Carbenoid Alkene Insertion Reactions of Oxiranyllithium

Lawrence M. Pratt, Binh Khanh Mai, and B. Ramu Ramachandran*
*Corresponding Author. E-mail: ramu@latech.edu

Supporing Information

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Table S1. The data used for constructing Table 2 in the paper.

Method	$\Delta G^{\ddagger}$	ΔG_{rxn}
B3LYP	18.32	-45.40
M06	16.83	-54.43
M06L	16.18	-51.53
M062X	21.45	-53.29
PBE0	17.38	-54.91
Avg.	18.03	-51.91
Std. dev.	2.07	3.87
MP2	20.18	-52.57
MP2//B3LYP	19.29	-47.96
MP2//M06	18.62	-48.30
MP2//M06L	19.00	-48.09
MP2//M062X	19.47	-48.60
MP2//PBE0	19.02	-48.12
Avg.	19.08	-48.22
Std. dev.	0.32	0.25
CCSD(T)//B3LYP	20.21	-47.61
CCSD(T)//M06	20.44	-52.88
CCSD(T)//M06L	19.88	-53.17
CCSD(T)//M062X	19.77	-53.05
CCSD(T)//PEBE0	19.88	-53.45
Avg.	20.04	-52.03
Std. dev.	0.28	2.48
CCSD(T)//MP2	19.50	-52.99

Table S2. Data used for constructing Table 3 in the paper

THF-solvated α-Li-CH2-O-CH3.2THF + ethylene

Method	$\Delta G^{\ddagger}_{CM}$	$\Delta G_{rxn;\,CM}$
B3LYP	26.00	-45.66
M06	20.92	-47.73
M06L	17.20	-50.07
M062X	26.25	-46.74
PBE0	21.81	-52.22
Avg.	22.44	-48.48
Std. dev.	3.79	2.65
MP2	31.34	-47.15
MP2//B3LYP	24.99	-50.89
MP2//M06	24.93	-50.15
MP2//M06L	23.63	-50.27
MP2//M062X	24.39	-50.67
MP2//PBE0	24.99	-51.02
Avg.	24.58	-50.60
Std. dev.	0.59	0.38

Table S3. Data used for constructing Table 4 in the paper.

Aggregates - non-polar; all relative to R

Method	RR d1	RS d1	RR d2	RS d2	RRRR	RRRS	RRSS
B3LYP	-41.01	-41.12	-40.29	-40.12	-93.93	-93.94	-93.17
M06	-40.61	-41.29	-40.64	-40.20	-103.57	-102.37	-101.08
M06L	-39.31	-39.57	-38.73	-38.52	-101.99	-101.29	-98.95
M062X	-44.28	-44.38	-43.49	-43.36	-113.31	-113.47	-110.07
PBE0	-42.69	-42.82	-41.87	-41.63	-103.24	-102.46	-101.23
Avg.	-41.58	-41.84	-41.00	-40.76	-103.21	-102.71	-100.90
Std. dev.	1.93	1.83	1.79	1.82	6.88	6.98	6.08
MP2	-42.97	-43.04	-42.14	-41.84	-107.14	-107.67	-107.71
MP2//B3LYP	-43.10	-43.16	-42.09	-41.93	-107.13	-106.90	-105.84
MP2//M06	-42.18	-43.28	-42.15	-41.65	-107.81	-106.76	-104.45
MP2//M06L	-42.79	-43.43	-42.31	-41.96	-107.38	-107.45	-103.78
MP2//M062X	-43.06	-43.18	-41.98	-42.16	-105.72	-106.99	-102.53
MP2//PBE0	-43.03	-43.08	-41.95	-41.82	-106.73	-107.60	-104.44
Avg.	-42.83	-43.23	-42.09	-41.90	-106.95	-107.14	-104.21
Std. dev.	0.38	0.14	0.14	0.19	0.79	0.36	1.20
CCSD(T)//B3LYP	-43.39	-43.43	-42.23	-42.14			
CCSD(T)//M06	-42.55	-43.66	-42.42	-42.00			
CCSD(T)//M06L	-43.03	-43.70	-42.44	-42.14			
CCSD(T)//M062X	-43.40	-43.51	-42.19	-42.46			
CCSD(T)//PEBE0	-43.35	-43.38	-42.13	-42.07			
Avg.	-43.14	-43.54	-42.28	-42.16			
Std. dev.	0.36	0.14	0.14	0.18			
CCSD(T)//MP2	-43.32	-43.37	-42.33	-42.08			

Table S4. Data used to construct Table 5 in the paper

Aggregates - THF; all relative to R.2THF

	dimer 1				dimer 2			
Method	RR.2THF	RS.2THF	RR.4THF	RS.4THF	RR.2THF	RS.2THF	RR.4THF	RS.4THF
B3LYP	-5.45	-5.00	-9.75	-10.13	-4.60	-5.64	-8.90	-10.24
M06	-5.89	-4.74	-18.70	-19.67	-3.60	-7.81	-16.39	-17.86
M06L	-6.04	-7.10	-24.18	-21.75	-4.81	-6.31	-18.07	-19.57
M062X	-5.80	-5.61	-22.09	-22.73	-4.34	-6.44	-20.30	-21.74
PBE0	-9.36	-8.60	-13.20	-12.74	-7.78	-8.47	-11.61	-13.50
Avg.	-6.51	-6.21	-17.58	-17.40	-5.03	-6.93	-15.06	-16.58
Std. dev.	1.61	1.62	6.03	5.63	1.61	1.16	4.70	4.66
MP2	-9.21	-9.10			-8.79	-10.68		
MP2//B3LYP	0.21	0.62	-22.17	-22.48	1.33	0.64	-21.76	-22.16
MP2//M06	-0.06	1.08	-22.59	-22.43	1.37	-1.99	-18.93	-20.10
MP2//M06L	-1.48	-2.85	-28.03	-26.67	-0.59	-0.86	-21.31	-23.37
MP2//M062X	-2.67	-2.41	-25.11	-26.78	-1.69	-2.86	-22.67	-24.31
MP2//PBE0	-10.21	-9.13	-26.10	-25.10	-8.53	-9.47	-22.47	-23.80
Avg.	-2.84	-2.54	-24.80	-24.69	-1.62	-2.91	-21.43	-22.75
Std. dev.	4.28	4.08	2.45	2.15	4.08	3.89	1.50	1.68

Table S5A. Data used to construct Tables 7 and 8 in the paper

Method	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}
	monomer		**RR d1**		**RR d2**		**RS d1**		**RS d2**	
B3LYP	18.32	-45.40	18.51	-54.08	17.42	-54.73	18.88	-53.90	17.26	-54.98
M06	16.83	-54.43	16.61	-62.53	16.64	-62.35	17.59	-61.70	15.95	-62.93
M06L	16.18	-51.53	17.14	-59.61	16.44	-60.13	17.70	-59.28	15.86	-60.41
M062X	21.45	-53.29	21.87	-61.52	20.76	-62.25	22.09	-61.37	20.52	-62.44
PBE0	17.38	-54.91	19.38	-62.22	17.86	-62.97	19.50	-62.02	17.62	-63.26
Avg.	18.03	-51.91	18.70	-59.99	17.82	-60.49	19.15	-59.65	17.44	-60.80
Std. dev.	2.07	3.87	2.08	3.49	1.74	3.39	1.83	3.39	1.89	3.44
MP2	20.18	-52.57	20.04	-61.46	18.87	-62.54	20.28	-61.65	18.62	-62.59
MP2//B3LYP	19.29	-47.96	17.73	-57.63	16.54	-59.05	18.18	-57.85	16.45	-58.88
MP2//M06	18.62	-48.30	16.38	-58.87	16.69	-59.24	18.23	-58.00	15.56	-59.41
MP2//M06L	19.00	-48.09	17.50	-58.15	17.31	-59.12	18.65	-57.86	16.15	-59.03
MP2//M062X	19.47	-48.60	18.26	-58.22	17.34	-59.76	18.67	-58.48	17.17	-59.16
MP2//PBE0	19.02	-48.12	17.65	-57.81	15.76	-59.39	17.56	-58.14	16.15	-59.07
Avg.	19.08	-48.22	17.50	-58.13	16.73	-59.31	18.26	-58.07	16.29	-59.11
Std. dev.	0.32	0.25	0.69	0.48	0.65	0.28	0.45	0.26	0.59	0.20
CCSD(T)//B3LYP	20.21	-47.61	18.82	-56.86	17.61	-58.10	18.94	-57.07	17.40	-58.10
CCSD(T)//M06	20.44	-52.88	19.78	-62.15	18.55	-63.39	20.36	-62.32	18.40	-63.32
CCSD(T)//M06L	19.88	-53.17	18.50	-63.39	18.83	-63.65	20.43	-62.52	17.62	-63.92
CCSD(T)//M062X	19.77	-53.05	19.20	-62.67	19.02	-63.52	20.42	-62.39	17.82	-63.50
CCSD(T)//PEBE0	19.88	-53.45	19.65	-62.69	18.74	-64.09	20.19	-62.92	18.51	-63.58
Avg.	20.04	-52.03	19.19	-61.55	18.55	-62.55	20.07	-61.44	17.95	-62.48
Std. dev.	0.28	2.48	0.54	2.66	0.55	2.50	0.64	2.46	0.48	2.46
CCSD(T)//MP2	19.50	-52.99	19.02	-62.32	17.59	-63.74	19.07	-62.61	17.50	-63.49

Table S5B. Activation barriers for tetramers in nonpolar media (Table 7)

Non-polar phase activation energies: tetramers

	RRRR	RRRS	RRSS
B3LYP	14.53	13.37	13.27
M06	11.62	11.71	10.61
M06L	14.53	12.45	11.00
M06-2X	15.44	16.89	14.11
PBE0	16.45	14.17	13.47
Avg.	14.52	13.72	12.49
Std. dev.	1.80	2.00	1.58
MP2	16.80	14.73	14.15
MP2//B3LYP	17.28	13.60	13.07
MP2//M06	17.39	14.40	12.03
MP2//M06L	16.85	13.75	11.07
MP2//M062X	16.34	15.13	11.28
MP2//PBE0	16.49	13.51	10.60
Avg.	16.87	14.08	11.61
Std. dev.	0.46	0.68	0.97

Table S6A. Data used to construct Table 9 in the paper.

THF-phase reaction and activation energies: monomer.2THF

Method	$\Delta G^{\ddagger}$	ΔG_{rxn}
B3LYP	20.10	-50.43
M06	18.05	-55.45
M06L	15.63	-53.73
M062X	21.77	-55.27
PBE0	18.43	-59.14
Avg.	18.80	-54.81
Std. dev.	2.30	3.15
MP2	19.39	-58.44
MP2//B3LYP	19.62	-51.59
MP2//M06	19.04	-50.36
MP2//M06L	17.95	-51.18
MP2//M062X	17.92	-51.99
MP2//PBE0	19.12	-52.25
Avg.	18.73	-51.47
Std. dev.	0.76	0.74
CCSD(T)//B3LYP	20.43	-53.63
CCSD(T)//M06	20.40	-56.35
CCSD(T)//M06L	20.18	-55.00
CCSD(T)//M062X	18.48	-55.89
CCSD(T)//PEBE0	17.89	-56.57
Avg.	19.47	-55.49
Std. dev.	1.20	1.20
CCSD(T)//MP2	19.00	-56.98

Table S6B. Additional data used to construct Table 9 in the paper.

THF-phase reaction and activation energies: Dimers.2THF

	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}
	RR d1		RR d2		RS d1		RS d2	
B3LYP	20.48	-54.54	18.54	-56.36	19.26	-55.45	20.09	-54.22
M06	18.16	-60.44	15.19	-62.79	16.32	-63.68	20.24	-56.62
M06L	16.71	-59.95	16.68	-59.65	16.90	-59.27	17.03	-56.79
M062X	22.91	-60.63	21.08	-61.18	21.46	-61.94	24.10	-56.76
PBE0	22.03	-61.68	19.16	-63.97	19.68	-63.05	20.49	-62.60
Avg.	20.06	-59.45	18.13	-60.79	18.72	-60.68	20.39	-57.40
Std. dev.	2.60	2.82	2.27	2.97	2.11	3.38	2.51	3.10
MP2	20.01	-63.07	18.63	-62.61	17.39	-63.52	20.66	-61.54
MP2//B3LYP	21.46	-61.54	18.98	-63.29	20.14	-62.50	19.61	-61.82
MP2//M06	20.28	-61.41	17.81	-63.00	17.96	-64.56	22.83	-57.29
MP2//M06L	18.82	-62.22	20.14	-61.65	19.05	-61.90	19.49	-60.11
MP2//M062X	19.35	-63.32	19.26	-62.25	17.85	-63.87	21.35	-59.07
MP2//PBE0	21.21	-61.20	18.39	-63.25	18.09	-63.11	19.73	-61.27
Avg.	20.22	-61.94	18.92	-62.69	18.62	-63.19	20.60	-59.91
Std. dev.	1.15	0.86	0.88	0.72	0.97	1.06	1.46	1.81

Table S6C. Activation free energies $\Delta G^{\ddagger}$ and reaction free energies $\Delta_r G°$ of cyclopropanation reaction of oxiranyllithium monomer and disolvated dimers with ethylene (kcal/mol) in THF solvent. Each species listed is solvated by 2 THF molecules.

THF-phase reaction and activation energies: Dimers.2THF

	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}
	RR d1		RR d2		RS d1		RS d2	
B3LYP	20.48	-54.54	18.54	-56.36	19.26	-55.45	20.09	-54.22
M06	18.16	-60.44	15.19	-62.79	16.32	-63.68	20.24	-56.62
M06L	16.71	-59.95	16.68	-59.65	16.90	-59.27	17.03	-56.79
M062X	22.91	-60.63	21.08	-61.18	21.46	-61.94	24.10	-56.76
PBE0	22.03	-61.68	19.16	-63.97	19.68	-63.05	20.49	-62.60
Avg.	20.06	-59.45	18.13	-60.79	18.72	-60.68	20.39	-57.40
Std. dev.	2.60	2.82	2.27	2.97	2.11	3.38	2.51	3.10
MP2	20.01	-63.07	18.63	-62.61	17.39	-63.52	20.66	-61.54
MP2//B3LYP	21.46	-61.54	18.98	-63.29	20.14	-62.50	19.61	-61.82
MP2//M06	20.28	-61.41	17.81	-63.00	17.96	-64.56	22.83	-57.29
MP2//M06L	18.82	-62.22	20.14	-61.65	19.05	-61.90	19.49	-60.11
MP2//M062X	19.35	-63.32	19.26	-62.25	17.85	-63.87	21.35	-59.07
MP2//PBE0	21.21	-61.20	18.39	-63.25	18.09	-63.11	19.73	-61.27
Avg.	20.22	-61.94	18.92	-62.69	18.62	-63.19	20.60	-59.91
Std. dev.	1.15	0.86	0.88	0.72	0.97	1.06	1.46	1.81

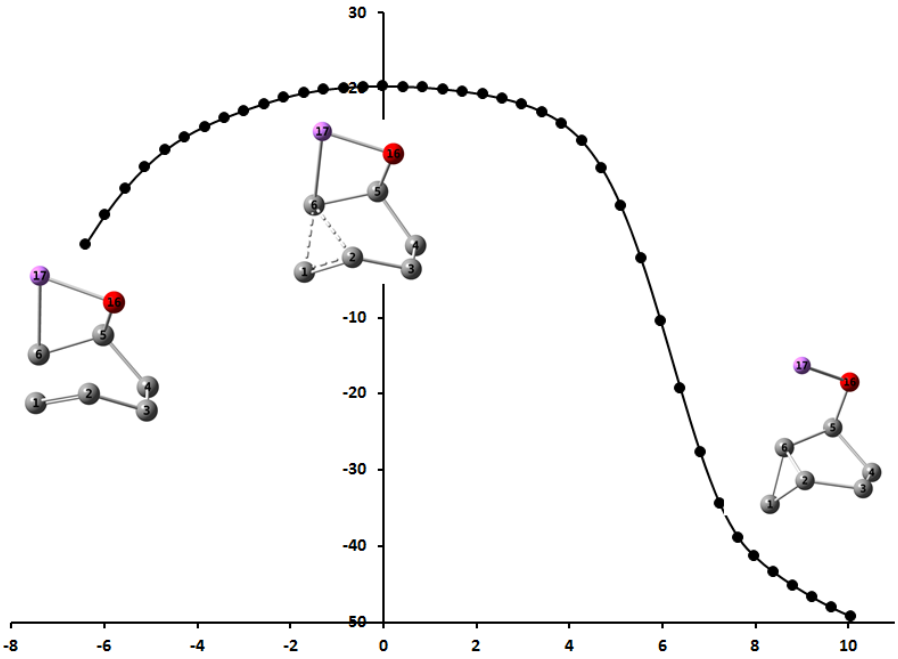

Figure S1. The M06-2X/6-31+G(d) IRC and associated structures for the concerted methylene transfer carbenoid reaction of lithio-2-epoxy-5-hexene. The vertical axis is Born-Oppenheimer energy relative to the reactant in kcal/mol. Hydrogens are not shown for clarity. $\Delta E^{\ddagger}$ = 20.4 kcal/mol.

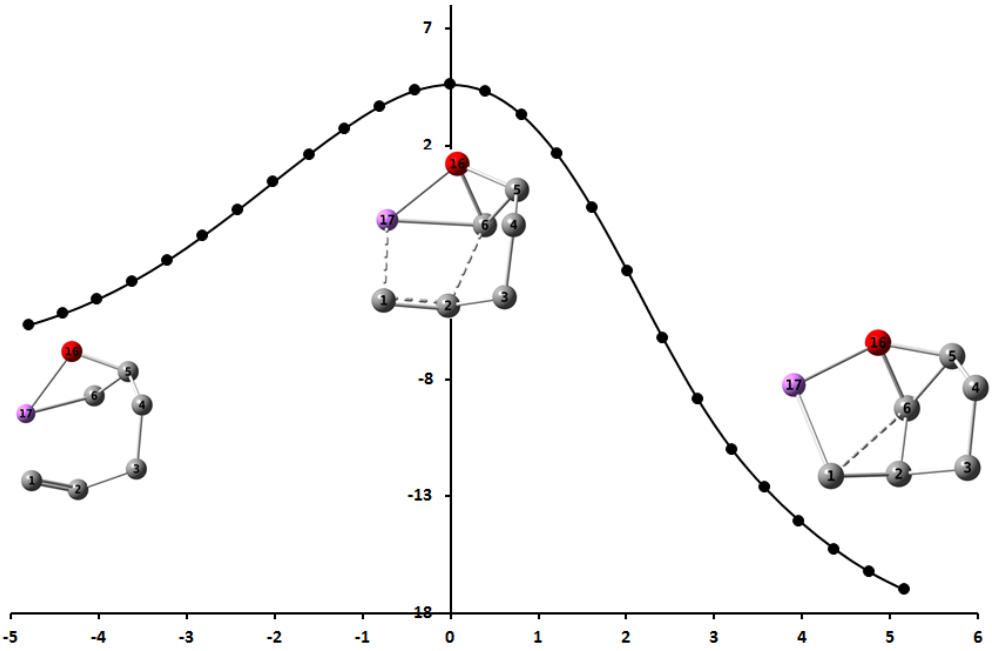

Figure S2. The M06-2X/6-31+G(d) IRC and associated structures for the stepwise carbolithiation carbenoid reaction of lithio-2-epoxy-5-hexene. The vertical axis is Born-Oppenheimer energy relative to the reactant in kcal/mol. Hydrogens are not shown for clarity. $\Delta E^{\ddagger}$ = 4.6 kcal/mol.

Table S7. M06-2X/6-31+G(d) geometry of α-lithio-dimethylether (CH_3-O-CH_2-Li).

