.42519069	-2.45223843	2.53655500
H	-10.95585004	-1.30859985	0.94301982
H	-10.05784278	0.43176950	-0.59157421
H	-7.65463015	1.01497848	-0.53639120
C	-2.93651548	-1.79356644	2.72287000
C	-2.24536093	-3.16847143	2.82917736
H	-2.65319418	-3.71068824	3.68911902
H	-2.39073080	-3.78780748	1.93457299
H	-1.17594131	-3.01776856	2.99376505
H	-4.02227614	-1.93162775	2.71931953
O	0.59129319	1.66263175	4.09993512
C	1.61136643	2.64464034	3.89265818
C	2.71464666	2.32404329	4.92348108
C	1.98057472	1.46044752	5.98852114
C	0.51545013	1.47805234	5.52395727
H	-0.02729687	2.32848004	5.96653742
H	-0.05032661	0.55980648	5.68299915
H	2.09166302	1.85463101	7.00368374
H	2.36705229	0.43661417	5.98445679
H	3.14240658	3.23817800	5.34790248
H	3.52238971	1.75829600	4.45180652
H	1.93455243	2.56989268	2.85405344
H	1.18590802	3.64543627	4.06564173
O	-1.23091125	-0.66355356	4.13111132
C	-2.53662019	-0.95278949	4.06309209
C	-3.48398678	0.27621100	4.27936146
H	-4.51318017	-0.04268652	4.03806535
C	-3.47367828	0.67058191	5.76439320
H	-4.14904190	1.51299505	5.96030592
H	-3.78587064	-0.16720384	6.40007051
H	-2.46410450	0.96366106	6.06998599
C	-3.11700238	1.49022595	3.41552849
H	-3.16131089	1.27984043	2.34008533
H	-3.79740330	2.32928623	3.60907917
H	-2.09747327	1.81618480	3.64326354
H	-2.85981518	-1.69300389	4.83758613
O	0.82443284	-1.43630727	-1.20975516
C	1.48609452	-2.55273538	-0.59422176
C	0.54893830	-3.75132063	-0.83057166
C	-0.27115640	-3.33814045	-2.08616783
C	0.26640173	-1.93477810	-2.43116231
H	-0.49448505	-1.22423343	-2.75628946
H	1.05819052	-1.99158701	-3.19315840
H	-1.33997277	-3.29497857	-1.85302673
H	-0.14511604	-4.03400522	-2.92135529
H	-0.10867371	-3.89734032	0.03144551
H	1.10975035	-4.67882525	-0.98112645
H	2.45893440	-2.70677162	-1.08456388
H	1.64672583	-2.29036875	0.45132620

Table 61. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,S*)-**6** from **5** D_{2d} tetramer

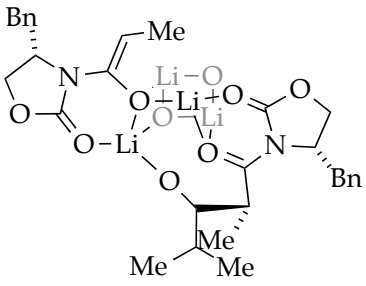


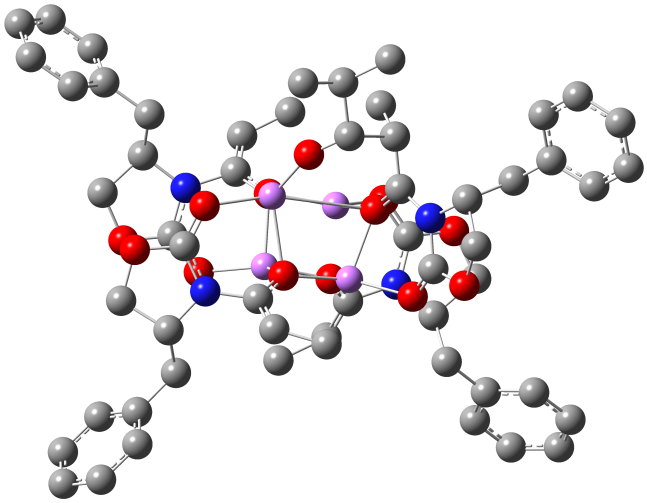
G = -3399.030426 Hartree
G_{MP2} = -2126262.914 kcal/mol
ΔG_{MP2} = -10.11563257 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -12.45772222 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-6.42317781	1.75048119	3.39115978
Li	0.00000000	0.00000000	2.71116570	H	-7.40950294	1.48140751	3.01036585
O	2.03422653	0.00000000	2.80836724	H	-6.53246339	2.51385160	4.16878656
C	2.71044244	0.71352022	2.07931518	C	-5.60534045	0.53632735	3.87114622
O	4.02638500	0.44280611	1.85833045	N	-4.28418011	0.85513112	3.30235110
C	4.53849157	1.33496012	0.84618632	C	-3.08234665	0.06029263	3.56048156
H	4.68770970	0.75258447	-0.06686070	O	-2.19734169	0.05318511	2.59827184
H	5.49642144	1.72817498	1.19097482	Li	-2.12202585	-1.15421291	1.04382305
C	3.45952512	2.42709255	0.66403950	O	-3.86648352	-1.69359070	0.37444609
N	2.33570996	1.82743275	1.39251214	C	-4.51280242	-0.86643899	-0.26355487
C	0.99340287	2.38078770	1.45644265	O	-5.87166623	-0.83097334	-0.18918592
C	0.87335236	3.72188844	1.58839266	C	-6.35209206	0.33493195	-0.89283179
H	1.78082923	4.30210313	1.73289566	H	-6.64433385	1.08360936	-0.14957436
C	-0.42321658	4.47923931	1.54131276	H	-7.22414010	0.04514503	-1.48042631
H	-0.75710077	4.81327935	2.53636477	C	-5.16413604	0.82050788	-1.74872167
H	-0.33169932	5.38460881	0.92625136	N	-4.06047326	0.10181400	-1.10014828
H	-1.23535383	3.88024991	1.11771127	C	-2.64972525	0.28267756	-1.40108250
O	0.03496402	1.48706903	1.33985988	C	-2.28965612	0.47579531	-2.68788486
Li	-1.88917120	1.42156733	1.24531406	H	-3.05176949	0.38663318	-3.45701763
O	-3.50228799	2.36676551	1.68583753	C	-0.88325517	0.77940446	-3.12406709
C	-4.37329194	1.86015846	2.39093476	H	-0.30449149	-0.12585271	-3.35840221
O	-5.65501130	2.31797847	2.31161104	H	-0.87764102	1.40655348	-4.02410752

H	-0.33013703	1.31839912	-2.34545362
O	-1.87277173	0.27328790	-0.34017831
C	-4.98416121	2.35035495	-1.73712304
H	-4.77739641	2.66358552	-0.70793416
H	-4.09509439	2.58913422	-2.33028474
C	-6.19884660	3.07551632	-2.27697454
C	-6.49136943	3.07108154	-3.64936113
C	-7.62390545	3.71867801	-4.14268901
C	-8.48512125	4.38801931	-3.27010575
C	-8.20282742	4.40583910	-1.90378612
C	-7.06944728	3.75432254	-1.41274731
H	-6.84752167	3.78032107	-0.34802353
H	-8.86190930	4.93172853	-1.21770385
H	-9.36532056	4.89669298	-3.65414008
H	-7.83055015	3.70692001	-5.20978902
H	-5.81872847	2.56563532	-4.33953691
H	-5.27485499	0.47440301	-2.78556850
O	-0.23214192	-1.50241524	1.26239451
C	0.38834639	-2.63366627	1.00735981
N	1.78321797	-2.49313557	0.61359759
C	2.22073050	-1.56382065	-0.26813379
O	1.57876020	-0.68512749	-0.84645842
O	3.55431671	-1.69116088	-0.48246502
C	4.09243798	-2.67143384	0.43155181
H	4.67313499	-2.13673527	1.18748002
H	4.74646677	-3.33898506	-0.13155209
C	2.86715667	-3.38577477	1.04506650
H	2.73425189	-4.37522200	0.58829493
C	2.94990683	-3.53819191	2.57610135
C	4.10932394	-4.41494404	2.99994065
C	5.26234618	-3.85854637	3.57057085
C	6.34228205	-4.66440150	3.93741030
C	6.28653870	-6.04411262	3.73800224
C	5.14190248	-6.61299697	3.17449835
C	4.06474784	-5.80495478	2.81134832
H	3.17172233	-6.25836514	2.38587268
H	5.08545099	-7.68805102	3.02384488
H	7.12501409	-6.67317641	4.02487188
H	7.22487862	-4.21301040	4.38334617
H	5.30701119	-2.78496326	3.73925355
H	2.00067436	-3.96270998	2.92001624
H	3.03468924	-2.53795890	3.01416030
C	-0.11434279	-3.88555312	1.09900006
C	-1.50431398	-4.19690725	1.58122756
H	-2.23425034	-4.27824786	0.76218607
H	-1.52893784	-5.14980224	2.12481532
H	-1.87447933	-3.42536581	2.26699922
H	0.50808021	-4.71879935	0.78586002
C	-3.01802360	-0.60981181	4.73858536
H	-3.80925956	-0.47444305	5.46875047
C	-1.91810024	-1.57179741	5.08965689
H	-2.32160631	-2.46843116	5.57836235
H	-1.37751196	-1.89826575	4.19538314
H	-1.17459731	-1.13828679	5.77373482
C	-6.15034555	-0.82892240	3.39368187
H	-6.25047066	-0.81492542	2.30336579
H	-5.39633719	-1.58568089	3.63371681
C	-7.47271181	-1.17071861	4.04581832
C	-8.67341917	-1.10455211	3.32599884
C	-9.89571544	-1.39153321	3.93786414
C	-9.93655213	-1.75018758	5.28532551
C	-8.74721405	-1.82661536	6.01413315
C	-7.52906872	-1.54065274	5.39855680
H	-6.60668584	-1.61805111	5.97084681
H	-8.76804379	-2.11615850	7.06162088
H	-10.88600372	-1.97583238	5.76330970
H	-10.81416396	-1.33964565	3.35892294
H	-8.64694188	-0.84226759	2.27056170
H	-5.55022240	0.54023805	4.96293261
C	3.13235419	2.72138598	-0.81245423
H	2.81235589	1.78547210	-1.28378965
H	2.27848092	3.40750133	-0.83412267
C	4.30902287	3.31837536	-1.55557103
C	4.70459389	4.64487743	-1.32414020
C	5.80163149	5.19253633	-1.98857594
C	6.52429970	4.42187625	-2.90241745
C	6.13859491	3.10361636	-3.14705551
C	5.04092649	2.55800941	-2.47784556
H	4.73935090	1.53309179	-2.68216405
H	6.68870643	2.49800125	-3.86265082
H	7.37685038	4.84876012	-3.42387614
H	6.08848658	6.22366280	-1.79850655
H	4.13864491	5.25783418	-0.62540291
H	3.77114973	3.35760019	1.15709664
O	0.00025370	0.91601613	4.59269241
C	-0.62939978	1.93491880	4.81617681
H	-1.23328808	2.39857540	4.01110581
C	-0.63420316	2.66076140	6.13991625
C	0.08000688	4.01698167	5.96967712
H	0.07160302	4.56599522	6.91786841
H	1.12139509	3.88409702	5.65897773
H	-0.42252527	4.63815756	5.21818250
H	-0.07571533	2.04098515	6.85074912
C	-2.08272412	2.84433630	6.62723329
H	-2.58494449	1.87984846	6.75373798
H	-2.09434765	3.37089961	7.58795829
H	-2.66565796	3.43903502	5.91267107

Table 62. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,S*)-**6** from **5** D_{2d} tetramer



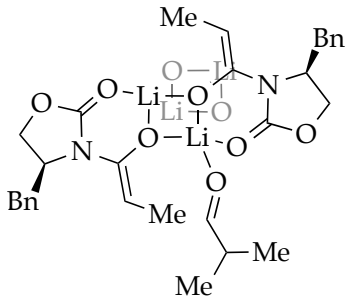


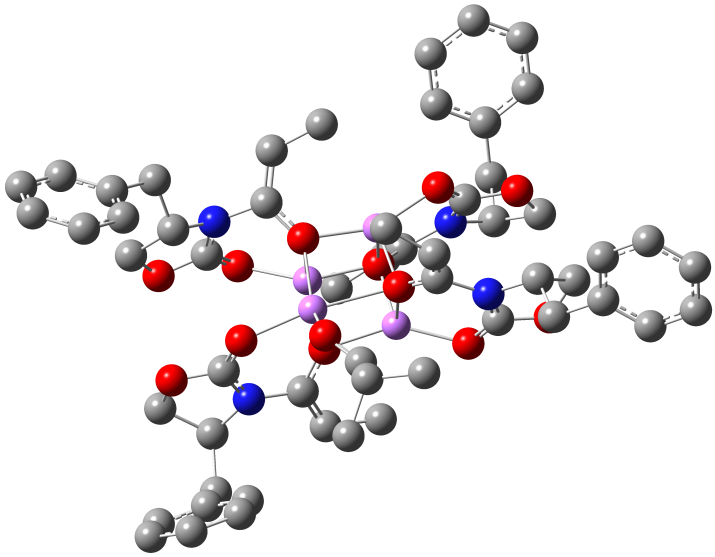
G = -3399.016367 Hartree
G_{MP2} = -2126253.014 kcal/mol
ΔG_{MP2} = -2.558143128 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -0.21605348 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-3.72685103	2.36596120	3.30666196
Li	0.00000000	0.00000000	2.80046440	C	-3.32858596	1.01334170	3.19038196
O	1.97259065	0.00000000	2.95152253	O	-2.82107224	0.63681315	2.12525078
C	2.71053915	0.61365148	2.19114918	Li	-2.30384316	-0.87846126	0.88024617
O	4.01902212	0.26727279	2.05048778	O	-3.95147213	-1.42525482	0.07563808
C	4.59777801	1.03046032	0.97048541	C	-4.47992842	-0.69730615	-0.75946979
H	4.70130068	0.36470916	0.10900452	O	-5.82331090	-0.71120813	-0.94287761
H	5.58201728	1.37877266	1.28714444	C	-6.18158335	0.31976127	-1.88304921
C	3.60058823	2.17667163	0.69704152	H	-6.61685558	1.15641056	-1.32506615
N	2.41113960	1.67076393	1.39107570	H	-6.92898303	-0.08268758	-2.56779954
C	1.11722490	2.34017058	1.41951018	C	-4.86275995	0.71951718	-2.57278366
C	1.12758603	3.68073790	1.58941501	N	-3.88959982	0.19154261	-1.60785189
H	2.08152470	4.15624339	1.79791974	C	-2.44549227	0.32950153	-1.72370031
C	-0.08656874	4.56358422	1.55308238	C	-1.89862898	0.38879437	-2.95679914
H	-0.59789029	4.62325920	2.52708537	H	-2.53973462	0.22815048	-3.81854662
H	0.18575230	5.58955993	1.27792108	C	-0.43678146	0.63411784	-3.21005975
H	-0.83025845	4.22075439	0.82570503	H	0.14977093	-0.29430398	-3.25213115
O	0.08464499	1.54151024	1.23743291	H	-0.28656028	1.15621554	-4.16293208
Li	-1.78606124	1.76266310	0.79656103	H	0.00732532	1.25428886	-2.42215833
O	-3.10038911	3.17195601	1.18354132	O	-1.81685925	0.42196138	-0.56874254
C	-3.56093532	3.31622497	2.30165860	C	-4.73194543	2.23225938	-2.82246044
O	-4.01098552	4.51019599	2.73486989	H	-4.82110792	2.75318503	-1.86167810
C	-4.26884140	4.43758455	4.15588454	H	-3.72183524	2.42544560	-3.19844037
H	-5.13351434	5.06269137	4.37754836	C	-5.77090999	2.73896362	-3.80147869
H	-3.38762427	4.81871336	4.68094030	C	-5.65728495	2.45757240	-5.17157893
C	-4.50810456	2.94577621	4.42004732	C	-6.62554300	2.89340093	-6.07563624