SCF Done: E(RM062X) = -161.845824046 A.U. after 8 cycles
Convg = 0.8159D-08 -V/T = 2.0087

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327798	-0.027326	0.000020
2	1	0	1.985069	0.848645	-0.000028
3	1	0	1.525991	-0.635258	0.892679
4	1	0	1.526047	-0.635398	-0.892530
5	8	0	-0.007923	0.410848	-0.000060
6	6	0	-1.063029	-0.639341	0.000006
7	1	0	-0.891298	-1.261364	-0.891779
8	1	0	-0.891228	-1.261314	0.891813
9	3	0	-1.593270	1.219303	0.000059

Table S8. M06-2X/6-31+G(d) geometry of α-lithio-dimethylether + ethylene TS

SCF Done: E(RM062X) = -240.363664628 A.U. after 1 cycles
Convg = 0.3622D-08 -V/T = 2.0089

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.344909	-0.214537	0.047038
2	1	0	3.210349	0.368696	-0.298813
3	1	0	2.580976	-0.601524	1.053152
4	1	0	2.261627	-1.088977	-0.629528
5	8	0	1.198361	0.547934	0.034653
6	6	0	-0.311083	-0.826181	-0.126765
7	1	0	0.052740	-0.953559	-1.141453
8	3	0	0.015983	1.723078	-0.186701
9	1	0	0.287831	-1.296077	0.648349
10	6	0	-1.786750	0.789759	0.042893
11	6	0	-1.767645	-0.745572	0.058702
12	1	0	-2.120345	-1.197399	0.990573
13	1	0	-2.311984	-1.182806	-0.784845
14	1	0	-2.015264	1.188411	1.034278
15	1	0	-2.457354	1.189720	-0.720042

Table S9. M06-2X/6-31+G(d) geometry of CH_3-O-Li product

SCF Done: E(RM062X) = -122.617912862 A.U. after 10 cycles
Convg = 0.2445D-08 -V/T = 2.0089

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.931885	-0.000002	-0.000006
2	1	0	1.350367	-0.742435	0.703811
3	1	0	1.350283	-0.238408	-0.994903
4	1	0	1.350353	0.980782	0.290933
5	8	0	-0.441156	0.000019	0.000044
6	3	0	-2.037689	-0.000026	-0.000053

Table S10. M06-2X/6-31+G(d) geometry of cyclopropane

SCF Done: E(RM062X) = -117.834253604 A.U. after 11 cycles
Convg = 0.3858D-08 -V/T = 2.0093

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.197254	-0.844530	0.000006
2	1	0	-0.331259	-1.417832	-0.911274
3	1	0	-0.331282	-1.417875	0.911254
4	6	0	0.830063	0.251434	-0.000004
5	6	0	-0.632759	0.593133	-0.000007
6	1	0	-1.062408	0.995658	0.911280
7	1	0	-1.062489	0.995670	-0.911249
8	1	0	1.393539	0.422102	0.911272
9	1	0	1.393598	0.422059	-0.911250

Table S11. M06-2X/6-31+G(d) geometry of lithiated 1,2-epoxy-5-hexene [H_2C=CH-(CH_2)$_2$-CH(O-Li)CH]

SCF Done: E(RM062X) = -316.580231848 A.U. after 9 cycles
Convg = 0.5512D-08 -V/T = 2.0088

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.041758	0.772914	0.207000
2	6	0	2.562988	-0.459283	0.035228
3	6	0	1.119615	-0.830725	-0.169908
4	6	0	0.142337	0.341055	-0.208375
5	6	0	-1.269553	-0.142703	-0.433608
6	6	0	-2.153298	-0.582575	0.672484
7	1	0	1.039265	-1.408710	-1.102851
8	1	0	3.262308	-1.296208	0.044481
9	1	0	2.397663	1.648320	0.210424
10	1	0	4.103673	0.947128	0.353119
11	1	0	0.163501	0.889647	0.741816
12	1	0	0.430271	1.044469	-1.002148
13	1	0	-1.422669	-0.579351	-1.427373
14	1	0	-1.659170	-0.367856	1.631066
15	1	0	0.816823	-1.525103	0.627284
16	8	0	-2.276621	0.795508	-0.060665
17	3	0	-3.860590	-0.102831	-0.069143

Table S12. M06-2X/6-31+G(d) geometry of the methylene transfer TS of lithiated 1,2-epoxy-5-hexene

```
SCF Done:  E(RM062X) =  -316.547773299     A.U. after    1 cycles
             Convg  =    0.2420D-08             -V/T =  2.0087
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.575162	-1.053843	0.159918
2	6	0	-1.186049	-0.128645	-0.766921
3	6	0	-0.887442	1.285803	-0.409593
4	6	0	0.144530	1.286896	0.751418
5	6	0	1.051377	0.073485	0.488245
6	6	0	0.346198	-1.256321	0.703595
7	1	0	-0.471551	1.803748	-1.273221
8	1	0	-0.968791	-0.455612	-1.781814
9	1	0	-1.967581	-0.711627	1.114325
10	1	0	-1.836813	-2.063462	-0.133522
11	1	0	0.709973	2.224366	0.743465
12	1	0	-0.361025	1.195641	1.721450
13	1	0	1.820078	0.053199	1.306503
14	1	0	0.016209	-1.339492	1.751254
15	1	0	-1.805777	1.795740	-0.090093
16	8	0	1.605826	0.134981	-0.770892
17	3	0	1.552650	-1.608867	-0.917063

Table S13. M06-2X/6-31+G(d) geometry of the carbolithiation TS of lithiated 1,2-epoxy-5-hexene

```
SCF Done:  E(RM062X) =  -316.572882495     A.U. after    9 cycles
             Convg  =    0.8267D-08             -V/T =  2.0086
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.952716	-0.693351	-0.469557
2	6	0	-1.232135	-0.060341	0.563767
3	6	0	-0.709936	1.354966	0.330706
4	6	0	0.518730	1.326215	-0.586993
5	6	0	1.455496	0.299630	0.027733
6	6	0	0.771122	-0.696052	0.858591
7	1	0	-1.514483	1.971216	-0.085850
8	1	0	-1.541640	-0.275729	1.584887
9	1	0	-2.022679	-0.210355	-1.442001
10	1	0	-2.749158	-1.388844	-0.214476
11	1	0	0.251153	1.025946	-1.607083
12	1	0	0.996750	2.309041	-0.647451
13	1	0	2.486898	0.589684	0.222414
14	1	0	1.338615	-1.162309	1.671662
15	1	0	-0.408129	1.796996	1.287715
16	8	0	1.367260	-1.038760	-0.468353

17	3	0	-0.292924	-1.843990	-0.456157

Table S14A. M06-2X/6-31+G(d) geometry of the lithiated alcohol **2**

SCF Done: E(RM062X) = -316.670200828 A.U. after 9 cycles
Convg = 0.4007D-08 -V/T = 2.0087

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.544858	1.417852	-0.599783
2	6	0	1.398271	0.547902	0.289062
3	6	0	1.537871	-0.923483	-0.086363
4	6	0	0.102224	-1.385641	-0.380871
5	6	0	-0.848965	-0.510397	0.482086
6	6	0	-0.019125	0.792433	0.680925
7	1	0	2.223333	-1.082000	-0.927111
8	1	0	2.210444	1.040277	0.815915
9	1	0	0.779882	2.478819	-0.606303
10	1	0	0.256208	1.007125	-1.568778
11	1	0	-0.162452	-1.215600	-1.431479
12	1	0	-0.050804	-2.450792	-0.187213
13	1	0	-0.924382	-0.964009	1.491203
14	1	0	-0.258921	1.453717	1.512982
15	1	0	1.949212	-1.459616	0.777417
16	8	0	-2.083610	-0.302335	-0.080687
17	3	0	-1.881483	1.326251	-0.513824

Table S14B. M06-2X/6-31+G(d) geometry of the lithiated alcohol precursor **3**

SCF Done: E(RM062X) = -316.619695518 A.U. after 10 cycles
Convg = 0.4005D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.154708	0.048536	0.081952
2	6	0	0.827138	0.431987	-0.601709
3	6	0	-0.035757	1.377469	0.281248
4	6	0	-1.506702	0.919194	0.177655
5	6	0	-1.413195	-0.528774	-0.242574
6	6	0	-0.071213	-0.782030	-0.771365
7	1	0	0.309390	1.299257	1.320293
8	1	0	0.929732	0.885261	-1.605685
9	1	0	2.680041	0.969848	0.372441
10	1	0	2.807066	-0.460385	-0.644943
11	1	0	-2.068553	1.055009	1.108037
12	1	0	-2.043324	1.456103	-0.614333
13	1	0	-2.291132	-1.091348	-0.549211
14	1	0	0.139358	-1.558298	-1.502507
15	1	0	0.090134	2.424742	-0.007003
16	8	0	-0.480556	-1.311503	0.531024

17	3	0	1.187287	-1.095482	1.441161

Table S15. M06-2X/6-31+G(d) geometry of oxiranyllithium monomer “R”

SCF Done: E(RM062X) = -160.626401893 A.U. after 9 cycles
Convg = 0.4297D-08 -V/T = 2.0083

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.890580	-0.093906	0.266162
2	6	0	0.214031	0.871933	0.046052
3	8	0	0.227252	-0.604589	-0.456236
4	1	0	-1.044169	-0.543327	1.249764
5	1	0	-1.799137	-0.067615	-0.337665
6	1	0	-0.007312	1.486769	-0.834603
7	3	0	1.697297	-0.235759	0.566371

Table S16. M06-2X/6-31+G(d) geometry of R + ethylene TS (concerted)

SCF Done: E(RM062X) = -239.148020725 A.U. after 14 cycles
Convg = 0.8976D-08 -V/T = 2.0087

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.967079	-0.781492	0.353408
2	6	0	0.215156	0.293776	-0.344827
3	8	0	2.075596	-0.086401	-0.156549
4	1	0	0.895113	-0.783576	1.453259
5	1	0	0.903196	-1.811950	-0.021923
6	1	0	0.040241	0.014218	-1.392515
7	3	0	1.719699	1.628842	-0.012102
8	6	0	-1.710402	0.647489	0.387843
9	1	0	-1.904563	1.624153	-0.041836
10	1	0	-1.444932	0.635056	1.440472
11	6	0	-2.099815	-0.485103	-0.247652
12	1	0	-2.001400	-1.459280	0.221413
13	1	0	-2.483626	-0.461968	-1.262795

Table S17. M06-2X/6-31+G(d) geometry of R + ethylene TS (hydrogen transfer)

SCF Done: E(RM062X) = -239.142629348 A.U. after 1 cycles
Convg = 0.1246D-08 -V/T = 2.0087
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.137339	-0.468082	-0.901314
2	6	0	-2.002569	-0.365411	0.383123
3	1	0	-1.669927	-0.898002	1.268844

4	1	0	-2.774802	-0.835705	-0.219021
5	6	0	-1.476671	0.827174	0.046289
6	1	0	-1.852013	1.388097	-0.803657
7	1	0	-0.769112	1.320853	0.712126
8	3	0	1.198051	1.346682	-0.800425
9	1	0	-0.408224	-1.371877	-1.198577
10	6	0	1.131845	-0.680314	0.146488
11	1	0	0.984109	-1.467495	0.909804
12	1	0	1.634689	-1.260972	-0.756417
13	8	0	1.815182	0.400607	0.555082

Table S18. M06-2X/6-31+G(d) geometry of R + ethylene product (concerted)

SCF Done: E(RM062X) = -239.273197126 A.U. after 8 cycles
Convg = 0.6549D-08 -V/T = 2.0088
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.914561	-0.794204	-0.115810
2	6	0	0.373567	-0.235863	0.511823
3	8	0	-1.935560	0.126390	-0.087369
4	1	0	-0.651029	-1.107477	-1.149790
5	1	0	-1.161850	-1.724027	0.431326
6	1	0	0.341090	-0.122736	1.596639
7	3	0	-1.125535	1.576104	0.242774
8	6	0	1.104270	0.876040	-0.245599
9	1	0	1.582360	1.693708	0.289597
10	1	0	0.752291	1.119345	-1.248455
11	6	0	1.715290	-0.494918	-0.078343
12	1	0	1.754602	-1.124021	-0.962514
13	1	0	2.572234	-0.580552	0.581403

Table S19. M06-2X/6-31+G(d) geometry of monomer R·2THF

SCF Done: E(RM062X) = -625.382206493 A.U. after 8 cycles
Convg = 0.5777D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.503142	2.381540	0.646450
2	6	0	-0.228106	2.322930	-0.645953
3	8	0	-0.584322	1.471714	0.599656
4	1	0	1.488485	1.910214	0.736144
5	1	0	0.355743	3.192992	1.362869
6	1	0	-0.968994	3.137048	-0.662275
7	3	0	-0.201443	0.373430	-0.947311
8	8	0	1.408108	-0.576773	-0.551734
9	8	0	-1.788674	-0.685295	-1.097720
10	6	0	2.599871	-0.082532	-1.188883
11	1	0	2.600850	-0.451907	-2.216921
12	1	0	2.563227	1.014249	-1.199535

13	6	0	1.675795	-0.905373	0.824662
14	1	0	0.970594	-0.350424	1.451455
15	1	0	1.508508	-1.981951	0.948552
16	6	0	-2.937178	0.145240	-0.858648
17	1	0	-2.661139	1.161308	-1.146936
18	1	0	-3.754573	-0.210124	-1.498464
19	6	0	-1.875372	-1.775210	-0.181381
20	1	0	-2.603820	-2.506449	-0.561346
21	1	0	-0.889633	-2.245601	-0.134590
22	6	0	3.742880	-0.614440	-0.334409
23	1	0	3.961205	-1.655316	-0.597612
24	1	0	4.657672	-0.027552	-0.446329
25	6	0	3.139077	-0.529198	1.071440
26	1	0	3.212208	0.494555	1.452210
27	1	0	3.620352	-1.196560	1.790526
28	6	0	-3.274315	-0.002609	0.638809
29	1	0	-3.063912	0.922664	1.177099
30	1	0	-4.328906	-0.259326	0.773509
31	6	0	-2.345975	-1.137292	1.124119
32	1	0	-2.850611	-1.853889	1.777527
33	1	0	-1.492740	-0.709741	1.657204

Table S20. M06-2X/6-31+G(d) geometry of R·2THF + ethylene TS (concerted)

SCF Done: E(RM062X) = -703.902732467 A.U. after 10 cycles
Convg = 0.5327D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.756305	1.647642	1.389500
2	6	0	0.865238	1.824032	-0.077078
3	8	0	-0.490919	1.130716	1.016535
4	1	0	1.445696	0.910404	1.840793
5	1	0	0.684166	2.526398	2.045459
6	1	0	0.425937	2.788643	-0.371517
7	3	0	-0.345331	0.149572	-0.531850
8	6	0	2.764448	1.917357	-0.826377
9	1	0	2.570067	1.732203	-1.877972
10	1	0	3.170837	1.076629	-0.269259
11	6	0	2.897038	3.188145	-0.357233
12	1	0	3.211754	3.383765	0.663144
13	1	0	2.631723	4.045992	-0.966865
14	8	0	0.469954	-1.581451	-0.366936
15	8	0	-2.130987	-0.042446	-1.211819
16	6	0	1.630527	-1.765607	-1.199932
17	1	0	1.332733	-2.351393	-2.073381
18	1	0	1.976716	-0.776481	-1.525234
19	6	0	0.786686	-1.882109	1.007821
20	1	0	0.326552	-1.107557	1.628338
21	1	0	0.354949	-2.861091	1.252520
22	6	0	-2.898620	1.108143	-0.817040
23	1	0	-2.214837	1.957843	-0.790073
24	1	0	-3.674713	1.276200	-1.574355

25	6	0	-2.785445	-1.176333	-0.638311
26	1	0	-3.679415	-1.412292	-1.234098
27	1	0	-2.087014	-2.014927	-0.681158
28	6	0	2.665853	-2.458412	-0.317473
29	1	0	2.529731	-3.545180	-0.346506
30	1	0	3.689475	-2.229978	-0.624424
31	6	0	2.309540	-1.912956	1.068288
32	1	0	2.700973	-0.897171	1.189769
33	1	0	2.683424	-2.530460	1.888731
34	6	0	-3.499270	0.774208	0.563176
35	1	0	-3.039272	1.387686	1.338882
36	1	0	-4.580653	0.939362	0.565233
37	6	0	-3.151553	-0.715574	0.770094
38	1	0	-3.973867	-1.294285	1.199200
39	1	0	-2.277826	-0.798812	1.423474

Table S21. M06-2X/6-31+G(d) geometry of R·2THF + ethylene product

SCF Done: E(RM062X) = -704.029862260 A.U. after 7 cycles
Convg = 0.5624D-08 -V/T = 2.0087

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.642700	2.099574	1.013431
2	6	0	1.411985	2.621590	-0.195516
3	8	0	-0.440537	1.339069	0.661499
4	1	0	1.389166	1.531600	1.627395
5	1	0	0.359883	2.970879	1.638241
6	1	0	0.845957	3.305663	-0.826552
7	3	0	-0.410562	0.230598	-0.677875
8	6	0	2.332549	1.668345	-0.911224
9	1	0	2.407925	1.697227	-1.994928
10	1	0	2.448515	0.678417	-0.472707
11	6	0	2.893011	2.834094	-0.131380
12	1	0	3.389046	2.612782	0.810198
13	1	0	3.333266	3.653886	-0.690336
14	8	0	0.575554	-1.394814	-0.384004
15	8	0	-2.215707	-0.186466	-1.191540
16	6	0	1.570377	-2.093722	-1.148710
17	1	0	1.064370	-2.769596	-1.844237
18	1	0	2.142124	-1.354978	-1.722955
19	6	0	0.831198	-1.539963	1.030324
20	1	0	0.568998	-0.586444	1.497835
21	1	0	0.179958	-2.335863	1.418277
22	6	0	-3.042053	0.934897	-0.824478
23	1	0	-2.443093	1.835375	-0.964488
24	1	0	-3.911738	0.947187	-1.493880
25	6	0	-2.698311	-1.298454	-0.433204
26	1	0	-3.625365	-1.669618	-0.894385
27	1	0	-1.934920	-2.079255	-0.472815
28	6	0	2.450660	-2.819125	-0.128404
29	1	0	2.059222	-3.823041	0.069020
30	1	0	3.483871	-2.915542	-0.470466

31	6	0	2.297464	-1.939527	1.117250
32	1	0	2.936844	-1.052489	1.048538
33	1	0	2.533472	-2.464091	2.046377
34	6	0	-3.441969	0.713592	0.646464
35	1	0	-2.930001	1.434149	1.285264
36	1	0	-4.524528	0.807381	0.773763
37	6	0	-2.950561	-0.716770	0.955479
38	1	0	-3.669695	-1.306812	1.530192
39	1	0	-2.008374	-0.658116	1.508435

Table S22. M06-2X/6-31+G(d) geometry of dimer 1 RR

SCF Done: E(RM062X) = -321.339792277 A.U. after 8 cycles
Convg = 0.3949D-08 -V/T = 2.0082

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.290650	0.262501	0.784070
2	6	0	-1.658880	0.646308	-0.507418
3	8	0	-2.092329	-0.781446	-0.154103
4	1	0	-1.683628	0.182560	1.687632
5	1	0	-3.343804	0.464591	0.977528
6	1	0	-2.436998	1.019655	-1.184272
7	3	0	-0.376122	-1.158971	-0.636013
8	3	0	0.376094	1.159277	-0.635691
9	6	0	1.658850	-0.646123	-0.507672
10	6	0	2.290786	-0.262847	0.783888
11	8	0	2.092213	0.781527	-0.153750
12	1	0	3.343989	-0.464940	0.977083
13	1	0	1.683895	-0.183414	1.687582
14	1	0	2.436918	-1.019046	-1.184820

Table S23. M06-2X/6-31+G(d) geometry of dimer 1 RR + ethylene TS

SCF Done: E(RHF) = -397.516772414 A.U. after 10 cycles
Convg = 0.7462D-08 -V/T = 2.0023

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.832799	0.058570	0.765613
2	8	0	2.406756	-1.161308	-0.148037
3	3	0	0.665046	-0.512139	-0.127043
4	3	0	1.513913	1.692321	0.771319
5	6	0	-1.320116	0.082373	0.279753
6	6	0	-1.350405	1.302415	-0.569759
7	8	0	-0.009381	1.398064	-0.092230
8	1	0	-1.952098	2.169997	-0.273870
9	1	0	-1.405982	1.144952	-1.653580
10	1	0	-1.617810	0.352194	1.305827
11	6	0	-3.809687	-0.462337	0.336882

12	6	0	-2.956980	-1.347417	-0.238568
13	1	0	-4.247626	0.354560	-0.229212
14	1	0	-4.071535	-0.530195	1.388648
15	1	0	-2.583751	-2.206875	0.306945
16	1	0	-2.766721	-1.334958	-1.306889
17	6	0	3.551388	-0.350111	-0.469697
18	1	0	4.485511	-0.910447	-0.419958
19	1	0	3.441175	0.235803	-1.383244
20	1	0	3.320963	-0.410593	1.629297

Table S24. M06-2X/6-31+G(d) geometry of dimer 1 RR + ethylene Product

SCF Done: E(RM062X) = -399.999784732 A.U. after 8 cycles
Convg = 0.2796D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.352964	-0.711915	-0.614072
2	8	0	3.142426	0.483719	-0.047078
3	3	0	1.572942	1.417047	-0.046776
4	3	0	0.272875	-0.558352	-0.501929
5	6	0	-2.237872	0.110164	-0.459836
6	6	0	-1.487107	1.254548	0.206491
7	8	0	-0.126244	1.130893	-0.003314
8	1	0	-1.734825	1.235252	1.285323
9	1	0	-1.879528	2.207104	-0.188030
10	1	0	-2.248056	0.144680	-1.548988
11	6	0	-3.422471	-0.521173	0.194464
12	1	0	-3.737740	-0.118845	1.152608
13	1	0	-4.229113	-0.887967	-0.431051
14	6	0	-2.114023	-1.270407	0.161499
15	1	0	-2.057669	-2.148601	-0.476273
16	1	0	-1.575637	-1.352237	1.104743
17	6	0	3.219591	-0.778664	0.593590
18	1	0	4.218478	-1.213477	0.550241
19	1	0	2.768986	-0.811964	1.587421
20	1	0	2.941702	-1.042246	-1.479548

Table S25. M06-2X/6-31+G(d) geometry of dimer 1 RR·2THF

SCF Done: E(RM062X) = -786.087892589 A.U. after 9 cycles
Convg = 0.4184D-08 -V/T = 2.0084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.937035	-1.148786	1.941220
2	6	0	-1.666285	-0.408954	1.696512
3	8	0	-3.015133	-0.020086	1.092120
4	1	0	-3.112846	-2.105547	1.445568
5	1	0	-3.495473	-1.025890	2.869883

6	1	0	-1.515284	0.297806	2.528913
7	3	0	-2.044775	-0.041523	-0.493265
8	3	0	-0.184243	-1.343640	0.518765
9	6	0	-0.901201	-1.477307	-1.573490
10	6	0	-1.361931	-2.895076	-1.537537
11	8	0	-0.156167	-2.605000	-0.859809
12	1	0	-1.225608	-3.557622	-2.393078
13	1	0	-2.192949	-3.178592	-0.888953
14	1	0	-0.346018	-1.321940	-2.513574
15	1	0	-1.652259	3.647082	-0.050125
16	6	0	-1.410838	2.598211	0.170133
17	8	0	-1.754258	1.805956	-0.970790
18	1	0	-2.019221	2.247650	1.005333
19	6	0	0.103288	2.394728	0.352739
20	6	0	-0.685357	1.989774	-1.898421
21	6	0	0.582224	1.914751	-1.041206
22	1	0	0.594736	3.318085	0.672433
23	1	0	0.286450	1.623080	1.105522
24	1	0	-0.797305	2.974176	-2.374861
25	1	0	-0.760583	1.205238	-2.653096
26	1	0	1.392056	2.526213	-1.450612
27	1	0	0.921283	0.875642	-0.986054
28	1	0	4.233591	0.910981	1.507711
29	6	0	3.327265	0.681479	0.942071
30	6	0	2.391889	-0.258760	1.703077
31	6	0	3.613194	-0.093169	-0.366559
32	1	0	2.811962	1.622609	0.727346
33	8	0	1.657412	-0.920077	0.679737
34	1	0	2.955943	-1.004614	2.282165
35	1	0	1.674713	0.237838	2.360436
36	6	0	2.591165	-1.249094	-0.353147
37	1	0	4.635156	-0.479867	-0.394066
38	1	0	3.478674	0.548834	-1.240836
39	1	0	3.065996	-2.206160	-0.103361
40	1	0	2.020946	-1.372644	-1.275615

Table S26. M06-2X/6-31+G(d) geometry of dimer 1 RR·2THF + ethylene TS

SCF Done: E(RM062X) = -864.603188185 A.U. after 9 cycles
Convg = 0.4443D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.037992	-2.449653	-0.580346
2	8	0	1.002733	-1.659432	-1.368274
3	3	0	0.899803	0.055973	-0.627546
4	3	0	-0.979244	-1.267670	0.838999
5	6	0	-0.637528	1.473552	-0.262855
6	6	0	-0.276134	1.671004	1.162986
7	8	0	-0.060709	0.285312	1.061206
8	1	0	-1.038726	1.937838	1.908946
9	1	0	0.642451	2.246099	1.351854
10	1	0	-1.702849	1.203148	-0.340728

11	6	0	-1.678406	3.695629	-0.852389
12	6	0	-0.547154	3.253691	-1.449555
13	1	0	-1.649783	4.244272	0.084646
14	1	0	-2.658031	3.492599	-1.275628
15	1	0	-0.571983	2.787422	-2.428375
16	1	0	0.433684	3.550920	-1.090943
17	6	0	3.160937	0.828021	1.038367
18	6	0	3.786229	-0.212102	-0.987878
19	6	0	4.618173	0.373656	1.148670
20	1	0	2.497323	0.297996	1.730678
21	1	0	3.038217	1.905314	1.183448
22	6	0	4.689190	-0.753837	0.113853
23	1	0	3.308619	-0.981096	-1.600061
24	1	0	4.326875	0.489777	-1.636509
25	1	0	5.295906	1.186689	0.866085
26	1	0	4.874704	0.051095	2.160658
27	1	0	5.704562	-0.955124	-0.236878
28	1	0	4.272014	-1.680015	0.523157
29	6	0	-3.542776	-1.987483	-0.002585
30	6	0	-3.578337	-0.094720	1.330678
31	6	0	-3.892464	-0.850034	-0.951777
32	1	0	-4.442433	-2.490640	0.380436
33	1	0	-2.845724	-2.722272	-0.408228
34	6	0	-4.328945	0.255638	0.026403
35	1	0	-2.829267	0.648470	1.616095
36	1	0	-4.266271	-0.247687	2.169988
37	1	0	-2.991267	-0.555860	-1.501167
38	1	0	-4.671734	-1.114919	-1.670686
39	1	0	-4.074577	1.255570	-0.334261
40	1	0	-5.410611	0.221679	0.187804
41	8	0	2.747760	0.501675	-0.300383
42	8	0	-2.879223	-1.322721	1.078191
43	6	0	1.434813	-2.644620	-0.444550
44	1	0	1.956082	-3.480256	-0.916368
45	1	0	1.947920	-2.246957	0.437407
46	1	0	-0.408907	-3.200098	-1.295799

Table S27. M06-2X/6-31+G(d) geometry of dimer 1 RR·2THF + ethylene Product

SCF Done: E(RM062X) = -864.741702349 A.U. after 7 cycles
Convg = 0.6002D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.082148	-1.602046	-1.732668
2	8	0	1.347626	-1.892728	-0.920686
3	3	0	1.343497	-0.012138	-0.776769
4	3	0	-1.060869	0.043998	-1.066336
5	6	0	-0.826315	3.101753	-0.488596
6	6	0	-0.208906	2.180568	0.548161
7	8	0	0.063995	0.927037	0.040233
8	1	0	-0.921246	2.129571	1.401161
9	1	0	0.700766	2.669980	0.948953

10	1	0	-0.175280	3.331722	-1.330630
11	6	0	-1.794212	4.168424	-0.073158
12	1	0	-2.027126	4.249164	0.985373
13	1	0	-1.789856	5.114019	-0.605641
14	6	0	-2.290090	2.945003	-0.803054
15	1	0	-2.626214	3.066541	-1.828381
16	1	0	-2.848392	2.207866	-0.230119
17	1	0	-4.026248	-1.506119	-1.489884
18	6	0	-3.354298	-1.728057	-0.656998
19	8	0	-2.715699	-0.502705	-0.264675
20	6	0	-2.668892	-0.394121	1.173035
21	1	0	-3.364014	0.399194	1.475889
22	6	0	4.116243	-0.616465	-0.749454
23	8	0	3.192688	0.461023	-0.545171
24	1	0	3.677923	-1.290918	-1.486915
25	6	0	3.349224	0.978456	0.792781
26	1	0	2.352434	1.004176	1.244741
27	1	0	3.738074	1.999547	0.729094
28	1	0	5.065295	-0.210731	-1.126933
29	6	0	4.308234	0.019808	1.517250
30	6	0	4.277674	-1.232414	0.631611
31	1	0	3.993827	-0.173824	2.545551
32	1	0	5.320500	0.436729	1.545365
33	1	0	3.399438	-1.849230	0.849685
34	1	0	5.177546	-1.845944	0.724131
35	1	0	-1.648817	-0.110955	1.449734
36	1	0	-2.581527	-2.431219	-0.993597
37	6	0	-3.114076	-1.757012	1.698402
38	6	0	-4.067495	-2.227003	0.595504
39	1	0	-5.042472	-1.738111	0.700062
40	1	0	-4.221070	-3.308840	0.585119
41	1	0	-3.586816	-1.688442	2.681287
42	1	0	-2.258442	-2.436872	1.773640
43	6	0	0.134865	-2.515753	-0.551814
44	1	0	0.156473	-3.601673	-0.663005
45	1	0	-0.271184	-2.176639	0.406970
46	1	0	0.185037	-2.202440	-2.645944

Table S28. M06-2X/6-31+G(d) geometry of dimer 1 RR·4THF

SCF Done: E(RM062X) = -1250.81849563 A.U. after 10 cycles
Convg = 0.2523D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.899222	-2.076692	1.770377
2	6	0	-0.016024	-0.875482	1.789929
3	8	0	-1.516633	-0.828796	1.500587
4	1	0	-0.870188	-2.757986	0.914358
5	1	0	-1.255578	-2.543613	2.691601
6	1	0	0.067028	-0.552491	2.843498
7	3	0	-1.252380	-0.247883	-0.313994
8	3	0	1.358489	-0.352481	0.264917

9	6	0	0.150932	-1.107629	-1.659955
10	6	0	0.839745	-2.427604	-1.555586
11	8	0	1.641352	-1.271831	-1.387950
12	1	0	1.102495	-3.009405	-2.441880
13	1	0	0.725396	-3.031715	-0.650683
14	1	0	0.092175	-0.853286	-2.733975
15	1	0	-4.967530	-0.142789	-0.443271
16	6	0	-4.073266	-0.622066	-0.017062
17	1	0	-3.671992	-0.010561	0.794788
18	8	0	-3.066644	-0.715924	-1.032973
19	6	0	-4.354630	-2.059133	0.399063
20	6	0	-3.054367	-2.043486	-1.594010
21	6	0	-4.219488	-2.789441	-0.940600
22	1	0	-3.581433	-2.387253	1.101989
23	1	0	-5.336091	-2.181712	0.864736
24	1	0	-2.086470	-2.498856	-1.356487
25	1	0	-3.143446	-1.957301	-2.680836
26	1	0	-4.016280	-3.858059	-0.834431
27	1	0	-5.135675	-2.671023	-1.530324
28	1	0	-0.398399	1.554102	1.584280
29	6	0	-1.099803	2.252697	1.126266
30	8	0	-1.512189	1.690869	-0.118073
31	1	0	-0.599358	3.216956	0.935363
32	6	0	-2.407831	2.438472	1.888161
33	6	0	-2.676761	2.406380	-0.527474
34	6	0	-3.395467	2.841194	0.771231
35	1	0	-2.686047	1.479206	2.335697
36	1	0	-2.335574	3.186899	2.681719
37	1	0	-3.259566	1.739259	-1.165760
38	1	0	-2.363642	3.279757	-1.116757
39	1	0	-4.363820	2.346723	0.886542
40	1	0	-3.575291	3.920173	0.767765
41	1	0	5.592156	-1.962459	-0.820244
42	6	0	4.593660	-1.899287	-0.379271
43	6	0	4.186921	-0.467012	-0.050939
44	6	0	4.490555	-2.565676	0.995984
45	1	0	3.865091	-2.331493	-1.072752
46	8	0	3.221367	-0.569843	1.005407
47	1	0	5.041426	0.120514	0.314207
48	1	0	3.714744	0.049796	-0.891695
49	6	0	3.244698	-1.893400	1.567993
50	1	0	5.371162	-2.327150	1.603778
51	1	0	4.389360	-3.652908	0.946498
52	1	0	3.247447	-1.798101	2.657185
53	1	0	2.328255	-2.415948	1.264643
54	1	0	0.349785	2.179867	-1.762669
55	6	0	1.408136	1.928543	-1.624242
56	8	0	1.580848	1.493853	-0.265346
57	1	0	1.664771	1.092931	-2.280256
58	6	0	2.319339	3.145765	-1.772892
59	6	0	2.321781	2.454730	0.488714
60	6	0	2.303754	3.726206	-0.355315
61	1	0	1.963763	3.844291	-2.534623
62	1	0	3.335794	2.833200	-2.039683
63	1	0	1.846953	2.558734	1.469205
64	1	0	3.344543	2.083279	0.636869
65	1	0	1.375916	4.285127	-0.185606

66	1	0	3.149028	4.385284	-0.141005

Table S29. M06-2X/6-31+G(d) geometry of dimer 1 RR·4THF + ethylene TS

SCF Done: E(RM062X) = -1329.33754491 A.U. after 9 cycles
Convg = 0.5607D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.420456	-1.508272	1.625074
2	8	0	-0.787322	-2.148999	0.955025
3	3	0	-1.128579	-0.669730	-0.217744
4	3	0	1.482605	-0.190663	0.387411
5	6	0	-0.493106	1.171290	-1.644941
6	6	0	0.316778	0.229369	-2.448239
7	8	0	0.480562	-0.320819	-1.165093
8	1	0	1.267018	0.542851	-2.908019
9	1	0	-0.245160	-0.422183	-3.132103
10	1	0	0.161234	1.954874	-1.226411
11	6	0	-0.867981	3.107694	-3.234102
12	6	0	-1.852391	2.301182	-2.757773
13	1	0	-0.285588	2.837195	-4.109867
14	1	0	-0.598260	4.029410	-2.725761
15	1	0	-2.506135	2.638171	-1.958487
16	1	0	-2.217211	1.457415	-3.337336
17	6	0	0.462810	-2.801938	0.870424
18	1	0	0.304909	-1.751036	2.695347
19	1	0	0.481945	-3.769039	1.378428
20	1	0	0.888895	-2.817102	-0.137361
21	1	0	4.935346	-3.579823	0.981453
22	6	0	4.727702	-2.745095	0.307276
23	6	0	3.879990	-1.659870	0.964967
24	6	0	3.851020	-3.129718	-0.888599
25	1	0	5.681904	-2.330275	-0.037121
26	1	0	4.460328	-0.914692	1.516254
27	8	0	3.215322	-0.990733	-0.115482
28	1	0	3.118615	-2.088588	1.630065
29	6	0	3.293895	-1.773286	-1.317121
30	1	0	4.401388	-3.627751	-1.690908
31	1	0	3.039485	-3.789877	-0.562972
32	1	0	3.973684	-1.263978	-2.013204
33	1	0	2.293086	-1.812201	-1.756102
34	8	0	2.204136	1.582435	0.738266
35	6	0	1.935354	2.653221	1.631643
36	6	0	2.812220	2.128028	-0.438435
37	1	0	1.198787	2.300032	2.358016
38	1	0	2.858335	2.930179	2.163771
39	6	0	1.461579	3.783878	0.723281
40	1	0	2.472898	1.522377	-1.283087
41	1	0	3.901141	2.032553	-0.349315
42	6	0	2.362998	3.604378	-0.514506
43	1	0	0.410113	3.630262	0.456815
44	1	0	1.562218	4.769723	1.184730

45	1	0	1.824937	3.813333	-1.442696
46	1	0	3.227946	4.272513	-0.465791
47	1	0	-2.247127	0.777659	4.421132
48	6	0	-1.775389	0.777333	3.434893
49	6	0	-2.488147	-0.140107	2.445035
50	6	0	-1.854917	2.123970	2.711548
51	1	0	-0.730136	0.464583	3.537762
52	1	0	-3.576723	-0.120430	2.597447
53	8	0	-2.210273	0.401382	1.140933
54	1	0	-2.130672	-1.171009	2.468731
55	6	0	-1.598690	1.694686	1.272187
56	1	0	-2.856206	2.558646	2.814007
57	1	0	-1.124303	2.858389	3.064611
58	1	0	-2.026904	2.353535	0.511869
59	1	0	-0.524300	1.585895	1.075715
60	1	0	-5.630873	-1.190563	-0.814454
61	6	0	-4.627712	-1.063658	-0.396936
62	6	0	-3.655820	-0.507405	-1.459574
63	6	0	-4.001816	-2.418721	0.003037
64	1	0	-4.699074	-0.388255	0.458887
65	8	0	-2.510845	-1.362214	-1.435441
66	1	0	-4.097901	-0.541646	-2.465214
67	1	0	-3.299055	0.502483	-1.251154
68	6	0	-2.987456	-2.665184	-1.111465
69	1	0	-4.738977	-3.221640	0.089278
70	1	0	-3.462790	-2.336069	0.951225
71	1	0	-3.460737	-3.107641	-2.001539
72	1	0	-2.129058	-3.266158	-0.807369

Table S30. M06-2X/6-31+G(d) geometry of dimer 1 RR·4THF + ethylene Product

SCF Done: E(RM062X) = -1329.47678098 A.U. after 9 cycles
Convg = 0.2747D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037113	-0.923907	-2.277642
2	6	0	0.194848	-2.421442	-2.066558
3	8	0	0.058942	-0.194772	-1.112943
4	1	0	0.840371	-0.614416	-2.982580
5	1	0	-0.910533	-0.768418	-2.841818
6	1	0	-0.578308	-2.873044	-1.445165
7	3	0	-1.218114	0.125493	0.137324
8	3	0	1.284216	0.515419	0.033206
9	6	0	-0.387930	1.382062	1.635461
10	6	0	0.142208	2.734070	1.276591
11	8	0	1.092698	1.719027	1.542368
12	1	0	0.173620	3.554435	1.996992
13	1	0	0.118322	3.064535	0.233451
14	1	0	-0.606431	1.391610	2.720305
15	6	0	1.566684	-3.012605	-1.932177
16	1	0	2.414431	-2.336306	-2.008733
17	1	0	1.714773	-3.834421	-1.237635

18	6	0	0.749580	-3.273719	-3.172218
19	1	0	1.046169	-2.769151	-4.088531
20	1	0	0.348052	-4.271390	-3.319750
21	1	0	-2.620562	-1.615996	2.764317
22	6	0	-3.053245	-1.141435	1.878673
23	8	0	-2.226753	-1.457047	0.748160
24	1	0	-3.035419	-0.053628	2.023964
25	6	0	-4.452664	-1.655164	1.536091
26	6	0	-3.026667	-1.958388	-0.332186
27	6	0	-4.462068	-1.571641	0.005856
28	1	0	-4.567773	-2.695566	1.859796
29	1	0	-5.239677	-1.061592	2.009002
30	1	0	-2.903549	-3.048530	-0.383861
31	1	0	-2.658208	-1.510220	-1.260168
32	1	0	-5.195747	-2.236404	-0.457607
33	1	0	-4.651584	-0.546557	-0.327112
34	1	0	-4.692646	3.076581	-1.268235
35	6	0	-3.751734	3.254161	-0.734676
36	6	0	-3.419345	2.072082	0.171240
37	6	0	-2.572202	3.226849	-1.710553
38	1	0	-3.838656	4.192030	-0.180301
39	1	0	-4.303943	1.596566	0.610054
40	8	0	-2.767413	1.111429	-0.671725
41	1	0	-2.725807	2.356685	0.973116
42	6	0	-2.362925	1.728088	-1.911328
43	1	0	-2.771652	3.749649	-2.649518
44	1	0	-1.687316	3.673342	-1.244934
45	1	0	-3.006152	1.336465	-2.710382
46	1	0	-1.324388	1.440291	-2.095797
47	1	0	-0.180083	-1.078420	2.631779
48	6	0	0.747265	-1.645879	2.740728
49	6	0	1.279011	-2.020643	1.353357
50	6	0	1.857739	-0.745609	3.334084
51	1	0	0.548884	-2.532465	3.350206
52	8	0	2.165207	-0.957022	0.997313
53	1	0	1.851654	-2.960498	1.379591
54	1	0	0.512715	-2.072892	0.578440
55	6	0	2.870450	-0.607375	2.185306
56	1	0	2.323459	-1.184263	4.221223
57	1	0	1.457097	0.235634	3.597244
58	1	0	3.719582	-1.297317	2.308888
59	1	0	3.242368	0.411972	2.059477
60	1	0	3.282742	2.445922	0.870435
61	6	0	3.725271	2.236562	-0.106131
62	8	0	2.772353	1.460923	-0.833816
63	1	0	3.887323	3.183956	-0.636747
64	6	0	5.023453	1.395671	-0.057548
65	6	0	3.497627	0.628581	-1.730983
66	6	0	4.690906	0.151457	-0.907776
67	1	0	5.300146	1.125889	0.965120
68	1	0	5.858998	1.955706	-0.487652
69	1	0	2.820427	-0.163778	-2.055722
70	1	0	3.816352	1.218050	-2.604541
71	1	0	4.372102	-0.680106	-0.272383
72	1	0	5.530027	-0.177637	-1.526352

Table S31. M06-2X/6-31+G(d) geometry of dimer 1 RS

SCF Done: E(RM062X) = -321.340052365 A.U. after 15 cycles
Convg = 0.3479D-08 -V/T = 2.0081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.655429	0.293263	-0.474660
2	6	0	1.594664	0.609155	0.520755
3	8	0	2.121248	-0.804729	0.244374
4	1	0	2.423863	0.293013	-1.541098
5	1	0	3.706491	0.475275	-0.252090
6	1	0	2.071809	0.911210	1.460930
7	3	0	0.344061	-1.166791	0.072837
8	3	0	-0.344019	1.166948	-0.072402
9	6	0	-1.594422	-0.609121	-0.520451
10	8	0	-2.121280	0.804671	-0.244553
11	6	0	-2.655640	-0.293258	0.474470
12	1	0	-3.706576	-0.475451	0.251458
13	1	0	-2.424533	-0.292794	1.541004
14	1	0	-2.071117	-0.911496	-1.460759