C	-7.72746726	3.62414049	-5.62525227
C	-7.84961788	3.91773448	-4.26693167
C	-6.87872632	3.47763480	-3.36486720
H	-6.97538788	3.72162065	-2.30906006
H	-8.69834807	4.49367315	-3.90735665
H	-8.48068863	3.96728176	-6.32925365
H	-6.51649426	2.66805936	-7.13326272
H	-4.79574764	1.90068156	-5.53421117
H	-4.76171299	0.18761554	-3.52899226
O	-0.51353538	-1.39744505	1.30791460
C	0.02130797	-2.58875603	1.12089265
N	1.45983831	-2.57515359	0.88922461
C	2.05317767	-1.76632885	-0.01848157
O	1.53604084	-0.89674177	-0.72309855
O	3.38384190	-2.01458898	-0.09069930
C	3.74922442	-2.94164128	0.95807541
H	4.27861836	-2.37639859	1.72929002
H	4.41250713	-3.69430570	0.52956443
C	2.41584673	-3.52152798	1.47919635
H	2.24811141	-4.52362320	1.06233889
C	2.32821700	-3.58721346	3.01510352
C	3.35158096	-4.53525579	3.60395313
C	4.48619375	-4.04933021	4.26815010
C	5.44082425	-4.92402197	4.79156251
C	5.27644249	-6.30303001	4.65767712
C	4.14846855	-6.80154463	4.00159355
C	3.19643821	-5.92479473	3.48212541
H	2.31346345	-6.32278275	2.98593776
H	4.00655743	-7.87458160	3.90068484
H	6.01711731	-6.98510665	5.06669128
H	6.31030737	-4.52599127	5.30844877
H	4.61402443	-2.97585051	4.38755214
H	1.31367887	-3.90701705	3.27738471
H	2.46008261	-2.57417882	3.40960749
C	-0.58495648	-3.79611809	1.13781355
C	-2.03709122	-4.02924499	1.44209542
H	-2.64636677	-4.14632667	0.53427269
H	-2.17303146	-4.94120068	2.03806283
H	-2.46918751	-3.20279533	2.01447397
H	0.01549648	-4.66806031	0.89313594
C	-3.38072540	0.16905978	4.39306051
H	-4.16029947	0.49911839	5.07970347
C	-3.51595997	-1.31780772	4.06782038
H	-4.29693904	-1.51337035	3.32428739
H	-2.56228481	-1.69146213	3.68650001
H	-3.76379761	-1.88037597	4.97301904
C	-6.00107228	2.54579513	4.34641102
H	-6.40805822	2.90166417	3.39191064
H	-6.06534149	1.45190774	4.32837471
C	-6.80873613	3.10179848	5.50070965
C	-7.69685569	4.16893899	5.31232091
C	-8.42466209	4.69309372	6.38285077
C	-8.27234849	4.15569271	7.66101368
C	-7.39196725	3.08984293	7.86173963
C	-6.66781781	2.56783779	6.79054229
H	-5.99263394	1.73105275	6.95766130
H	-7.27235303	2.66075331	8.85283058
H	-8.83872688	4.56034558	8.49520513
H	-9.11243715	5.51750487	6.21511667
H	-7.83042537	4.58520453	4.31588602
H	-4.07371639	2.64939358	5.37537685
C	3.35757716	2.43845110	-0.80042541
H	2.99603629	1.50905598	-1.25444410
H	2.55347370	3.17877300	-0.88145538
C	4.60325640	2.93042783	-1.50713261
C	5.06594663	4.24120458	-1.31430561
C	6.22864200	4.69049561	-1.93989912
C	6.95105280	3.83504711	-2.77504037
C	6.49928381	2.53116798	-2.98075336
C	5.33550721	2.08451485	-2.35117611
H	4.98341789	1.07011289	-2.52489456
H	7.04938249	1.85997709	-3.63525598
H	7.85518861	4.18516985	-3.26592824
H	6.56766708	5.71094738	-1.78059339
H	4.50237414	4.91877645	-0.67597838
H	3.94688828	3.10370513	1.17385738
O	-0.90016000	0.13864979	4.32983358
C	-1.89390463	0.46468694	5.13223888
H	-1.95379632	1.55998648	5.37638912
C	-1.86385959	-0.27439335	6.50999719
C	-0.53107881	0.06019202	7.19728949
H	-0.41601189	-0.50624243	8.13009868
H	0.30410989	-0.17143449	6.53274433
H	-0.47928559	1.12924526	7.44757585
H	-1.86719638	-1.35137261	6.29592195
C	-3.04132439	0.05822061	7.43710462
H	-3.99592805	-0.34467852	7.07638449
H	-2.87804867	-0.35744757	8.43877584
H	-3.15380199	1.14603609	7.55812124

Table 63. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,R*)-**6** from **5** D_{2d} tetramer



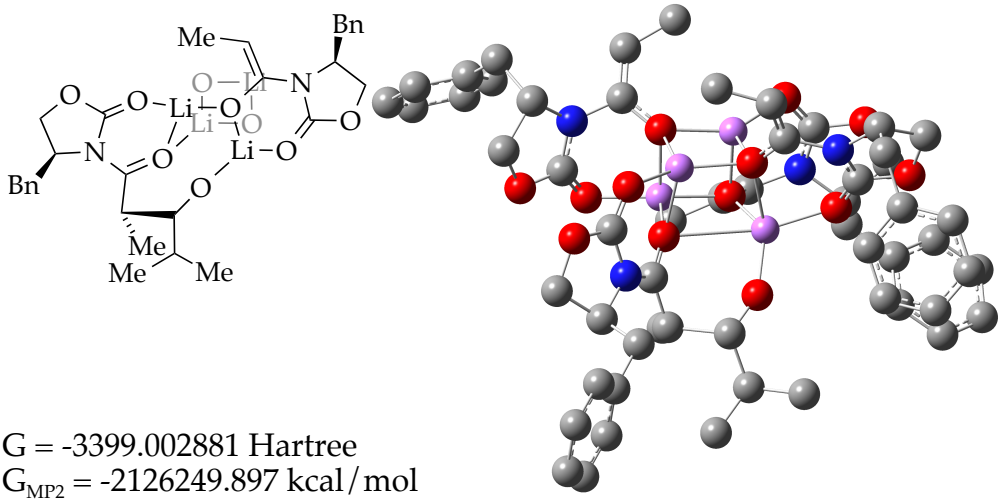


G = -3399.015586 Hartree
G_{MP2} = -2126255.63 kcal/mol
ΔG_{MP2} = -2.831781333 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -7.970548406 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-5.45841943	2.86442763	1.84287759
Li	0.00000000	0.00000000	2.70878580	C	-6.45483959	2.03153925	2.47488381
O	2.00008535	0.00000000	2.85189427	H	-6.84828650	1.33735360	1.72625062
C	2.76279667	0.73433528	2.23790626	H	-7.25227216	2.67509447	2.84877265
O	4.09232502	0.45058682	2.18349739	C	-5.68112000	1.30382761	3.57922609
C	4.71015933	1.30250621	1.20212205	H	-6.01286790	0.26759465	3.66980470
H	4.80586143	0.73526117	0.27146330	N	-4.32263821	1.33499278	3.01586778
H	5.69628552	1.58189122	1.57637715	C	-3.29588438	0.33609771	3.30034120
C	3.74735088	2.49449798	1.06159466	O	-2.25234094	0.37959858	2.51864261
H	3.61483082	2.77034707	0.01093793	Li	-2.24872973	-0.86051447	1.01168091
N	2.50058873	1.88382023	1.54291043	O	-4.05553136	-1.04913027	0.35313421
C	1.17456407	2.34484966	1.17895040	C	-4.51455334	-0.24739050	-0.45232659
C	1.01916829	3.58377109	0.65171464	O	-5.84055048	0.06503107	-0.43419697
H	1.87131965	4.24058851	0.54261123	C	-6.08141417	1.13348079	-1.37277310
C	-0.31998965	4.10614290	0.19879097	H	-6.14497226	2.07328587	-0.81441496
H	-1.00393812	4.32039980	1.03331961	H	-7.02960170	0.92887804	-1.87293423
H	-0.19850876	5.04108775	-0.35893855	C	-4.86794735	1.10336535	-2.31772474
H	-0.84263975	3.40701756	-0.46880639	H	-4.51174700	2.11342550	-2.54026172
O	0.21013824	1.46784254	1.35707333	N	-3.88632200	0.44096785	-1.45048002
Li	-1.71145074	1.67488737	1.18662804	C	-2.44825251	0.62148480	-1.53486541
O	-3.24592496	2.77529935	1.49807976	C	-1.89369825	1.00284468	-2.70906098
C	-4.22754177	2.32948450	2.08410761	H	-2.51435812	1.08494642	-3.59221068

C	-0.42727261	1.30399573	-2.86743449
H	0.16981845	0.40969571	-3.09877671
H	-0.26385400	2.01897847	-3.68278380
H	0.00177944	1.74697107	-1.96066457
O	-1.81372137	0.44277208	-0.39772977
C	-5.15971708	0.37628774	-3.65997207
H	-5.94217767	0.95915090	-4.16385576
H	-4.27102471	0.44351062	-4.29420787
C	-5.59007788	-1.06975515	-3.54150414
C	-6.93771380	-1.43627147	-3.65650282
C	-7.33176327	-2.77008124	-3.53748357
C	-6.37859477	-3.76157439	-3.30339382
C	-5.03066489	-3.41158662	-3.19756786
C	-4.63931100	-2.07811938	-3.31915199
H	-3.58721241	-1.81401916	-3.24580790
H	-4.27980719	-4.17791388	-3.02459088
H	-6.68225109	-4.80087933	-3.21084779
H	-8.38206846	-3.03339600	-3.63229277
H	-7.68633304	-0.67143297	-3.85465476
O	-0.41253416	-1.44997717	1.32470727
C	0.10799117	-2.60912951	0.96653065
N	1.55026222	-2.60447329	0.73338591
C	2.11357677	-1.65073156	-0.05085780
O	1.54710936	-0.84453695	-0.78974520
O	3.46296909	-1.65625488	0.07082828
C	3.84636420	-2.69988619	0.99363587
H	4.60077515	-2.29283134	1.66593745
H	4.26870288	-3.52832646	0.41331270
C	2.54352222	-3.10141190	1.70944262
H	2.43376206	-2.52660822	2.63700921
C	2.44679840	-4.60150013	2.01773163
H	1.44544154	-4.80157665	2.41387224
H	2.53958888	-5.16591443	1.08178231
C	3.50620443	-5.04629428	3.00679199
C	4.59128961	-5.83360759	2.60042398
C	5.57592295	-6.22517453	3.51028514
C	5.49041170	-5.83165537	4.84574319
C	4.41237735	-5.04844080	5.26518399
C	3.42991749	-4.66187723	4.35435825
H	2.59038430	-4.05834540	4.69282485
H	4.33402875	-4.74092543	6.30471336
H	6.25469837	-6.13554315	5.55605144
H	6.40703608	-6.83988453	3.17420828
H	4.66098694	-6.15207098	1.56243496
C	-0.53761057	-3.78316542	0.79353815
C	-2.00286914	-3.98843745	1.06062693
H	-2.62439761	-3.83176448	0.16637210
H	-2.19999692	-5.01024578	1.40809058
H	-2.37380504	-3.30653439	1.83465229
H	0.03358132	-4.62177163	0.40899943
C	-3.53537225	-0.55835253	4.29834199
H	-4.44684084	-0.47843048	4.87930313
C	-2.67342228	-1.75927042	4.57262364
H	-3.24210079	-2.69198317	4.44334546
H	-1.81635942	-1.79941336	3.89645350
H	-2.28039688	-1.77444073	5.60000193
C	-5.75856966	2.01933105	4.95085098
H	-5.00594651	1.57391796	5.60952942
H	-5.47348459	3.06890374	4.80620910
C	-7.13140486	1.93465638	5.58318514
C	-7.59462426	0.72593212	6.12522423
C	-8.86826036	0.63305248	6.68529897
C	-9.70471928	1.75143508	6.71590543
C	-9.25601380	2.96092415	6.18526573
C	-7.98020609	3.04890799	5.62390283
H	-7.63390060	3.99842831	5.22099552
H	-9.89609218	3.83896357	6.20998633
H	-10.69644756	1.68029520	7.15423823
H	-9.20656881	-0.31201304	7.10198800
H	-6.94846066	-0.14954990	6.11492728
C	4.21772436	3.75681131	1.83604379
H	5.14001920	4.09110219	1.34275494
H	3.48200560	4.55183938	1.68698684
C	4.46872718	3.57735459	3.31676297
C	5.76611586	3.39220187	3.81393145
C	5.99743534	3.23541001	5.18133178
C	4.92938651	3.27118750	6.07792873
C	3.63305380	3.46781778	5.59740071
C	3.40418217	3.61882968	4.22957676
H	2.39459537	3.78476284	3.86168148
H	2.79793630	3.51608975	6.29072586
H	5.10602633	3.15657070	7.14406243
H	7.01196462	3.09479019	5.54499516
H	6.60800382	3.38694732	3.12434607
O	-0.15321313	0.19591588	4.74913640
C	-0.75956217	1.04984763	5.37209968
H	-1.25407685	1.88200289	4.83192450
C	-0.83871674	1.09339349	6.88081616
C	0.15934846	2.15740510	7.38590754
H	0.11649125	2.22101179	8.47883545
H	1.18449314	1.90694740	7.09499318
H	-0.08172199	3.14989094	6.98451632
H	-0.52233902	0.10920452	7.24523695
C	-2.26947523	1.39829580	7.34974233
H	-2.97141585	0.63470616	7.00123622
H	-2.31038500	1.43518866	8.44389422
H	-2.60972866	2.37009931	6.97056906

Table 64. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,R*)-**6** from **5** D_{2d} tetramer