Table S32. M06-2X/6-31+G(d) geometry of dimer 1 RS + ethylene TS

SCF Done: E(RM062X) = -399.858971851 A.U. after 9 cycles
Convg = 0.2592D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.897934	-1.134213	0.554859
2	6	0	2.960572	0.312106	0.213248
3	8	0	2.400771	-0.765794	-0.722807
4	1	0	3.782552	-1.768794	0.496439
5	1	0	2.139564	-1.499866	1.250227
6	3	0	0.697462	-0.108373	-0.860096
7	3	0	1.557913	1.715098	0.742057
8	6	0	-1.146570	0.048791	0.114106
9	6	0	-1.389620	1.480847	-0.212538
10	8	0	0.009918	1.526625	-0.071133
11	1	0	-1.908203	2.129387	0.504613
12	1	0	-1.726823	1.697651	-1.234425
13	1	0	-1.164271	-0.071105	1.208866
14	1	0	3.960842	0.528036	-0.184788
15	6	0	-3.531472	-0.729834	0.549961
16	6	0	-2.837000	-1.280905	-0.464696
17	1	0	-4.112837	0.177675	0.413387
18	1	0	-3.522188	-1.163067	1.545797
19	1	0	-2.311982	-2.222648	-0.347512
20	1	0	-2.911354	-0.894838	-1.476597

Table S33. M06-2X/6-31+G(d) geometry of dimer 1 RS + ethylene Product

SCF Done: E(RM062X) = -399.999595118 A.U. after 9 cycles
Convg = 0.3088D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.157352	-0.505804	0.682715
2	6	0	2.780086	0.337435	-0.483680
3	8	0	2.163930	-1.041187	-0.174842
4	1	0	4.075770	-1.093475	0.683208
5	1	0	2.802122	-0.245134	1.681594
6	3	0	0.505530	-0.296501	-0.297562
7	3	0	1.452995	1.936091	-0.289441
8	6	0	-1.929930	-0.102772	0.548257
9	6	0	-1.522313	1.306726	0.146067
10	8	0	-0.159077	1.374488	-0.079137
11	1	0	-1.842712	2.004429	0.938336
12	1	0	-2.095822	1.576271	-0.761499
13	1	0	-1.585795	-0.412161	1.534981
14	1	0	3.492265	0.142381	-1.295593
15	6	0	-3.214196	-0.701717	0.075705
16	6	0	-1.915696	-1.175332	-0.526366
17	1	0	-3.853651	-0.084725	-0.548665
18	1	0	-3.743442	-1.382705	0.733457
19	1	0	-1.585008	-2.180715	-0.280762
20	1	0	-1.709942	-0.860553	-1.548403

Table S34. M06-2X/6-31+G(d) geometry of dimer 1 RS·2THF

SCF Done: E(RM062X) = -786.085220886 A.U. after 8 cycles
Convg = 0.5236D-08 -V/T = 2.0084
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.922987	2.445875	0.277372
2	6	0	0.150971	1.636784	-0.713001
3	8	0	-0.408956	2.128217	0.618057
4	1	0	1.675564	1.958011	0.904913
5	1	0	1.093632	3.514910	0.138667
6	1	0	-0.267590	2.316515	-1.468811
7	3	0	-0.772764	0.307386	0.803378
8	3	0	0.968403	-0.312218	-0.893522
9	6	0	0.072577	-1.624154	0.668979
10	8	0	0.496959	-2.112711	-0.715289
11	1	0	-3.015358	2.151578	-0.175046
12	6	0	-3.183102	1.107398	-0.447331
13	8	0	-2.661957	0.285282	0.614321
14	1	0	-2.616929	0.884032	-1.359914
15	6	0	-4.650568	0.708290	-0.576603
16	6	0	-3.595691	-0.741034	0.968271
17	6	0	-4.609323	-0.769020	-0.171300

18	1	0	-5.267489	1.277474	0.127600
19	1	0	-5.038226	0.871349	-1.585107
20	1	0	-4.071128	-0.469398	1.919341
21	1	0	-3.040581	-1.674287	1.100042
22	1	0	-5.579393	-1.164677	0.139476
23	1	0	-4.233049	-1.380101	-0.999767
24	1	0	4.550958	-0.987894	1.808423
25	6	0	3.815913	-0.509888	1.155974
26	6	0	3.467427	-1.347257	-0.068242
27	6	0	4.335664	0.793860	0.517784
28	1	0	2.901496	-0.327359	1.731154
29	8	0	2.890028	-0.390519	-0.961159
30	1	0	4.366854	-1.776003	-0.534617
31	1	0	2.727346	-2.131448	0.095408
32	6	0	3.704539	0.785319	-0.894438
33	1	0	5.427343	0.786018	0.448083
34	1	0	4.047109	1.677713	1.091927
35	1	0	4.471197	0.723263	-1.676383
36	1	0	3.055342	1.639740	-1.097308
37	6	0	-0.806361	-2.399931	-0.257615
38	1	0	-0.990284	-3.466232	-0.115408
39	1	0	-1.600819	-1.883891	-0.806262
40	1	0	0.538299	-2.324414	1.377485

Table S35. M06-2X/6-31+G(d) geometry of dimer 1 RS·2THF + ethylene TS

SCF Done: E(RM062X) = -864.607882002 A.U. after 9 cycles
Convg = 0.7030D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246799	-1.515253	2.180598
2	6	0	-0.687532	-1.825955	0.788038
3	8	0	-1.407286	-0.854240	1.715817
4	1	0	-0.444209	-2.197530	3.008925
5	1	0	0.610605	-0.856053	2.342918
6	3	0	-1.095986	0.441044	0.385720
7	3	0	0.412568	-1.132859	-0.860157
8	6	0	0.717894	1.505242	0.090827
9	6	0	0.415401	1.880155	-1.314152
10	8	0	-0.041514	0.551131	-1.325722
11	1	0	1.228077	2.065410	-2.031766
12	1	0	-0.387665	2.618276	-1.455660
13	1	0	1.715364	1.040044	0.136341
14	1	0	-1.294450	-2.744542	0.817490
15	6	0	2.157522	3.397211	0.898016
16	6	0	0.945377	3.133736	1.441621
17	1	0	2.262227	4.031030	0.022266
18	1	0	3.065777	2.958688	1.302237
19	1	0	0.852074	2.579639	2.369561
20	1	0	0.054481	3.660198	1.113070
21	6	0	-3.193905	0.495066	-1.476302
22	6	0	-3.923643	0.378732	0.676144

23	6	0	-3.576027	-0.978341	-1.307770
24	1	0	-2.305005	0.665087	-2.085639
25	1	0	-4.036942	1.090056	-1.856886
26	6	0	-4.180506	-1.031565	0.117487
27	1	0	-3.564266	0.383048	1.705367
28	1	0	-4.812849	1.018122	0.587829
29	1	0	-4.272523	-1.313766	-2.080801
30	1	0	-2.676254	-1.599006	-1.358977
31	1	0	-5.248878	-1.264163	0.106896
32	1	0	-3.668122	-1.777140	0.729349
33	6	0	2.870247	-2.202629	0.136780
34	6	0	3.152488	-0.645596	-1.565225
35	6	0	3.618798	-1.044811	0.785165
36	1	0	3.557038	-2.994097	-0.195534
37	1	0	2.077386	-2.634259	0.751841
38	6	0	4.135859	-0.264203	-0.437338
39	1	0	2.544633	0.191407	-1.918937
40	1	0	3.666713	-1.101159	-2.418865
41	1	0	2.917145	-0.437581	1.366530
42	1	0	4.421798	-1.377443	1.447634
43	1	0	4.151043	0.814479	-0.261110
44	1	0	5.152061	-0.577699	-0.693873
45	8	0	-2.891517	0.930796	-0.148196
46	8	0	2.247062	-1.609731	-1.005678

Table S36. M06-2X/6-31+G(d) geometry of dimer 1 RS·2THF + ethylene Product

SCF Done: E(RM062X) = -864.745491877 A.U. after 7 cycles
Convg = 0.7654D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.987373	-1.409598	1.997285
2	6	0	0.202968	-1.912527	0.828404
3	8	0	-0.397193	-1.129694	1.996091
4	1	0	1.295108	-2.065359	2.813765
5	1	0	1.625150	-0.527322	1.876599
6	3	0	-1.000853	0.056545	0.685510
7	3	0	0.778791	-0.740437	-0.827860
8	6	0	-0.374853	2.904122	0.437057
9	6	0	-0.108668	2.168637	-0.863963
10	8	0	-0.036186	0.805678	-0.668613
11	1	0	0.820038	2.572243	-1.314096
12	1	0	-0.925025	2.439234	-1.567856
13	1	0	0.422655	2.816068	1.174713
14	1	0	-0.071561	-2.960690	1.022113
15	6	0	-1.169435	4.174379	0.451247
16	6	0	-1.781591	2.901355	0.978794
17	1	0	-1.533810	4.547533	-0.502125
18	1	0	-0.904739	4.947310	1.165473
19	1	0	-1.936750	2.813988	2.049776
20	1	0	-2.548226	2.424102	0.372081
21	6	0	-3.161545	-0.108504	-1.083206

22	6	0	-3.229425	-1.696355	0.643058
23	6	0	-3.586493	-1.460190	-1.683718
24	1	0	-2.260993	0.303007	-1.550273
25	1	0	-3.965871	0.634335	-1.119000
26	6	0	-3.073405	-2.476243	-0.654381
27	1	0	-2.579977	-2.028294	1.455805
28	1	0	-4.274729	-1.683647	0.983227
29	1	0	-4.677050	-1.520379	-1.762961
30	1	0	-3.167095	-1.614048	-2.680921
31	1	0	-3.636839	-3.413115	-0.659779
32	1	0	-2.012038	-2.693318	-0.814427
33	6	0	3.530077	-1.640636	-0.462437
34	6	0	3.176786	0.656940	-0.897173
35	6	0	4.521876	-0.826244	0.365563
36	1	0	4.036070	-2.212572	-1.249411
37	1	0	2.906526	-2.313831	0.133004
38	6	0	4.621044	0.468614	-0.447165
39	1	0	2.565800	1.151863	-0.131729
40	1	0	3.065597	1.198298	-1.839747
41	1	0	4.109467	-0.619409	1.359148
42	1	0	5.479494	-1.337974	0.489268
43	1	0	4.990988	1.317688	0.132687
44	1	0	5.277270	0.326309	-1.313065
45	8	0	-2.831549	-0.363597	0.296825
46	8	0	2.669735	-0.676492	-1.093229

Table S37. M06-2X/6-31+G(d) geometry of dimer 1 RS·4THF

SCF Done: E(RM062X) = -1250.81690264 A.U. after 9 cycles
Convg = 0.4272D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.385912	-2.060225	-1.616661
2	6	0	-0.019618	-0.620485	-1.617557
3	8	0	1.423241	-1.103162	-1.577689
4	1	0	0.276130	-2.645739	-0.696856
5	1	0	0.386067	-2.665489	-2.526746
6	1	0	-0.184069	-0.317829	-2.667462
7	3	0	1.497963	-0.047147	0.006188
8	3	0	-1.069355	-0.134569	0.209445
9	6	0	0.450656	-0.210639	1.861578
10	8	0	-1.028235	-0.015634	2.163525
11	1	0	5.167443	0.049955	-0.332159
12	6	0	4.233142	-0.449245	-0.623777
13	1	0	3.718296	0.149704	-1.379109
14	8	0	3.385457	-0.526679	0.534796
15	6	0	4.478695	-1.891949	-1.053955
16	6	0	3.325675	-1.879199	1.012683
17	6	0	4.446873	-2.622592	0.291772
18	1	0	3.653635	-2.226168	-1.690758
19	1	0	5.422185	-2.013915	-1.592895
20	1	0	2.342137	-2.296409	0.758521

21	1	0	3.429518	-1.858461	2.100909
22	1	0	4.245513	-3.693283	0.202055
23	1	0	5.397363	-2.491667	0.822122
24	1	0	0.950840	2.397935	-2.057252
25	6	0	0.999484	2.652513	-0.995487
26	8	0	1.970786	1.788720	-0.394376
27	1	0	0.017727	2.471493	-0.538202
28	6	0	1.507332	4.057550	-0.696633
29	6	0	2.632771	2.463653	0.688215
30	6	0	2.043292	3.878685	0.728518
31	1	0	2.318471	4.323174	-1.384064
32	1	0	0.723611	4.816132	-0.770712
33	1	0	3.706201	2.468734	0.465954
34	1	0	2.466245	1.895366	1.608564
35	1	0	2.785521	4.629319	1.012147
36	1	0	1.217385	3.927417	1.446376
37	1	0	-2.769987	-4.297763	1.551692
38	6	0	-2.354457	-3.473820	0.965775
39	6	0	-2.998908	-2.128975	1.286852
40	6	0	-2.618043	-3.615382	-0.547941
41	1	0	-1.280590	-3.408440	1.169461
42	8	0	-2.697616	-1.336060	0.137893
43	1	0	-4.092860	-2.222145	1.382235
44	1	0	-2.586036	-1.618356	2.156913
45	6	0	-2.933358	-2.170216	-0.998644
46	1	0	-3.469216	-4.274372	-0.742665
47	1	0	-1.753116	-4.023304	-1.076700
48	1	0	-3.986808	-2.067135	-1.296599
49	1	0	-2.289892	-1.813624	-1.805037
50	1	0	-3.173446	2.694074	1.259047
51	6	0	-3.225034	1.688383	0.821185
52	8	0	-2.129465	1.542841	-0.098806
53	1	0	-3.098643	0.945240	1.611417
54	6	0	-4.488756	1.507886	-0.014277
55	6	0	-2.612060	1.561517	-1.449964
56	6	0	-4.046294	2.075416	-1.366255
57	1	0	-5.353171	2.022125	0.414039
58	1	0	-4.720216	0.441177	-0.109374
59	1	0	-1.941360	2.189766	-2.043760
60	1	0	-2.575185	0.541450	-1.851926
61	1	0	-4.062988	3.171224	-1.343642
62	1	0	-4.659407	1.737499	-2.205804
63	6	0	-0.115913	1.004174	2.521605
64	1	0	-0.042809	1.161388	3.599545
65	1	0	-0.228513	1.929444	1.946302
66	1	0	0.816521	-0.885876	2.652587

Table S38. M06-2X/6-31+G(d) geometry of dimer 1 RS·4THF + ethylene TS

SCF Done: E(RM062X) = -1329.33775689 A.U. after 9 cycles
Convg = 0.3940D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.040692	0.636565	-2.134567
2	8	0	-0.416393	0.917037	-1.771789
3	3	0	-0.894129	0.231162	-0.019629
4	3	0	1.973674	-0.195843	-0.473633
5	6	0	-0.762097	-1.205775	1.849764
6	6	0	0.600003	-0.681332	2.106187
7	8	0	0.613093	-0.679951	0.700396
8	1	0	1.379555	-1.323245	2.544022
9	1	0	0.644887	0.324838	2.553350
10	1	0	-0.706062	-2.297564	1.693425
11	6	0	-1.378565	-2.139165	4.115246
12	6	0	-2.020693	-1.081567	3.564384
13	1	0	-0.465374	-2.010711	4.688658
14	1	0	-1.729966	-3.156121	3.968359
15	1	0	-2.987130	-1.199203	3.083331
16	1	0	-1.732569	-0.062747	3.808134
17	1	0	4.617487	3.259834	-1.301125
18	6	0	4.244401	2.863035	-0.353656
19	6	0	4.259316	1.334101	-0.322678
20	6	0	2.763107	3.167335	-0.106823
21	1	0	4.857244	3.272028	0.457735
22	1	0	5.185801	0.911348	0.076409
23	8	0	3.176836	0.945067	0.542609
24	1	0	4.069169	0.908236	-1.315103
25	6	0	2.403694	2.097966	0.917387
26	1	0	2.581719	4.181346	0.260546
27	1	0	2.186597	3.006922	-1.024394
28	1	0	2.692983	2.399379	1.933573
29	1	0	1.348901	1.807118	0.915037
30	8	0	3.131506	-1.739264	-0.784604
31	6	0	2.517679	-2.638807	-1.706397
32	6	0	3.282400	-2.449521	0.448484
33	1	0	2.121476	-2.039011	-2.528978
34	1	0	3.277132	-3.338209	-2.087983
35	6	0	1.457616	-3.360723	-0.875648
36	1	0	3.268867	-1.704988	1.248214
37	1	0	4.257392	-2.955143	0.443303
38	6	0	2.120345	-3.463752	0.514305
39	1	0	0.561397	-2.737336	-0.804197
40	1	0	1.188555	-4.333612	-1.296355
41	1	0	1.409481	-3.207313	1.303502
42	1	0	2.499365	-4.471693	0.707841
43	1	0	-4.530568	-1.116945	-3.281062
44	6	0	-3.720287	-1.249500	-2.559500
45	6	0	-3.337523	0.051065	-1.861835
46	6	0	-4.097277	-2.129102	-1.364706
47	1	0	-2.851660	-1.666219	-3.082443
48	1	0	-4.229040	0.658403	-1.649084
49	8	0	-2.742527	-0.342175	-0.615839
50	1	0	-2.608604	0.654580	-2.406300
51	6	0	-3.042126	-1.722572	-0.339084
52	1	0	-5.101266	-1.872437	-1.007590
53	1	0	-4.072694	-3.199778	-1.582864
54	1	0	-3.365775	-1.800787	0.701090
55	1	0	-2.120587	-2.306845	-0.456240
56	1	0	-3.874808	3.500568	1.204143

57	6	0	-3.336494	2.711164	0.671905
58	6	0	-2.375050	1.964529	1.619895
59	6	0	-2.409156	3.287641	-0.422166
60	1	0	-4.076063	2.027405	0.248154
61	8	0	-1.114238	1.919383	0.947508
62	1	0	-2.247352	2.503188	2.569226
63	1	0	-2.659677	0.929992	1.820569
64	6	0	-1.016007	3.116967	0.179497
65	1	0	-2.635800	4.328143	-0.669440
66	1	0	-2.466375	2.692535	-1.337764
67	1	0	-0.754226	3.951607	0.848654
68	1	0	-0.230818	2.969891	-0.564667
69	6	0	-0.121575	-0.124224	-2.685458
70	1	0	-0.339617	-1.131573	-2.309153
71	1	0	-0.510688	0.054226	-3.691923
72	1	0	1.289453	1.417199	-2.874285

Table S39. M06-2X/6-31+G(d) geometry of dimer 1 RS·4THF + ethylene Product

SCF Done: E(RM062X) = -1329.48017105 A.U. after 11 cycles
Convg = 0.3536D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.849972	-0.530352	2.042793
2	6	0	1.019490	-1.978281	2.471903
3	8	0	0.498004	-0.389213	0.717907
4	1	0	0.097873	-0.080158	2.730879
5	1	0	1.799848	-0.001812	2.277744
6	1	0	1.753950	-2.535153	1.890313
7	3	0	1.506912	0.578086	-0.464036
8	3	0	-0.893350	0.380719	-0.230145
9	6	0	0.183286	1.373164	-1.966186
10	8	0	-1.343320	1.360115	-1.877357
11	6	0	-0.170167	-2.758892	2.953878
12	1	0	-1.122076	-2.234839	3.003907
13	1	0	-0.249960	-3.811646	2.697838
14	6	0	0.905358	-2.342084	3.923830
15	1	0	0.671154	-1.540670	4.620114
16	1	0	1.558281	-3.110205	4.325916
17	1	0	1.462417	-1.061205	-2.379787
18	6	0	2.433944	-1.432070	-2.040332
19	8	0	3.017940	-0.406530	-1.223224
20	1	0	3.080715	-1.606262	-2.911506
21	6	0	2.364517	-2.657672	-1.138833
22	6	0	3.759070	-1.004441	-0.143020
23	6	0	3.673909	-2.518564	-0.355471
24	1	0	1.506496	-2.557797	-0.464075
25	1	0	2.289078	-3.594562	-1.698230
26	1	0	3.288457	-0.698665	0.798116
27	1	0	4.782466	-0.618779	-0.171617
28	1	0	3.678650	-3.067995	0.589744
29	1	0	4.517146	-2.872167	-0.959827

30	1	0	2.522770	5.067094	-0.050903
31	6	0	2.003552	4.204486	-0.480762
32	6	0	2.919175	2.962361	-0.464076
33	6	0	0.813352	3.793299	0.401434
34	1	0	1.695144	4.468778	-1.495344
35	1	0	3.942479	3.210301	-0.158370
36	8	0	2.360417	2.046434	0.488500
37	1	0	2.954711	2.442340	-1.426162
38	6	0	1.438276	2.754880	1.323364
39	1	0	0.376949	4.633965	0.948318
40	1	0	0.033764	3.316327	-0.199439
41	1	0	1.989523	3.224106	2.151718
42	1	0	0.721687	2.029645	1.713321
43	1	0	-0.459268	-2.654197	-2.046384
44	6	0	-1.397747	-3.051231	-1.643048
45	6	0	-1.638581	-2.445185	-0.265327
46	6	0	-2.602150	-2.527212	-2.449404
47	1	0	-1.332763	-4.142545	-1.628070
48	8	0	-2.144341	-1.143070	-0.564545
49	1	0	-2.400514	-3.012244	0.294517
50	1	0	-0.744248	-2.302823	0.344535
51	6	0	-3.058853	-1.282062	-1.653068
52	1	0	-3.401204	-3.273494	-2.487829
53	1	0	-2.332233	-2.276711	-3.478642
54	1	0	-4.072697	-1.417971	-1.250097
55	1	0	-3.022522	-0.352411	-2.224359
56	1	0	-2.341156	2.938369	-0.318929
57	6	0	-2.774686	2.471330	0.566543
58	8	0	-1.826365	1.531256	1.067031
59	1	0	-2.972448	3.230496	1.338899
60	6	0	-4.010686	1.625955	0.275160
61	6	0	-2.536590	0.651052	1.943309
62	6	0	-3.982542	0.576937	1.406791
63	1	0	-3.882079	1.150144	-0.701021
64	1	0	-4.932549	2.213434	0.259373
65	1	0	-2.013550	-0.308103	1.923671
66	1	0	-2.501267	1.061791	2.961261
67	1	0	-4.213934	-0.423774	1.033341
68	1	0	-4.701161	0.820180	2.194902
69	6	0	-0.704794	0.726756	-2.970818
70	1	0	-0.925573	1.193303	-3.932897
71	1	0	-0.797643	-0.365287	-2.983608
72	1	0	0.433300	2.379783	-2.347246

Table S40. M06-2X/6-31+G(d) geometry of dimer 2 RR

SCF Done: E(RM062X) = -321.338554774 A.U. after 14 cycles
Convg = 0.8308D-08 -V/T = 2.0081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.633017	0.144732	0.447915
2	6	0	-1.678070	0.601942	-0.600848

3	8	0	-1.819889	-0.852239	-0.141265
4	1	0	-2.424392	0.336543	1.502022
5	1	0	-3.691939	0.015866	0.225253
6	1	0	-2.206179	0.651013	-1.560454
7	3	0	-0.000005	-0.783500	-0.000078
8	3	0	0.000019	1.673191	-0.000062
9	6	0	1.678032	0.601895	0.600885
10	6	0	2.633067	0.144762	-0.447831
11	8	0	1.819868	-0.852250	0.141184
12	1	0	3.691969	0.015871	-0.225089
13	1	0	2.424543	0.336690	-1.501938
14	1	0	2.206053	0.650865	1.560544

Table S41. M06-2X/6-31+G(d) geometry of dimer 2 RR + ethylene TS

SCF Done: E(RM062X) = -399.860645395 A.U. after 9 cycles
Convg = 0.5420D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.546830	-0.394875	0.792465
2	8	0	-3.166449	0.182248	-0.492661
3	3	0	-1.711120	1.270440	-0.379755
4	3	0	-0.480345	-0.132627	1.175903
5	6	0	1.244422	-0.027463	-0.005619
6	6	0	1.392089	1.454201	0.012793
7	8	0	-0.010359	1.378516	0.068543
8	1	0	1.753122	1.981731	-0.878980
9	1	0	1.836900	1.887905	0.918058
10	1	0	1.130857	-0.355980	-1.050931
11	6	0	3.605774	-0.714834	-0.634489
12	6	0	3.107644	-1.091792	0.559831
13	1	0	4.107019	0.240076	-0.764854
14	1	0	3.508038	-1.343472	-1.514612
15	1	0	2.669881	-2.073106	0.706775
16	1	0	3.277704	-0.502176	1.455327
17	6	0	-2.947877	-1.214710	-0.383043
18	1	0	-3.874682	-1.788475	-0.382609
19	1	0	-2.184836	-1.609306	-1.056622
20	1	0	-3.366468	-0.399912	1.521323

Table S42. M06-2X/6-31+G(d) geometry of dimer 2 RR + ethylene Product

SCF Done: E(RM062X) = -399.999593972 A.U. after 8 cycles
Convg = 0.8365D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.779175	0.340642	-0.470843
2	8	0	-2.159186	-1.041779	-0.189189

3	3	0	-0.507496	-0.284012	-0.326571
4	3	0	-1.455172	1.942834	-0.269384
5	6	0	1.917286	-0.106713	0.547712
6	6	0	1.521456	1.307336	0.149652
7	8	0	0.161379	1.383424	-0.091465
8	1	0	2.106876	1.579591	-0.749419
9	1	0	1.835975	1.998573	0.949902
10	1	0	1.558995	-0.420968	1.527845
11	6	0	3.204627	-0.708701	0.087480
12	1	0	3.855069	-0.090671	-0.524380
13	1	0	3.722047	-1.396710	0.747329
14	6	0	1.911684	-1.171958	-0.534213
15	1	0	1.572842	-2.177226	-0.299556
16	1	0	1.720451	-0.849269	-1.556601
17	6	0	-3.138191	-0.516766	0.691064
18	1	0	-4.056916	-1.103877	0.699267
19	1	0	-2.766619	-0.268678	1.687236
20	1	0	-3.504382	0.156567	-1.273635

Table S43. M06-2X/6-31+G(d) geometry of dimer 2 RR·2THF

SCF Done: E(RM062X) = -786.085877111 A.U. after 9 cycles
Convg = 0.3492D-08 -V/T = 2.0084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.553012	-1.202256	2.962553
2	6	0	-0.241935	-1.236335	1.699423
3	8	0	1.264173	-0.993402	1.755874
4	1	0	0.500300	-0.328256	3.614665
5	1	0	0.839623	-2.120370	3.476383
6	1	0	-0.348490	-2.290449	1.392888
7	3	0	0.815516	0.556337	0.811638
8	3	0	-1.543190	0.394447	1.368305
9	6	0	-0.550623	2.248053	1.081396
10	6	0	-0.010078	2.922866	-0.131803
11	8	0	0.935070	2.429846	0.804173
12	1	0	0.002284	4.010113	-0.218201
13	1	0	-0.012446	2.400374	-1.093066
14	1	0	-0.799201	3.020324	1.823860
15	8	0	1.350045	0.118825	-1.009233
16	6	0	2.600374	0.748015	-1.306800
17	6	0	3.627730	-0.169787	-0.647926
18	6	0	3.013720	-1.573797	-0.848017
19	6	0	1.549783	-1.282111	-1.238457
20	1	0	2.562163	1.761246	-0.902513
21	1	0	2.729541	0.785093	-2.398430
22	1	0	4.623391	-0.070036	-1.087435
23	1	0	3.694474	0.065484	0.418658
24	1	0	3.523742	-2.128470	-1.640635
25	1	0	3.061010	-2.157613	0.072797
26	1	0	1.362789	-1.487404	-2.301249
27	1	0	0.821062	-1.816270	-0.627026

28	8	0	-3.140099	0.069616	0.348091
29	6	0	-3.041799	0.757419	-0.903959
30	6	0	-2.093799	-0.115518	-1.725256
31	6	0	-2.425658	-1.545935	-1.237452
32	6	0	-3.287380	-1.317092	0.020276
33	1	0	-2.667215	1.762052	-0.699296
34	1	0	-4.042423	0.813887	-1.355924
35	1	0	-2.237737	0.012212	-2.801383
36	1	0	-1.056853	0.142434	-1.482768
37	1	0	-2.977795	-2.117678	-1.988301
38	1	0	-1.515713	-2.098352	-0.991164
39	1	0	-4.349172	-1.515627	-0.174843
40	1	0	-2.963907	-1.895243	0.888051

Table S44. M06-2X/6-31+G(d) geometry of dimer 2 RR·2THF + ethylene TS

SCF Done: E(RM062X) = -864.608392755 A.U. after 9 cycles
Convg = 0.9088D-08 -V/T = 2.0085
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.619427	0.688470	1.416385
2	8	0	-1.050168	-0.417345	2.378955
3	3	0	-1.225738	-1.367927	0.788408
4	3	0	0.407990	0.097534	-0.359085
5	6	0	1.659731	-1.651326	-0.027403
6	6	0	0.962382	-2.498316	-1.030660
7	8	0	-0.133819	-1.714278	-0.626325
8	1	0	0.812231	-3.569930	-0.844215
9	1	0	1.246373	-2.331545	-2.079223
10	1	0	1.539801	-2.111760	0.967836
11	6	0	3.814772	-2.900773	0.307547
12	6	0	3.804018	-1.657785	-0.223855
13	1	0	3.689657	-3.783029	-0.313153
14	1	0	3.916824	-3.059918	1.376725
15	1	0	4.021142	-0.782822	0.381196
16	1	0	3.807593	-1.511267	-1.300326
17	6	0	0.141932	0.299262	2.640163
18	1	0	0.090294	0.891800	3.555043
19	1	0	1.058477	-0.286315	2.540309
20	1	0	-1.257705	1.551792	1.674881
21	8	0	1.086407	1.636278	-1.348108
22	6	0	0.596498	2.852438	-0.770399
23	6	0	1.490681	3.126004	0.457321
24	6	0	2.670668	2.141863	0.277592
25	6	0	2.504691	1.669308	-1.165307
26	1	0	-0.455910	2.697077	-0.524764
27	1	0	0.683915	3.650128	-1.519727
28	1	0	1.826212	4.166666	0.468746
29	1	0	0.953711	2.928040	1.387917
30	1	0	3.645274	2.601281	0.461515
31	1	0	2.554179	1.282714	0.948054
32	1	0	2.941165	2.379248	-1.882814
33	1	0	2.882085	0.663654	-1.356084

34	8	0	-3.031298	-1.249254	0.170412
35	6	0	-3.769670	-0.126416	0.667924
36	6	0	-3.619145	0.984757	-0.392679
37	6	0	-2.971167	0.266650	-1.597486
38	6	0	-3.145412	-1.210959	-1.254178
39	1	0	-3.352326	0.127674	1.644015
40	1	0	-4.818331	-0.428674	0.785152
41	1	0	-4.594041	1.407848	-0.650854
42	1	0	-2.983876	1.794822	-0.027467
43	1	0	-3.432823	0.531068	-2.552429
44	1	0	-1.902936	0.499190	-1.655195
45	1	0	-4.141252	-1.579732	-1.540027
46	1	0	-2.368777	-1.859119	-1.662348

Table S45. M06-2X/6-31+G(d) geometry of dimer 2 RR·2THF + ethylene Product

SCF Done: E(RM062X) = -864.745318358 A.U. after 9 cycles
Convg = 0.2237D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354857	1.162761	1.652665
2	8	0	2.166917	2.190799	0.856486
3	3	0	1.640327	1.246933	-0.659570
4	3	0	-0.180777	0.228878	0.572168
5	6	0	-1.686229	2.283727	-0.861756
6	6	0	-1.081543	1.223153	-1.767238
7	8	0	0.037045	0.632968	-1.208333
8	1	0	-0.857652	1.685348	-2.746420
9	1	0	-1.882507	0.476208	-1.967351
10	1	0	-1.045415	3.148682	-0.694052
11	6	0	-3.162844	2.534646	-0.851033
12	6	0	-2.510517	1.841352	0.320271
13	1	0	-3.778020	1.928452	-1.511412
14	1	0	-3.521563	3.548585	-0.707639
15	1	0	-2.425709	2.384511	1.257045
16	1	0	-2.698326	0.774311	0.428559
17	6	0	1.212177	2.640413	1.797679
18	1	0	1.657484	3.175888	2.637501
19	1	0	0.347202	3.147108	1.362887
20	1	0	2.043038	0.811199	2.436954
21	8	0	-1.252523	-1.359458	0.731048
22	6	0	-2.193500	-1.789081	1.712302
23	6	0	-3.523868	-1.983850	0.957212
24	6	0	-3.109021	-2.001164	-0.534246
25	6	0	-1.580023	-2.043446	-0.481006
26	1	0	-2.228835	-1.025618	2.492633
27	1	0	-1.840056	-2.731101	2.151767
28	1	0	-4.010080	-2.914738	1.259700
29	1	0	-4.219403	-1.165828	1.161464
30	1	0	-3.524378	-2.852632	-1.078788
31	1	0	-3.439036	-1.086842	-1.036127
32	1	0	-1.209781	-3.077257	-0.412754

33	1	0	-1.068286	-1.516637	-1.290317
34	8	0	3.012104	-0.025224	-1.055723
35	6	0	3.884563	-0.376568	0.024192
36	6	0	3.282395	-1.646775	0.659762
37	6	0	2.202650	-2.094245	-0.351853
38	6	0	2.505889	-1.250241	-1.588639
39	1	0	3.926352	0.482227	0.696438
40	1	0	4.883446	-0.570259	-0.388463
41	1	0	4.050979	-2.412167	0.799765
42	1	0	2.837165	-1.426434	1.632272
43	1	0	2.231766	-3.167202	-0.562134
44	1	0	1.205656	-1.844126	0.024295
45	1	0	3.282502	-1.712741	-2.215431
46	1	0	1.626549	-1.003144	-2.185874

Table S46. M06-2X/6-31+G(d) geometry of dimer 2 RR·4THF

SCF Done: E(RM062X) = -1250.81667492 A.U. after 9 cycles
Convg = 0.3498D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.172186	0.940786	-2.161313
2	6	0	-0.010490	0.103734	-1.743610
3	8	0	-1.449716	-0.378165	-1.736551
4	1	0	-1.544678	1.720525	-1.490177
5	1	0	-1.403531	1.117737	-3.214097
6	1	0	0.434671	-0.326413	-2.660007
7	3	0	-0.874769	-0.689015	0.196567
8	3	0	1.351392	0.335604	-0.125137
9	6	0	0.719138	-0.350492	1.787756
10	6	0	0.634235	-1.715617	2.389168
11	8	0	-0.582233	-1.037358	2.154462
12	1	0	0.841196	-1.879840	3.449038
13	1	0	0.784551	-2.597024	1.761129
14	1	0	0.910113	0.361594	2.613742
15	8	0	-0.775870	-2.689436	-0.171261
16	6	0	-1.922607	-3.262755	0.455095
17	6	0	-3.018762	-3.109559	-0.598770
18	6	0	-2.252159	-3.333691	-1.921019
19	6	0	-0.771217	-3.192772	-1.508924
20	1	0	-2.090389	-2.721291	1.388320
21	1	0	-1.723270	-4.323291	0.674935
22	1	0	-3.844905	-3.811182	-0.454568
23	1	0	-3.415427	-2.089829	-0.562744
24	1	0	-2.448069	-4.326896	-2.336217
25	1	0	-2.521108	-2.582395	-2.665097
26	1	0	-0.262589	-4.167523	-1.507683
27	1	0	-0.211152	-2.486571	-2.122048
28	8	0	3.095960	-0.424058	-0.510574
29	6	0	4.023398	-0.052106	0.518037
30	6	0	4.823914	-1.316669	0.801209
31	6	0	3.737320	-2.386994	0.659736

32	6	0	2.901674	-1.852904	-0.505261
33	1	0	3.463682	0.274526	1.405152
34	1	0	4.619010	0.783643	0.141636
35	1	0	5.603389	-1.451655	0.042669
36	1	0	5.293819	-1.304975	1.787943
37	1	0	4.132206	-3.387287	0.463874
38	1	0	3.130209	-2.420805	1.570061
39	1	0	3.246931	-2.236444	-1.472378
40	1	0	1.831095	-2.060430	-0.392630
41	8	0	1.804795	2.237923	-0.037171
42	6	0	2.233935	2.737379	-1.307135
43	6	0	1.740445	4.177819	-1.330949
44	6	0	0.363646	4.028257	-0.671471
45	6	0	0.590407	2.905408	0.352798
46	1	0	1.774282	2.142119	-2.108761
47	1	0	3.320025	2.627755	-1.352387
48	1	0	2.396751	4.809507	-0.722416
49	1	0	1.690294	4.593812	-2.340400
50	1	0	0.007064	4.950280	-0.204589
51	1	0	-0.373173	3.715839	-1.418916
52	1	0	0.742324	3.283143	1.369835
53	1	0	-0.227156	2.174483	0.359225
54	8	0	-2.267357	0.641524	0.770690
55	6	0	-3.526141	0.931668	0.178466
56	6	0	-3.724831	2.436061	0.411910
57	6	0	-2.886607	2.711837	1.685910
58	6	0	-2.252148	1.347813	2.008625
59	1	0	-4.305591	0.348418	0.693070
60	1	0	-3.479370	0.627756	-0.868445
61	1	0	-3.337368	3.006276	-0.437888
62	1	0	-4.780096	2.693755	0.534132
63	1	0	-2.114290	3.461402	1.486161
64	1	0	-3.494685	3.077619	2.517478
65	1	0	-1.219207	1.388740	2.355847
66	1	0	-2.845851	0.788493	2.744613

Table S47. M06-2X/6-31+G(d) geometry of dimer 2 RR·4THF + ethylene TS

SCF Done: E(RM062X) = -1329.34118030 A.U. after 9 cycles
Convg = 0.7215D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745540	-0.177544	1.830315
2	8	0	-0.752693	-0.152729	2.150449
3	3	0	-0.934131	0.194351	0.295809
4	3	0	1.381406	-0.381204	-0.232592
5	6	0	-0.295088	-2.128480	-0.878857
6	6	0	-0.230655	-1.459915	-2.196677
7	8	0	-0.199190	-0.339107	-1.343856
8	1	0	-1.093770	-1.460015	-2.879722
9	1	0	0.699648	-1.602657	-2.766530
10	1	0	-1.348568	-2.162720	-0.552212

11	6	0	-0.978856	-4.492178	-1.530696
12	6	0	0.182556	-4.184711	-0.899765
13	1	0	-1.066714	-4.450446	-2.612547
14	1	0	-1.874714	-4.748595	-0.971581
15	1	0	0.288367	-4.337945	0.170313
16	1	0	1.110125	-4.054580	-1.450536
17	6	0	0.014847	-1.295202	2.495446
18	1	0	0.074185	-1.457350	3.573842
19	1	0	-0.222626	-2.191322	1.915383
20	1	0	1.206617	0.436168	2.628540
21	8	0	2.999959	-1.516669	-0.378827
22	6	0	4.231508	-0.847000	-0.124341
23	6	0	4.235441	-0.655759	1.390785
24	6	0	3.570320	-1.955805	1.892230
25	6	0	2.878589	-2.525028	0.634094
26	1	0	4.229777	0.078271	-0.702469
27	1	0	5.065666	-1.488287	-0.448514
28	1	0	5.238897	-0.500241	1.796668
29	1	0	3.613320	0.207767	1.649127
30	1	0	4.312566	-2.660183	2.279612
31	1	0	2.845773	-1.750448	2.683815
32	1	0	3.377624	-3.436617	0.277487
33	1	0	1.810748	-2.712933	0.756712
34	8	0	2.186567	1.339210	-0.846743
35	6	0	2.404772	2.405585	0.087322
36	6	0	2.024182	3.698003	-0.641188
37	6	0	2.186777	3.306303	-2.113984
38	6	0	1.701624	1.862372	-2.089174
39	1	0	3.468018	2.395291	0.362762
40	1	0	1.800324	2.213671	0.978441
41	1	0	0.978404	3.948262	-0.436803
42	1	0	2.649702	4.543659	-0.343381
43	1	0	1.605526	3.934447	-2.794647
44	1	0	3.240674	3.352380	-2.411661
45	1	0	0.608279	1.790956	-2.101211
46	1	0	2.105729	1.235889	-2.889320
47	8	0	-0.749838	2.162076	0.190202
48	6	0	-1.714175	2.707108	-0.711150
49	6	0	-2.937511	3.101779	0.145392
50	6	0	-2.446628	2.909475	1.596608
51	6	0	-0.930414	2.833066	1.436193
52	1	0	-1.917636	1.941279	-1.464247
53	1	0	-1.274841	3.585149	-1.208392
54	1	0	-3.226122	4.139072	-0.047724
55	1	0	-3.796911	2.462248	-0.069090
56	1	0	-2.759586	3.716091	2.264690
57	1	0	-2.805359	1.959548	2.002738
58	1	0	-0.479743	3.837250	1.374084
59	1	0	-0.426932	2.242907	2.203571
60	8	0	-2.896446	0.009488	0.110348
61	6	0	-3.669865	-0.588746	1.148487
62	6	0	-3.929714	-2.006164	0.644337
63	6	0	-4.084541	-1.805277	-0.878300
64	6	0	-3.453405	-0.418141	-1.134718
65	1	0	-4.609969	-0.025941	1.267289
66	1	0	-3.081015	-0.531253	2.065649
67	1	0	-3.060314	-2.633943	0.864852