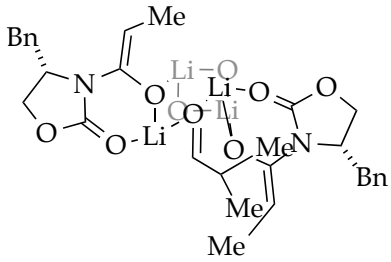


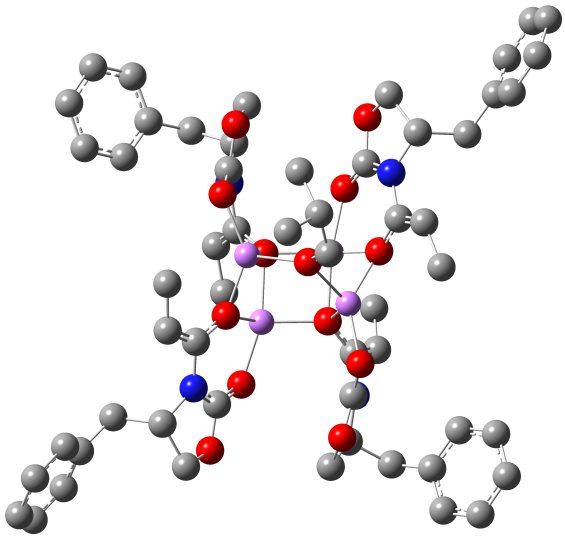
G = -3399.002881 Hartree
G_{MP2} = -2126249.897 kcal/mol
ΔG_{MP2} = 2.901640594 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -2.237126478 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	1.87044736	2.31970643	-4.92833876
O	0.00000000	0.00000000	1.94879940	H	0.92015639	2.43528780	-5.45157094
C	0.99312128	0.00000000	2.66156717	N	1.77943175	1.20523464	-3.95931873
O	0.87472245	0.26787452	3.98838684	C	0.63152489	0.77834141	-3.24711262
C	2.13474130	0.03634640	4.63788886	O	0.70793858	-0.28050197	-2.61007039
H	2.08424715	-0.92746433	5.15529586	Li	-0.21137670	-2.05905027	-2.31228676
H	2.29243976	0.83847765	5.36098829	O	-0.16477584	-2.67806965	-4.14890785
C	3.17033506	0.02932919	3.49999344	C	0.93770193	-3.00466500	-4.58106470
H	3.86016546	-0.80975387	3.62649336	O	1.36314628	-2.59426707	-5.80214964
N	2.30540750	-0.23037191	2.34289579	C	2.74293694	-2.97888732	-5.97750064
C	2.80226431	-0.74339776	1.08295216	H	3.36314402	-2.08211596	-5.88229308
C	4.11864402	-1.05774902	0.97102299	H	2.84408590	-3.39579898	-6.98095860
H	4.79430332	-0.91029003	1.80240664	C	3.03107935	-4.00789268	-4.86096715
C	4.70826750	-1.63124662	-0.29162894	H	3.94889361	-3.75336188	-4.32141249
H	4.84842274	-0.88311596	-1.08758402	N	1.88340819	-3.77201697	-3.97465943
H	5.69642285	-2.06019105	-0.09187946	C	1.86744648	-4.00518886	-2.53696348
H	4.09527847	-2.44253878	-0.71002555	C	2.23516655	-5.21101694	-2.05482004
O	1.90728173	-0.88832389	0.12834652	H	2.41943270	-6.01883816	-2.75269112
Li	2.27996718	-1.16520076	-1.74006952	C	2.36276058	-5.51476429	-0.58707219
O	3.33355219	-0.41186818	-3.23467462	H	1.41445937	-5.84731450	-0.14135351
C	2.95910589	0.46308505	-3.99425728	H	3.09657744	-6.31130553	-0.41611910
O	3.71056088	0.85566531	-5.04244799	H	2.69012951	-4.63928893	-0.01433029
C	2.94345252	1.75891629	-5.87266914	O	1.51530529	-2.94729875	-1.83008020
H	2.51612802	1.18194170	-6.69881763	Li	0.92274757	-2.60736888	-0.00882919
H	3.62044788	2.51939733	-6.26096665	O	0.35151810	-3.47958610	1.60626595

C	-0.64135453	-2.95606623	2.11504086
O	-0.69003020	-2.68424318	3.43706575
C	-1.95393206	-2.05656676	3.74606177
H	-1.74984650	-1.17521134	4.35374359
H	-2.55485911	-2.77225679	4.31812830
C	-2.59389351	-1.71927863	2.38274242
H	-2.39747956	-0.67268818	2.12567989
N	-1.78891022	-2.58016472	1.49300359
C	-1.84181233	-2.51049958	0.03760490
C	-2.87902523	-3.12193535	-0.57471093
C	-3.12206761	-3.08841872	-2.05822793
H	-2.61520394	-3.90701316	-2.59161153
H	-4.19145864	-3.17916231	-2.28387084
H	-2.77755793	-2.14900750	-2.50790536
H	-3.55846750	-3.70217639	0.04047554
O	-0.85059095	-1.84608192	-0.53297847
C	-4.10535845	-1.98773450	2.32913422
H	-4.43748835	-1.83528215	1.29653662
H	-4.29066982	-3.04074036	2.57492523
C	-4.87888816	-1.08416525	3.26859554
C	-5.45939796	-1.58436474	4.44134099
C	-6.15565099	-0.74478037	5.31369037
C	-6.28142877	0.61407507	5.02525565
C	-5.70966874	1.12596209	3.85796607
C	-5.01731313	0.28404019	2.98843579
H	-4.58227043	0.69160274	2.07835891
H	-5.80536371	2.18257931	3.62194745
H	-6.82336402	1.26955457	5.70181383
H	-6.60168485	-1.15515348	6.21607933
H	-5.37438135	-2.64484665	4.66919577
C	3.17399491	-5.45667685	-5.39352944
H	4.07385499	-5.46666606	-6.02292349
H	3.39180904	-6.11044285	-4.54334993
C	1.99556447	-5.98303888	-6.18512620
C	2.06570943	-6.09318635	-7.58104663
C	0.98180187	-6.56769867	-8.32196788
C	-0.19500105	-6.94282703	-7.67393057
C	-0.27649514	-6.84643684	-6.28314053
C	0.80877543	-6.37418535	-5.54474788
H	0.73468790	-6.31154740	-4.46264152
H	-1.18659403	-7.14295668	-5.76868422
H	-1.04088879	-7.31326737	-8.24672882
H	1.06036104	-6.64796411	-9.40306963
H	2.98553374	-5.81745156	-8.09362724
C	-0.56933076	1.62764077	-3.21034628
H	-0.55284261	2.37712996	-4.00297499
C	-1.85383962	0.79135973	-3.26465402
H	-1.83426510	0.05878348	-4.07971073
H	-1.98689784	0.26439750	-2.31615409
H	-2.71942937	1.44245769	-3.41851995
C	2.28173522	3.64897548	-4.25661187
H	1.55643450	3.87013881	-3.46617119
H	3.25032609	3.50261252	-3.76275464
C	2.36351750	4.79370180	-5.24497253
C	1.19480364	5.36739595	-5.76833795
C	1.26298342	6.40391279	-6.69882879
C	2.50357008	6.88719036	-7.12135023
C	3.67321240	6.33029711	-6.60384500
C	3.60151024	5.29142766	-5.67326418
H	4.51802180	4.87221358	-5.26311323
H	4.64298336	6.70609980	-6.91877123
H	2.55690610	7.69705308	-7.84364301
H	0.34692696	6.83924827	-7.08885619
H	0.22333998	5.00956465	-5.43383714
C	4.00095817	1.33438268	3.37460619
H	4.71389510	1.33999293	4.20943823
H	4.59108847	1.25971447	2.45528299
C	3.20480608	2.62159663	3.38123217
C	3.17912435	3.43801656	4.52091753
C	2.43847536	4.62107398	4.54302346
C	1.70645740	5.00625960	3.41958563
C	1.72804437	4.20668240	2.27497659
C	2.47565795	3.02903994	2.25321495
H	2.48671640	2.42143929	1.35240058
H	1.15878726	4.49354813	1.39566766
H	1.12504387	5.92436210	3.43392289
H	2.43565223	5.23989930	5.43678332
H	3.75539709	3.14927561	5.39818409
O	-0.42418750	1.58918757	-0.72610972
C	-0.48146284	2.43510377	-1.73704320
H	0.43630105	3.07142291	-1.85478904
C	-1.67983434	3.43898136	-1.64782411
C	-1.53496542	4.23538001	-0.34240643
H	-2.40574118	4.88201539	-0.17543684
H	-1.42601327	3.55545819	0.50537846
H	-0.64624225	4.88222114	-0.38072745
H	-2.59357995	2.83557536	-1.56804237
C	-1.81259390	4.39634980	-2.84086240
H	-2.10809465	3.88729485	-3.76634064
H	-2.57195716	5.16226058	-2.64146708
H	-0.86781734	4.92617369	-3.03031834

Table 65. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,R*)-**6** from **5** D_{2d} tetramer



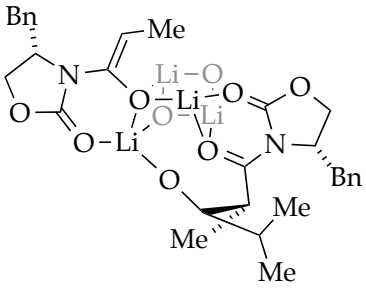


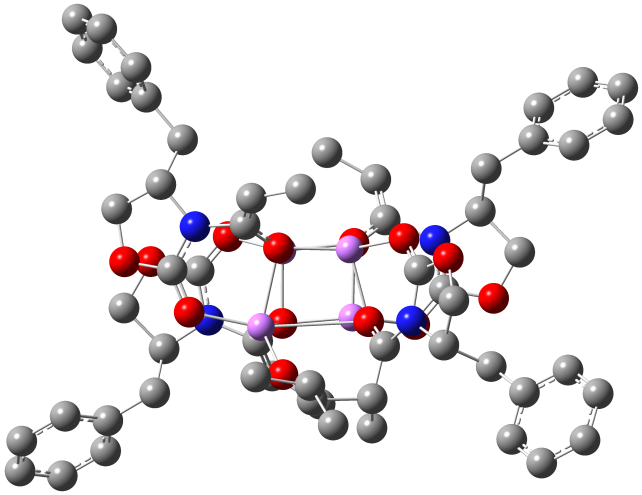
G = -3399.005379 Hartree
G_{MP2} = -2126242.921 kcal/mol
ΔG_{MP2} = 9.877340194 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -1.529003127 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-5.84026636	-1.70929935	1.75809995
Li	0.00000000	0.00000000	3.29458670	H	-5.57191226	-2.30066442	0.87545927
O	1.57333031	0.00000000	4.35246982	H	-6.91416199	-1.77927457	1.93582290
C	2.10600768	1.08460854	4.58943594	C	-4.99037403	-2.07364704	2.97900139
O	3.43538290	1.17311066	4.81265259	H	-4.63611558	-3.10374123	2.90316156
C	3.80929676	2.56536249	4.90016543	N	-3.87138781	-1.13382825	2.80133585
H	4.31464344	2.84676101	3.97277985	C	-2.62066075	-1.19970663	3.55230149
H	4.49135439	2.66803015	5.74607142	C	-2.35207021	-2.34579828	4.25114408
C	2.48419818	3.33519345	5.09008972	H	-3.05932954	-3.16717935	4.22419834
H	2.41783029	4.17451806	4.39214520	C	-1.23865380	-2.46445815	5.25772137
N	1.51656747	2.30881603	4.67899997	H	-0.58362707	-1.58814330	5.25256334
C	0.20067518	2.57123604	4.12038935	H	-1.63416463	-2.55896548	6.28066304
C	-0.61844659	3.46298707	4.72056520	H	-0.60842983	-3.35159731	5.09389410
H	-0.33044051	3.89898690	5.66854477	O	-1.87524342	-0.15262596	3.46704125
C	-1.95282190	3.85558397	4.14520296	C	-5.72045474	-1.85602056	4.32720710
H	-2.75030391	3.14119896	4.40229471	H	-4.96796857	-1.89871285	5.12124317
H	-2.27084612	4.83509170	4.52049071	H	-6.13703335	-0.84128766	4.33204514
H	-1.91928644	3.92542371	3.05010393	C	-6.81376158	-2.87276890	4.57271248
O	-0.06318286	1.90543888	3.01343719	C	-6.49343717	-4.19151668	4.92974346
Li	-1.85634873	1.36790494	2.24475180	C	-7.49319266	-5.14232317	5.13212757
O	-3.73267753	1.00136134	1.80589691	C	-8.83677042	-4.79038710	4.98236924
C	-4.27802391	-0.06844021	2.04300988	C	-9.17061423	-3.48185292	4.63287110
O	-5.50783960	-0.33071201	1.50376437	C	-8.16593073	-2.53321194	4.42983652

H	-8.43507125	-1.51126383	4.17078084
H	-10.21316953	-3.19537262	4.52234087
H	-9.61657497	-5.52981312	5.14309689
H	-7.22402436	-6.15716900	5.41307656
H	-5.45032646	-4.47191551	5.06220429
O	-1.02032773	1.60783093	0.48219084
C	-1.58958081	2.24187751	-0.52378707
N	-2.49286865	1.42347720	-1.31846820
C	-2.26019171	0.10111104	-1.53081483
O	-1.19985988	-0.51254390	-1.41020682
O	-3.38915077	-0.53261215	-1.92128364
C	-4.50309034	0.38238693	-1.83085412
H	-5.10784163	0.10165932	-0.96485449
H	-5.08612388	0.27868876	-2.74778570
C	-3.87391265	1.78409510	-1.66903853
H	-4.31786034	2.31508053	-0.82222561
C	-4.03385299	2.66145516	-2.93801647
H	-5.11268668	2.82278812	-3.06540090
H	-3.60414262	3.64652734	-2.73254997
C	-3.45405988	2.08350363	-4.21170410
C	-4.29242214	1.55978114	-5.20571974
C	-3.76680063	1.01417084	-6.37845506
C	-2.38644492	0.98499398	-6.57651994
C	-1.53916818	1.51031932	-5.59847847
C	-2.06692074	2.05715095	-4.42863381
H	-1.39704006	2.46759615	-3.67804833
H	-0.46251572	1.49789552	-5.74595447
H	-1.97320768	0.56111156	-7.48788710
H	-4.43669394	0.61639389	-7.13647394
H	-5.37138769	1.59016049	-5.06541645
C	-1.43678184	3.54794263	-0.84056455
H	-1.89578095	3.92731913	-1.74495813
C	-0.62696698	4.51650611	-0.02201638
H	0.40877541	4.61701001	-0.38068848
H	-1.06868256	5.52037063	-0.05082109
H	-0.57566922	4.21790487	1.03152066
Li	0.77588247	2.12712690	1.26604053
O	2.41104459	3.13366451	1.52339673
C	3.49727924	2.73986248	1.11074446
O	4.63904260	3.38253971	1.51156385
C	5.77704953	2.62963949	1.04606202
H	6.13024457	1.98967437	1.86256477
H	6.56285459	3.33164780	0.76345786
C	5.22536999	1.81691833	-0.12955587
H	5.66994857	0.81974633	-0.15695317
N	3.81294468	1.72150402	0.26293158
C	2.87807338	0.73618009	-0.27539993
C	3.34253014	-0.15443672	-1.19059743
C	2.46678907	-1.21174322	-1.80327961
H	2.38623866	-2.11915166	-1.18125382
H	1.44612617	-0.85227035	-1.98205779
H	2.86642801	-1.53444096	-2.77241330
H	4.38324453	-0.14513030	-1.48778635
O	1.67235645	0.81206142	0.19803769
C	5.40061027	2.52274325	-1.49805116
H	4.75978591	2.00761934	-2.22058206
H	5.02129793	3.54794236	-1.40572073
C	6.83810799	2.53774713	-1.96976180
C	7.60769511	3.70783199	-1.91631378
C	8.94265809	3.71019250	-2.32680613
C	9.53156325	2.53668517	-2.79797548
C	8.77578933	1.36350161	-2.86032290
C	7.44283543	1.36618225	-2.45094470
H	6.85949054	0.44987225	-2.51484057
H	9.22370182	0.44623427	-3.23366897
H	10.56954051	2.53599819	-3.11957893
H	9.51931350	4.63039770	-2.28140770
H	7.15195883	4.62991339	-1.56132607
C	2.30655024	3.87668105	6.53260633
H	3.11635039	4.60138971	6.69096998
H	1.37618926	4.45119678	6.57441533
C	2.33428327	2.83357742	7.62949561
C	3.46537727	2.67764196	8.44262342
C	3.50263141	1.70859788	9.44692786
C	2.40170971	0.87818080	9.65620942
C	1.26424274	1.02821227	8.85984204
C	1.22902047	1.99811942	7.85774796
H	0.33663602	2.10943046	7.24761025
H	0.39862437	0.39085140	9.01998049
H	2.42670832	0.12322596	10.43754740
H	4.38977005	1.60703500	10.06675067
H	4.32332510	3.33112397	8.29607321
O	-0.04212030	-1.34926349	1.67171787
C	-0.06366073	-2.50966424	2.08260297
C	-0.53045406	-3.71773612	1.30970013
H	-0.92226585	-4.41236047	2.06508254
C	0.72114977	-4.37763432	0.67890303
H	0.43954349	-5.32875010	0.21494275
H	1.14988477	-3.73185510	-0.09444917
H	1.49776523	-4.58267482	1.42495235
C	-1.61682037	-3.41762271	0.27493005
H	-1.91290318	-4.34371072	-0.23062730
H	-2.50281621	-2.99406374	0.75990260
H	-1.28134899	-2.70469816	-0.48203704
H	0.37688418	-2.72443978	3.07088644