68	1	0	-4.809852	-2.462080	1.105081
69	1	0	-3.570067	-2.588279	-1.441844
70	1	0	-5.137573	-1.810402	-1.174237
71	1	0	-2.636417	-0.426971	-1.859211
72	1	0	-4.211768	0.312851	-1.451171

Table S48. M06-2X/6-31+G(d) geometry of dimer 2 RR·4THF + ethylene Product

SCF Done: E(RM062X) = -1329.47994422 A.U. after 8 cycles
Convg = 0.7333D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.561778	-0.422600	2.009337
2	8	0	0.833145	0.168589	2.222232
3	3	0	1.106231	0.205357	0.342987
4	3	0	-1.316372	-0.217335	0.012254
5	6	0	-1.121067	3.080247	-1.248823
6	6	0	-0.478924	1.799204	-1.756105
7	8	0	-0.103318	0.941039	-0.749985
8	1	0	0.382159	2.088782	-2.398311
9	1	0	-1.210870	1.332438	-2.453334
10	1	0	-0.526406	3.617141	-0.510316
11	6	0	-1.941477	3.913998	-2.191425
12	6	0	-2.611668	3.150529	-1.078386
13	1	0	-2.067334	3.539502	-3.204519
14	1	0	-1.891090	4.995689	-2.115905
15	1	0	-3.015695	3.720996	-0.246531
16	1	0	-3.179082	2.260795	-1.339188
17	6	0	-0.299362	0.890619	2.672317
18	1	0	-0.329895	1.008382	3.757722
19	1	0	-0.495308	1.813335	2.117390
20	1	0	-0.661247	-1.180745	2.809868
21	8	0	-3.278808	0.104070	0.019098
22	6	0	-4.062389	-1.077058	0.162309
23	6	0	-3.889893	-1.457490	1.631895
24	6	0	-3.819232	-0.080413	2.329254
25	6	0	-3.559728	0.906795	1.170509
26	1	0	-3.683213	-1.809558	-0.551957
27	1	0	-5.112762	-0.843025	-0.070189
28	1	0	-4.704235	-2.085765	2.003121
29	1	0	-2.943199	-1.991940	1.761319
30	1	0	-4.756330	0.160137	2.840000
31	1	0	-3.009855	-0.050231	3.062123
32	1	0	-4.444419	1.523382	0.958550
33	1	0	-2.697958	1.559240	1.326326
34	8	0	-1.308153	-1.877928	-1.042342
35	6	0	-1.027484	-3.120992	-0.384276
36	6	0	-0.128549	-3.921243	-1.334587
37	6	0	-0.394154	-3.258624	-2.692388
38	6	0	-0.606715	-1.804650	-2.287856
39	1	0	-1.987005	-3.624974	-0.208715
40	1	0	-0.556160	-2.903982	0.579387

41	1	0	0.920751	-3.792695	-1.054210
42	1	0	-0.361401	-4.989290	-1.324617
43	1	0	0.430560	-3.383305	-3.399633
44	1	0	-1.305356	-3.663217	-3.147306
45	1	0	0.338251	-1.270460	-2.134762
46	1	0	-1.229380	-1.232051	-2.980191
47	8	0	1.757981	-1.652206	-0.029209
48	6	0	2.898476	-1.693920	-0.888856
49	6	0	4.140305	-1.712077	0.028857
50	6	0	3.542879	-1.870228	1.442730
51	6	0	2.127239	-2.360061	1.155773
52	1	0	2.846981	-0.823139	-1.546311
53	1	0	2.841729	-2.604016	-1.504921
54	1	0	4.795662	-2.550003	-0.226566
55	1	0	4.711767	-0.786030	-0.059154
56	1	0	4.109732	-2.560574	2.072852
57	1	0	3.482423	-0.900816	1.945727
58	1	0	2.109243	-3.442751	0.946319
59	1	0	1.397878	-2.115297	1.928158
60	8	0	2.900255	1.118953	0.211757
61	6	0	3.072866	2.040752	1.290482
62	6	0	2.247096	3.246207	0.860027
63	6	0	2.555454	3.322908	-0.645279
64	6	0	2.947316	1.874256	-1.007283
65	1	0	4.140250	2.294598	1.384668
66	1	0	2.721131	1.549446	2.199262
67	1	0	1.187332	3.022237	1.019680
68	1	0	2.506126	4.160973	1.399759
69	1	0	1.696590	3.665996	-1.227227
70	1	0	3.389153	4.005702	-0.837087
71	1	0	2.242847	1.407612	-1.700068
72	1	0	3.963985	1.816314	-1.418687

Table S49. M06-2X/6-31+G(d) geometry of dimer 2 RS

SCF Done: E(RM062X) = -321.337431332 A.U. after 9 cycles
Convg = 0.4332D-08 -V/T = 2.0081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.368675	-0.271791	0.706289
2	6	0	-1.795252	0.808577	-0.141718
3	8	0	-1.793093	-0.675003	-0.524203
4	1	0	-1.833841	-0.615446	1.593413
5	1	0	-3.443945	-0.443858	0.746772
6	1	0	-2.604173	1.251930	-0.736243
7	3	0	0.000050	-0.455756	-0.793896
8	3	0	-0.000039	1.780158	0.262016
9	6	0	1.795244	0.808602	-0.141709
10	8	0	1.793113	-0.675018	-0.524200
11	6	0	2.368658	-0.271775	0.706295
12	1	0	3.443930	-0.443832	0.746813
13	1	0	1.833809	-0.615434	1.593410

14	1	0	2.604167	1.251927	-0.736248

Table S50. M06-2X/6-31+G(d) geometry of dimer 2 RS + ethylene TS

SCF Done: E(RM062X) = -399.860705396 A.U. after 9 cycles
Convg = 0.5045D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.476589	-0.939336	-0.297036
2	8	0	-3.317834	0.335545	-0.481443
3	3	0	-1.664601	1.091343	-0.584555
4	3	0	-0.424178	-0.831932	0.230330
5	6	0	1.462914	-0.067902	-0.240737
6	6	0	1.307203	1.239943	0.454837
7	8	0	-0.023705	1.055094	0.044877
8	1	0	1.758482	2.144928	0.029201
9	1	0	1.431301	1.229685	1.545967
10	1	0	1.665375	0.122669	-1.305874
11	6	0	3.991888	-0.214787	-0.357851
12	6	0	3.314748	-1.145219	0.343602
13	1	0	4.307206	0.720406	0.096120
14	1	0	4.231447	-0.357692	-1.407386
15	1	0	3.060873	-2.106898	-0.088807
16	1	0	3.147659	-1.038574	1.410921
17	6	0	-3.571808	-0.520902	0.619568
18	1	0	-3.334587	-0.089976	1.593871
19	1	0	-4.555632	-0.987843	0.573147
20	1	0	-2.883609	-1.650827	-1.026257

Table S51. M06-2X/6-31+G(d) geometry of dimer 2 RS + ethylene Product

SCF Done: E(RM062X) = -399.999784589 A.U. after 8 cycles
Convg = 0.6565D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.213604	-0.781115	0.595163
2	6	0	-2.353782	-0.709909	-0.617149
3	8	0	-3.141797	0.483024	-0.042594
4	1	0	-4.212108	-1.217230	0.556330
5	1	0	-2.757428	-0.816347	1.586395
6	3	0	-1.573493	1.418086	-0.047182
7	3	0	-0.273408	-0.555479	-0.510146
8	6	0	2.238469	0.111490	-0.458792
9	6	0	1.486055	1.254205	0.208541
10	8	0	0.125965	1.132458	-0.007253
11	1	0	1.880864	2.207857	-0.180901
12	1	0	1.729440	1.230749	1.288290
13	1	0	2.252502	0.149516	-1.547768

14	1	0	-2.946637	-1.038807	-1.480297
15	6	0	3.420264	-0.522657	0.197814
16	6	0	2.111426	-1.270896	0.157815
17	1	0	3.732491	-0.123523	1.158281
18	1	0	4.228833	-0.888159	-0.425966
19	1	0	2.056831	-2.147112	-0.482814
20	1	0	1.569605	-1.355318	1.098869

Table S52. M06-2X/6-31+G(d) geometry of dimer 2 RS·2THF

SCF Done: E(RM062X) = -786.086597242 A.U. after 9 cycles
Convg = 0.2060D-08 -V/T = 2.0084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.736639	-0.798022	2.472772
2	6	0	-0.114073	-1.253036	1.193160
3	8	0	0.653999	-0.587436	2.329850
4	1	0	-1.336447	0.116454	2.493277
5	1	0	-0.984445	-1.500286	3.270027
6	1	0	0.113368	-2.327652	1.291972
7	3	0	1.258418	0.710099	1.138386
8	3	0	-0.498511	-0.126297	-0.514987
9	6	0	0.116305	1.877037	-0.492645
10	8	0	0.994271	2.475254	0.597802
11	6	0	-0.347419	2.908993	0.480607
12	1	0	-0.434449	3.958876	0.198391
13	1	0	-0.992279	2.625004	1.315800
14	1	0	0.419394	2.396110	-1.417424
15	8	0	-2.107895	-0.547038	-1.476829
16	6	0	-2.831330	-1.615644	-0.851845
17	6	0	-3.669129	-0.960455	0.266020
18	6	0	-3.552910	0.553634	-0.025341
19	6	0	-2.977687	0.588430	-1.439545
20	1	0	-2.097301	-2.336421	-0.486957
21	1	0	-3.467614	-2.091165	-1.609141
22	1	0	-4.706631	-1.302809	0.225310
23	1	0	-3.268189	-1.205915	1.252167
24	1	0	-4.506451	1.081233	0.055540
25	1	0	-2.839203	1.023134	0.660218
26	1	0	-3.759009	0.464711	-2.203039
27	1	0	-2.377831	1.473326	-1.661506
28	8	0	2.892779	0.100313	0.372713
29	6	0	3.114539	-1.310197	0.314304
30	6	0	2.632216	-1.739857	-1.081999
31	6	0	2.628010	-0.420375	-1.895556
32	6	0	3.219512	0.605248	-0.922095
33	1	0	2.563811	-1.762220	1.140736
34	1	0	4.189628	-1.496866	0.441908
35	1	0	3.295783	-2.492290	-1.516308
36	1	0	1.627719	-2.166689	-1.021393
37	1	0	3.210477	-0.490096	-2.817862
38	1	0	1.608045	-0.127752	-2.164132

39	1	0	4.313844	0.659310	-1.011456
40	1	0	2.794457	1.607319	-1.001628

Table S53. M06-2X/6-31+G(d) geometry of dimer 2 RS·2THF + ethylene TS

SCF Done: E(RM062X) = -864.607497540 A.U. after 8 cycles
Convg = 0.5857D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.200386	-2.037446	-1.073181
2	8	0	-0.355102	-2.881503	0.085586
3	3	0	-0.601510	-1.189449	0.834174
4	3	0	0.939911	-0.037662	-0.815513
5	6	0	-0.217010	1.663927	-0.180158
6	6	0	0.159908	1.731506	1.253847
7	8	0	0.354103	0.359334	1.027777
8	1	0	-0.595368	1.944025	2.024089
9	1	0	1.086538	2.275376	1.494385
10	1	0	-1.288508	1.415422	-0.256901
11	6	0	-1.278319	3.916100	-0.569234
12	6	0	-0.141031	3.543613	-1.201427
13	1	0	-1.257798	4.377324	0.413928
14	1	0	-2.254518	3.744132	-1.013375
15	1	0	-0.156328	3.170647	-2.219481
16	1	0	0.833952	3.825380	-0.814603
17	6	0	0.840576	-3.278601	-0.550992
18	1	0	1.731733	-3.218775	0.077966
19	1	0	0.748069	-4.227535	-1.081552
20	1	0	-0.413135	-2.322447	-1.943351
21	8	0	2.847692	0.229190	-1.057904
22	6	0	3.578066	-0.945447	-0.701633
23	6	0	3.516917	-0.958355	0.824017
24	6	0	3.578039	0.543274	1.183323
25	6	0	3.289376	1.251419	-0.157668
26	1	0	4.611532	-0.848621	-1.065942
27	1	0	3.094062	-1.794067	-1.188066
28	1	0	2.556553	-1.374094	1.145986
29	1	0	4.322776	-1.543597	1.274475
30	1	0	2.824040	0.789094	1.933874
31	1	0	4.560538	0.829794	1.568784
32	1	0	2.494267	1.998586	-0.112723
33	1	0	4.195439	1.711850	-0.573058
34	8	0	-2.514932	-1.098086	0.936661
35	6	0	-3.214334	-1.723585	-0.145191
36	6	0	-3.536945	-0.555245	-1.067202
37	6	0	-3.926817	0.544952	-0.062020
38	6	0	-3.202594	0.122921	1.236976
39	1	0	-4.128527	-2.195087	0.244465
40	1	0	-2.554364	-2.485214	-0.561808
41	1	0	-2.632670	-0.276975	-1.620068
42	1	0	-4.331594	-0.779420	-1.783230
43	1	0	-3.620252	1.539751	-0.395023

44	1	0	-5.009701	0.562130	0.093063
45	1	0	-2.453318	0.842882	1.575141
46	1	0	-3.910006	-0.064900	2.053341

Table S54. M06-2X/6-31+G(d) geometry of dimer 2 RS·2THF + ethylene Product

SCF Done: E(RM062X) = -864.738872442 A.U. after 7 cycles
Convg = 0.5745D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.177151	-2.641738	0.655221
2	6	0	-0.750982	-2.327222	0.383628
3	8	0	-1.827827	-2.428808	-0.701439
4	1	0	-2.511948	-3.660647	0.856975
5	1	0	-2.826097	-1.875460	1.089060
6	3	0	-1.322767	-0.633635	-1.024623
7	3	0	0.539624	-0.653711	0.553489
8	6	0	1.770526	2.135888	-0.350731
9	6	0	0.597986	1.664585	-1.193150
10	8	0	0.056056	0.482199	-0.740178
11	1	0	0.941621	1.579329	-2.242434
12	1	0	-0.149818	2.488392	-1.192205
13	1	0	2.642557	1.482897	-0.382785
14	1	0	-0.201883	-3.280808	0.320383
15	6	0	2.040230	3.603394	-0.193010
16	6	0	1.486071	2.808489	0.962300
17	1	0	1.369446	4.292521	-0.699099
18	1	0	3.069222	3.943137	-0.130691
19	1	0	2.138453	2.625109	1.811344
20	1	0	0.440554	2.956109	1.222587
21	8	0	2.414283	-1.082653	0.626423
22	6	0	3.571940	-0.576083	1.303742
23	6	0	4.712786	-0.633874	0.285221
24	6	0	4.265127	-1.772986	-0.636836
25	6	0	2.761011	-1.539817	-0.692819
26	1	0	3.765947	-1.219930	2.169139
27	1	0	3.357179	0.438377	1.654264
28	1	0	4.772404	0.303849	-0.278321
29	1	0	5.681716	-0.810677	0.758473
30	1	0	4.731907	-1.737466	-1.624070
31	1	0	4.483195	-2.745122	-0.181382
32	1	0	2.490257	-0.761001	-1.417981
33	1	0	2.167577	-2.434681	-0.895626
34	8	0	-2.971783	0.347761	-0.857236
35	6	0	-2.906837	1.483089	0.005786
36	6	0	-3.604571	1.003971	1.273424
37	6	0	-4.757238	0.151107	0.709026
38	6	0	-4.262195	-0.251786	-0.699559
39	1	0	-3.442970	2.324855	-0.457389
40	1	0	-1.850053	1.729174	0.126130
41	1	0	-2.910030	0.386011	1.852761
42	1	0	-3.952231	1.823808	1.907246

43	1	0	-4.970124	-0.720177	1.333544
44	1	0	-5.675972	0.740761	0.637578
45	1	0	-4.130985	-1.327682	-0.834549
46	1	0	-4.926550	0.131273	-1.483565

Table S55. M06-2X/6-31+G(d) geometry of dimer 2 RS·4THF

SCF Done: E(RM062X) = -1250.81697247 A.U. after 9 cycles
Convg = 0.3306D-08 -V/T = 2.0085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.668449	-1.456832	-2.076326
2	6	0	-0.469524	-0.516996	-1.841999
3	8	0	0.999669	-0.134019	-1.693960
4	1	0	0.916957	-2.218694	-1.330802
5	1	0	1.006579	-1.711233	-3.084104
6	1	0	-0.752848	-0.112228	-2.832119
7	3	0	1.501432	0.086749	0.165831
8	3	0	-1.303532	-0.269916	0.063171
9	6	0	-0.043372	-0.301276	1.790714
10	8	0	1.432340	-0.150651	2.086164
11	6	0	0.800816	-1.378438	2.391640
12	1	0	0.776680	-1.596698	3.461147
13	1	0	1.124354	-2.222926	1.775580
14	1	0	-0.554788	0.224840	2.618888
15	8	0	-2.541180	1.253683	0.099709
16	6	0	-3.170594	1.810966	-1.049333
17	6	0	-4.672112	1.480525	-0.910640
18	6	0	-4.815861	1.006267	0.555201
19	6	0	-3.465311	1.369433	1.174361
20	1	0	-2.687548	1.370661	-1.924847
21	1	0	-3.000856	2.897672	-1.053879
22	1	0	-5.285354	2.361716	-1.117589
23	1	0	-4.974524	0.696904	-1.610410
24	1	0	-5.652695	1.480887	1.074104
25	1	0	-4.948985	-0.077718	0.599631
26	1	0	-3.455514	2.405095	1.548489
27	1	0	-3.138497	0.690944	1.964807
28	8	0	2.027429	2.002061	0.130029
29	6	0	1.646491	2.681466	-1.068699
30	6	0	0.163617	2.982737	-0.856450
31	6	0	0.067608	3.215833	0.670242
32	6	0	1.447897	2.768451	1.192692
33	1	0	1.847886	2.017678	-1.909861
34	1	0	2.242465	3.603124	-1.155269
35	1	0	-0.179942	3.837160	-1.447064
36	1	0	-0.416972	2.099291	-1.141797
37	1	0	-0.123854	4.264041	0.919071
38	1	0	-0.731205	2.604492	1.097346
39	1	0	2.099212	3.632590	1.386722
40	1	0	1.412428	2.128504	2.074790
41	8	0	3.258761	-0.791561	-0.055408

42	6	0	3.954765	-0.423699	-1.242760
43	6	0	5.362893	-0.979274	-1.032152
44	6	0	5.564995	-0.835156	0.493986
45	6	0	4.151666	-0.517765	1.027139
46	1	0	3.964768	0.674040	-1.328529
47	1	0	3.412089	-0.843062	-2.091152
48	1	0	5.392351	-2.032249	-1.326772
49	1	0	6.114861	-0.441411	-1.615309
50	1	0	5.962867	-1.754987	0.929763
51	1	0	6.260376	-0.026899	0.736113
52	1	0	3.837072	-1.131116	1.872315
53	1	0	4.051332	0.539696	1.304629
54	8	0	-2.801830	-1.566229	0.542475
55	6	0	-3.294014	-2.040506	-0.714363
56	6	0	-2.416827	-3.254876	-1.088597
57	6	0	-1.589636	-3.514348	0.189627
58	6	0	-2.344762	-2.717803	1.248994
59	1	0	-3.213830	-1.214183	-1.425450
60	1	0	-4.349720	-2.325418	-0.594840
61	1	0	-3.038144	-4.116529	-1.349940
62	1	0	-1.767734	-3.021236	-1.935318
63	1	0	-1.500775	-4.575354	0.437844
64	1	0	-0.586398	-3.090997	0.081057
65	1	0	-3.213124	-3.274452	1.634256
66	1	0	-1.727286	-2.370966	2.079763

Table S56. M06-2X/6-31+G(d) geometry of dimer 2 RS·4THF + ethylene TS

SCF Done: E(RM062X) = -1329.33678146 A.U. after 9 cycles
Convg = 0.5679D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.089332	0.724677	-1.859905
2	8	0	-1.403765	0.635288	-2.152596
3	3	0	-1.705586	0.201423	-0.336533
4	3	0	0.869514	-0.435943	-0.213368
5	6	0	0.151966	-0.944758	1.927051
6	6	0	-0.631071	-2.102143	1.427364
7	8	0	-0.818802	-1.248783	0.336821
8	1	0	-1.567413	-2.394319	1.927677
9	1	0	-0.044859	-3.001857	1.178545
10	1	0	-0.534784	-0.233531	2.419116
11	6	0	0.406290	-1.466792	4.361715
12	6	0	1.448775	-1.499399	3.494904
13	1	0	-0.246673	-2.324058	4.494471
14	1	0	0.160652	-0.568499	4.920298
15	1	0	2.170482	-0.690486	3.448427
16	1	0	1.757099	-2.435579	3.037716
17	6	0	-0.517955	-0.216351	-2.852241
18	1	0	-0.602051	-1.275586	-2.589925
19	1	0	-0.493102	-0.021701	-3.926558
20	1	0	0.424008	1.619643	-2.418826