Table 66. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,R*)-**6** from **5** D_{2d} tetramer



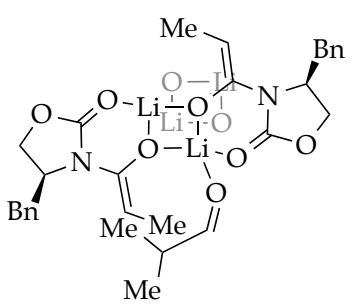


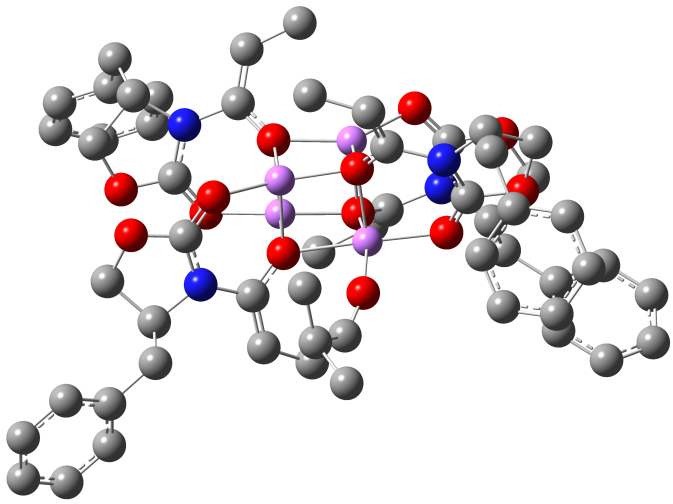
G = -3399.015094 Hartree
G_{MP2} = -2126252.022 kcal/mol
ΔG_{MP2} = 0.776340132 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -10.63000319 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-3.88711630	2.41452661	-3.19196083
Li	0.00000000	0.00000000	-2.78808210	C	-3.36465866	1.09284294	-3.19473608
O	1.97770507	0.00000000	-2.95852207	O	-2.76840016	0.69559365	-2.18202072
C	2.72302878	0.59546613	-2.19049891	Li	-2.30580695	-0.83662001	-0.92099834
O	4.02550045	0.22789634	-2.04629177	O	-3.97655309	-1.35570534	-0.14139263
C	4.61057665	0.97655010	-0.95888487	C	-4.49917298	-0.63009677	0.69959695
H	4.69694600	0.30482554	-0.10018435	O	-5.84445075	-0.62568358	0.87258464
H	5.60235061	1.30971645	-1.26805572	C	-6.19590412	0.39406930	1.82720553
C	3.63067268	2.13765635	-0.68493838	H	-6.62982601	1.23954337	1.28163857
N	2.43681675	1.65155234	-1.38463106	H	-6.94374982	-0.01421587	2.50815443
C	1.14944133	2.33138464	-1.41026629	C	-4.87453314	0.78055947	2.52082310
C	1.16389923	3.67226772	-1.57663068	N	-3.90253777	0.23986763	1.56223446
H	2.11822018	4.14842382	-1.78190969	C	-2.45784370	0.35846054	1.69041987
C	-0.05457405	4.55051800	-1.54184709	C	-1.92068271	0.41465098	2.92814075
H	-0.58635716	4.57568634	-2.50599228	H	-2.57005828	0.26677686	3.78588316
H	0.21756133	5.58548994	-1.30345483	C	-0.45719729	0.64082205	3.19041123
H	-0.78102123	4.22635529	-0.78795699	H	0.11777379	-0.29476869	3.23361658
O	0.11178171	1.53973439	-1.23209388	H	-0.30581738	1.15920704	4.14507350
Li	-1.75578234	1.78673639	-0.82118387	H	-0.00130592	1.25732825	2.40627544
O	-3.10023605	3.17471036	-1.10355915	O	-1.81782515	0.43786503	0.54156198
C	-3.72588645	3.31153945	-2.13956040	C	-4.72668920	2.29285925	2.76526715
O	-4.39912308	4.44895975	-2.40889660	H	-4.80819323	2.81107112	1.80230347
C	-4.85448646	4.42195995	-3.77945821	H	-3.71441753	2.47502027	3.14092272
H	-5.82502456	4.91567128	-3.82702705	C	-5.76015058	2.81542095	3.74160458
H	-4.12912039	4.96801144	-4.39063877	C	-5.65889546	2.52558334	5.11097032
C	-4.90786672	2.93050395	-4.12983282	C	-6.62238705	2.97684158	6.01248238

C	-7.70700110	3.73207539	5.56046408
C	-7.81648673	4.03452293	4.20304388
C	-6.85045196	3.57878327	3.30347354
H	-6.93654875	3.83003288	2.24844208
H	-8.65141272	4.62960276	3.84228927
H	-8.45643027	4.08722923	6.26255005
H	-6.52302758	2.74437295	7.06952195
H	-4.81054182	1.94984773	5.47522868
H	-4.78283489	0.25100636	3.47909366
O	-0.51559930	-1.38322051	-1.31961881
C	0.00033373	-2.58435981	-1.14437983
N	1.43458912	-2.59465067	-0.89109953
C	2.02993082	-1.79464271	0.02350544
O	1.51737240	-0.92304023	0.72885877
O	3.35780109	-2.05590059	0.10289125
C	3.72158074	-2.98167964	-0.94733413
H	4.26352747	-2.41854451	-1.71118855
H	4.37278454	-3.74404646	-0.51743797
C	2.38658878	-3.54406757	-1.48360171
H	2.20653566	-4.54859016	-1.07808822
C	2.31106065	-3.59320500	-3.02084732
C	3.33643139	-4.53803544	-3.61135823
C	4.47396288	-4.04765804	-4.26734971
C	5.43064192	-4.91877115	-4.79296376
C	5.26572959	-6.29864512	-4.66904792
C	4.13509290	-6.80152319	-4.02090961
C	3.18081039	-5.92836471	-3.49950343
H	2.29575074	-6.32990070	-3.00990755
H	3.99283137	-7.87522573	-3.92780472
H	6.00802843	-6.97801089	-5.07963649
H	6.30230298	-4.51721373	-5.30341309
H	4.60249871	-2.97331077	-4.37808589
H	1.29764920	-3.90586903	-3.29544971
H	2.45016495	-2.57648044	-3.40320983
C	-0.62482556	-3.78086452	-1.19547465
C	-2.07474849	-3.97686723	-1.53595991
H	-2.71604937	-4.04693323	-0.64540803
H	-2.22190384	-4.90088034	-2.10963616
H	-2.46086203	-3.15399650	-2.14643793
H	-0.04524803	-4.66841358	-0.95694863
C	-3.41469424	0.31033221	-4.43110421
H	-4.14917997	0.69173349	-5.14049853
C	-3.61447972	-1.18704541	-4.18148761
H	-4.47234432	-1.39925371	-3.53255243
H	-2.71180173	-1.60086749	-3.72591691
H	-3.77295670	-1.69685978	-5.13759519
C	-1.86140037	0.45572375	-5.15866853
O	-0.91651834	0.13614714	-4.30743393
C	-1.70680707	1.85094222	-5.84895687
H	-1.96486585	2.63514905	-5.11923327
C	-0.23749835	2.06274315	-6.24225991
H	-0.09218441	3.05277980	-6.69356872
H	0.08069243	1.30936016	-6.97479839
H	0.40914383	1.96700634	-5.36793118
C	-2.59926505	2.00050906	-7.09142813
H	-2.47818003	2.98937477	-7.55052009
H	-3.66885117	1.86572680	-6.88419681
H	-2.32670815	1.25366223	-7.84813363
H	-2.01169659	-0.29304078	-5.97575115
C	-6.29174973	2.28619445	-3.87585913
H	-6.59221701	2.50779444	-2.84436679
H	-6.18055237	1.19824040	-3.94684979
C	-7.34819823	2.77133049	-4.84598993
C	-8.32606066	3.69255686	-4.44792463
C	-9.28393882	4.15671108	-5.35191490
C	-9.27662118	3.70457479	-6.67152897
C	-8.30990891	2.78285361	-7.08033285
C	-7.35576960	2.32075539	-6.17455542
H	-6.61529286	1.59302999	-6.50057964
H	-8.30205276	2.41889365	-8.10412754
H	-10.02207492	4.06252509	-7.37617535
H	-10.03726277	4.86701268	-5.02205812
H	-8.34705173	4.03947647	-3.41680241
H	-4.59330150	2.77021122	-5.16030939
C	3.38665485	2.39776016	0.81267182
H	3.00998636	1.47210345	1.26229784
H	2.59329093	3.14950451	0.89379057
C	4.63768416	2.86918814	1.52391743
C	5.11417375	4.17678184	1.34372429
C	6.28326865	4.60686936	1.97089595
C	6.99823435	3.73476616	2.79509691
C	6.53238523	2.43399051	2.98878674
C	5.36218029	2.00662509	2.35779614
H	4.99921527	0.99451005	2.52212607
H	7.07660065	1.75026291	3.63519448
H	7.90754612	4.06958919	3.28711329
H	6.63310832	5.62511918	1.82126944
H	4.55655178	4.86685343	0.71363674
H	3.99210749	3.06130522	-1.15751073

Table 67. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,S*)-**6** from **5** D_{2d} tetramer



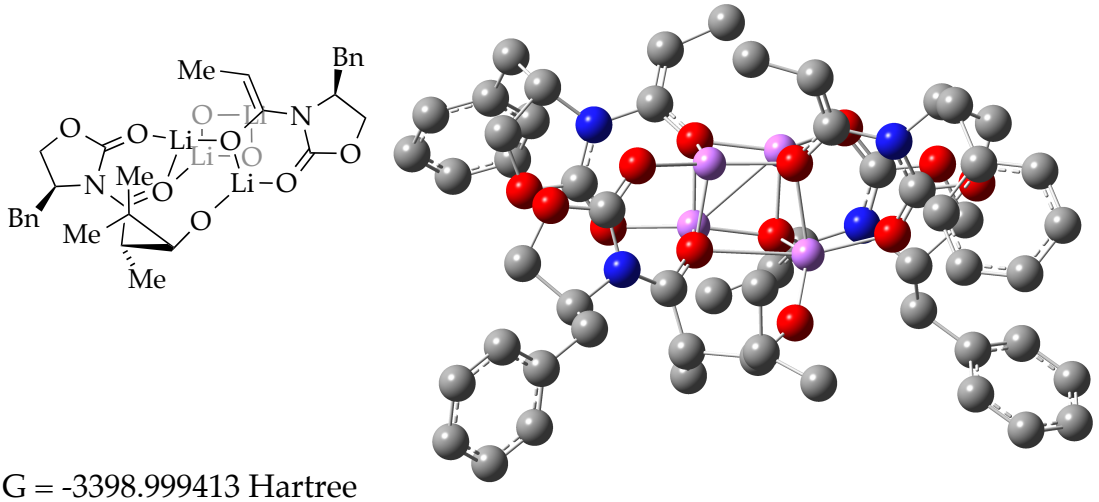


G = -3399.016015 Hartree
G_{MP2} = -2126257.688 kcal/mol
ΔG_{MP2} = -4.889474051 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = -9.661641118 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	0.27397654	0.20016564	-6.78810880
O	0.00000000	0.00000000	1.97101150	H	0.78433276	1.86173523	-7.23029480
C	1.03129947	0.00000000	2.63197589	C	-0.41487790	1.72988456	-5.37807635
O	0.97213543	-0.07735951	3.98949181	H	-1.41196796	1.31030080	-5.52803945
C	2.30465226	-0.25731178	4.50563727	N	0.16061270	1.18436592	-4.13908956
H	2.45368837	-1.32367894	4.70301139	C	-0.61405045	0.86261783	-2.94790578
H	2.38391519	0.31423293	5.43173707	C	-1.87861783	1.35566761	-2.84564347
C	3.21967336	0.25718325	3.38375090	H	-2.26516427	2.00965675	-3.61873049
H	4.09008417	-0.39317918	3.25911749	C	-2.84295552	0.94275192	-1.76804558
N	2.33512590	0.08250695	2.22607967	H	-2.41554409	0.17026738	-1.12183197
C	2.81274054	-0.08784904	0.86767710	H	-3.15252383	1.78152808	-1.12494649
C	4.12044767	0.13094992	0.58564589	H	-3.76641638	0.53036854	-2.19888484
H	4.79822914	0.47676304	1.35510454	O	-0.01465610	0.08101197	-2.09546548
C	4.68870153	-0.07862616	-0.79405251	Li	-0.29967829	-1.85248001	-2.20238218
H	4.44836582	0.74130877	-1.48850723	O	-0.42206120	-2.36613049	-4.05777788
H	5.78146688	-0.15029418	-0.75543637	C	0.59454042	-2.59683174	-4.70378703
H	4.32530616	-1.00613759	-1.25651918	O	0.65051150	-2.29818864	-6.03140773
O	1.90900893	-0.49741887	0.00726989	C	1.99721746	-2.51495120	-6.50252704
Li	1.87281694	-0.41890267	-1.92714780	H	2.50004784	-1.54426587	-6.55891001
O	2.33749016	0.54479689	-3.52014489	H	1.93263198	-2.96335996	-7.49541906
C	1.47804422	0.87611834	-4.33095805	C	2.63425457	-3.44097139	-5.45108272
O	1.79964990	1.00565862	-5.64833582	H	3.65590048	-3.13105735	-5.21260825
C	0.57971079	1.17808277	-6.40545214	N	1.77463440	-3.14771924	-4.29716303

C	2.18028276	-3.25267994	-2.90567774
C	3.12829573	-4.15134451	-2.55429879
H	3.50745902	-4.84603724	-3.29282162
C	3.67924948	-4.25686227	-1.15724255
H	3.06233345	-4.88817815	-0.50106692
H	4.68547273	-4.69211695	-1.16825130
H	3.75736880	-3.27634071	-0.67164197
O	1.59618456	-2.38751225	-2.10620430
Li	1.31155908	-2.37347546	-0.19811719
O	1.23140108	-3.49144480	1.36691746
C	0.25990822	-3.27153888	2.09023909
O	0.40370623	-3.14235780	3.43161193
C	-0.89456261	-2.92048496	4.02356480
H	-0.79907424	-2.11560912	4.75167365
H	-1.20071498	-3.84515725	4.52604581
C	-1.82287030	-2.56879833	2.84522663
H	-1.88142399	-1.48069620	2.72593397
N	-1.03781770	-3.11860632	1.72050996
C	-1.38029089	-2.90125658	0.31568492
C	-2.39100734	-3.64015888	-0.19356742
C	-2.92247457	-3.48212605	-1.59155936
H	-2.82980867	-2.44837268	-1.94731668
H	-2.40224679	-4.12077543	-2.32140902
H	-3.98577686	-3.74721588	-1.64081928
H	-2.82058878	-4.41516217	0.43228776
O	-0.66073430	-1.99139623	-0.31000208
C	-3.23723021	-3.15060170	2.98582281
H	-3.78376006	-2.93681565	2.06113610
H	-3.16785763	-4.24192728	3.07276323
C	-3.97346375	-2.57520536	4.17945714
C	-4.20437556	-3.34500038	5.32709510
C	-4.86704772	-2.80723923	6.43260795
C	-5.30950641	-1.48463203	6.40758296
C	-5.08796636	-0.70605835	5.26909184
C	-4.42813313	-1.24768806	4.16653689
H	-4.26800192	-0.63544831	3.28162781
H	-5.43314638	0.32412524	5.23789812
H	-5.82654291	-1.06384038	7.26584635
H	-5.03942766	-3.42425958	7.31075511
H	-3.87093804	-4.38032051	5.35138774
C	2.66293479	-4.92973390	-5.89603620
H	3.29981126	-4.97195772	-6.78970647
H	3.17589179	-5.51544535	-5.12785188
C	1.31483560	-5.54883371	-6.19419326
C	0.86781457	-5.71038037	-7.51245025
C	-0.38120238	-6.27172956	-7.78345770
C	-1.20346612	-6.68424785	-6.73468359
C	-0.76567491	-6.53926287	-5.41638648
C	0.48380729	-5.97991061	-5.14830395
H	0.82201819	-5.87819775	-4.12010228
H	-1.39552096	-6.86619618	-4.59336777
H	-2.17604999	-7.12231055	-6.94230490
H	-0.70801473	-6.39039003	-8.81329210
H	1.50932286	-5.40555734	-8.33722752
C	-0.47656070	3.27786718	-5.36505558
H	-1.02054414	3.59008362	-4.46712807
H	0.54667750	3.66119979	-5.26701732
C	-1.13257798	3.85318051	-6.60229035
C	-2.51756266	3.73548185	-6.79527374
C	-3.12638820	4.24157505	-7.94306317
C	-2.35938317	4.87879973	-8.92138646
C	-0.98211041	5.00684176	-8.74103926
C	-0.37612794	4.49711693	-7.59060515
H	0.69717866	4.61022005	-7.45264989
H	-0.37698250	5.50636537	-9.49302241
H	-2.83356377	5.27563479	-9.81487178
H	-4.20093419	4.14234861	-8.07206486
H	-3.12646693	3.24899210	-6.03585267
C	3.71903032	1.71518185	3.58562994
H	4.50422742	1.67720616	4.35187877
H	4.20156377	2.03370678	2.65626701
C	2.67000775	2.72768785	3.99451835
C	2.61095280	3.19624560	5.31442964
C	1.64457895	4.12309972	5.70931661
C	0.71490697	4.59717428	4.78407069
C	0.76568888	4.14306873	3.46444992
C	1.73737756	3.22311169	3.06937761
H	1.76386330	2.88088318	2.03831904
H	0.04256595	4.50474647	2.73798488
H	-0.04115176	5.31671997	5.08685087
H	1.62101384	4.47420429	6.73773600
H	3.33826021	2.83846630	6.04081488
O	0.11254866	2.16060193	-0.10318604
C	-0.38315900	3.13781099	-0.63467762
C	0.40019048	4.26746416	-1.27006900
H	-0.00108272	4.34608333	-2.29295537
C	1.90346782	3.99186547	-1.32988584
H	2.11628067	3.05691167	-1.85667432
H	2.41812956	4.80827607	-1.84870897
H	2.32862460	3.90859374	-0.32428422
C	0.05982776	5.58718767	-0.54481125
H	0.45601068	5.58392008	0.47728324
H	0.50579376	6.43551531	-1.07434290
H	-1.02241472	5.75585151	-0.49203752
H	-1.48329185	3.26720237	-0.64328571

Table 68. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,S*)-**6** from **5** D_{2d} tetramer

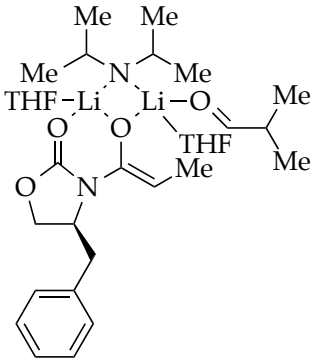


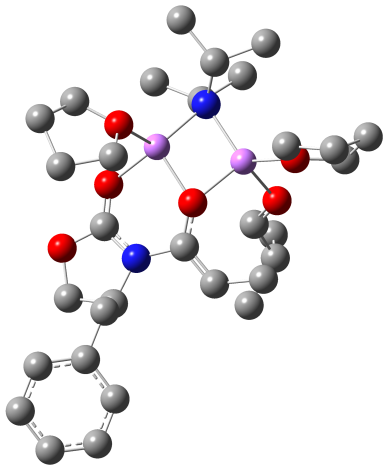
G = -3398.999413 Hartree
G_{MP2} = -2126249.961 kcal/mol
ΔG_{MP2} = -1.93514677 kcal/mol vs. **5** D_{2d} tetramer and isobutyraldehyde
ΔG_{MP2} = 2.837020297 kcal/mol vs. **5** D_{2d} tetramer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	1.40441843	1.18001847	-4.21525662
O	0.00000000	0.00000000	1.95951270	C	0.43295532	0.78689332	-3.25936435
C	0.95974281	0.00000000	2.71598256	C	-0.86160850	1.47080999	-3.19631615
O	0.76723697	0.00826473	4.06211309	H	-0.97168342	2.22107808	-3.98360017
C	2.02432467	-0.22863516	4.71765698	C	-2.03015312	0.47245655	-3.22859780
H	2.07472417	-1.28806042	4.98962454	H	-2.01683604	-0.13371882	-2.31926614
H	2.05674934	0.39174702	5.61453554	H	-2.97521740	1.02554522	-3.25241329
C	3.08325017	0.15051379	3.66996244	H	-1.99613893	-0.18699909	-4.10424275
H	3.89614335	-0.58142315	3.66244478	O	0.73437648	-0.11868136	-2.46566655
N	2.30156558	-0.00116674	2.43585029	Li	0.25090795	-2.07864649	-2.28161953
C	2.89874385	-0.24475158	1.14057701	O	0.47298684	-2.57228465	-4.13643001
C	4.24964730	-0.20289402	1.01329947	C	1.60260592	-2.80620696	-4.55736557
H	4.87719249	0.04367271	1.85865963	O	1.96071440	-2.43822349	-5.81696184
C	4.93911801	-0.48698277	-0.29592842	C	3.36853568	-2.70345596	-6.00266946
H	4.79004938	0.30561082	-1.04615627	H	3.90502164	-1.75223872	-5.93954503
H	6.02124901	-0.57380791	-0.14997248	H	3.49345350	-3.13881493	-6.99560624
H	4.61136237	-1.43380232	-0.75121977	C	3.74744587	-3.66894293	-4.86190663
O	2.05928114	-0.53433508	0.16881243	H	4.68563480	-3.37123882	-4.38431381
Li	2.48691326	-0.68414307	-1.70036114	N	2.64424086	-3.41530147	-3.92573808
O	3.30659052	0.11561395	-3.33202877	C	2.72160971	-3.55176773	-2.47925168
C	2.68927707	0.64638438	-4.23785673	C	3.45380517	-4.55051944	-1.94007368
O	3.22732226	0.81280714	-5.46421633	H	3.88158238	-5.30449558	-2.58882119
C	2.18785458	1.23983354	-6.37970406	C	3.68716729	-4.68958140	-0.45944932
H	1.79016396	0.34902091	-6.87473404	H	2.85916780	-5.19680675	0.05578620
H	2.63685621	1.91289347	-7.10945220	H	4.59530195	-5.27106528	-0.26307684
C	1.15005939	1.91715543	-5.47308641	H	3.81267680	-3.71535790	0.02921279
H	0.13681465	1.70832865	-5.82094143	O	2.08524548	-2.60611424	-1.81719692

Li	1.42838931	-2.40312349	0.00834436
O	1.03612724	-3.44477429	1.57814056
C	-0.04228914	-3.14623469	2.09528017
O	-0.14484373	-2.93628546	3.42640412
C	-1.51070568	-2.58765888	3.74645072
H	-1.48768463	-1.71669690	4.40059026
H	-1.96189902	-3.43763748	4.27055272
C	-2.19345068	-2.31308273	2.39075426
H	-2.18741107	-1.23815032	2.17890795
N	-1.23885796	-2.97532936	1.47744220
C	-1.30214156	-2.86898668	0.02388572
C	-2.20309765	-3.64787870	-0.61374328
C	-2.44729670	-3.61271915	-2.09695950
H	-2.26853113	-2.61485516	-2.51591858
H	-1.80773426	-4.31665150	-2.65148303
H	-3.48515169	-3.87849810	-2.33191377
H	-2.76164597	-4.36524126	-0.02193557
O	-0.45660046	-2.00997474	-0.51776747
C	-3.62983492	-2.84854996	2.30621642
H	-3.98097548	-2.71143252	1.27772576
H	-3.62113064	-3.92798065	2.50227364
C	-4.55760973	-2.14562939	3.27766101
C	-5.04750626	-2.80210330	4.41411665
C	-5.88601683	-2.14557178	5.31769434
C	-6.24662529	-0.81619808	5.09764925
C	-5.76660444	-0.15002944	3.96742311
C	-4.93212437	-0.80971226	3.06591583
H	-4.56933898	-0.28405702	2.18527493
H	-6.04457226	0.88475493	3.78533055
H	-6.89916882	-0.30287298	5.79892033
H	-6.25813993	-2.67509925	6.19107180
H	-4.77657507	-3.84130265	4.58865471
C	3.88718434	-5.13960977	-5.34152109
H	4.71059988	-5.14937897	-6.06809634
H	4.22000974	-5.75168153	-4.49814289
C	2.64582300	-5.74276377	-5.96208525
C	2.52043009	-5.86572288	-7.35253193
C	1.36914420	-6.40982375	-7.92478326
C	0.32314960	-6.84374747	-7.11023094
C	0.43948280	-6.73772010	-5.72250276
C	1.59162779	-6.19529185	-5.15297927
H	1.67760930	-6.12437959	-4.07161980
H	-0.36626645	-7.08205102	-5.07981583
H	-0.57392614	-7.26872196	-7.55236190
H	1.29354729	-6.49902168	-9.00538083
H	3.33852026	-5.54532586	-7.99502030
C	1.36680690	3.43937481	-5.32403996
H	0.71664204	3.80266573	-4.52186018
H	2.39863130	3.61398287	-4.99617071
C	1.08921586	4.19150200	-6.60927051
C	-0.22834378	4.38633318	-7.05011785
C	-0.49084697	5.05722182	-8.24413656
C	0.56260625	5.54833678	-9.01885145
C	1.87730311	5.36708293	-8.58918621
C	2.13625510	4.69345577	-7.39352133
H	3.16367901	4.56924281	-7.05754551
H	2.70325865	5.75400204	-9.17990787
H	0.35840380	6.07427881	-9.94734505
H	-1.51837160	5.20248600	-8.56646488
H	-1.05710810	4.02063167	-6.44703558
C	3.69602867	1.56429098	3.86776418
H	4.36104780	1.49915484	4.73907430
H	4.33040345	1.77930105	3.00235938
C	2.70536101	2.69031912	4.07043535
C	2.44078259	3.19008969	5.35339548
C	1.51749957	4.21848616	5.54891110
C	0.84356033	4.76728078	4.45767000
C	1.10622737	4.28815299	3.17269183
C	2.03236565	3.26270948	2.98060247
H	2.23714063	2.90575719	1.97469342
H	0.59165911	4.71231506	2.31526600
H	0.12299901	5.56723078	4.60569613
H	1.32905637	4.59170509	6.55232609
H	2.97293187	2.77707766	6.20849602
O	-0.81268333	1.46787543	-0.67875053
C	-1.00250071	2.27383852	-1.70067216
C	-0.16762557	3.59468643	-1.66433361
H	-0.27667133	4.10403410	-2.63657471
C	1.31994046	3.36692772	-1.37241888
H	1.82924090	2.82000059	-2.17386793
H	1.84747176	4.32031800	-1.24440466
H	1.42953957	2.78208771	-0.45393494
C	-0.77834248	4.51338627	-0.59275441
H	-0.74382347	4.01681672	0.38312261
H	-0.23569362	5.46478443	-0.52423611
H	-1.82872469	4.73976596	-0.81370803
H	-2.06488613	2.59684275	-1.83486238

Table 69. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,S*)-**6** from LDA **5** mixed dimer with three THF