21	8	0	2.611524	0.579838	0.302847
22	6	0	2.741373	1.375170	1.482079
23	6	0	2.828092	2.846441	1.015732
24	6	0	2.684901	2.755625	-0.514746
25	6	0	3.130799	1.324789	-0.791923
26	1	0	3.649603	1.070716	2.020293
27	1	0	1.869903	1.154971	2.103794
28	1	0	2.048708	3.464540	1.470967
29	1	0	3.793978	3.281191	1.290147
30	1	0	1.638544	2.856334	-0.821150
31	1	0	3.282631	3.501612	-1.045267
32	1	0	2.711348	0.897799	-1.707157
33	1	0	4.230519	1.241942	-0.811847
34	8	0	1.940946	-1.923311	-0.928821
35	6	0	2.473860	-2.053911	-2.240426
36	6	0	4.003021	-1.901882	-2.097661
37	6	0	4.254842	-2.043992	-0.577621
38	6	0	2.892320	-2.477478	-0.028977
39	1	0	2.001570	-1.287290	-2.860021
40	1	0	2.210296	-3.044922	-2.635987
41	1	0	4.526319	-2.669975	-2.673552
42	1	0	4.342216	-0.928986	-2.463576
43	1	0	5.040733	-2.767951	-0.346790
44	1	0	4.532488	-1.081765	-0.140038
45	1	0	2.788928	-3.573349	-0.024206
46	1	0	2.663107	-2.079440	0.962332
47	8	0	-1.922804	1.872171	0.634781
48	6	0	-2.679408	2.755026	-0.211066
49	6	0	-1.659928	3.755319	-0.735486
50	6	0	-0.767841	3.940772	0.495694
51	6	0	-0.713447	2.520914	1.067775
52	1	0	-3.454338	3.245903	0.393931
53	1	0	-3.151014	2.147851	-0.985888
54	1	0	-1.097007	3.300709	-1.558019
55	1	0	-2.117865	4.685331	-1.082903
56	1	0	0.224468	4.333394	0.256532
57	1	0	-1.241911	4.625941	1.207975
58	1	0	0.128408	1.948194	0.659581
59	1	0	-0.676556	2.492882	2.162147
60	8	0	-3.605555	-0.297906	-0.369034
61	6	0	-3.781538	-1.233671	-1.443883
62	6	0	-4.716788	-2.300111	-0.888051
63	6	0	-4.230725	-2.381103	0.562104
64	6	0	-3.953267	-0.912722	0.882442
65	1	0	-2.804969	-1.662682	-1.703843
66	1	0	-4.170637	-0.682938	-2.303272
67	1	0	-5.757559	-1.958547	-0.929243
68	1	0	-4.638473	-3.248635	-1.425442
69	1	0	-4.955762	-2.829481	1.246389
70	1	0	-3.299508	-2.955843	0.607334
71	1	0	-4.844149	-0.405706	1.272770
72	1	0	-3.123129	-0.767161	1.581540

Table S57. M06-2X/6-31+G(d) geometry of dimer 2 RS·4THF + ethylene Product

SCF Done: E(RM062X) = -1329.47833033 A.U. after 9 cycles

Convg = 0.2808D-08 -V/T = 2.0086

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.746005	1.590581	-2.504157
2	6	0	-0.203460	0.479112	-2.189982
3	8	0	1.317983	0.332916	-2.190113
4	1	0	0.946061	1.908847	-3.529860
5	1	0	0.934376	2.371694	-1.760315
6	3	0	1.625501	0.177638	-0.317264
7	3	0	-1.047241	0.222022	-0.233201
8	6	0	-0.697329	-0.130359	3.093950
9	6	0	0.367005	0.594702	2.286402
10	8	0	0.343453	0.303883	0.943241
11	1	0	1.347959	0.341648	2.746318
12	1	0	0.230380	1.682832	2.481857
13	1	0	-0.680875	-1.215528	2.985675
14	1	0	-0.509748	0.043947	-3.161160
15	6	0	-1.067696	0.413680	4.444585
16	6	0	-2.041283	0.508045	3.298782
17	1	0	-0.570088	1.326186	4.764078
18	1	0	-1.290760	-0.280945	5.248283
19	1	0	-2.924146	-0.122736	3.340528
20	1	0	-2.206590	1.477608	2.837076
21	8	0	-2.355911	1.693343	0.091506
22	6	0	-1.556226	2.870751	0.311875
23	6	0	-2.037622	3.905196	-0.706281
24	6	0	-2.551237	3.023082	-1.848954
25	6	0	-3.158862	1.851703	-1.083698
26	1	0	-0.505207	2.593698	0.168294
27	1	0	-1.697809	3.190265	1.349050
28	1	0	-2.855259	4.504633	-0.289689
29	1	0	-1.237057	4.583323	-1.013269
30	1	0	-3.279172	3.527505	-2.490314
31	1	0	-1.717295	2.665797	-2.460321
32	1	0	-4.194957	2.058454	-0.779024
33	1	0	-3.123979	0.909745	-1.640960
34	8	0	-2.339656	-1.255917	-0.276968
35	6	0	-3.369250	-1.367776	0.715997
36	6	0	-4.466576	-2.238437	0.092939
37	6	0	-4.227670	-2.045514	-1.408472
38	6	0	-2.706175	-1.970987	-1.457987
39	1	0	-3.712837	-0.353248	0.948359
40	1	0	-2.933973	-1.805379	1.620102
41	1	0	-4.321465	-3.290348	0.362277
42	1	0	-5.466649	-1.939386	0.416387
43	1	0	-4.633372	-2.855273	-2.020299
44	1	0	-4.663480	-1.099107	-1.748540
45	1	0	-2.259310	-2.976105	-1.426982
46	1	0	-2.296862	-1.425230	-2.312020
47	8	0	3.281093	1.180612	-0.072009
48	6	0	3.839244	0.885917	1.216612
49	6	0	5.332332	0.673113	0.980261
50	6	0	5.333411	0.072277	-0.428945

51	6	0	4.234649	0.885430	-1.106362
52	1	0	3.367185	-0.027242	1.602143
53	1	0	3.603988	1.716557	1.887337
54	1	0	5.862682	1.632270	0.987253
55	1	0	5.784186	0.022124	1.732968
56	1	0	6.295964	0.160983	-0.939506
57	1	0	5.044333	-0.983025	-0.388839
58	1	0	4.620469	1.834976	-1.499492
59	1	0	3.708862	0.356288	-1.905559
60	8	0	2.428587	-1.669630	-0.213511
61	6	0	1.807522	-2.412872	0.841021
62	6	0	0.518877	-2.999674	0.235537
63	6	0	0.730153	-2.846983	-1.290419
64	6	0	2.197163	-2.430151	-1.400887
65	1	0	1.620819	-1.721406	1.664294
66	1	0	2.501223	-3.203692	1.161126
67	1	0	0.386257	-4.044403	0.532869
68	1	0	-0.352018	-2.423759	0.560161
69	1	0	0.513855	-3.762098	-1.849625
70	1	0	0.105980	-2.036565	-1.680033
71	1	0	2.870209	-3.301533	-1.400845
72	1	0	2.411092	-1.788029	-2.256450

Table S58. M06-2X/6-31+G(d) geometry of tetramer RRRR

```
SCF Done:  E(RM062X) =  -642.743925567     A.U. after   10 cycles
             Convg  =    0.1491D-08             -V/T =  2.0081
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.234935	-1.345358	-1.175949
2	3	0	-0.879154	-0.799570	1.041254
3	6	0	-1.235199	1.345389	1.175852
4	6	0	1.235073	-1.345276	1.176157
5	6	0	2.724007	-1.312853	1.143094
6	3	0	0.879290	-0.799416	-1.041584
7	6	0	1.235171	1.345471	-1.175990
8	1	0	0.935211	-2.281691	1.672334
9	1	0	-0.935413	2.281742	1.672185
10	6	0	-2.724134	1.312650	1.143084
11	3	0	-0.879079	0.799568	-1.040934
12	3	0	0.879146	0.799553	1.041324
13	6	0	-2.723870	-1.312823	-1.143228
14	6	0	2.724106	1.312760	-1.143042
15	1	0	0.935431	2.281912	-1.672177
16	1	0	3.304759	-2.083080	1.649033
17	1	0	3.250833	-0.364718	1.022928
18	1	0	-3.250655	-0.364664	-1.023065
19	1	0	-3.304564	-2.082950	-1.649384
20	1	0	-3.250792	0.364435	1.022821
21	1	0	-3.304941	2.082654	1.649299
22	1	0	3.304960	2.082868	-1.649046
23	1	0	3.250774	0.364534	-1.022890

24	8	0	2.067421	1.785111	0.018001
25	1	0	-0.935011	-2.281727	-1.672176
26	8	0	-2.067590	1.785230	-0.017953
27	8	0	-2.067298	-1.785213	0.017873
28	8	0	2.067153	-1.785065	-0.017910

Table S59. M06-2X/6-31+G(d) geometry of tetramer RRRR + ethyelene TS

SCF Done: E(RM062X) = -721.271019107 A.U. after 10 cycles
Convg = 0.4160D-08 -V/T = 2.0083

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.161277	-0.831631	1.481116
2	3	0	0.375148	-0.903246	-1.371002
3	6	0	2.519075	-1.088494	-1.006977
4	6	0	-0.254387	1.142466	-1.704596
5	6	0	-0.333100	2.616367	-1.482329
6	3	0	-0.648672	0.562083	0.730685
7	6	0	1.379305	1.034462	1.517959
8	1	0	-0.949717	0.907764	-2.528965
9	1	0	3.489501	-0.755772	-1.402618
10	6	0	2.524866	-2.583670	-0.986411
11	3	0	1.355636	-1.047941	0.913696
12	3	0	1.695353	0.945321	-0.780804
13	6	0	-1.345324	-1.896809	0.949421
14	6	0	1.142172	2.502017	1.613511
15	1	0	2.117051	0.774372	2.294845
16	1	0	-0.931575	3.241434	-2.144768
17	1	0	0.481752	3.147870	-0.987449
18	1	0	-1.065134	-1.991328	2.078853
19	1	0	-1.773960	-2.880402	0.694520
20	1	0	1.584878	-3.139219	-0.951207
21	1	0	3.360500	-3.139385	-1.410683
22	1	0	1.593412	3.081459	2.418420
23	1	0	0.230654	2.941159	1.204243
24	8	0	2.082602	2.066932	0.649835
25	1	0	-3.005597	-1.240991	2.053048
26	8	0	2.847260	-1.913365	0.216190
27	8	0	-0.280454	-1.537711	0.183074
28	8	0	-1.115311	1.795969	-0.637765
29	6	0	-4.350289	-0.980894	-0.134524
30	1	0	-5.204920	-0.722006	0.485149
31	1	0	-4.249280	-2.025807	-0.417329
32	6	0	-3.469179	-0.055577	-0.532184
33	1	0	-2.627931	-0.304251	-1.175865
34	1	0	-3.565978	0.992419	-0.268502

Table S60. M06-2X/6-31+G(d) geometry of tetramer RRRS

SCF Done: E(RM062X) = -642.741965694 A.U. after 9 cycles
Convg = 0.7329D-08 -V/T = 2.0081
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.277386	1.801773	0.094383
2	3	0	0.775515	0.423861	1.594195
3	6	0	1.427141	-1.565912	1.113462
4	6	0	-1.358899	0.751891	1.660530
5	6	0	-2.813041	0.739091	1.346571
6	3	0	-0.820822	1.054992	-0.884353
7	6	0	-0.888392	-1.052464	-1.385235
8	1	0	-1.199386	1.532723	2.424236
9	1	0	1.345109	-2.628559	1.380894
10	6	0	2.876469	-1.200293	1.161031
11	3	0	1.132296	-0.392129	-0.905364
12	3	0	-0.753353	-1.174755	0.879654
13	6	0	2.226494	2.091238	-1.003987
14	6	0	-2.368872	-1.139955	-1.545389
15	1	0	-0.436894	-1.771711	-2.087298
16	1	0	-3.512776	1.353216	1.912836
17	1	0	-3.263746	-0.144906	0.893130
18	1	0	3.112942	1.467239	-1.129394
19	1	0	2.331093	3.095412	-1.413398
20	1	0	3.181621	-0.154915	1.255568
21	1	0	3.616149	-1.915400	1.518768
22	1	0	-2.804112	-1.764605	-2.324335
23	1	0	-3.008919	-0.313893	-1.229262
24	8	0	-1.788340	-1.881817	-0.493020
25	1	0	0.672641	2.711438	0.250935
26	8	0	2.336974	-1.535904	-0.101682
27	8	0	1.020597	1.448995	-1.410756
28	8	0	-1.982273	1.499457	0.486299

Table S61. M06-2X/6-31+G(d) geometry of tetramer RRRS + ethyelene TS

```
SCF Done:  E(RM062X) =  -721.272126767     A.U. after    9 cycles
             Convg  =    0.6838D-08             -V/T =  2.0083
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.151950	-0.575714	0.186274
2	3	0	0.576881	0.142325	-0.974294
3	6	0	-0.379742	2.092342	-1.214061
4	6	0	-0.795530	-1.535119	-1.231383
5	6	0	-1.957231	-2.464856	-1.201491
6	3	0	-0.861858	-0.944327	1.062129
7	6	0	-2.486601	0.539820	1.106931
8	1	0	0.037229	-2.061463	-1.725041
9	1	0	-0.940591	2.710180	-1.928759
10	6	0	0.927075	2.771233	-0.953234
11	3	0	-0.560575	1.507935	0.975511
12	3	0	-1.795335	0.381746	-1.092663
13	6	0	2.054857	0.202270	1.447649

14	6	0	-3.622711	-0.421265	1.037578
15	1	0	-2.860401	1.449906	1.605068
16	1	0	-1.909899	-3.428931	-1.707229
17	1	0	-2.968250	-2.071364	-1.085734
18	1	0	2.434770	1.232289	1.421040
19	1	0	2.290439	-0.268765	2.409125
20	1	0	1.776391	2.205846	-0.557747
21	1	0	1.212436	3.661181	-1.512822
22	1	0	-4.570382	-0.191238	1.523595
23	1	0	-3.433412	-1.488695	0.914005
24	8	0	-3.379352	0.369050	-0.109140
25	1	0	2.052470	-1.645370	0.435624
26	8	0	-0.116937	2.998833	-0.027159
27	8	0	0.675073	0.117441	1.132675
28	8	0	-1.153536	-2.411046	-0.036796
29	6	0	4.281651	-0.579914	-0.668533
30	1	0	4.385519	0.499926	-0.614520
31	1	0	4.020955	-0.991386	-1.637912
32	6	0	4.610263	-1.371562	0.366985
33	1	0	4.565196	-2.454196	0.290565
34	1	0	4.924326	-0.958601	1.321767

Table S62. M06-2X/6-31+G(d) geometry of tetramer RRSS

SCF Done: E(RM062X) = -642.736498873 A.U. after 9 cycles
Convg = 0.4388D-08 -V/T = 2.0081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.631048	0.635678	1.524400
2	3	0	-1.285649	0.798421	-0.767872
3	6	0	-0.702942	-1.635301	-1.041444
4	6	0	0.702856	1.636112	-1.040921
5	6	0	2.138334	2.003899	-0.865518
6	3	0	0.449699	1.103179	0.997245
7	6	0	1.631239	-0.636121	1.523902
8	1	0	0.338751	2.179218	-1.926714
9	1	0	-0.338638	-2.177554	-1.927686
10	6	0	-2.138271	-2.003809	-0.866304
11	3	0	-0.449725	-1.103452	0.997012
12	3	0	1.285720	-0.798018	-0.768038
13	6	0	-3.093607	0.724153	1.252904
14	6	0	3.093812	-0.724901	1.252607
15	1	0	1.445304	-1.190670	2.461823
16	1	0	2.599361	2.762857	-1.496162
17	1	0	2.629722	1.884033	0.104210
18	1	0	-3.573937	0.000700	0.593496
19	1	0	-3.763912	1.182731	1.978958
20	1	0	-2.629739	-1.884808	0.103497
21	1	0	-2.599002	-2.762488	-1.497496
22	1	0	3.763895	-1.183838	1.978637
23	1	0	3.574436	-0.001418	0.593447
24	8	0	2.260012	-1.654657	0.590623

25	1	0	-1.445381	1.190043	2.462473
26	8	0	-1.863342	-0.796148	-1.543474
27	8	0	-2.259939	1.654285	0.591285
28	8	0	1.862865	0.796839	-1.543593

Table S63. M06-2X/6-31+G(d) geometry of tetramer RRSS+ ethyelene TS

SCF Done: E(RM062X) = -721.270171005 A.U. after 9 cycles
Convg = 0.4367D-08 -V/T = 2.0083

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.052913	-1.251449	1.505711
2	3	0	1.001578	-1.073445	-0.853944
3	6	0	2.629909	0.863229	-0.883044
4	6	0	-1.938285	-0.630432	-0.210648
5	6	0	-1.775395	0.119732	-1.481857
6	3	0	-0.532011	0.223087	1.048604
7	6	0	0.175868	2.249933	1.310732
8	1	0	-1.756850	-1.698528	-0.410822
9	1	0	2.987822	1.477667	-1.723090
10	6	0	3.742499	-0.061673	-0.516656
11	3	0	1.784261	0.759845	1.083682
12	3	0	0.626370	1.671015	-0.860042
13	6	0	1.893362	-2.469102	1.324512
14	6	0	-1.172175	2.782055	0.940537
15	1	0	0.616008	2.937326	2.046209
16	1	0	-1.898900	-0.389299	-2.444822
17	1	0	-2.214098	1.125663	-1.521593
18	1	0	2.844696	-2.409804	0.794839
19	1	0	1.826942	-3.297731	2.029068
20	1	0	3.782136	-0.521141	0.474794
21	1	0	4.717098	0.024805	-0.995616
22	1	0	-1.587424	3.648313	1.454141
23	1	0	-1.926956	2.120422	0.506279
24	8	0	-0.094519	3.098676	0.082980
25	1	0	0.371382	-1.464246	2.350185
26	8	0	2.739002	-0.571580	-1.368075
27	8	0	0.753422	-2.344095	0.497373
28	8	0	-0.423194	0.126705	-1.047506
29	6	0	-4.326507	-1.563613	-0.588792
30	1	0	-4.228363	-2.639931	-0.481542
31	1	0	-4.570592	-1.187854	-1.578702
32	6	0	-4.141451	-0.733974	0.452142
33	1	0	-4.297734	0.336933	0.360734
34	1	0	-3.947867	-1.109989	1.451050

Table S64. M06-2X/6-31+G(d) geometry of tetramer RRRR·4THF

SCF Done: E(RM062X) = -1572.22613464 A.U. after 17 cycles
Convg = 0.5951D-08 -V/T = 2.0084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.577981	-1.253332	1.261105
2	3	0	-0.829523	-1.387411	0.939557
3	6	0	-0.981041	-1.835392	-1.205835
4	6	0	-1.149516	0.731880	1.447730
5	6	0	-1.328062	2.212039	1.479611
6	3	0	1.178188	0.788126	0.621689
7	6	0	0.869865	1.084430	-1.504960
8	1	0	-1.452443	0.349343	2.439994
9	1	0	-1.564307	-1.763526	-2.138377
10	6	0	-0.781340	-3.285279	-0.922211
11	3	0	1.196486	-1.073242	-0.922089
12	3	0	-1.255482	0.309754	-0.697085
13	6	0	1.739412	-2.726112	1.419611
14	6	0	0.598232	2.549740	-1.434518
15	1	0	1.274094	0.866836	-2.507438
16	1	0	-1.791464	2.707868	2.334965
17	1	0	-1.412423	2.767557	0.543336
18	1	0	1.584959	-3.387605	0.563493
19	1	0	2.396574	-3.140688	2.186537
20	1	0	-0.553130	-3.619359	0.092236
21	1	0	-1.264259	-4.045205	-1.538424
22	1	0	0.889857	3.218943	-2.247241
23	1	0	0.527572	3.042823	-0.459755
24	8	0	-0.495324	1.718951	-1.758955
25	1	0	2.135207	-0.775083	2.088059
26	8	0	0.268153	-2.610025	-1.588832
27	8	0	0.562753	-2.150529	1.951750
28	8	0	-0.033357	1.716835	1.755789
29	8	0	-2.475231	-2.236054	1.590607
30	6	0	-2.746960	-2.139185	2.990694
31	6	0	-3.852260	-1.068383	3.146938
32	6	0	-4.213699	-0.697316	1.693459
33	6	0	-3.673730	-1.883582	0.902283
34	1	0	-1.804570	-1.888949	3.484634
35	1	0	-3.085428	-3.118513	3.352425
36	1	0	-4.714493	-1.483117	3.677751
37	1	0	-3.501167	-0.198821	3.708692
38	1	0	-5.285919	-0.540688	1.544384
39	1	0	-3.678469	0.205360	1.383031
40	1	0	-4.367908	-2.737719	0.926001
41	1	0	-3.406988	-1.649687	-0.130911
42	8	0	-3.108506	0.598108	-1.369253
43	6	0	-3.618810	1.908609	-1.114064
44	6	0	-4.724604	2.083704	-2.144484
45	6	0	-4.066333	1.456699	-3.379249
46	6	0	-3.212090	0.327158	-2.780973
47	1	0	-2.818983	2.647043	-1.264951
48	1	0	-3.949845	1.936581	-0.072752
49	1	0	-5.611581	1.515765	-1.842625
50	1	0	-5.008848	3.128736	-2.292600
51	1	0	-4.787210	1.086323	-4.112291
52	1	0	-3.423579	2.192546	-3.872665