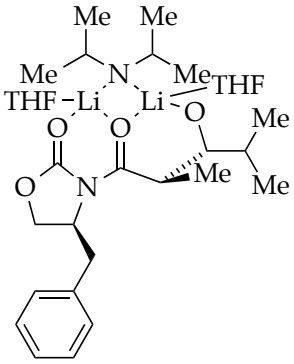


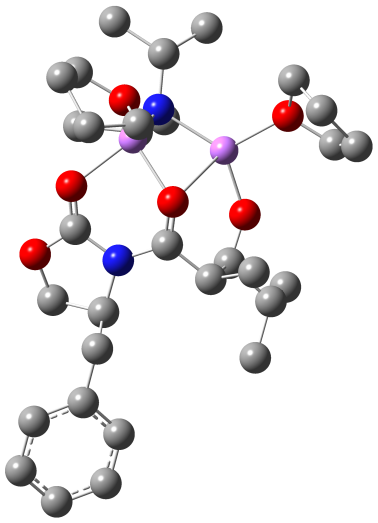
G = -1787.934854 Hartree
G_{MP2} = -1118239.454 kcal/mol
ΔG_{MP2} = -1.953107779 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -6.174167071 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.70444616	-1.19294485	-0.45336289
Li	0.00000000	0.00000000	2.51047440	H	3.11967699	-2.82232129	-0.09420273
N	1.57076076	0.00000000	1.24282335	O	-0.29342132	-1.58483309	3.75381888
C	2.33667709	1.25126730	1.21659268	C	-0.64372302	-2.65975522	3.29136529
H	1.57853299	2.02776914	1.00811192	C	-1.01275200	-3.86115149	4.12614272
C	2.98588796	1.69183394	2.55920379	H	-1.14293685	-3.51137495	5.15700015
H	3.86866289	1.09629404	2.81351655	C	0.16157515	-4.86318599	4.07657083
H	3.30558118	2.74380601	2.51141186	H	-0.08314822	-5.75415926	4.66547991
H	2.26556429	1.58953712	3.37794451	H	0.36394510	-5.18624945	3.04823047
C	3.39072202	1.42071355	0.09450780	H	1.07858380	-4.42400675	4.48237144
H	3.73429894	2.46352281	0.04092187	C	-2.31597670	-4.49576797	3.61246511
H	4.27716454	0.79829829	0.26498446	H	-2.58375121	-5.36015188	4.22993967
H	2.97299653	1.14896666	-0.88117122	H	-3.14489625	-3.78128226	3.63475846
C	2.27091285	-1.28937041	1.23437634	H	-2.20099347	-4.84604013	2.57927930
H	1.48397029	-2.02952986	1.47009048	H	-0.66005372	-2.80813971	2.19480268
C	3.36040807	-1.51531860	2.31138021	O	-0.33541037	1.49125642	3.82645403
H	3.65319752	-2.57423009	2.35167651	C	-0.62688691	2.84366128	3.41273909
H	4.27012340	-0.94039597	2.10150207	C	-0.86135589	3.62723479	4.70660174
H	2.99718707	-1.22243226	3.30324749	C	0.06107387	2.89418422	5.69373310
C	2.82471257	-1.76345491	-0.13862484	C	-0.08834977	1.43774520	5.24788298
H	2.05785447	-1.66333990	-0.91502784	H	-0.94262137	0.94778935	5.73209656

H	0.80528341	0.83050349	5.41650859
H	-0.21834911	3.04129116	6.74143977
H	1.09729596	3.22781913	5.56567644
H	-1.90727562	3.53986566	5.02403162
H	-0.62539163	4.69025580	4.59942351
H	0.23353732	3.23057858	2.85285477
H	-1.49553108	2.81215371	2.74897644
O	-1.49413065	-0.10529611	1.22926342
C	-2.56261767	-0.83524320	1.22216138
N	-2.83396784	-1.54392590	-0.03698696
C	-4.18260580	-1.91565655	-0.48787226
C	-3.83832772	-2.78823865	-1.70374059
H	-3.78252280	-3.85196431	-1.44531763
H	-4.52312748	-2.65670726	-2.54312344
O	-2.53036356	-2.34702300	-2.10464184
C	-1.92623634	-1.73854024	-1.04046964
O	-0.73758606	-1.45109482	-1.09668494
H	-4.69076284	-2.51458835	0.27103631
C	-5.04173408	-0.67291325	-0.82274483
H	-5.00476241	-0.01267116	0.05048447
H	-4.57053066	-0.13981307	-1.65796689
C	-6.47359362	-1.02237513	-1.16206725
C	-7.37653467	-1.37740222	-0.14803695
C	-8.69140931	-1.72992572	-0.45009123
C	-9.13021782	-1.73265310	-1.77637317
C	-8.24533480	-1.37703515	-2.79445630
C	-6.92900156	-1.02557384	-2.48737189
H	-6.24932743	-0.73731360	-3.28670645
H	-8.57861275	-1.36820682	-3.82893912
H	-10.15544433	-2.00446067	-2.01252602
H	-9.37614407	-1.99682545	0.35072933
H	-7.04655837	-1.36528149	0.88884777
C	-3.46669113	-1.00969924	2.22865304
H	-4.29971916	-1.68956843	2.08443679
C	-3.41820374	-0.25774533	3.52885358
H	-2.56144696	0.41999061	3.55790587
H	-4.32942022	0.34025946	3.68642999
H	-3.33476859	-0.92666205	4.39902087
O	-0.24439353	1.55196256	-1.30783467
C	0.32688502	1.39046932	-2.63006202
C	-0.67581749	2.01597807	-3.61004422
C	-2.00276597	1.90926111	-2.84108793
C	-1.54498015	2.16373276	-1.40524485
H	-2.17551845	1.71172995	-0.63603028
H	-1.45491783	3.24131809	-1.20419071
H	-2.41704421	0.89841227	-2.93644637
H	-2.75842554	2.62602759	-3.17759950
H	-0.69076696	1.49716229	-4.57310168
H	-0.43042611	3.06814287	-3.79690966
H	1.30712098	1.87623719	-2.64695952
H	0.45704137	0.31771748	-2.80855850

Table 70. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,S*)-**6** from LDA **5** mixed dimer with three THF



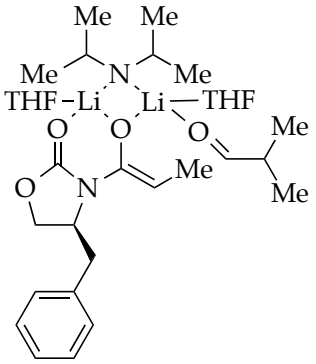


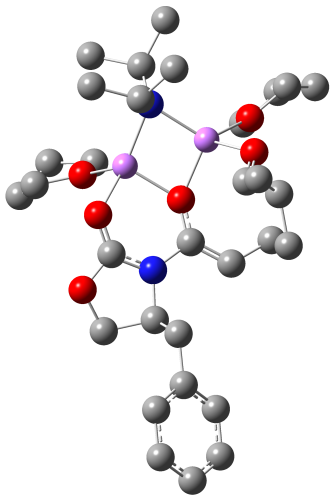
G = -1787.924983 Hartree
G_{MP2} = -1118238.639 kcal/mol
ΔG_{MP2} = -1.138351555 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -5.359410847 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*R,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-1.02530182	-1.23330931	3.67153475
Li	0.00000000	0.00000000	2.83891880	C	-1.73535047	-2.34035209	3.44572014
N	1.41728246	0.00000000	1.37485377	C	-2.42039984	-2.90413837	4.73368760
C	2.23851959	1.21610089	1.27153323	H	-3.05399703	-2.10195356	5.13720207
H	1.52090665	1.99305647	0.95054564	C	-1.32690682	-3.20217421	5.77041420
C	2.84714054	1.77101888	2.58863609	H	-1.76320608	-3.50339342	6.73122113
H	3.70671867	1.18472439	2.92871580	H	-0.67883879	-4.02085159	5.42742585
H	3.19693034	2.80406048	2.44519740	H	-0.70048148	-2.32067922	5.92271066
H	2.10213953	1.77314417	3.39100496	C	-3.28617821	-4.15154084	4.50272952
C	3.34661724	1.22915325	0.18834098	H	-3.61179915	-4.58299605	5.45706595
H	3.70562208	2.25360127	0.01450094	H	-4.19222564	-3.93966838	3.92149059
H	4.21658821	0.63166027	0.48408486	H	-2.71802508	-4.93288827	3.97668854
H	2.97608768	0.82940925	-0.76285406	H	-1.12971961	-3.19309231	3.03817265
C	2.06021368	-1.30680547	1.60463174	O	-0.45685344	1.72488306	3.79673684
H	1.20983406	-1.99141022	1.77684219	C	-0.62858775	3.04316067	3.26951241
C	2.93639021	-1.44944251	2.87397581	C	-2.13279285	3.30350662	3.39417794
H	3.15408408	-2.50763567	3.07519630	C	-2.50581663	2.56147777	4.70301482
H	3.89912309	-0.93686205	2.76628119	C	-1.30424484	1.61820586	4.95998600
H	2.42883915	-1.03852611	3.75430523	H	-1.55967804	0.56060208	5.03959648
C	2.83148355	-1.93286681	0.40967211	H	-0.73275486	1.93434738	5.84356900
H	2.25680328	-1.84117500	-0.51826085	H	-3.44038370	2.00404777	4.59217788
H	3.80682205	-1.46207179	0.24863117	H	-2.63700584	3.26021136	5.53556981
H	3.01795843	-3.00180025	0.59100817	H	-2.65554718	2.86051468	2.54000401

H	-2.37395222	4.37079261	3.42344330
H	-0.04657357	3.76218756	3.86680159
H	-0.24650776	3.04389176	2.24633307
O	-1.73906531	-0.56983725	0.81807986
C	-2.08860556	-1.72542837	1.06388694
N	-1.62164282	-2.78474740	0.24665164
C	-2.08174779	-4.18888078	0.28503860
C	-0.94647891	-4.85465592	-0.50332561
H	-0.12553593	-5.17971526	0.14320253
H	-1.27842527	-5.68364534	-1.12834787
O	-0.45307824	-3.80720819	-1.36716127
C	-0.74147202	-2.60649305	-0.82299866
O	-0.27432398	-1.57222290	-1.25668231
H	-2.10186987	-4.55148703	1.31342364
C	-3.46639651	-4.35830633	-0.38485079
H	-4.17512459	-3.68617874	0.11261096
H	-3.38914774	-4.02177605	-1.42599983
C	-3.97109647	-5.78539780	-0.33292288
C	-4.40688168	-6.34495653	0.87778869
C	-4.85114267	-7.66554948	0.93439824
C	-4.86969917	-8.45023570	-0.22113146
C	-4.44347041	-7.90461372	-1.43205531
C	-3.99740856	-6.58226259	-1.48503122
H	-3.67667356	-6.16016425	-2.43519646
H	-4.46022730	-8.50475697	-2.33780234
H	-5.21827260	-9.47834606	-0.17727046
H	-5.18730055	-8.08073086	1.88065958
H	-4.40547526	-5.74107776	1.78293224
C	-2.87126827	-2.08157041	2.27693334
H	-3.41864784	-3.01337696	2.12585455
C	-3.82678250	-0.95758842	2.68132921
H	-3.24953894	-0.10170634	3.03609587
H	-4.45789789	-0.63375112	1.84574748
H	-4.48353424	-1.29444935	3.48934356
O	-0.41710859	1.55081712	-1.18610118
C	0.38024004	1.66329614	-2.39428357
C	-0.57356818	2.15665056	-3.49056912
C	-1.94210370	1.67412706	-2.98336175
C	-1.79587215	1.86790514	-1.47584739
H	-2.41849350	1.20585703	-0.87045762
H	-1.99256636	2.90983479	-1.18602530
H	-2.08447926	0.61227186	-3.21501361
H	-2.78239216	2.23630725	-3.40218026
H	-0.31171909	1.75806326	-4.47501306
H	-0.55675141	3.25101921	-3.55378783
H	1.21044158	2.34783408	-2.19889522
H	0.78504921	0.67104017	-2.62213019

Table 71. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,R*)-**6** from LDA **5** mixed dimer with three THF



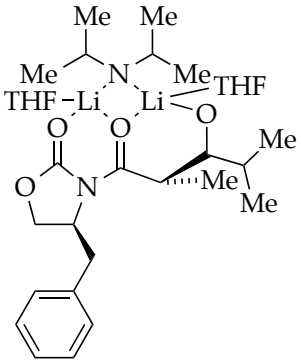


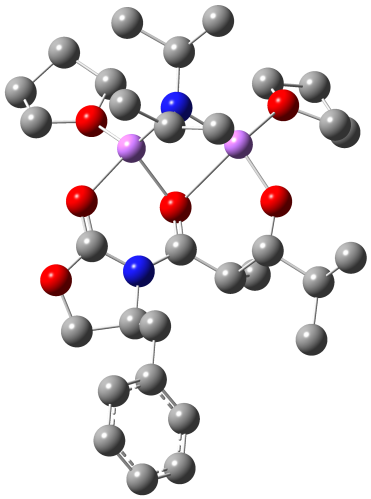
G = -1787.931664 Hartree
G_{MP2} = -1118235.818 kcal/mol
ΔG_{MP2} = 1.682961577 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -6.022391042 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.85026579	-1.03413732	2.39118575
O	0.00000000	0.00000000	1.93586870	H	-3.71257359	-1.39711350	1.38114791
C	0.84537702	0.00000000	2.91454756	H	-2.96551763	-1.88581937	2.92236317
N	0.54357933	0.94978369	3.99139468	N	-1.60182376	1.15907247	-0.36078309
C	1.28722295	1.04040249	5.25469787	C	-1.24661369	2.55248969	-0.65581564
C	0.24190260	1.73369839	6.13488751	H	-0.51467585	2.81118811	0.13178045
H	-0.40291886	1.01636062	6.65606511	C	-0.48953996	2.82094361	-1.98751550
H	0.66949249	2.43095784	6.85704323	H	-1.15061459	2.79024706	-2.85995022
O	-0.55842480	2.47850130	5.19943700	H	-0.02461448	3.81807773	-1.97163009
C	-0.44272501	1.89855108	3.96568657	H	0.30082810	2.07750992	-2.14062469
O	-1.16488740	2.27162926	3.05086281	C	-2.36403517	3.61649533	-0.51110538
Li	-1.62676756	0.98356236	1.65279854	H	-1.93788740	4.62958896	-0.50998153
O	-3.20467027	0.14861662	2.66344289	H	-3.08347131	3.57082046	-1.33732456
C	-3.68166179	-1.19777714	2.45714968	H	-2.91371447	3.47960633	0.42709493
C	-5.06511631	-1.26754455	3.11951468	C	-2.67503364	0.49568530	-1.10394542
C	-4.98164437	-0.15934611	4.18139755	H	-2.59940243	-0.56459060	-0.79622992
C	-4.14553663	0.89704794	3.45987315	C	-2.56202150	0.46328657	-2.64913708
H	-3.57349389	1.55391203	4.11814989	H	-3.26334749	-0.26873537	-3.07488849
H	-4.76777445	1.51646301	2.79873864	H	-2.80092963	1.43420143	-3.09860228
H	-4.45504577	-0.51869589	5.07376371	H	-1.54780783	0.18985557	-2.96164713
H	-5.96115686	0.21778716	4.49090004	C	-4.13066856	0.89905288	-0.73498747
H	-5.27690683	-2.25603853	3.53834215	H	-4.25338902	0.92235531	0.35321217

H	-4.40022776	1.88657061	-1.12310935
H	-4.85264158	0.17864714	-1.14837714
H	1.51388087	0.03701079	5.62253250
C	2.59169140	1.86550993	5.10813697
H	3.16517272	1.43839240	4.27930038
H	2.31669075	2.88719706	4.81792730
C	3.42147273	1.88884771	6.37337341
C	4.13224679	0.74950603	6.78156798
C	4.87732443	0.75313440	7.96027823
C	4.92797609	1.90088205	8.75497978
C	4.23045887	3.04246198	8.35967202
C	3.48411736	3.03370804	7.17926634
H	2.95099787	3.93139707	6.87324913
H	4.26832503	3.94304923	8.96697873
H	5.51063327	1.90559475	9.67218116
H	5.42324229	-0.13893743	8.25621206
H	4.10831443	-0.14663048	6.16467324
C	1.95334966	-0.78239242	3.05745003
H	2.57321545	-0.68865314	3.94126106
C	2.32074115	-1.87421823	2.09202225
H	1.70409708	-1.83115626	1.19074808
H	3.37317183	-1.80980350	1.77625541
H	2.19541531	-2.87658480	2.53374119
O	0.09887665	-1.85320275	-0.80692774
C	-0.61525214	-3.01233175	-0.32474159
C	-0.50710910	-4.07191956	-1.43151300
C	0.76637129	-3.64530574	-2.18020925
C	0.67338153	-2.12267251	-2.10095973
H	0.01404910	-1.71961491	-2.88186088
H	1.63485076	-1.60656746	-2.14809908
H	0.80549497	-4.01303325	-3.21007285
H	1.66062462	-3.99931908	-1.65383304
H	-1.37411922	-4.01919411	-2.10014325
H	-0.45347056	-5.08796640	-1.02912916
H	-0.13830757	-3.33566180	0.60732800
H	-1.64854888	-2.72310401	-0.10768814
O	1.89806551	0.61183581	-0.48442398
C	2.45444912	1.43922210	0.22045909
H	1.91461215	1.87651984	1.08149480
C	3.85264015	1.95109645	-0.01973004
C	3.77083402	3.43736704	-0.42603758
H	3.30553414	4.03883806	0.36423395
H	4.77785589	3.83282559	-0.59867171
H	3.18761624	3.57107063	-1.34291069
C	4.71262201	1.75946294	1.24262425
H	4.29611517	2.31468591	2.09155529
H	4.77786955	0.70454754	1.52814992
H	5.72754609	2.13204140	1.06528272
H	4.27176101	1.36882509	-0.84861906

Table 72. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,R*)-**6** from LDA **5** mixed dimer with three THF



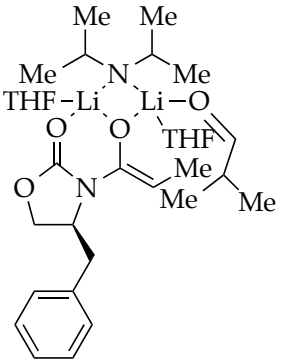


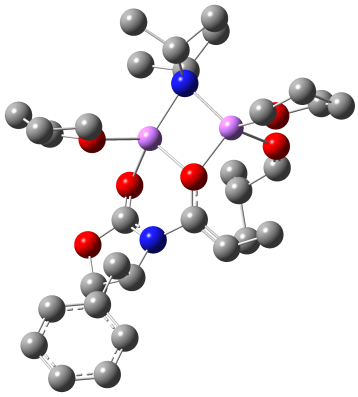
G = -1787.922574 Hartree
G_{MP2} = -1118236.553 kcal/mol
ΔG_{MP2} = 0.947782527 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -6.757570092 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*S,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.58726042	2.12987640	2.02214671
O	0.00000000	0.00000000	2.51962820	H	-3.91829782	0.59026310	1.20218014
C	1.15788039	0.00000000	2.93904615	H	-4.02427724	-0.42202553	2.66732682
N	1.59527635	1.08428602	3.74776786	N	-0.79952483	1.86576753	0.12913657
C	2.87787254	1.21071710	4.47503610	C	0.32678429	2.81388557	0.04266924
C	2.43021001	2.10910867	5.63640718	H	0.91497189	2.62223332	0.95978369
H	2.07442920	1.53491640	6.49866311	C	1.34019365	2.56887769	-1.10843027
H	3.19394349	2.81827127	5.95495337	H	0.92089189	2.80964566	-2.09046858
O	1.31828227	2.85486026	5.09789265	H	2.23553024	3.19376858	-0.97298195
C	0.77583936	2.17074644	4.06737693	H	1.66336706	1.52146824	-1.11766175
O	-0.26272717	2.52103171	3.54576235	C	-0.01002234	4.32303936	0.10281615
Li	-1.16634854	1.56510553	2.04800030	H	0.90432618	4.91555728	0.24623500
O	-2.98163936	1.35855462	2.87335481	H	-0.47834652	4.67771803	-0.82294612
C	-4.06550151	0.60693546	2.28529925	H	-0.69042211	4.54259541	0.93372604
C	-5.34831917	1.31915458	2.71971301	C	-1.95400494	2.02258685	-0.76367165
C	-4.94695839	1.89104492	4.08840761	H	-2.51791477	1.07911135	-0.64681903
C	-3.49141101	2.29726149	3.84936323	C	-1.67336229	2.12376250	-2.28264151
H	-2.86073999	2.23906090	4.73961034	H	-2.60735024	2.03317524	-2.85514614
H	-3.41570275	3.30996117	3.43371998	H	-1.22239567	3.08573266	-2.55251204
H	-5.00770846	1.11481702	4.86057962	H	-0.99526449	1.32789153	-2.60974525
H	-5.56781032	2.73455013	4.40466641	C	-2.97622854	3.12980737	-0.37884381
H	-6.20716888	0.64282542	2.76529359	H	-3.20584944	3.08145248	0.69247900

H	-2.60410447	4.13656650	-0.59263008
H	-3.91661931	3.00433805	-0.93640606
H	3.19848362	0.23529711	4.84456331
C	3.98788425	1.85043038	3.61020902
H	4.11697792	1.24033587	2.71017388
H	3.63938397	2.83449287	3.27413919
C	5.29878591	1.98408266	4.35759122
C	6.08595079	0.85359883	4.62535757
C	7.28244750	0.96681628	5.33292229
C	7.71511368	2.21557486	5.78480843
C	6.94567183	3.34868562	5.51989940
C	5.74741505	3.23157660	4.81218063
H	5.16051980	4.12208644	4.59685869
H	7.27847271	4.32623457	5.85839290
H	8.64904778	2.30466865	6.33289152
H	7.88108942	0.08036492	5.52488297
H	5.76798091	-0.12136616	4.26263026
C	2.12849102	-1.07406020	2.58740226
H	2.99772899	-1.03739930	3.24658766
C	1.45960063	-2.45287897	2.65976369
H	0.74967041	-2.55009966	1.83572323
H	2.21259871	-3.24133688	2.56571463
H	0.92699025	-2.60546700	3.60559489
O	-1.11740759	-1.45519819	-0.90874038
C	-2.42517615	-1.92225950	-0.52397948
C	-2.48168792	-3.41087902	-0.89860647
C	-0.99823104	-3.81174711	-0.87777270
C	-0.32664832	-2.55498211	-1.42535058
H	-0.36231432	-2.53140969	-2.52395185
H	0.69374252	-2.38620398	-1.07562854
H	-0.78322209	-4.70165179	-1.47765780
H	-0.66469709	-4.00185768	0.14956820
H	-2.89396145	-3.53727479	-1.90666067
H	-3.10154288	-3.99030040	-0.20716456
H	-2.53910040	-1.77352490	0.55773766
H	-3.18328717	-1.32226445	-1.03895221
O	1.61812915	-0.79957649	0.18921186
C	2.63754622	-0.76873175	1.05137425
H	3.12942912	0.23519461	1.12572977
C	3.78096179	-1.76662678	0.66534663
C	4.29619176	-1.39248150	-0.73255027
H	4.79537577	-0.41367188	-0.71368338
H	5.02304240	-2.12938255	-1.09753105
H	3.46496118	-1.33080291	-1.43813608
C	4.95198873	-1.83445314	1.65641055
H	5.38109315	-0.83790322	1.83163096
H	4.66639157	-2.25749464	2.62746443
H	5.75966005	-2.46201180	1.25968359
H	3.31965409	-2.76153905	0.59498607

Table 73. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*R,R*)-**6** from LDA **5** mixed dimer with three THF



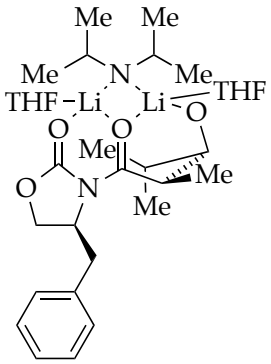


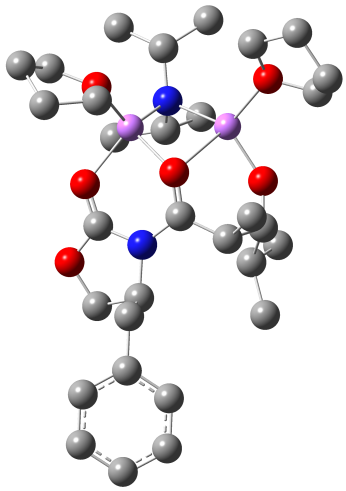
G = -1787.93281 Hartree
G_{MP2} = -1118239.503 kcal/mol
ΔG_{MP2} = -2.001858613 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -6.53130097 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.07400803	-2.78670353	4.25601622
O	0.00000000	0.00000000	1.93989790	N	-1.60815550	-1.19089269	-0.35234877
C	0.86219514	0.00000000	2.90700148	C	-2.81958464	-0.43944817	-0.69214531
N	0.60140705	-0.97601693	3.97793963	H	-2.88793277	0.33336914	0.09770654
C	0.65652203	-0.64570120	5.40569771	C	-2.78860321	0.37546935	-2.01681301
C	0.42666091	-2.03849253	6.01628996	H	-2.90012654	-0.25873204	-2.90180022
H	1.36977240	-2.54589600	6.24858572	H	-3.60624680	1.11172745	-2.03998476
H	-0.20546258	-2.02732525	6.90587075	H	-1.83887256	0.91290257	-2.10578500
O	-0.24819432	-2.78278851	4.98435429	C	-4.17113727	-1.19513293	-0.62450244
C	-0.02298484	-2.16855203	3.78388739	H	-5.01528285	-0.49316093	-0.68877101
O	-0.37517197	-2.69799450	2.73425005	H	-4.28215260	-1.90651889	-1.45086886
Li	-1.36044558	-1.33341289	1.63387516	H	-4.26036795	-1.75462343	0.31363704
O	-2.91879316	-1.17940228	2.96682295	C	-1.30317917	-2.44509638	-1.05076927
C	-3.63185811	-2.35966802	3.41616332	H	-0.25439019	-2.65734763	-0.77996116
C	-5.03187525	-1.88005304	3.82438777	C	-1.31393222	-2.42323290	-2.59836559
C	-4.79766885	-0.39674360	4.15523549	H	-0.85785076	-3.33847424	-3.00171930
C	-3.75062893	-0.01263102	3.11110434	H	-2.33146981	-2.36914510	-3.00339950
H	-3.10559621	0.81968344	3.40563767	H	-0.75089693	-1.56462923	-2.98142076
H	-4.21765701	0.22540552	2.14639244	C	-2.07751467	-3.70294118	-0.56588872
H	-4.38771761	-0.28619215	5.16669924	H	-2.03541244	-3.77914772	0.52729892
H	-5.70500216	0.21108451	4.08670186	H	-3.13084771	-3.68874610	-0.86556088
H	-5.43789483	-2.45256910	4.66376107	H	-1.63229310	-4.61981104	-0.97976945
H	-5.72963456	-1.97271496	2.98423476	H	1.64523659	-0.26877897	5.67865417
H	-3.64702996	-3.08989019	2.60167995	C	-0.41167098	0.40702382	5.78480351

H	-0.26253145	1.26299689	5.11665923	C	2.63785637	-3.95493910	-0.20601651
H	-1.40158259	-0.01044701	5.56370876	H	3.58437056	-4.05576023	-0.75267321
C	-0.32498777	0.84267237	7.23024861	H	2.59789319	-4.75070622	0.54516796
C	0.69283335	1.71291349	7.65016112	H	1.81419953	-4.11487211	-0.90946941
C	0.80134351	2.09708674	8.98625747	C	3.66377208	-2.37747671	1.51398158
C	-0.10992551	1.61801318	9.93058751	H	3.53150920	-1.43625440	2.05745824
C	-1.12997176	0.75615228	9.52699472	H	3.65230547	-3.19847435	2.23941510
C	-1.23393452	0.37306948	8.18797364	H	4.64938067	-2.37409708	1.03040879
H	-2.03929643	-0.29044903	7.87916792	H	3.55070897	-1.51892628	-1.16714724
H	-1.84856552	0.38352703	10.25238055	O	0.11285002	1.91721269	-0.67574672
H	-0.02773567	1.91914838	10.97143467	C	-0.73610078	2.96952350	-0.16426552
H	1.59424832	2.77561506	9.29015437	C	-0.61118739	4.13082971	-1.15764318
H	1.39925121	2.09936730	6.91823982	C	0.79163092	3.90942394	-1.74551437
C	1.95278130	0.79254813	3.08563608	C	0.86057292	2.38405491	-1.81691728
H	2.59033970	0.61403423	3.94714055	H	1.87013614	1.97420298	-1.74409650
C	2.33714510	1.91229567	2.16120506	H	0.39058129	2.00284262	-2.73399166
H	1.66855218	1.95080788	1.29711204	H	1.55931024	4.29398451	-1.06367971
H	2.30313097	2.89419142	2.66004232	H	0.93248899	4.38245775	-2.72220099
H	3.36357377	1.79728983	1.78117903	H	-0.73110914	5.10560801	-0.67526541
O	1.80354487	-0.61958433	-0.76116799	H	-1.36945063	4.04556369	-1.94460323
C	2.62510569	-1.49622870	-0.55100645	H	-1.75418116	2.57944979	-0.07718965
C	2.53030566	-2.58237829	0.48669642	H	-0.37523615	3.24145398	0.83460569
H	1.56333808	-2.49457179	0.99154989				

Table 74. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*R,R*)-**6** from LDA **5** mixed dimer with three THF



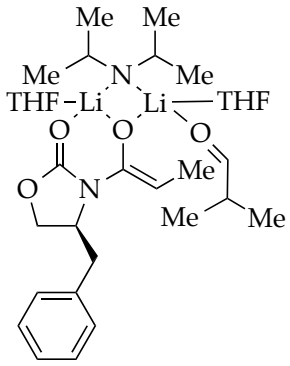


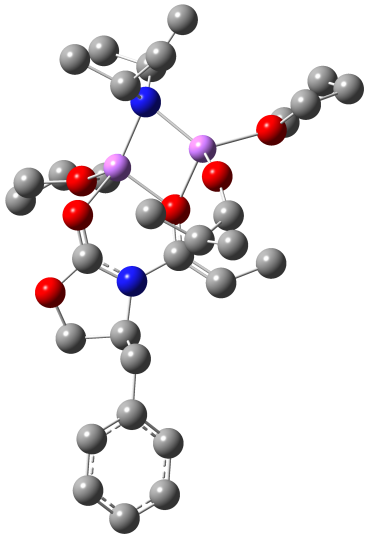
G = -1787.923007 Hartree
G_{MP2} = -1118237.143 kcal/mol
ΔG_{MP2} = 0.358166598 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -4.171275759 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*R,R*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.58051682	-1.54485469	4.02487542
O	0.00000000	0.00000000	2.47464250	H	-4.40001188	-2.59706676	2.20357967
C	1.15079854	0.00000000	2.91988682	H	-3.11766922	-3.19930217	3.28321254
N	1.60660256	-1.12499448	3.65438118	N	-0.91225560	-1.83355722	0.05465841
C	2.82008343	-1.18313433	4.49520342	C	-2.18478787	-1.93453700	-0.67432899
C	2.90570596	-2.69679863	4.72558204	H	-2.86497444	-1.26281697	-0.12006664
H	3.50314501	-3.20065996	3.95929424	C	-2.20324770	-1.38590905	-2.12821162
H	3.27090060	-2.96617053	5.71668189	H	-1.68894919	-2.04831831	-2.83165671
O	1.54102293	-3.15248687	4.60692041	H	-3.23823801	-1.27520454	-2.48519684
C	0.83762297	-2.27284283	3.86228765	H	-1.72051948	-0.40404556	-2.17311050
O	-0.28882410	-2.51553060	3.47792588	C	-2.89191472	-3.31263802	-0.66943052
Li	-1.19213049	-1.52085864	1.97492852	H	-3.92780870	-3.21908146	-1.02576851
O	-2.99154764	-1.19245815	2.78577924	H	-2.39043051	-4.03223730	-1.32690989
C	-3.79650375	-2.36181589	3.08423710	H	-2.91390300	-3.74253484	0.33889565
C	-4.62681735	-1.99777821	4.32028188	C	0.18519954	-2.76844638	-0.24644519
C	-3.73596387	-0.95777062	5.01806319	H	1.05233570	-2.34187052	0.28919208
C	-3.14920017	-0.20390046	3.82541791	C	0.64577356	-2.86706209	-1.72105131
H	-2.16947444	0.24259902	4.01128079	H	1.60356149	-3.40116448	-1.79137779
H	-3.83367213	0.57939152	3.47090314	H	-0.07391415	-3.41504329	-2.34082963
H	-2.93868431	-1.45497507	5.58275469	H	0.78149129	-1.87140078	-2.15864112
H	-4.28586267	-0.30296848	5.70095805	C	0.05008360	-4.20862929	0.32275828
H	-4.84497817	-2.86979241	4.94367774	H	-0.26379834	-4.18227342	1.37244485