53	1	0	-3.679412	-0.657216	-2.884906
54	1	0	-2.205790	0.296743	-3.211392
55	8	0	2.859749	1.735808	1.102127
56	6	0	3.506363	2.628421	0.193994
57	6	0	3.120743	4.055189	0.644237
58	6	0	2.407343	3.834087	1.996657
59	6	0	2.808294	2.407839	2.361218
60	1	0	3.166713	2.372158	-0.811763
61	1	0	4.592198	2.469537	0.259615
62	1	0	4.012648	4.678490	0.755837
63	1	0	2.464784	4.542568	-0.081894
64	1	0	2.701554	4.562618	2.756882
65	1	0	1.320645	3.872207	1.876040
66	1	0	3.804642	2.370425	2.827378
67	1	0	2.081685	1.887427	2.986930
68	8	0	2.946867	-1.364301	-1.764804
69	6	0	3.985832	-0.560224	-1.181900
70	6	0	5.196621	-1.483329	-1.020753
71	6	0	4.532530	-2.858544	-0.901246
72	6	0	3.388760	-2.721261	-1.898092
73	1	0	3.625998	-0.190095	-0.214266
74	1	0	4.176258	0.290705	-1.845013
75	1	0	5.832390	-1.448276	-1.912773
76	1	0	5.805447	-1.216376	-0.153176
77	1	0	5.204006	-3.688326	-1.137591
78	1	0	4.134224	-2.999997	0.109668
79	1	0	3.737430	-2.882458	-2.927691
80	1	0	2.528315	-3.366072	-1.706559

Table S65. M06-2X/6-31+G(d) geometry of tetramer RRRS·4THF

SCF Done: E(RM062X) = -1572.22276695 A.U. after 17 cycles
Convg = 0.7094D-08 -V/T = 2.0084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.193379	0.977848	1.854051
2	3	0	-0.762586	0.277507	1.623309
3	6	0	-0.763261	-1.825027	1.055578
4	6	0	-1.405199	1.657944	0.046753
5	6	0	-1.602771	2.474650	-1.185225
6	3	0	1.139863	1.135614	-0.896916
7	6	0	0.509161	-0.634922	-1.982800
8	1	0	-1.624915	2.319081	0.908510
9	1	0	-1.422919	-2.662390	0.773717
10	6	0	-0.229395	-2.123647	2.418051
11	3	0	1.246961	-1.209200	0.019993
12	3	0	-1.359239	-0.413794	-0.590670
13	6	0	2.481874	0.257799	2.010727
14	6	0	0.136482	0.198227	-3.160174
15	1	0	0.834372	-1.617962	-2.362363
16	1	0	-1.999981	3.490632	-1.134304
17	1	0	-1.767003	1.977819	-2.143425

18	1	0	2.473883	-0.789007	2.331351
19	1	0	3.419167	0.778190	2.232730
20	1	0	0.156705	-1.316571	3.045291
21	1	0	-0.583683	-2.992912	2.974151
22	1	0	0.302675	-0.164400	-4.175496
23	1	0	0.123784	1.288654	-3.079707
24	8	0	-0.917848	-0.460661	-2.490620
25	1	0	1.416490	2.060057	1.851898
26	8	0	0.594611	-2.461241	1.318786
27	8	0	2.056947	0.436294	0.664224
28	8	0	-0.282540	2.370199	-0.681832
29	8	0	2.478002	2.299651	-1.786776
30	6	0	2.110461	3.680754	-1.806993
31	6	0	2.462677	4.185439	-0.404150
32	6	0	3.629919	3.259152	0.025716
33	6	0	3.754716	2.275709	-1.147867
34	1	0	1.049248	3.742976	-2.048571
35	1	0	2.703202	4.187229	-2.583025
36	1	0	2.738251	5.243472	-0.405575
37	1	0	1.599492	4.049261	0.253425
38	1	0	4.562485	3.804678	0.194131
39	1	0	3.374564	2.720370	0.942215
40	1	0	4.512971	2.605916	-1.872645
41	1	0	3.957356	1.246878	-0.849824
42	8	0	2.882002	-2.254627	-0.453438
43	6	0	4.182421	-1.784619	-0.099046
44	6	0	4.633519	-2.632705	1.112121
45	6	0	3.542199	-3.719264	1.225485
46	6	0	2.856899	-3.645547	-0.134905
47	1	0	4.093428	-0.718617	0.118352
48	1	0	4.853913	-1.924493	-0.957075
49	1	0	5.619624	-3.070242	0.931171
50	1	0	4.698916	-2.031467	2.022875
51	1	0	3.949692	-4.710506	1.441602
52	1	0	2.810580	-3.460702	1.996599
53	1	0	3.417170	-4.198860	-0.904206
54	1	0	1.814853	-3.966313	-0.124486
55	8	0	-2.246692	0.376289	2.884919
56	6	0	-2.523199	1.604446	3.560396
57	6	0	-3.781728	2.203531	2.892620
58	6	0	-4.192216	1.141696	1.852518
59	6	0	-3.476366	-0.112456	2.346162
60	1	0	-1.632235	2.231301	3.465543
61	1	0	-2.695321	1.392556	4.623326
62	1	0	-4.570316	2.359372	3.634747
63	1	0	-3.571834	3.167159	2.421354
64	1	0	-5.275913	1.007681	1.787843
65	1	0	-3.810545	1.408322	0.862142
66	1	0	-4.043447	-0.615476	3.143933
67	1	0	-3.232759	-0.829285	1.556705
68	8	0	-3.126899	-1.288781	-0.907680
69	6	0	-4.016091	-0.420482	-1.625750
70	6	0	-4.679484	-1.296616	-2.682944
71	6	0	-3.547961	-2.272187	-3.018421
72	6	0	-2.921186	-2.507362	-1.647585
73	1	0	-3.425379	0.382489	-2.084091
74	1	0	-4.717400	0.011919	-0.906280

75	1	0	-5.535592	-1.831495	-2.255334
76	1	0	-5.025620	-0.719751	-3.544508
77	1	0	-3.896555	-3.199174	-3.481687
78	1	0	-2.815576	-1.792853	-3.675159
79	1	0	-3.414810	-3.322217	-1.103096
80	1	0	-1.845782	-2.702831	-1.696478

Table S66. M06-2X/6-31+G(d) geometry of tetramer RRSS·4THF

SCF Done: E(RM062X) = -1572.22051739 A.U. after 16 cycles
Convg = 0.5753D-08 -V/T = 2.0084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.466916	1.183271	-1.220081
2	3	0	1.301707	0.838248	-1.059383
3	6	0	0.895677	-1.602916	-1.123607
4	6	0	0.354498	1.767533	1.370381
5	6	0	1.600829	1.442563	2.112454
6	3	0	-1.478643	0.833591	0.979688
7	6	0	-1.537668	-1.295431	1.467418
8	1	0	0.573253	2.661265	0.752291
9	1	0	1.293296	-2.577443	-0.775214
10	6	0	1.316341	-1.449782	-2.546022
11	3	0	-1.108396	-0.861647	-0.654886
12	3	0	0.848268	-1.074087	1.027742
13	6	0	-1.343874	1.010286	-2.695492
14	6	0	-1.266821	-1.085965	2.920525
15	1	0	-2.276645	-2.112270	1.384716
16	1	0	2.469269	2.108832	2.105018
17	1	0	1.558839	0.796488	2.991871
18	1	0	-1.243621	0.003832	-3.109092
19	1	0	-1.762220	1.734963	-3.396318
20	1	0	0.785888	-0.762124	-3.206021
21	1	0	1.833289	-2.257838	-3.067810
22	1	0	-1.831173	-1.626960	3.681162
23	1	0	-0.850518	-0.134678	3.260765
24	8	0	-0.362342	-1.909810	2.205750
25	1	0	-1.925231	2.174470	-1.039092
26	8	0	2.116755	-0.819712	-1.561886
27	8	0	-0.205726	1.493699	-2.008961
28	8	0	1.427032	0.742166	0.888378
29	8	0	-3.107923	1.807284	1.420689
30	6	0	-2.867443	3.198622	1.675342
31	6	0	-4.179352	3.893404	1.330988
32	6	0	-4.650284	3.062282	0.133472
33	6	0	-4.232411	1.648468	0.541795
34	1	0	-2.046991	3.542728	1.031135
35	1	0	-2.560198	3.296419	2.719046
36	1	0	-4.887868	3.805440	2.162474
37	1	0	-4.045170	4.952777	1.097644
38	1	0	-5.723451	3.140980	-0.058801
39	1	0	-4.112622	3.367423	-0.770966

40	1	0	-5.024214	1.131742	1.097359
41	1	0	-3.922018	1.031008	-0.307871
42	8	0	2.536154	2.290970	-1.426292
43	6	0	2.082491	3.644115	-1.544601
44	6	0	2.840065	4.403150	-0.461974
45	6	0	4.200142	3.698607	-0.497042
46	6	0	3.798709	2.242203	-0.746784
47	1	0	0.995854	3.637798	-1.431973
48	1	0	2.336353	4.018427	-2.545965
49	1	0	2.902192	5.476384	-0.661106
50	1	0	2.355565	4.253472	0.510240
51	1	0	4.801621	4.080801	-1.329455
52	1	0	4.775888	3.817149	0.424673
53	1	0	4.509087	1.694057	-1.373223
54	1	0	3.650780	1.693342	0.190439
55	8	0	2.522171	-1.812783	1.661733
56	6	0	2.601627	-3.166649	2.099863
57	6	0	3.322256	-3.920305	0.967966
58	6	0	4.058644	-2.802128	0.188005
59	6	0	3.750209	-1.534220	0.992808
60	1	0	1.582551	-3.502077	2.301941
61	1	0	3.184981	-3.199895	3.031391
62	1	0	4.007828	-4.672344	1.368306
63	1	0	2.603688	-4.434397	0.323792
64	1	0	5.134535	-2.981757	0.111749
65	1	0	3.654256	-2.692959	-0.821730
66	1	0	4.524724	-1.335033	1.748946
67	1	0	3.593108	-0.649646	0.373592
68	8	0	-2.199212	-2.222325	-1.514690
69	6	0	-1.659924	-3.533415	-1.296581
70	6	0	-2.860089	-4.465824	-1.399640
71	6	0	-3.952471	-3.619777	-0.736660
72	6	0	-3.600900	-2.204523	-1.206384
73	1	0	-1.203007	-3.575063	-0.296936
74	1	0	-0.885575	-3.698183	-2.049625
75	1	0	-3.103195	-4.656578	-2.450999
76	1	0	-2.694016	-5.423758	-0.900332
77	1	0	-4.965445	-3.913255	-1.023910
78	1	0	-3.868810	-3.689599	0.353132
79	1	0	-4.139460	-1.926713	-2.119719
80	1	0	-3.779488	-1.442867	-0.439657

Table S67. M06-2X/6-31+G(d) geometry of THF-solvated α-lithio-dimethylether: CH_3-O-CH_2-Li·2THF

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SCF Done:  E(RM062X) =  -626.589464152     A.U. after    7 cycles
             Convg  =    0.5433D-08             -V/T =  2.0086
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.042340	2.428872	0.966051
2	1	0	-0.346285	2.536852	2.013978

3	1	0	0.729981	1.632526	0.897358
4	1	0	0.437890	3.368407	0.638131
5	8	0	-1.159220	2.127929	0.205718
6	6	0	-0.796622	1.908077	-1.212760
7	1	0	-1.772934	1.993881	-1.723892
8	1	0	-0.260642	2.827561	-1.527775
9	3	0	-0.032875	0.003926	-1.311880
10	6	0	-2.523022	-1.225996	-1.000740
11	6	0	-1.163326	-1.007861	0.912228
12	6	0	-3.251448	-0.309820	-0.028527
13	1	0	-2.471181	-0.832314	-2.019800
14	6	0	-2.608979	-0.696049	1.307691
15	1	0	-0.746968	-1.868024	1.448013
16	1	0	-3.025553	0.735171	-0.254064
17	1	0	-2.656005	0.114853	2.037945
18	6	0	2.134070	-1.641738	-0.133007
19	6	0	2.751254	0.444535	-0.894127
20	6	0	2.667144	-0.935922	1.110137
21	1	0	1.257218	-2.271930	0.030711
22	6	0	3.358823	0.311086	0.519280
23	1	0	3.499466	0.261054	-1.674585
24	1	0	3.345366	-1.563729	1.693377
25	1	0	4.441645	0.171444	0.460148
26	1	0	2.255454	1.399810	-1.080555
27	1	0	3.169147	1.200359	1.125000
28	1	0	1.830617	-0.642358	1.752570
29	1	0	2.918440	-2.231738	-0.628850
30	1	0	-0.518758	-0.134270	1.056082
31	1	0	-2.955683	-2.234870	-1.022723
32	1	0	-4.333281	-0.466927	-0.042879
33	1	0	-3.092620	-1.583082	1.731792
34	8	0	-1.176170	-1.316349	-0.499179
35	8	0	1.740388	-0.571023	-0.988001

Table S68. M06-2X/6-31+G(d) geometry of the carbolithiation TS for THF-solvated α-lithio-dimethylether + ethylene

SCF Done: E(RM062X) = -705.105312471 A.U. after 9 cycles
Convg = 0.4808D-08 -V/T = 2.0087

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.409947	1.253259	2.232620
2	1	0	0.902117	1.266478	3.211471
3	1	0	2.159700	0.439085	2.258844
4	1	0	1.990188	2.200569	2.170652
5	8	0	0.519399	1.138359	1.188296
6	6	0	0.815763	2.612769	-0.139236
7	1	0	0.982372	3.141272	0.798967
8	3	0	-0.114327	0.113938	-0.122523
9	1	0	1.707885	2.166033	-0.567633
10	6	0	-0.821092	1.796058	-1.200796
11	6	0	-0.145525	3.157826	-1.108286

12	1	0	0.333642	3.457057	-2.047255
13	1	0	-0.759686	3.984310	-0.735934
14	1	0	-0.948750	1.422202	-2.220228
15	1	0	-1.738258	1.753180	-0.609470
16	6	0	1.584904	-1.930880	0.359039
17	6	0	2.172918	-0.675365	-1.540689
18	6	0	3.102858	-1.713584	0.362618
19	1	0	1.100133	-1.479337	1.231014
20	6	0	3.260615	-0.455051	-0.498102
21	1	0	2.502322	-1.376236	-2.320370
22	1	0	3.497897	-1.595411	1.374734
23	1	0	3.034631	0.439245	0.093091
24	6	0	-2.444655	-0.371394	1.311291
25	6	0	-2.236420	-1.805537	-0.484324
26	6	0	-3.680171	-0.125984	0.414853
27	1	0	-2.698150	-0.982091	2.186697
28	6	0	-3.324931	-0.825754	-0.912676
29	1	0	-1.533849	-2.084775	-1.273030
30	1	0	-4.574105	-0.568120	0.864538
31	1	0	-4.182314	-1.321836	-1.374982
32	1	0	4.256650	-0.352358	-0.936546
33	1	0	3.616319	-2.559083	-0.108325
34	1	0	1.300024	-2.985588	0.299466
35	1	0	1.798969	0.237957	-2.012320
36	1	0	-1.936870	0.538881	1.640145
37	1	0	-3.872008	0.939768	0.269378
38	1	0	-2.910675	-0.106768	-1.625888
39	1	0	-2.666041	-2.715221	-0.038111
40	8	0	1.084000	-1.255697	-0.813808
41	8	0	-1.501454	-1.095062	0.508111

Table S69. M06-2X/6-31+G(d) geometry of CH_3-O-Li·2THF

SCF Done: E(RM062X) = -587.372763934 A.U. after 8 cycles
Convg = 0.1736D-08 -V/T = 2.0086
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.020574	2.696964	0.097190
2	1	0	-0.989389	3.050429	-0.325678
3	1	0	-0.056747	2.948417	1.178174
4	1	0	0.754878	3.356428	-0.344075
5	8	0	0.217293	1.370268	-0.129280
6	3	0	0.072872	-0.214254	-0.644323
7	6	0	-2.520221	0.347623	-1.060013
8	6	0	-2.148539	-1.539367	0.307828
9	6	0	-3.044475	0.668514	0.330196
10	1	0	-3.331252	0.126170	-1.766056
11	1	0	-1.861003	1.120509	-1.461376
12	6	0	-3.317488	-0.735068	0.880513
13	1	0	-1.299870	-1.565199	1.004124
14	1	0	-2.412430	-2.566004	0.039124
15	1	0	-2.251210	1.166008	0.898955
16	1	0	-3.933192	1.304543	0.310108

17	1	0	-3.348469	-0.776387	1.972080
18	1	0	-4.269378	-1.117102	0.495040
19	6	0	2.726893	-1.133154	-0.911486
20	6	0	1.968543	-0.708213	1.211434
21	6	0	3.268489	0.259354	-0.599559
22	1	0	2.393078	-1.275316	-1.942692
23	1	0	3.452217	-1.920699	-0.660664
24	6	0	2.990262	0.404152	0.910626
25	1	0	2.400040	-1.515454	1.817129
26	1	0	1.061071	-0.325951	1.682766
27	1	0	4.326898	0.359127	-0.854655
28	1	0	2.689771	1.009225	-1.145142
29	1	0	3.898115	0.268267	1.505994
30	1	0	2.557447	1.382518	1.124351
31	8	0	1.584907	-1.265616	-0.060268
32	8	0	-1.729266	-0.848603	-0.884816

Table S70. M06-2X/6-31+G(d) geometry of oxiranyllithium monomer R·3THF

SCF Done: E(RM062X) = -857.748297844 A.U. after 7 cycles
Convg = 0.7007D-08 -V/T = 2.0086

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.309448	2.322032	-0.601505
2	6	0	0.554299	2.071704	0.585969
3	8	0	0.594851	1.238893	-0.708314
4	1	0	-1.367392	2.037318	-0.572321
5	1	0	-0.104942	3.129381	-1.309285
6	1	0	1.420194	2.754017	0.516019
7	3	0	0.170733	0.106448	0.947988
8	8	0	-1.569125	-0.517780	0.346552
9	6	0	-1.960563	-0.641089	-1.030036
10	6	0	-3.391390	-0.105352	-1.108380
11	6	0	-3.910193	-0.367310	0.308745
12	6	0	-2.671425	-0.064664	1.143561
13	1	0	-1.915778	-1.704321	-1.297592
14	1	0	-1.243841	-0.080540	-1.637807
15	1	0	-3.386336	0.970236	-1.315496
16	1	0	-3.977887	-0.601446	-1.886011
17	1	0	-4.764546	0.257686	0.580967
18	1	0	-4.196927	-1.418862	0.424287
19	1	0	-2.558444	1.014603	1.321853
20	1	0	-2.627214	-0.590662	2.099897
21	8	0	1.700439	-1.091724	0.649381
22	6	0	1.880090	-1.524905	-0.703444
23	6	0	2.983942	-0.639954	-1.315322
24	6	0	3.470663	0.229090	-0.138063
25	6	0	2.924563	-0.501861	1.085307
26	1	0	0.915674	-1.414709	-1.203948
27	1	0	2.165423	-2.584954	-0.695044
28	1	0	3.790151	-1.258059	-1.722012
29	1	0	2.585733	-0.013322	-2.115190

30	1	0	4.559133	0.328538	-0.104660
31	1	0	3.019764	1.220929	-0.199788
32	1	0	3.606213	-1.296282	1.428426
33	1	0	2.684015	0.161832	1.921199
34	6	0	0.706204	-1.213396	3.660378
35	6	0	-0.293382	0.852069	3.696565
36	6	0	1.611465	-0.321873	4.542982
37	1	0	1.248578	-1.834710	2.944660
38	1	0	0.062923	-1.856102	4.276199
39	6	0	1.094607	1.105624	4.270157
40	1	0	-1.034250	0.650039	4.486602
41	1	0	-0.635973	1.642150	3.026017
42	1	0	1.498944	-0.587601	5.598322
43	1	0	2.669312	-0.432025	4.288073
44	1	0	1.081951	1.733363	5.164985
45	1	0	1.690140	1.604079	3.497720
46	8	0	-0.117730	-0.323780	2.905524