H	-0.67653269	-4.81313310	-0.22994119
H	1.01461489	-4.73517772	0.27111054
H	3.68720201	-0.83349763	3.93682113
C	2.64913310	-0.37154463	5.80212971
H	2.38981825	0.65891198	5.53270311
H	1.79389004	-0.78056737	6.35421558
C	3.88931893	-0.38946273	6.67103200
C	5.01910394	0.36292085	6.31659654
C	6.17335136	0.33104569	7.09837968
C	6.21688250	-0.45403609	8.25289508
C	5.09860115	-1.20269725	8.62005844
C	3.94487547	-1.16934976	7.83385368
H	3.07283466	-1.74688709	8.13372115
H	5.11985053	-1.81041418	9.52065345
H	7.11497209	-0.47732088	8.86384889
H	7.03719894	0.92301645	6.80849229
H	4.99257219	0.98713815	5.42569062
C	2.10417831	1.09407731	2.60951126
H	2.96069608	1.09427917	3.28624623
C	1.40467615	2.45851598	2.64781834
H	0.64994183	2.50323025	1.85981110
H	0.91864723	2.65437581	3.61162166
H	2.14048256	3.25015930	2.47021987
O	1.66249264	0.67625247	0.20265743
C	2.66482537	0.86496780	1.05388370
C	3.78243907	-0.23112781	1.01492996
H	3.39556497	-1.14158767	1.50101272
C	4.09276292	-0.59221951	-0.44432725
H	4.47569350	0.28356231	-0.98517409
H	4.85441544	-1.38062600	-0.50067445
H	3.18945872	-0.92915505	-0.95541843
C	5.07695156	0.21043405	1.71743872
H	4.93664036	0.48507234	2.77115614
H	5.83561330	-0.58122277	1.68591729
H	5.50138576	1.08929350	1.21512142
H	3.19509110	1.83991455	0.90221973
O	-1.07502024	1.57941016	-0.70335328
C	-2.40901281	1.99805027	-0.35272115
C	-2.50232994	3.48644189	-0.72373722
C	-1.03207296	3.93487003	-0.67508026
C	-0.31308212	2.69827372	-1.20992229
H	0.70979109	2.55491513	-0.85654888
H	-0.32989317	2.67507866	-2.30923632
H	-0.72458072	4.13724619	0.35807267
H	-0.83412774	4.83070250	-1.27200821
H	-3.15177933	4.04517545	-0.04258268
H	-2.89961581	3.60435557	-1.73874434
H	-3.12967519	1.37352106	-0.89033532
H	-2.54596124	1.83661548	0.72394141

Table 75. Geometric coordinates and thermally corrected MP2 energies for IRC derived reactants leading to (*S,S*)-**6** from LDA **5** mixed dimer with three THF



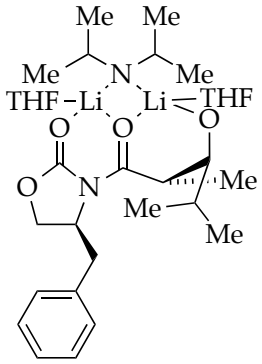


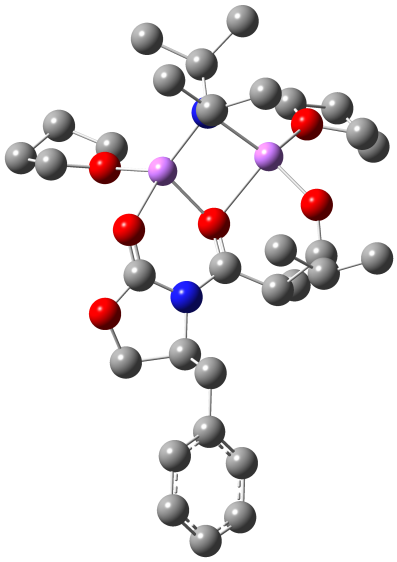
G = -1787.929557 Hartree
G_{MP2} = -1118235.511 kcal/mol
ΔG_{MP2} = 1.990613531 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -6.484736567 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.47382112	1.75328680	4.90729562
O	0.00000000	0.00000000	1.94436310	H	-5.14110030	-0.94002336	4.54281314
C	0.92776819	0.00000000	2.84008441	H	-5.70360632	0.03817787	3.17778532
N	0.83590704	1.07743400	3.83145021	H	-3.72684041	-0.80600147	2.12707949
C	1.51799883	1.08722881	5.13200798	H	-2.88089467	-1.01563771	3.67826132
C	0.57213565	1.99981760	5.92206224	N	-1.61338894	1.15293923	-0.37167491
H	-0.22519987	1.43795237	6.42228391	C	-1.20857313	2.41311298	-1.01162178
H	1.08035228	2.63697977	6.64729574	H	-0.41543361	2.80414923	-0.35225230
O	-0.01907469	2.84042909	4.91250383	C	-0.52312471	2.29187580	-2.40144434
C	0.04969497	2.19028021	3.71027137	H	-1.23080631	2.04881420	-3.20142531
O	-0.53342296	2.64043545	2.73367393	H	-0.03466299	3.23824018	-2.67649739
Li	-1.42272708	1.27248758	1.62091755	H	0.24774326	1.51264802	-2.38188794
O	-2.93417055	0.91908550	2.95924549	C	-2.25944644	3.54794542	-1.08284032
C	-3.56699153	-0.36966601	3.11805928	H	-1.78226475	4.49848228	-1.35930517
C	-4.87509141	-0.11126185	3.87963426	H	-3.03415365	3.34768177	-1.83296797
C	-4.57356181	1.19714154	4.62862128	H	-2.75216757	3.68691808	-0.11360937
C	-3.71171008	1.94355861	3.61103696	C	-2.80695151	0.44138609	-0.83172569
H	-3.01354370	2.66213163	4.04561301	H	-2.76813521	-0.52713655	-0.29572208
H	-4.33216870	2.45905727	2.86458186	C	-2.87861448	0.06024903	-2.33211511
H	-3.99884962	0.99650852	5.54093309	H	-3.68752004	-0.66238088	-2.51419566

H	-3.07859951	0.93192315	-2.96580955
H	-1.93551972	-0.38735176	-2.66538229
C	-4.18167813	1.04108669	-0.41962469
H	-4.17065660	1.31282907	0.64126902
H	-4.43608577	1.93812060	-0.99270797
H	-4.98991091	0.31152208	-0.57988078
H	1.53840405	0.07382489	5.54005028
C	2.95684610	1.66038164	5.04913208
H	3.50343271	1.10144768	4.28302430
H	2.89064828	2.69854018	4.70111781
C	3.69335124	1.59819046	6.37012256
C	4.14361296	0.36951238	6.87756001
C	4.80180062	0.29845294	8.10483362
C	5.02498297	1.45909061	8.84951558
C	4.58683344	2.68799718	8.35583969
C	3.92655764	2.75429900	7.12691149
H	3.59698025	3.71809578	6.74469780
H	4.76095710	3.59801394	8.92400044
H	5.54041576	1.40523110	9.80458200
H	5.14542149	-0.66283852	8.47790290
H	3.98363041	-0.53968860	6.30125682
C	1.95050765	-0.89473685	2.97969244
H	2.65350108	-0.78587376	3.79733795
C	2.06745185	-2.14338114	2.14982658
H	1.49976547	-2.05931512	1.21896262
H	3.11398536	-2.35659064	1.88692283
H	1.69756431	-3.03614867	2.68094848
O	0.19100156	-1.81441653	-0.90888674
C	-0.71907020	-2.91706016	-0.70246026
C	-0.80684872	-3.64069951	-2.04817912
C	0.58856977	-3.38569497	-2.63993449
C	0.87546819	-1.95657119	-2.17265944
H	0.47614813	-1.21229062	-2.87314971
H	1.93694252	-1.75040069	-2.00995620
H	0.62176549	-3.48305284	-3.72923391
H	1.31875399	-4.08338520	-2.21269363
H	-1.57760480	-3.18132151	-2.67716584
H	-1.04362910	-4.70320431	-1.93692255
H	-0.30809356	-3.56439188	0.08320894
H	-1.67445171	-2.51048706	-0.36080749
O	1.87817951	0.75396874	-0.21156450
C	2.95009658	0.73915110	0.37114889
C	3.69205762	1.97613794	0.82591759
C	5.06785592	2.01439832	0.12513321
H	5.67329795	2.83320035	0.52743217
H	5.62581533	1.08160660	0.27031747
H	4.95217141	2.17892005	-0.95249625
C	2.88272863	3.25772553	0.62102882
H	1.91586759	3.20413366	1.13006951
H	3.43482739	4.12128797	1.00840308
H	2.68427621	3.42778026	-0.44224279
H	3.87735319	1.81914827	1.89967083
H	3.46958700	-0.22146095	0.55166058

Table 76. Geometric coordinates and thermally corrected MP2 energies for IRC derived products leading to (*S,S*)-**6** from LDA **5** mixed dimer with three THF





G = -1787.916425 Hartree
G_{MP2} = -1118232.469 kcal/mol
ΔG_{MP2} = 5.032631344 kcal/mol vs. **5** LDA mixed dimer with three THF and isobutyraldehyde
ΔG_{MP2} = -3.442718754 kcal/mol vs. **5** LDA mixed dimer transition state leading to (*S,S*)-**6**

Atom	X	Y	Z	Atom	X	Y	Z

Li	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.26901720
C	1.07426693	0.00000000	2.87767923
N	1.24685024	0.91833153	3.94810413
C	2.21333603	0.81267874	5.06247810
C	1.39420625	1.48966935	6.17321703
H	0.77550864	0.77852212	6.73084524
H	2.00152246	2.07246407	6.86532429
O	0.51960934	2.39686988	5.46724838
C	0.34731588	1.95399934	4.20115550
O	-0.46806499	2.44799559	3.44961533
Li	-1.36325255	1.41523569	1.95034998
O	-2.99911471	0.95967171	3.05719657
C	-3.84837524	-0.18230986	2.79929277
C	-5.24866170	0.21233565	3.28400427
C	-4.93872745	1.25115087	4.37412848
C	-3.73184491	1.97465870	3.77924122
H	-3.05624894	2.41206619	4.51746427
H	-4.04260504	2.75927023	3.07633255
H	-4.66483929	0.75562633	5.31343414
H	-5.77450365	1.92767354	4.57628464
H	-5.81959384	-0.64596781	3.65067407
H	-5.81633290	0.67608001	2.46958896
H	-3.80885790	-0.40876763	1.72975555
H	-3.44813996	-1.03786137	3.35778846
N	-1.33796007	1.57828308	-0.01142516
C	-0.60291623	2.79718846	-0.38968593
H	0.13222269	2.93062746	0.42362805
C	0.26562607	2.70654516	-1.67486581
H	-0.33731193	2.69778066	-2.58875234
H	0.94582122	3.56818140	-1.74182990
H	0.88005268	1.79869504	-1.66378564
C	-1.39740917	4.12543669	-0.42466664
H	-0.71217503	4.98192302	-0.48890505
H	-2.06576398	4.18343293	-1.29220318
H	-2.00588347	4.24534300	0.47976793
C	-2.57083552	1.21770117	-0.71932532
H	-2.79027286	0.19087374	-0.37300892
C	-2.50112986	1.10702040	-2.26212402
H	-3.40817190	0.62738091	-2.65790781
H	-2.42536078	2.09083021	-2.73929961
H	-1.63560371	0.51112566	-2.57020825
C	-3.84747119	2.02397788	-0.34647552
H	-3.93693523	2.11311382	0.74233811
H	-3.84060441	3.03610768	-0.76258298
H	-4.75121359	1.52194247	-0.72395456
H	2.39237343	-0.23929392	5.29504387
C	3.55229145	1.53351112	4.78588380

H	3.98452629	1.12681073	3.86715608
H	3.34440225	2.59250926	4.59294601
C	4.52912900	1.38772125	5.93459900
C	5.18025911	0.16606150	6.16307862
C	6.06307600	0.01436353	7.23176017
C	6.31330160	1.08616383	8.09183013
C	5.67851153	2.30879086	7.87225073
C	4.79362310	2.45616921	6.80180086
H	4.31401437	3.41732974	6.62856688
H	5.87444845	3.15166325	8.52954097
H	7.00401017	0.97002917	8.92243346
H	6.56169522	-0.93835641	7.38878216
H	5.00521861	-0.67055571	5.48938468
C	2.17904757	-0.90740757	2.50083889
H	3.01575428	-0.84609454	3.20215514
C	1.66910424	-2.35541738	2.40433702
H	0.96551316	-2.43651113	1.57214441
H	2.51297978	-3.02620514	2.21096842
H	1.17014264	-2.69056053	3.32226948
O	-0.68488542	-1.72014175	-0.95242026
C	-1.88644969	-2.50784578	-0.86266000
C	-1.52289259	-3.92655652	-1.35202350
C	0.01579175	-3.92624746	-1.31317934
C	0.33399445	-2.47146589	-1.64519652
H	0.25470673	-2.28723862	-2.72761621
H	1.28694168	-2.09194188	-1.27219699
H	0.46194013	-4.63298449	-2.02003088
H	0.37983992	-4.16969886	-0.30804030
H	-1.87471585	-4.07809977	-2.37881433
H	-1.97067833	-4.70792966	-0.73009719
H	-2.21049568	-2.49903476	0.18464256
H	-2.67314396	-2.04638993	-1.47053518
O	1.79112568	-0.36516557	0.08117159
C	2.76071560	-0.51380077	0.97525680
C	3.79816297	0.65332942	1.01666435
C	4.68130069	0.56079225	-0.23883517
H	5.44175746	1.35146961	-0.25155948
H	5.19846584	-0.40541776	-0.29266421
H	4.06260923	0.66219901	-1.13675583
C	3.15747384	2.04332148	1.09467243
H	2.55170587	2.18246650	1.99672054
H	3.92446613	2.82807944	1.09038642
H	2.50236227	2.19878981	0.23373452
H	4.45385454	0.50021019	1.89086447
H	3.37663750	-1.43461546	0.8141097